Full wwPDB EM Validation Report

Mar 31, 2025 – 06:38 PM JST

PDB ID	:	7C9R / pdb_00007c9r
EMDB ID	:	EMD-30314
Title	:	STRUCTURE OF PHOTOSYNTHETIC LH1-RC SUPER-COMPLEX OF THIORHODOVIBRIO STRAIN 970
Authors	:	Tani, K.; Kanno, R.; Makino, Y.; Hall, M.; Takenouchi, M.; Imanishi, M.; Yu, L.-J.; Overmann, J.; Madigan, M.T.; Kimura, Y.; Mizoguchi, A.; Humbel, B.M.; Wang-Otomo, Z.-Y.
Deposited on	:	2020-06-07
Resolution	:	2.82 Å(reported)
Based on initial model	:	5Y5S

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 (i) 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 (1)) were used in the production of this report:

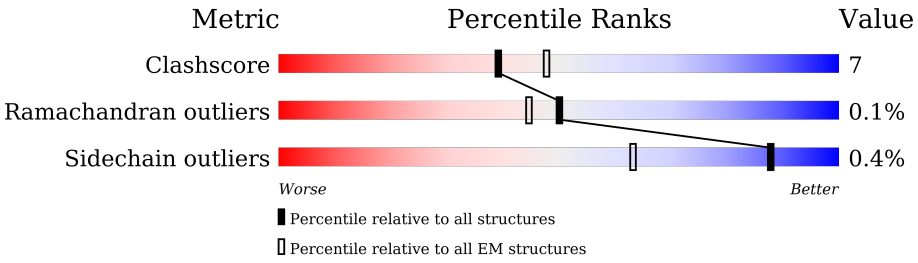
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.82 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	C	396	67% 11% • 21%
2	L	273	86% 13% •
3	M	324	90% 8% • •
4	H	258	82% 17% •
5	A	73	86% 10% •
5	D	73	95% • •
5	F	73	90% 8% •
5	I	73	99% •

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Mol	Chain	Length	Quality of chain
5	K	73	93% 5%
5	O	73	93% 7%
6	4	46	89% 7%
6	B	46	80% 13% 7%
6	P	46	89% 9%
7	0	46	76% 11% 11%
7	2	46	83% 7% 11%
7	6	46	87% 7% 7%
7	8	46	78% 11% 9%
7	E	46	89% 9%
7	G	46	83% 7% 11%
7	J	46	85% 11%
7	N	46	87% 9%
7	R	46	93%
7	T	46	83% 11% 7%
7	V	46	85% 9% 7%
7	X	46	89% 11%
7	Z	46	89% 9%
8	Q	81	84% 12%
9	1	77	86% 8% 6%
9	3	77	88% 6% 5%
9	5	77	90% 6%
9	7	77	88% 6% 5%
9	S	77	84% 8% 6%
9	U	77	87% 6% 6%

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Mol	Chain	Length	Quality of chain
9	W	77	
9	Y	77	
10	9	86	

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 29228 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	311	Total	C	N	O	S	0	0
			2433	1536	423	458	16		

- Molecule 2 is a protein called L subunit of the reaction center.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	272	Total	C	N	O	S	0	0
			2161	1459	350	344	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	318	Total	C	N	O	S	0	0
			2535	1700	408	416	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	257	Total	C	N	O	S	0	0
			2017	1298	348	366	5		

- Molecule 5 is a protein called Alpha subunit 1 of light-harvesting 1 complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	70	Total	C	N	O	S	0	0
			563	373	89	96	5		
5	D	72	Total	C	N	O	S	0	0
			580	382	93	100	5		
5	F	72	Total	C	N	O	S	0	0
			580	382	93	100	5		
5	I	73	Total	C	N	O	S	0	0
			588	387	94	101	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	72	Total	C	N	O	S	0	0
			580	382	93	100	5		
5	O	73	Total	C	N	O	S	0	0
			588	387	94	101	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	43	Total	C	N	O	S	0	0
			352	236	55	58	3		
6	P	42	Total	C	N	O	S	0	0
			343	230	53	57	3		
6	4	44	Total	C	N	O	S	0	0
			361	241	56	61	3		

- Molecule 7 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	42	Total	C	N	O	S	0	0
			343	230	53	58	2		
7	G	41	Total	C	N	O	S	0	0
			337	227	52	56	2		
7	J	41	Total	C	N	O	S	0	0
			337	227	52	56	2		
7	N	42	Total	C	N	O	S	0	0
			343	230	53	58	2		
7	R	44	Total	C	N	O	S	0	0
			361	241	56	62	2		
7	T	43	Total	C	N	O	S	0	0
			352	236	55	59	2		
7	V	43	Total	C	N	O	S	0	0
			352	236	55	59	2		
7	X	41	Total	C	N	O	S	0	0
			337	227	52	56	2		
7	Z	42	Total	C	N	O	S	0	0
			343	230	53	58	2		
7	2	41	Total	C	N	O	S	0	0
			337	227	52	56	2		
7	6	43	Total	C	N	O	S	0	0
			352	236	55	59	2		
7	8	42	Total	C	N	O	S	0	0
			343	230	53	58	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	0	41	Total	C	N	O	S	0	0
			337	227	52	56	2		

- Molecule 8 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	78	Total	C	N	O	S	0	0
			628	416	101	107	4		

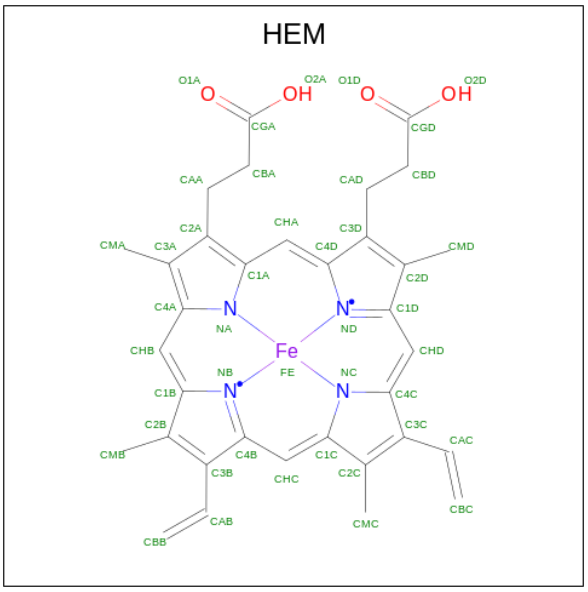
- Molecule 9 is a protein called LHC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	72	Total	C	N	O	S	0	0
			579	382	92	99	6		
9	U	72	Total	C	N	O	S	0	0
			576	382	91	98	5		
9	W	73	Total	C	N	O	S	0	0
			584	386	92	101	5		
9	Y	73	Total	C	N	O	S	0	0
			584	386	92	101	5		
9	1	72	Total	C	N	O	S	0	0
			576	382	91	98	5		
9	3	73	Total	C	N	O	S	0	0
			584	386	93	100	5		
9	5	74	Total	C	N	O	S	0	0
			589	389	94	101	5		
9	7	73	Total	C	N	O	S	0	0
			584	386	93	100	5		

- Molecule 10 is a protein called Alpha subunit 2 of light-harvesting 1 complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	84	Total	C	N	O	S	0	0
			668	440	113	111	4		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 13 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
13	C	1	Total	Ca	0
			1	1	
13	A	1	Total	Ca	0
			1	1	
13	D	1	Total	Ca	0
			1	1	
13	F	1	Total	Ca	0
			1	1	

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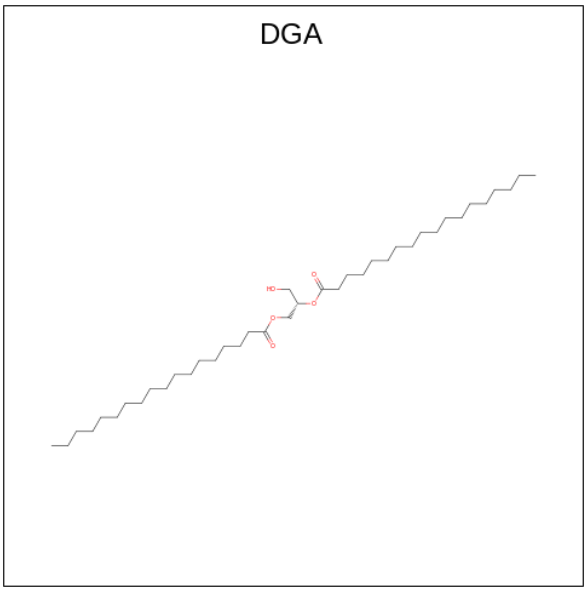
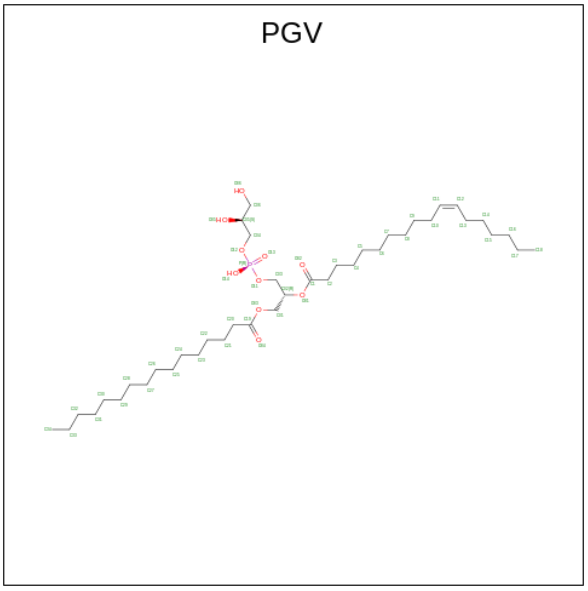
Mol	Chain	Residues	Atoms	AltConf
13	I	1	Total Ca 1 1	0
13	K	1	Total Ca 1 1	0
13	O	1	Total Ca 1 1	0
13	Q	1	Total Ca 1 1	0
13	S	1	Total Ca 1 1	0
13	U	1	Total Ca 1 1	0
13	W	1	Total Ca 1 1	0
13	Y	1	Total Ca 1 1	0
13	1	1	Total Ca 1 1	0
13	3	1	Total Ca 1 1	0
13	5	1	Total Ca 1 1	0
13	7	1	Total Ca 1 1	0
13	9	1	Total Ca 1 1	0

- Molecule 14 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			AltConf
14	C	1	Total	C	O	0
			32	28	4	

- Molecule 15 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	O	P	0
			16	9	6	1	
15	L	1	Total	C	O	P	0
			47	36	10	1	

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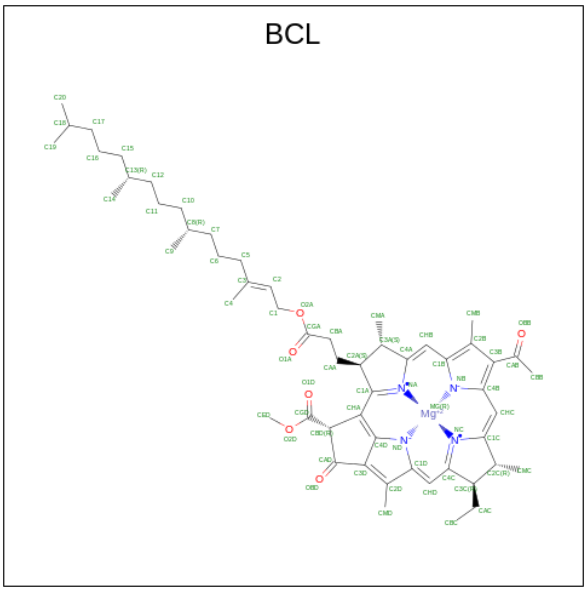
Mol	Chain	Residues	Atoms				AltConf
15	M	1	Total	C	O	P	0
			39	28	10	1	
15	H	1	Total	C	O	P	0
			36	25	10	1	
15	A	1	Total	C	O	P	0
			23	12	10	1	
15	D	1	Total	C	O	P	0
			43	32	10	1	
15	F	1	Total	C	O	P	0
			34	25	8	1	
15	F	1	Total	C	O	P	0
			37	26	10	1	
15	I	1	Total	C	O	P	0
			41	32	8	1	
15	K	1	Total	C	O	P	0
			36	25	10	1	
15	K	1	Total	C	O	P	0
			19	10	8	1	
15	K	1	Total	C	O	P	0
			43	34	8	1	
15	O	1	Total	C	O	P	0
			44	33	10	1	
15	Q	1	Total	C	O	P	0
			38	27	10	1	
15	Y	1	Total	C	O	P	0
			27	18	8	1	
15	1	1	Total	C	O	P	0
			26	17	8	1	
15	3	1	Total	C	O	P	0
			47	36	10	1	
15	5	1	Total	C	O	P	0
			47	36	10	1	
15	9	1	Total	C	O	P	0
			47	36	10	1	

- Molecule 16 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
16	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
16	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
16	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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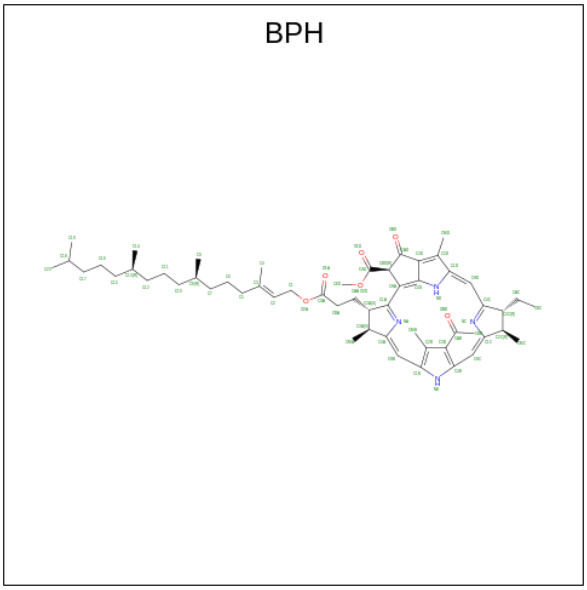
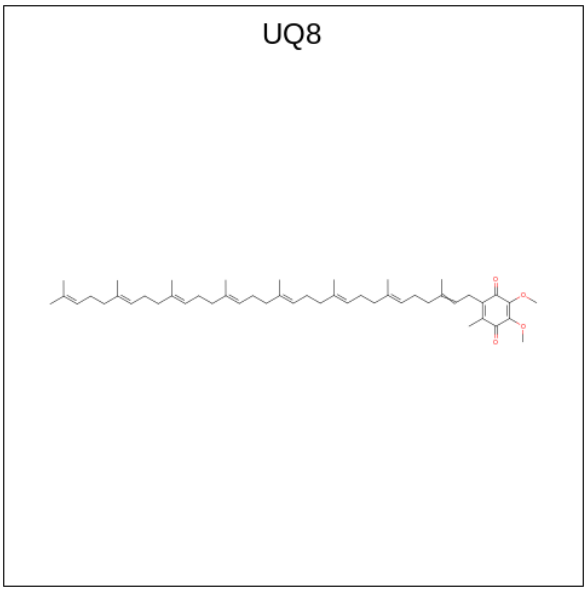
Mol	Chain	Residues	Atoms					AltConf
16	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 17 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



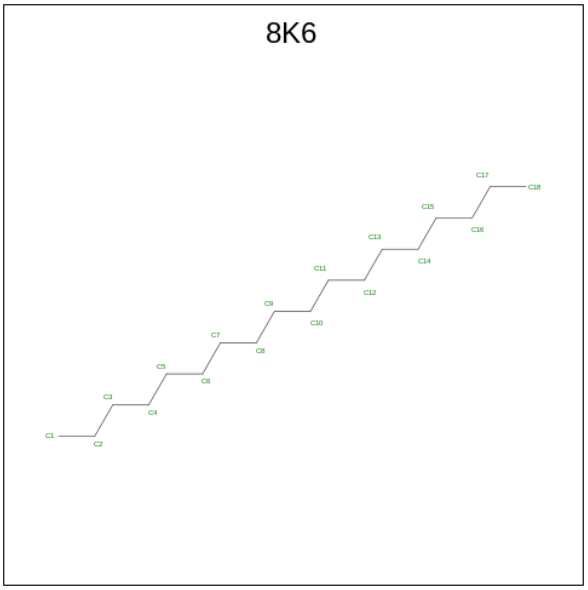
Mol	Chain	Residues	Atoms				AltConf
17	L	1	Total	C	N	O	0
			65	55	4	6	
17	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 18 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms	AltConf
18	L	1	Total C O 33 29 4	0
18	L	1	Total C O 33 29 4	0

- Molecule 19 is Octadecane (CCD ID: 8K6) (formula: $C_{18}H_{38}$).

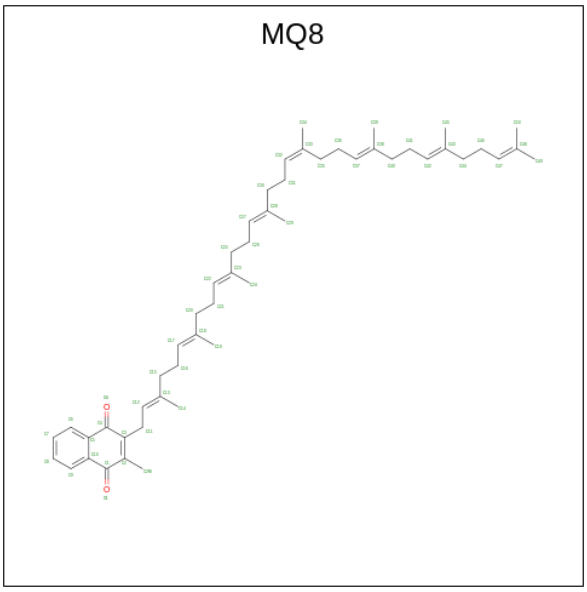


Mol	Chain	Residues	Atoms	AltConf
19	L	1	Total C 18 18	0
19	5	1	Total C 15 15	0

- Molecule 20 is FE (III) ION (CCD ID: FE) (formula: Fe).

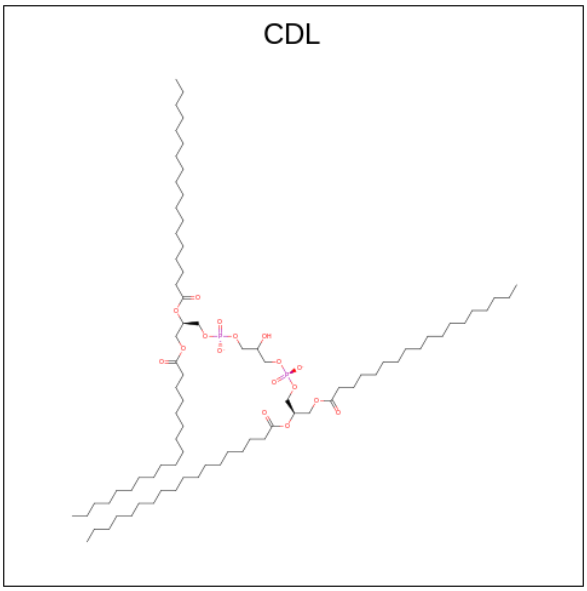
Mol	Chain	Residues	Atoms	AltConf
20	M	1	Total Fe 1 1	0

- Molecule 21 is MENAQUINONE 8 (CCD ID: MQ8) (formula: $C_{51}H_{72}O_2$).



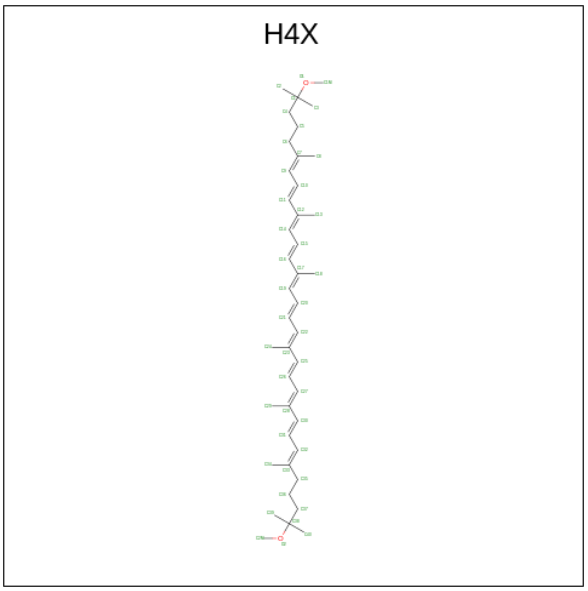
Mol	Chain	Residues	Atoms	AltConf
21	M	1	Total C O 53 51 2	0

- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
22	H	1	Total	C	O	P	0
			73	54	17	2	
22	S	1	Total	C	O	P	0
			74	55	17	2	
22	Y	1	Total	C	O	P	0
			30	14	14	2	

- Molecule 23 is (6 {E},8 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},24 {E},26 {E})-2,31-dimethoxy-2,6,10,14,19,23,27,31-octamethyl-dotriaconta-6,8,10,12,14,16,18,20,22,24,26-undecaene (CCD ID: H4X) (formula: $C_{42}H_{64}O_2$).



Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			44	42	2	
23	E	1	Total	C	O	0
			44	42	2	
23	G	1	Total	C	O	0
			44	42	2	
23	K	1	Total	C	O	0
			44	42	2	
23	K	1	Total	C	O	0
			44	42	2	
23	O	1	Total	C	O	0
			44	42	2	
23	O	1	Total	C	O	0
			44	42	2	
23	P	1	Total	C	O	0
			44	42	2	

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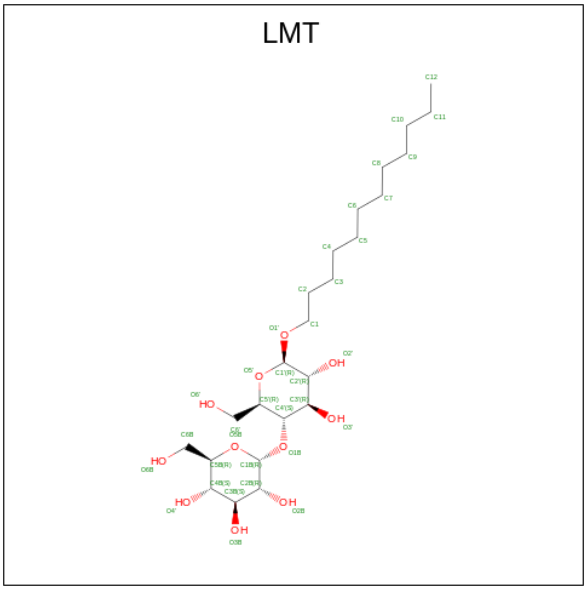
Mol	Chain	Residues	Atoms	AltConf
23	Q	1	Total C O 44 42 2	0
23	U	1	Total C O 44 42 2	0
23	V	1	Total C O 44 42 2	0
23	Z	1	Total C O 44 42 2	0
23	2	1	Total C O 44 42 2	0
23	4	1	Total C O 44 42 2	0
23	5	1	Total C O 44 42 2	0
23	6	1	Total C O 44 42 2	0
23	7	1	Total C O 44 42 2	0

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



Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total C O 35 24 11	0
24	B	1	Total C O 35 24 11	0

Continued on next page...

Continued from previous page...

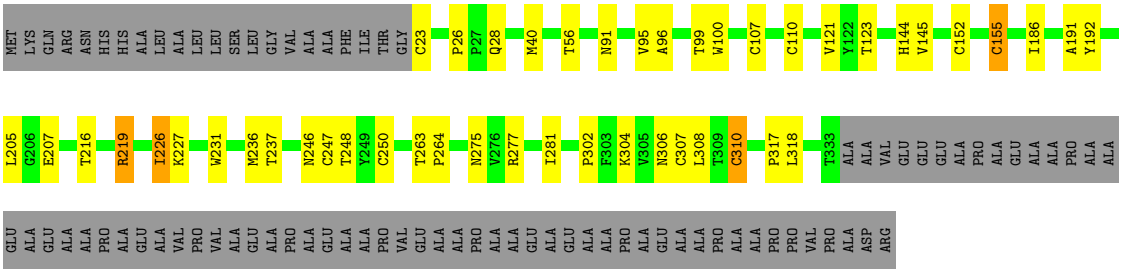
Mol	Chain	Residues	Atoms			AltConf
24	E	1	Total	C	O	0
			35	24	11	
24	G	1	Total	C	O	0
			35	24	11	
24	J	1	Total	C	O	0
			35	24	11	
24	N	1	Total	C	O	0
			35	24	11	
24	P	1	Total	C	O	0
			35	24	11	
24	R	1	Total	C	O	0
			35	24	11	
24	T	1	Total	C	O	0
			35	24	11	
24	V	1	Total	C	O	0
			35	24	11	
24	X	1	Total	C	O	0
			35	24	11	
24	Z	1	Total	C	O	0
			35	24	11	
24	2	1	Total	C	O	0
			35	24	11	
24	4	1	Total	C	O	0
			35	24	11	
24	6	1	Total	C	O	0
			35	24	11	
24	8	1	Total	C	O	0
			35	24	11	
24	8	1	Total	C	O	0
			35	24	11	
24	0	1	Total	C	O	0
			35	24	11	

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

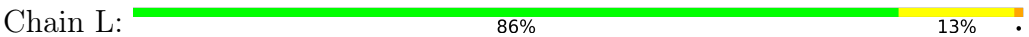
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

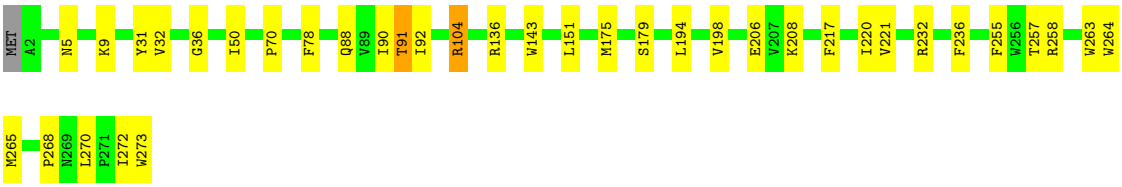
Chain C:



• Molecule 2: L subunit of the reaction center

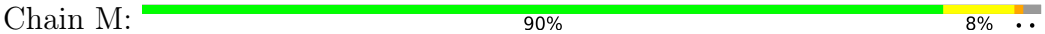
Chain L:





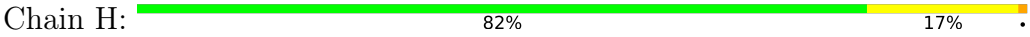
• Molecule 3: Reaction center protein M chain

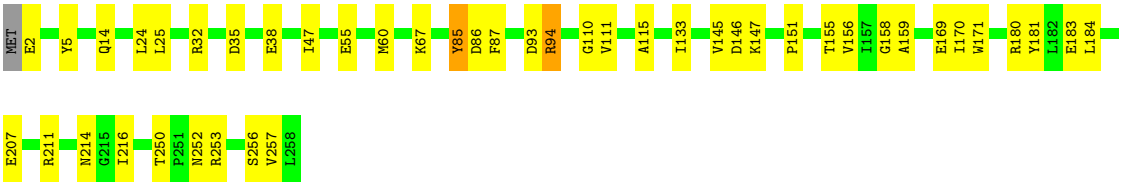
Chain M:



• Molecule 4: Photosynthetic reaction center, subunit H, bacterial

Chain H:



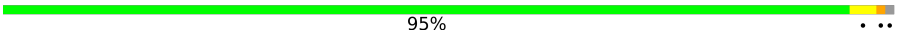


• Molecule 5: Alpha subunit 1 of light-harvesting 1 complex

Chain A:

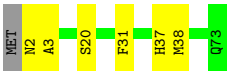
• Molecule 5: Alpha subunit 1 of light-harvesting 1 complex

Chain D:



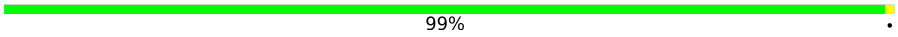
• Molecule 5: Alpha subunit 1 of light-harvesting 1 complex

Chain F:



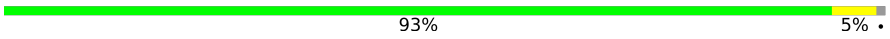
• Molecule 5: Alpha subunit 1 of light-harvesting 1 complex

Chain I:



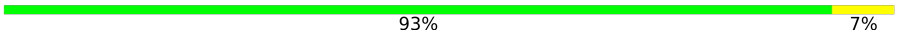
• Molecule 5: Alpha subunit 1 of light-harvesting 1 complex

Chain K:



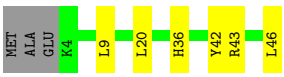
• Molecule 5: Alpha subunit 1 of light-harvesting 1 complex

Chain O:



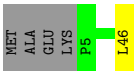
• Molecule 6: Antenna complex alpha/beta subunit

Chain B:



• Molecule 6: Antenna complex alpha/beta subunit

Chain P:

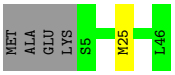


• Molecule 6: Antenna complex alpha/beta subunit

Chain 4:

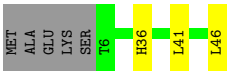
• Molecule 7: Antenna complex alpha/beta subunit

Chain E:



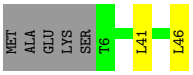
• Molecule 7: Antenna complex alpha/beta subunit

Chain G:



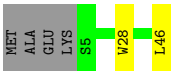
• Molecule 7: Antenna complex alpha/beta subunit

Chain J:



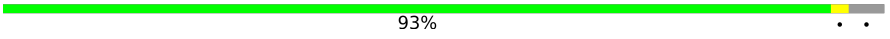
• Molecule 7: Antenna complex alpha/beta subunit

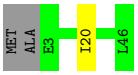
Chain N:



• Molecule 7: Antenna complex alpha/beta subunit

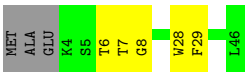
Chain R:





• Molecule 7: Antenna complex alpha/beta subunit

Chain T:



• Molecule 7: Antenna complex alpha/beta subunit

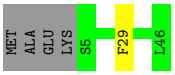
Chain V:

• Molecule 7: Antenna complex alpha/beta subunit

Chain X:

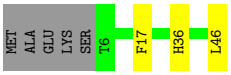
• Molecule 7: Antenna complex alpha/beta subunit

Chain Z:



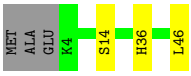
• Molecule 7: Antenna complex alpha/beta subunit

Chain 2:



• Molecule 7: Antenna complex alpha/beta subunit

Chain 6:

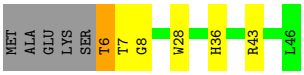


• Molecule 7: Antenna complex alpha/beta subunit

Chain 8:

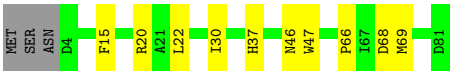
• Molecule 7: Antenna complex alpha/beta subunit

Chain 0:



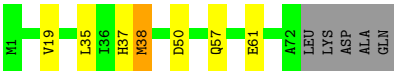
• Molecule 8: Antenna complex alpha/beta subunit

Chain Q:



• Molecule 9: LHC domain-containing protein

Chain S:



• Molecule 9: LHC domain-containing protein

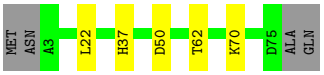
Chain U:

• Molecule 9: LHC domain-containing protein

Chain W:

• Molecule 9: LHC domain-containing protein

Chain Y:

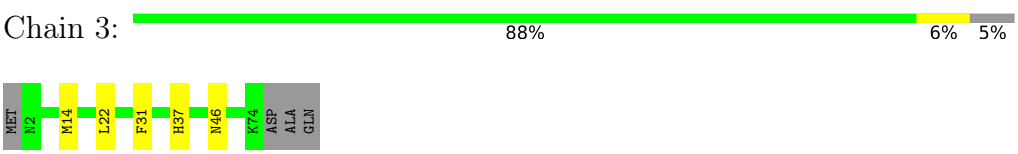


• Molecule 9: LHC domain-containing protein

Chain 1:

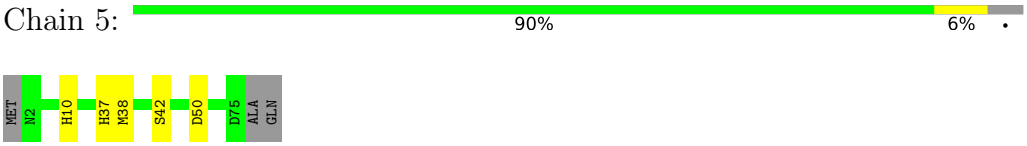
• Molecule 9: LHC domain-containing protein

Chain 3:



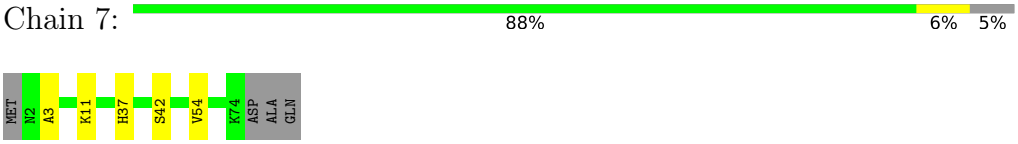
• Molecule 9: LHC domain-containing protein

Chain 5:



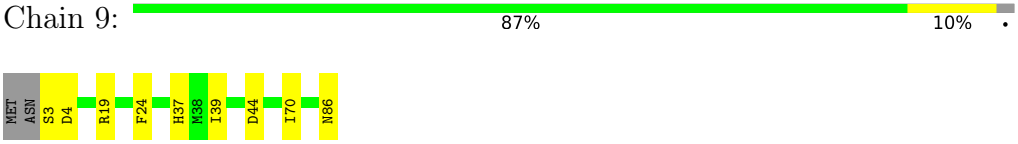
• Molecule 9: LHC domain-containing protein

Chain 7:



• Molecule 10: Alpha subunit 2 of light-harvesting 1 complex

Chain 9:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	105234	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H4X, FE, HEM, BPH, MG, UQ8, CA, PGV, 8K6, BCL, CDL, DGA, 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	C	0.75	3/2503 (0.1%)	0.95	7/3423 (0.2%)
2	L	0.67	1/2244 (0.0%)	0.92	5/3068 (0.2%)
3	M	0.63	0/2633	0.90	4/3599 (0.1%)
4	H	0.49	0/2069	0.87	3/2811 (0.1%)
5	A	0.67	0/579	0.83	0/787
5	D	0.62	0/596	0.85	1/810 (0.1%)
5	F	0.64	1/596 (0.2%)	0.79	0/810
5	I	0.56	0/604	0.76	0/820
5	K	0.57	0/596	0.76	0/810
5	O	0.64	0/604	0.81	0/820
6	4	0.59	0/374	0.67	0/506
6	B	1.07	3/365 (0.8%)	0.91	2/494 (0.4%)
6	P	0.58	0/356	0.70	0/482
7	0	0.64	0/349	0.83	1/474 (0.2%)
7	2	0.51	0/349	0.63	0/474
7	6	0.60	0/364	0.67	0/493
7	8	0.63	0/355	0.74	1/482 (0.2%)
7	E	0.62	0/355	0.66	0/482
7	G	0.62	0/349	0.65	0/474
7	J	0.60	0/349	0.71	1/474 (0.2%)
7	N	0.58	0/355	0.64	0/482
7	R	0.60	0/373	0.70	0/505
7	T	0.56	0/364	0.64	0/493
7	V	0.57	0/364	0.73	0/493
7	X	0.55	0/349	0.67	0/474
7	Z	0.53	0/355	0.61	0/482
8	Q	0.51	0/649	0.78	0/881
9	1	0.64	1/592 (0.2%)	0.74	0/805
9	3	0.57	0/600	0.76	0/816
9	5	0.61	0/605	0.73	0/823
9	7	0.67	0/600	0.95	2/816 (0.2%)
9	S	0.63	0/595	0.84	1/808 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	U	0.64	1/592 (0.2%)	0.75	0/805
9	W	0.59	0/600	0.75	0/816
9	Y	0.57	0/600	0.75	0/816
10	9	0.52	0/690	0.94	0/941
All	All	0.63	10/24872 (0.0%)	0.82	28/33849 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
5	A	0	1
5	K	0	1
7	0	0	1
9	1	0	1
All	All	0	5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	219	ARG	CZ-NH1	20.04	1.59	1.33
6	B	42	TYR	CZ-OH	14.18	1.61	1.37
1	C	219	ARG	NE-CZ	11.86	1.48	1.33
6	B	42	TYR	CE2-CZ	6.24	1.46	1.38
6	B	42	TYR	CD2-CE2	5.96	1.48	1.39
9	U	43	SER	CA-CB	-5.27	1.45	1.52
9	1	68	GLU	CD-OE2	5.15	1.31	1.25
2	L	179	SER	CA-CB	-5.07	1.45	1.52
1	C	219	ARG	CD-NE	5.06	1.55	1.46
5	F	20	SER	CB-OG	-5.00	1.35	1.42

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	219	ARG	NE-CZ-NH1	-13.16	113.72	120.30
1	C	219	ARG	NE-CZ-NH2	10.65	125.63	120.30
3	M	216	PHE	CB-CG-CD1	10.00	127.80	120.80
6	B	43	ARG	NE-CZ-NH2	-7.75	116.42	120.30
9	7	3	ALA	N-CA-CB	-7.72	99.29	110.10
7	J	41	LEU	CB-CG-CD1	7.27	123.36	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	160	LEU	CB-CG-CD1	-6.63	99.73	111.00
2	L	136	ARG	NE-CZ-NH1	6.29	123.44	120.30
6	B	42	TYR	CG-CD1-CE1	6.22	126.28	121.30
1	C	186	ILE	C-N-CA	-6.14	109.41	122.30
1	C	155	CYS	CB-CA-C	-6.13	98.14	110.40
7	0	43	ARG	NE-CZ-NH2	-5.89	117.36	120.30
3	M	160	LEU	CA-CB-CG	5.79	128.63	115.30
4	H	94	ARG	CD-NE-CZ	5.63	131.48	123.60
5	D	37	HIS	CG-ND1-CE1	5.50	115.90	108.20
1	C	310	CYS	CB-CA-C	-5.35	99.70	110.40
1	C	246	ASN	CB-CA-C	-5.33	99.74	110.40
4	H	85	TYR	CD1-CE1-CZ	-5.32	115.01	119.80
9	S	38	MET	CG-SD-CE	5.32	108.71	100.20
4	H	85	TYR	CB-CA-C	5.32	121.03	110.40
2	L	104	ARG	CG-CD-NE	-5.31	100.64	111.80
1	C	219	ARG	CD-NE-CZ	5.28	131.00	123.60
2	L	232	ARG	NE-CZ-NH2	-5.19	117.70	120.30
9	7	54	VAL	CA-CB-CG1	5.19	118.68	110.90
2	L	5	ASN	CB-CA-C	-5.12	100.17	110.40
7	8	20	ILE	CG1-CB-CG2	-5.03	100.34	111.40
2	L	91	THR	OG1-CB-CG2	-5.02	98.46	110.00
3	M	216	PHE	CB-CG-CD2	-5.01	117.29	120.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	0	6	THR	Peptide
9	1	15	ILE	Mainchain
5	A	68	GLU	Mainchain
1	C	219	ARG	Sidechain
5	K	42	SER	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2433	0	2339	58	0
2	L	2161	0	2138	31	0
3	M	2535	0	2502	23	0
4	H	2017	0	2015	39	0
5	A	563	0	565	7	0
5	D	580	0	579	2	0
5	F	580	0	579	4	0
5	I	588	0	591	1	0
5	K	580	0	579	7	0
5	O	588	0	591	6	0
6	4	361	0	354	3	0
6	B	352	0	348	4	0
6	P	343	0	336	1	0
7	0	337	0	332	10	0
7	2	337	0	332	3	0
7	6	352	0	350	3	0
7	8	343	0	337	5	0
7	E	343	0	337	1	0
7	G	337	0	332	3	0
7	J	337	0	332	1	0
7	N	343	0	337	2	0
7	R	361	0	356	2	0
7	T	352	0	350	4	0
7	V	352	0	350	3	0
7	X	337	0	332	0	0
7	Z	343	0	337	1	0
8	Q	628	0	617	8	0
9	1	576	0	578	5	0
9	3	584	0	584	5	0
9	5	589	0	586	5	0
9	7	584	0	584	3	0
9	S	579	0	583	8	0
9	U	576	0	578	4	0
9	W	584	0	582	4	0
9	Y	584	0	582	6	0
10	9	668	0	673	8	0
11	C	172	0	120	30	0
12	C	1	0	0	0	0
13	1	1	0	0	0	0
13	3	1	0	0	0	0
13	5	1	0	0	0	0
13	7	1	0	0	0	0
13	9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	1	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	F	1	0	0	0	0
13	I	1	0	0	0	0
13	K	1	0	0	0	0
13	O	1	0	0	0	0
13	Q	1	0	0	0	0
13	S	1	0	0	0	0
13	U	1	0	0	0	0
13	W	1	0	0	0	0
13	Y	1	0	0	0	0
14	C	32	0	45	6	0
15	1	26	0	25	0	0
15	3	47	0	65	4	0
15	5	47	0	65	4	0
15	9	47	0	65	2	0
15	A	23	0	18	0	0
15	C	16	0	11	0	0
15	D	43	0	59	0	0
15	F	71	0	83	2	0
15	H	36	0	42	1	0
15	I	41	0	53	0	0
15	K	98	0	117	3	0
15	L	47	0	62	3	0
15	M	39	0	48	1	0
15	O	44	0	61	5	0
15	Q	38	0	46	1	0
15	Y	27	0	27	6	0
16	1	66	0	74	6	0
16	2	66	0	74	4	0
16	3	132	0	148	14	0
16	5	132	0	148	11	0
16	7	127	0	135	9	0
16	9	132	0	148	9	0
16	A	66	0	74	9	0
16	B	66	0	74	4	0
16	D	132	0	148	8	0
16	F	132	0	148	10	0
16	I	66	0	74	4	0
16	J	66	0	73	4	0
16	K	132	0	147	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	L	132	0	148	5	0
16	M	132	0	148	7	0
16	O	132	0	147	8	0
16	Q	132	0	147	12	0
16	S	66	0	74	6	0
16	T	66	0	74	4	0
16	U	132	0	147	9	0
16	W	66	0	74	3	0
16	X	66	0	74	4	0
16	Y	132	0	148	8	0
17	L	65	0	76	7	0
17	M	65	0	76	7	0
18	L	66	0	78	8	0
19	5	15	0	29	0	0
19	L	18	0	38	1	0
20	M	1	0	0	0	0
21	M	53	0	72	2	0
22	H	73	0	90	3	0
22	S	74	0	95	1	0
22	Y	30	0	17	0	0
23	2	44	0	0	0	0
23	4	44	0	0	0	0
23	5	44	0	0	0	0
23	6	44	0	0	0	0
23	7	44	0	0	0	0
23	B	44	0	0	0	0
23	E	44	0	0	1	0
23	G	44	0	0	0	0
23	K	88	0	0	1	0
23	O	88	0	0	1	0
23	P	44	0	0	0	0
23	Q	44	0	0	0	0
23	U	44	0	0	0	0
23	V	44	0	0	0	0
23	Z	44	0	0	0	0
24	0	35	0	46	1	0
24	2	35	0	46	2	0
24	4	35	0	46	3	0
24	6	35	0	46	2	0
24	8	70	0	92	5	0
24	B	70	0	92	3	0
24	E	35	0	46	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	G	35	0	46	1	0
24	J	35	0	46	2	0
24	N	35	0	46	3	0
24	P	35	0	46	2	0
24	R	35	0	46	2	0
24	T	35	0	46	2	0
24	V	35	0	46	1	0
24	X	35	0	46	2	0
24	Z	35	0	46	1	0
All	All	29228	0	28934	406	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 (406) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:CYS:SG	11:C:403:HEM:HAB	1.52	1.47
1:C:247:CYS:SG	11:C:403:HEM:CAB	2.07	1.42
1:C:307:CYS:SG	11:C:404:HEM:HAB	1.66	1.36
1:C:155:CYS:SG	11:C:402:HEM:HAC	1.73	1.29
1:C:310:CYS:SG	11:C:404:HEM:CAC	2.28	1.21
1:C:307:CYS:SG	11:C:404:HEM:CAB	2.28	1.20
1:C:310:CYS:SG	11:C:404:HEM:HAC	1.93	1.07
1:C:250:CYS:SG	11:C:403:HEM:CAC	2.45	1.03
1:C:110:CYS:SG	11:C:401:HEM:HAC	1.99	1.01
1:C:155:CYS:SG	11:C:402:HEM:CAC	2.51	0.99
1:C:250:CYS:SG	11:C:403:HEM:CBC	2.54	0.96
17:M:404:BPH:HHC	17:M:404:BPH:HBB3	1.49	0.93
1:C:247:CYS:SG	11:C:403:HEM:CBB	2.57	0.93
1:C:152:CYS:SG	11:C:402:HEM:HAB	2.09	0.92
4:H:94:ARG:HD2	7:0:8:GLY:HA3	1.50	0.91
4:H:47:ILE:HG21	6:B:9:LEU:HD11	1.54	0.90
1:C:152:CYS:SG	11:C:402:HEM:CAB	2.60	0.90
16:M:403:BCL:HMB1	16:M:403:BCL:HBB3	1.53	0.88
16:L:301:BCL:HMB1	16:L:301:BCL:HBB3	1.54	0.86
1:C:307:CYS:CB	11:C:404:HEM:HAB	2.05	0.86
16:L:301:BCL:HMB1	16:L:301:BCL:CBB	2.06	0.85
16:M:403:BCL:HMB1	16:M:403:BCL:CBB	2.07	0.85
17:L:302:BPH:HHC	17:L:302:BPH:CBB	2.07	0.84
7:8:18:HIS:HE2	24:8:101:LMT:H6D	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:CYS:HB3	11:C:401:HEM:HAB	1.59	0.83
4:H:93:ASP:OD2	10:9:19:ARG:NH1	2.10	0.83
1:C:144:HIS:HD1	1:C:275:ASN:HD22	1.27	0.82
21:M:405:MQ8:H501	22:H:302:CDL:H631	1.63	0.80
16:9:103:BCL:CBB	16:9:103:BCL:HMB1	2.13	0.79
4:H:94:ARG:HD2	7:0:8:GLY:CA	2.11	0.79
1:C:110:CYS:SG	11:C:401:HEM:CAC	2.71	0.78
3:M:73:LEU:HD11	9:S:35:LEU:HD12	1.64	0.78
2:L:88:GLN:CD	18:L:306:UQ8:H4M	2.04	0.78
17:L:302:BPH:HHC	17:L:302:BPH:HBB3	1.63	0.77
16:S:103:BCL:CBB	16:S:103:BCL:HMB1	2.14	0.77
4:H:94:ARG:CD	7:0:8:GLY:HA3	2.14	0.77
16:I:102:BCL:HBB3	16:I:102:BCL:HMB1	1.66	0.76
16:U:102:BCL:CBB	16:U:102:BCL:HMB1	2.16	0.76
1:C:307:CYS:SG	11:C:404:HEM:CBB	2.74	0.75
1:C:107:CYS:CB	11:C:401:HEM:HAB	2.17	0.75
16:U:102:BCL:HMB1	16:U:102:BCL:HBB3	1.68	0.75
2:L:31:TYR:O	2:L:104:ARG:NH1	2.21	0.73
2:L:198:VAL:HG23	2:L:208:LYS:HB2	1.69	0.73
4:H:47:ILE:HG21	6:B:9:LEU:CD1	2.18	0.73
2:L:272:ILE:HA	9:W:39:VAL:HG22	1.71	0.73
16:W:102:BCL:HMB1	16:W:102:BCL:HBB3	1.69	0.73
16:M:402:BCL:HMB1	16:M:402:BCL:HBB2	1.68	0.72
16:J:101:BCL:CBB	16:J:101:BCL:HMB1	2.20	0.72
15:F:104:PGV:H21	15:F:104:PGV:H202	1.70	0.71
16:K:108:BCL:HMB1	16:K:108:BCL:CBB	2.21	0.71
16:9:103:BCL:ND	24:0:101:LMT:H101	2.06	0.71
16:D:103:BCL:HMB1	16:D:103:BCL:CBB	2.21	0.70
16:W:102:BCL:HMB1	16:W:102:BCL:CBB	2.20	0.70
1:C:250:CYS:SG	11:C:403:HEM:HAC	2.32	0.70
1:C:145:VAL:HG23	1:C:145:VAL:O	1.92	0.69
16:J:101:BCL:HMB1	16:J:101:BCL:HBB3	1.74	0.69
16:A:102:BCL:CBB	16:A:102:BCL:HMB1	2.22	0.68
16:I:102:BCL:HMB1	16:I:102:BCL:CBB	2.22	0.68
16:9:103:BCL:HMB1	16:9:103:BCL:HBB3	1.75	0.68
1:C:23:CYS:HA	14:C:407:DGA:HG2	1.76	0.68
2:L:92:ILE:HG21	18:L:306:UQ8:H15B	1.75	0.67
3:M:73:LEU:HD11	9:S:35:LEU:CD1	2.23	0.67
5:K:38:MET:HE3	15:K:101:PGV:H51	1.77	0.67
21:M:405:MQ8:C50	22:H:302:CDL:H631	2.24	0.67
16:K:105:BCL:CBB	16:K:105:BCL:HMB1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:PRO:HG2	10:9:70:ILE:HD13	1.75	0.66
9:5:37:HIS:CE1	16:5:104:BCL:HMD1	2.30	0.66
16:S:103:BCL:HMB1	16:S:103:BCL:HBB3	1.78	0.66
16:D:103:BCL:ND	24:E:102:LMT:H101	2.11	0.65
16:3:104:BCL:CBB	16:3:104:BCL:HMB1	2.26	0.65
9:5:10:HIS:O	7:6:14:SER:OG	2.14	0.65
2:L:220:ILE:HG22	2:L:221:VAL:HG23	1.79	0.64
17:M:404:BPH:HHC	17:M:404:BPH:CBB	2.25	0.64
16:Q:104:BCL:CBB	16:Q:104:BCL:HMB1	2.28	0.64
16:1:102:BCL:CBB	16:1:102:BCL:HMB1	2.28	0.64
2:L:206:GLU:HG2	4:H:67:LYS:HD3	1.80	0.64
1:C:263:THR:HG22	10:9:86:ASN:HD21	1.62	0.64
14:C:407:DGA:HB41	15:Y:105:PGV:H011	1.80	0.64
5:A:26:PHE:HE1	16:A:102:BCL:H52	1.62	0.64
3:M:241:ARG:NH1	4:H:38:GLU:OE1	2.32	0.63
4:H:94:ARG:HB3	7:0:8:GLY:HA3	1.78	0.63
16:K:108:BCL:HMB1	16:K:108:BCL:HBB3	1.79	0.63
16:7:103:BCL:CBB	16:7:103:BCL:HMB1	2.29	0.63
18:L:306:UQ8:H1MA	18:L:306:UQ8:H10	1.79	0.62
5:F:37:HIS:CE1	16:F:105:BCL:HMD1	2.33	0.62
7:J:46:LEU:HD13	24:N:101:LMT:H42	1.79	0.62
1:C:100:TRP:HB3	1:C:152:CYS:HB2	1.80	0.62
2:L:236:PHE:HB2	15:L:305:PGV:H281	1.82	0.62
9:U:37:HIS:CE1	16:U:103:BCL:HMD1	2.34	0.62
16:W:102:BCL:ND	24:X:102:LMT:H101	2.15	0.62
10:9:37:HIS:CE1	16:9:104:BCL:HMD1	2.35	0.62
5:A:26:PHE:CE1	16:A:102:BCL:H52	2.35	0.61
5:A:37:HIS:CE1	16:B:103:BCL:HMD1	2.35	0.61
9:3:37:HIS:CE1	16:3:104:BCL:HMD1	2.35	0.61
4:H:146:ASP:O	4:H:147:LYS:HB2	2.00	0.61
4:H:94:ARG:NH1	7:0:8:GLY:O	2.33	0.61
16:A:102:BCL:ND	24:B:104:LMT:H101	2.16	0.60
16:1:102:BCL:HMB1	16:1:102:BCL:HBB2	1.84	0.60
16:7:102:BCL:HMB1	16:7:102:BCL:HBB3	1.83	0.60
1:C:207:GLU:HG2	1:C:277:ARG:HD3	1.83	0.60
15:Q:101:PGV:H202	22:S:101:CDL:HA62	1.84	0.60
16:2:102:BCL:CBB	16:2:102:BCL:HMB1	2.31	0.60
16:D:103:BCL:HMB1	16:D:103:BCL:HBB3	1.84	0.60
1:C:121:VAL:HG12	1:C:123:THR:H	1.66	0.59
16:2:102:BCL:HMB1	16:2:102:BCL:HBB3	1.85	0.59
16:U:103:BCL:HMB1	16:U:103:BCL:CBB	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:104:BCL:HMB1	16:3:104:BCL:HBB3	1.84	0.59
6:P:46:LEU:HD13	24:R:101:LMT:H42	1.83	0.59
2:L:104:ARG:NH2	3:M:255:CYS:O	2.34	0.58
5:I:37:HIS:CE1	16:J:101:BCL:HMD1	2.38	0.58
16:O:105:BCL:CBB	16:O:105:BCL:HMB1	2.34	0.58
15:M:406:PGV:H42	5:O:38:MET:SD	2.44	0.58
16:X:101:BCL:HMB1	16:X:101:BCL:HBB3	1.85	0.57
9:5:38:MET:HG3	15:5:101:PGV:H231	1.85	0.57
16:S:103:BCL:ND	24:T:102:LMT:H101	2.19	0.57
7:T:6:THR:HG22	7:T:8:GLY:H	1.70	0.57
16:K:105:BCL:HMB1	16:K:105:BCL:HBB3	1.86	0.57
14:C:407:DGA:HG11	14:C:407:DGA:HA42	1.86	0.57
16:Q:103:BCL:ND	24:R:101:LMT:H101	2.20	0.57
3:M:73:LEU:CD1	9:S:35:LEU:HD12	2.33	0.57
9:W:37:HIS:CE1	16:X:101:BCL:HMD1	2.40	0.57
16:X:101:BCL:HMB1	16:X:101:BCL:CBB	2.34	0.57
15:3:101:PGV:O12	15:3:101:PGV:O06	2.16	0.57
16:F:105:BCL:CBB	16:F:105:BCL:HMB1	2.34	0.57
9:Y:37:HIS:CE1	16:Y:104:BCL:HMD1	2.40	0.56
2:L:255:PHE:HZ	15:3:101:PGV:H212	1.71	0.56
15:5:101:PGV:H51	15:5:101:PGV:O01	2.05	0.56
1:C:227:LYS:O	1:C:231:TRP:HD1	1.88	0.56
16:O:105:BCL:H42	16:Q:103:BCL:H171	1.88	0.55
1:C:307:CYS:CA	11:C:404:HEM:HAB	2.36	0.55
18:L:306:UQ8:H4MA	18:L:306:UQ8:H3MB	1.88	0.55
4:H:24:LEU:O	4:H:25:LEU:HB3	2.06	0.55
16:A:102:BCL:HMB1	16:A:102:BCL:HBB3	1.89	0.55
1:C:247:CYS:HG	11:C:403:HEM:CAB	2.13	0.55
15:5:101:PGV:H91	15:5:101:PGV:H202	1.89	0.54
9:5:42:SER:O	15:5:101:PGV:H061	2.07	0.54
1:C:191:ALA:HB3	1:C:237:THR:CG2	2.37	0.54
3:M:53:LEU:O	8:Q:20:ARG:NH1	2.41	0.54
5:O:37:HIS:CE1	16:O:105:BCL:HMD1	2.43	0.54
16:M:402:BCL:H11	17:M:404:BPH:H203	1.89	0.54
1:C:192:TYR:HB3	2:L:265:MET:CE	2.37	0.54
3:M:101:ALA:HB3	8:Q:66:PRO:HB3	1.89	0.54
16:Y:102:BCL:HMB1	16:Y:102:BCL:HBB3	1.89	0.54
5:K:37:HIS:CE1	16:K:108:BCL:HMD1	2.43	0.53
16:F:103:BCL:CBB	16:F:103:BCL:HMB1	2.38	0.53
16:O:104:BCL:ND	24:P:102:LMT:H101	2.23	0.53
16:A:102:BCL:C1D	24:B:104:LMT:H101	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:304:BCL:CBB	16:L:304:BCL:HMB1	2.38	0.53
7:G:46:LEU:HD13	24:J:102:LMT:H42	1.91	0.53
16:Q:103:BCL:HMB1	16:Q:103:BCL:HBB3	1.90	0.53
1:C:26:PRO:HG2	15:3:101:PGV:H201	1.91	0.53
3:M:55:GLY:HA3	15:O:102:PGV:H012	1.91	0.53
16:Q:103:BCL:HMB1	16:Q:103:BCL:CBB	2.39	0.53
16:Q:104:BCL:HMB1	16:Q:104:BCL:HBB3	1.91	0.53
4:H:250:THR:HB	4:H:253:ARG:HG3	1.91	0.53
9:W:58:LEU:HD11	9:Y:70:LYS:HG3	1.91	0.53
16:1:102:BCL:ND	24:2:103:LMT:H101	2.24	0.53
9:1:37:HIS:CE1	16:2:102:BCL:HMD1	2.44	0.52
16:3:103:BCL:HMB1	16:3:103:BCL:HBB3	1.91	0.52
16:7:102:BCL:ND	24:8:102:LMT:H101	2.23	0.52
16:F:103:BCL:ND	24:G:102:LMT:H101	2.24	0.52
5:A:49:ASP:OD1	10:9:44:ASP:N	2.43	0.52
5:O:31:PHE:CE2	15:O:102:PGV:H281	2.45	0.52
15:Y:105:PGV:H62	15:Y:105:PGV:H201	1.90	0.52
5:A:6:PHE:CE1	24:B:102:LMT:H6E	2.45	0.52
16:U:102:BCL:ND	24:V:102:LMT:H101	2.24	0.52
4:H:155:THR:OG1	4:H:207:GLU:OE1	2.24	0.51
4:H:94:ARG:O	7:0:7:THR:O	2.28	0.51
17:L:302:BPH:H121	16:L:304:BCL:H172	1.93	0.51
5:D:57:GLN:O	5:D:61:GLU:HG2	2.10	0.51
9:7:37:HIS:CE1	16:7:103:BCL:HMD1	2.45	0.51
23:O:106:H4X:C6	7:R:20:ILE:HD12	2.41	0.51
17:L:302:BPH:HHC	17:L:302:BPH:HBB2	1.90	0.51
16:S:103:BCL:H142	7:T:28:TRP:HZ3	1.75	0.51
16:Y:104:BCL:HMB1	16:Y:104:BCL:HBB3	1.92	0.51
16:5:104:BCL:CBB	16:5:104:BCL:HMB1	2.41	0.51
16:Y:104:BCL:HMB1	16:Y:104:BCL:CBB	2.41	0.51
16:7:102:BCL:HMB1	16:7:102:BCL:CBB	2.40	0.51
1:C:100:TRP:HE3	1:C:152:CYS:HG	1.57	0.51
1:C:216:THR:HB	4:H:5:TYR:CZ	2.46	0.51
7:8:18:HIS:HE2	24:8:101:LMT:C6'	2.19	0.51
16:S:103:BCL:HMB1	16:S:103:BCL:HBB2	1.91	0.50
16:5:103:BCL:ND	24:6:102:LMT:H101	2.27	0.50
7:V:6:THR:HG22	7:V:8:GLY:H	1.77	0.50
16:Y:102:BCL:HMB1	16:Y:102:BCL:CBB	2.42	0.50
16:5:103:BCL:CBB	16:5:103:BCL:HMB1	2.41	0.50
3:M:37:SER:HB3	3:M:40:LEU:HB2	1.94	0.50
4:H:146:ASP:O	4:H:147:LYS:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:16:MET:CE	5:O:23:TRP:CZ2	2.95	0.50
4:H:151:PRO:HD2	4:H:170:ILE:HD11	1.92	0.49
1:C:96:ALA:HA	1:C:99:THR:HG22	1.94	0.49
4:H:85:TYR:OH	4:H:110:GLY:HA3	2.12	0.49
2:L:273:TRP:CD1	2:L:273:TRP:C	2.86	0.49
2:L:273:TRP:CD1	3:M:88:LYS:HB2	2.47	0.49
3:M:127:LEU:HB3	15:O:102:PGV:H331	1.93	0.49
4:H:145:VAL:HG12	4:H:146:ASP:O	2.13	0.49
16:K:105:BCL:C1D	24:N:101:LMT:H101	2.43	0.49
9:S:37:HIS:CE1	16:T:101:BCL:HMD1	2.48	0.49
1:C:310:CYS:SG	11:C:404:HEM:CBC	2.98	0.49
4:H:85:TYR:OH	4:H:110:GLY:O	2.30	0.49
5:K:16:MET:HE1	5:O:23:TRP:CZ2	2.48	0.49
5:K:38:MET:CE	15:K:101:PGV:H51	2.42	0.49
16:O:104:BCL:H62	16:O:104:BCL:H41	1.47	0.49
16:7:103:BCL:HMB1	16:7:103:BCL:HBB3	1.95	0.48
17:M:404:BPH:HBC3	17:M:404:BPH:HHD	1.94	0.48
2:L:9:LYS:HE2	4:H:115:ALA:HB1	1.95	0.48
2:L:143:TRP:NE1	18:L:306:UQ8:H4MB	2.28	0.48
17:M:404:BPH:CBB	17:M:404:BPH:CHC	2.92	0.48
16:U:103:BCL:HMB1	16:U:103:BCL:HBB3	1.94	0.48
4:H:171:TRP:HB2	4:H:181:TYR:HB2	1.95	0.48
8:Q:15:PHE:HD1	9:S:19:VAL:HG22	1.77	0.48
16:3:103:BCL:HMB1	16:3:103:BCL:CBB	2.43	0.48
1:C:247:CYS:SG	11:C:403:HEM:HBB1	2.52	0.48
8:Q:30:ILE:HG13	16:Q:103:BCL:H43	1.96	0.48
1:C:110:CYS:HA	1:C:123:THR:OG1	2.13	0.48
5:K:38:MET:SD	15:K:101:PGV:H31	2.54	0.47
1:C:250:CYS:SG	11:C:403:HEM:HBC1	2.50	0.47
16:F:105:BCL:HMB1	16:F:105:BCL:HBB3	1.96	0.47
16:A:102:BCL:H8	16:A:102:BCL:H51	1.57	0.47
9:3:46:ASN:HD21	15:3:101:PGV:H041	1.78	0.47
10:9:3:SER:OG	10:9:4:ASP:N	2.47	0.47
2:L:268:PRO:HA	2:L:273:TRP:HE1	1.80	0.47
2:L:273:TRP:HB2	3:M:84:ARG:HG3	1.95	0.47
4:H:252:ASN:HD21	6:4:3:GLU:HA	1.79	0.47
16:A:102:BCL:HMD1	6:B:36:HIS:CE1	2.49	0.47
16:Q:103:BCL:H111	16:Q:103:BCL:H72	1.53	0.47
16:3:103:BCL:ND	24:4:102:LMT:H101	2.29	0.47
16:5:103:BCL:HMB1	16:5:103:BCL:HBB3	1.96	0.47
17:L:302:BPH:H9C3	17:L:302:BPH:H6C1	1.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:305:PGV:O13	3:M:2:PRO:HB3	2.15	0.47
1:C:40:MET:HG2	1:C:248:THR:HB	1.96	0.47
1:C:310:CYS:SG	11:C:404:HEM:C3C	3.05	0.47
16:B:103:BCL:CBB	16:B:103:BCL:HMB1	2.45	0.47
16:S:103:BCL:C1D	24:T:102:LMT:H101	2.45	0.47
15:Y:105:PGV:H241	15:Y:105:PGV:C7	2.45	0.47
7:6:46:LEU:HD13	24:8:102:LMT:H42	1.96	0.47
1:C:306:ASN:HB3	1:C:308:LEU:H	1.81	0.46
5:F:2:ASN:O	5:F:3:ALA:HB3	2.16	0.46
7:V:46:LEU:HD13	24:X:102:LMT:H42	1.97	0.46
7:2:46:LEU:HD13	24:4:102:LMT:H42	1.96	0.46
16:K:105:BCL:H72	16:K:105:BCL:H111	1.54	0.46
16:5:103:BCL:H111	16:5:103:BCL:H71	1.59	0.46
14:C:407:DGA:HB22	14:C:407:DGA:HB51	1.54	0.46
16:F:103:BCL:HMB1	16:F:103:BCL:HBB3	1.98	0.46
8:Q:37:HIS:CE1	16:Q:104:BCL:HMD1	2.50	0.46
16:Q:103:BCL:H202	16:Q:103:BCL:H161	1.84	0.46
3:M:277:ILE:HG13	17:M:404:BPH:HAC2	1.98	0.46
3:M:309:SER:O	3:M:310:GLU:HB3	2.15	0.46
15:Y:105:PGV:C7	15:Y:105:PGV:H222	2.46	0.46
1:C:191:ALA:HB3	1:C:237:THR:HG21	1.97	0.46
16:3:103:BCL:H71	16:3:103:BCL:H111	1.63	0.46
1:C:236:MET:HB3	11:C:403:HEM:C4B	2.50	0.45
2:L:143:TRP:CD1	18:L:306:UQ8:H4MB	2.51	0.45
16:Q:104:BCL:HMB1	16:Q:104:BCL:HBB2	1.98	0.45
16:U:102:BCL:H41	16:U:102:BCL:H62	1.64	0.45
3:M:73:LEU:HD23	3:M:73:LEU:HA	1.80	0.45
2:L:194:LEU:HD22	2:L:217:PHE:HE2	1.81	0.45
16:3:103:BCL:HMD1	6:4:36:HIS:CE1	2.52	0.45
16:O:105:BCL:HMB1	16:O:105:BCL:HBB3	1.98	0.45
16:D:104:BCL:CBB	16:D:104:BCL:HMB1	2.47	0.45
16:Y:102:BCL:ND	24:Z:102:LMT:H101	2.32	0.45
1:C:110:CYS:CB	11:C:401:HEM:HAC	2.46	0.45
15:O:102:PGV:H72	8:Q:22:LEU:HD13	1.98	0.45
16:M:403:BCL:HAA2	16:M:403:BCL:HBD	1.99	0.44
16:9:104:BCL:CBB	16:9:104:BCL:HMB1	2.47	0.44
3:M:264:SER:OG	4:H:35:ASP:OD1	2.26	0.44
16:D:103:BCL:HMB1	16:D:103:BCL:HBB2	1.99	0.44
16:I:102:BCL:C1D	24:J:102:LMT:H101	2.47	0.44
9:7:11:LYS:HE3	7:8:11:GLU:OE2	2.17	0.44
1:C:91:ASN:O	1:C:95:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:169:GLU:HB3	4:H:183:GLU:HB3	1.99	0.44
5:K:38:MET:HE2	23:K:103:H4X:O2	2.18	0.44
16:3:104:BCL:H152	16:3:104:BCL:H112	1.77	0.44
16:5:103:BCL:C1D	24:6:102:LMT:H101	2.48	0.44
3:M:245:ALA:O	3:M:249:MET:HG2	2.18	0.44
15:Y:105:PGV:H42	15:Y:105:PGV:C19	2.47	0.44
16:O:104:BCL:HMB1	16:O:104:BCL:HBB3	2.00	0.44
16:Q:104:BCL:H93	16:Q:104:BCL:H111	1.81	0.44
1:C:192:TYR:HB3	2:L:265:MET:HE1	2.00	0.44
4:H:133:ILE:HD12	4:H:180:ARG:HG3	2.00	0.44
7:N:46:LEU:HD13	24:P:102:LMT:H42	2.00	0.44
4:H:87:PHE:HB2	4:H:111:VAL:CG1	2.47	0.44
16:F:103:BCL:OBB	16:F:103:BCL:HHC	2.17	0.44
16:3:103:BCL:C1D	24:4:102:LMT:H101	2.48	0.44
9:3:22:LEU:HD23	9:3:22:LEU:HA	1.85	0.43
16:L:304:BCL:H11	3:M:210:TYR:HB3	1.98	0.43
16:D:104:BCL:H92	16:D:104:BCL:H62	1.76	0.43
16:5:104:BCL:H93	16:5:104:BCL:H111	1.77	0.43
4:H:14:GLN:NE2	15:H:301:PGV:O13	2.52	0.43
5:F:38:MET:HG2	15:F:104:PGV:H211	1.99	0.43
16:F:103:BCL:HAA2	16:F:103:BCL:HBD	1.99	0.43
16:5:103:BCL:H62	16:5:103:BCL:H41	1.60	0.43
15:9:101:PGV:H291	15:9:101:PGV:H321	1.68	0.43
1:C:56:THR:HB	1:C:318:LEU:HD23	2.00	0.43
4:H:94:ARG:HB3	7:0:7:THR:O	2.18	0.43
5:F:31:PHE:HD1	5:F:31:PHE:HA	1.69	0.43
17:L:302:BPH:O2A	17:L:302:BPH:H4C3	2.18	0.43
4:H:24:LEU:O	4:H:25:LEU:CB	2.64	0.43
16:A:102:BCL:HMB1	16:A:102:BCL:HBB2	1.97	0.43
16:2:102:BCL:H92	16:2:102:BCL:H62	1.77	0.43
15:O:102:PGV:H262	15:O:102:PGV:H231	1.70	0.43
16:5:103:BCL:OBB	16:5:103:BCL:HHC	2.18	0.43
16:7:102:BCL:C1D	24:8:102:LMT:H101	2.48	0.43
18:L:306:UQ8:H25	19:L:307:8K6:H181	2.01	0.43
16:I:102:BCL:H162	16:I:102:BCL:H203	1.76	0.43
10:9:24:PHE:HB2	15:9:101:PGV:H212	2.00	0.43
16:M:403:BCL:HHC	16:M:403:BCL:OBB	2.19	0.43
16:B:103:BCL:HMB1	16:B:103:BCL:HBB3	2.01	0.43
2:L:78:PHE:HB3	9:7:42:SER:OG	2.18	0.42
2:L:175:MET:CE	2:L:264:TRP:CZ2	3.02	0.42
16:1:102:BCL:C1D	24:2:103:LMT:H101	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:0:6:THR:HG23	7:0:8:GLY:N	2.34	0.42
1:C:145:VAL:O	1:C:145:VAL:CG2	2.61	0.42
14:C:407:DGA:HG11	14:C:407:DGA:CA4	2.49	0.42
2:L:50:ILE:HD13	2:L:90:ILE:HD13	2.01	0.42
1:C:302:PRO:O	1:C:304:LYS:NZ	2.51	0.42
16:F:105:BCL:H152	16:F:105:BCL:H112	1.85	0.42
9:W:22:LEU:HD23	9:W:22:LEU:HA	1.87	0.42
16:D:103:BCL:H72	16:D:103:BCL:H111	1.73	0.42
7:G:41:LEU:HD23	7:G:41:LEU:HA	1.90	0.42
9:Y:62:THR:HG22	9:1:73:LEU:CD2	2.49	0.42
1:C:205:LEU:O	1:C:281:ILE:HD11	2.20	0.42
18:L:306:UQ8:H16A	18:L:306:UQ8:H10A	2.01	0.42
4:H:32:ARG:NH1	4:H:35:ASP:OD2	2.53	0.42
2:L:88:GLN:HA	2:L:91:THR:HG22	2.02	0.42
9:Y:22:LEU:HD23	9:Y:22:LEU:HA	1.87	0.42
16:3:103:BCL:HHD	16:3:103:BCL:HAC1	1.91	0.42
16:9:103:BCL:OBB	16:9:103:BCL:HHC	2.19	0.42
2:L:151:LEU:H	2:L:151:LEU:HG	1.72	0.42
9:U:22:LEU:HD23	9:U:22:LEU:HA	1.85	0.42
16:3:104:BCL:H91	16:3:104:BCL:H111	1.83	0.42
3:M:73:LEU:HD12	9:S:38:MET:CE	2.49	0.42
16:T:101:BCL:H92	16:T:101:BCL:H62	1.90	0.42
9:U:47:TRP:CE2	16:U:102:BCL:H2C	2.55	0.42
16:9:103:BCL:H2	7:0:28:TRP:CH2	2.55	0.42
4:H:24:LEU:HG	4:H:25:LEU:H	1.85	0.42
16:K:105:BCL:H43	7:N:28:TRP:CZ2	2.54	0.42
8:Q:46:ASN:OD1	8:Q:47:TRP:N	2.53	0.42
16:T:101:BCL:OBB	16:T:101:BCL:HHC	2.19	0.42
1:C:28:GLN:HG2	2:L:257:THR:HG21	2.02	0.41
1:C:155:CYS:HG	11:C:402:HEM:CAC	2.29	0.41
4:H:156:VAL:HG21	4:H:184:LEU:HD13	2.01	0.41
5:D:37:HIS:CE1	16:D:104:BCL:HMD1	2.54	0.41
16:F:103:BCL:HMD1	7:G:36:HIS:CE1	2.56	0.41
9:5:50:ASP:N	9:5:50:ASP:OD1	2.53	0.41
4:H:158:GLY:O	4:H:159:ALA:HB3	2.20	0.41
16:M:403:BCL:H192	16:M:403:BCL:H161	1.93	0.41
17:M:404:BPH:H6C1	17:M:404:BPH:H4C1	1.46	0.41
7:E:25:MET:HG3	23:E:101:H4X:C20	2.51	0.41
16:1:102:BCL:HMD1	7:2:36:HIS:CE1	2.56	0.41
2:L:32:VAL:O	2:L:36:GLY:HA3	2.19	0.41
4:H:55:GLU:HG3	4:H:60:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:22:LEU:HD23	5:A:22:LEU:HA	1.85	0.41
6:B:46:LEU:HD13	24:E:102:LMT:H42	2.03	0.41
16:K:105:BCL:H62	16:K:105:BCL:H41	1.31	0.41
9:S:57:GLN:O	9:S:61:GLU:HG3	2.19	0.41
16:3:104:BCL:HMB1	16:3:104:BCL:HBB2	2.02	0.41
16:5:103:BCL:HMD1	7:6:36:HIS:CE1	2.56	0.41
2:L:270:LEU:HD23	2:L:270:LEU:HA	1.92	0.41
16:J:101:BCL:H152	16:J:101:BCL:H112	1.94	0.41
16:O:104:BCL:HMB1	16:O:104:BCL:CBB	2.50	0.41
7:T:29:PHE:CE1	16:T:101:BCL:H11	2.55	0.41
16:X:101:BCL:H92	16:X:101:BCL:H62	1.96	0.41
9:S:50:ASP:OD1	9:S:50:ASP:N	2.54	0.41
9:Y:50:ASP:N	9:Y:50:ASP:OD1	2.54	0.41
9:3:31:PHE:HD1	9:3:31:PHE:HA	1.69	0.41
1:C:107:CYS:HB2	11:C:401:HEM:HAB	1.98	0.41
2:L:70:PRO:HG3	2:L:88:GLN:HE21	1.86	0.41
15:L:305:PGV:H131	15:L:305:PGV:H102	1.68	0.41
4:H:93:ASP:OD1	4:H:93:ASP:O	2.39	0.41
16:K:108:BCL:H141	16:K:108:BCL:H162	1.85	0.41
5:O:22:LEU:HD23	5:O:22:LEU:HA	1.82	0.41
9:U:50:ASP:OD1	9:U:50:ASP:N	2.53	0.41
1:C:317:PRO:O	1:C:318:LEU:HB2	2.21	0.41
4:H:158:GLY:O	4:H:214:ASN:HA	2.21	0.41
16:K:105:BCL:ND	24:N:101:LMT:H101	2.35	0.41
7:T:6:THR:HG22	7:T:7:THR:N	2.36	0.41
15:Y:105:PGV:H42	15:Y:105:PGV:O03	2.20	0.41
9:1:50:ASP:N	9:1:50:ASP:OD1	2.54	0.41
3:M:33:LYS:HA	3:M:34:PRO:HD3	1.94	0.40
16:7:103:BCL:H11	7:8:29:PHE:CE1	2.56	0.40
3:M:60:SER:O	3:M:61:LEU:HB2	2.21	0.40
3:M:99:PRO:HG3	8:Q:68:ASP:OD1	2.21	0.40
16:B:103:BCL:H62	16:B:103:BCL:H92	1.88	0.40
7:V:6:THR:HG22	7:V:7:THR:N	2.36	0.40
16:Y:104:BCL:H11	7:Z:29:PHE:CE1	2.56	0.40
10:9:39:ILE:HD13	10:9:39:ILE:HG21	1.85	0.40
16:9:104:BCL:OBB	16:9:104:BCL:HHC	2.21	0.40
1:C:226:ILE:H	1:C:226:ILE:HG12	1.67	0.40
14:C:407:DGA:OG2	2:L:263:TRP:NE1	2.54	0.40
22:H:302:CDL:H141	22:H:302:CDL:H781	2.03	0.40
16:1:102:BCL:H142	16:1:102:BCL:H111	1.89	0.40
7:8:16:GLU:O	7:8:20:ILE:HD12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:194:LEU:HD22	2:L:217:PHE:CE2	2.56	0.40
17:L:302:BPH:H9C1	17:L:302:BPH:H112	1.64	0.40
4:H:2:GLU:N	4:H:2:GLU:OE1	2.54	0.40
7:R:20:ILE:HG21	7:R:20:ILE:HD13	1.81	0.40
16:U:102:BCL:H112	16:U:102:BCL:H71	1.96	0.40
9:Y:62:THR:HG22	9:1:73:LEU:HD21	2.04	0.40
9:1:18:PRO:HB3	7:2:17:PHE:CZ	2.55	0.40
16:3:103:BCL:H203	16:3:103:BCL:H162	1.95	0.40
16:7:102:BCL:H72	16:7:102:BCL:H111	1.73	0.40
5:A:67:LEU:HD23	5:A:67:LEU:HA	1.97	0.40
16:Y:104:BCL:H92	16:Y:104:BCL:H62	1.95	0.40
9:3:14:MET:CE	6:4:11:GLU:HG3	2.51	0.40
16:9:103:BCL:HMD1	7:0:36:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	309/396 (78%)	287 (93%)	22 (7%)	0	100	100
2	L	270/273 (99%)	251 (93%)	19 (7%)	0	100	100
3	M	316/324 (98%)	303 (96%)	13 (4%)	0	100	100
4	H	255/258 (99%)	231 (91%)	21 (8%)	3 (1%)	11	32
5	A	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
5	D	70/73 (96%)	70 (100%)	0	0	100	100
5	F	70/73 (96%)	68 (97%)	2 (3%)	0	100	100
5	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
5	K	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
5	O	71/73 (97%)	69 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	4	42/46 (91%)	40 (95%)	2 (5%)	0	100	100
6	B	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
6	P	40/46 (87%)	40 (100%)	0	0	100	100
7	0	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
7	2	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
7	6	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
7	8	40/46 (87%)	38 (95%)	1 (2%)	1 (2%)	4	15
7	E	40/46 (87%)	39 (98%)	1 (2%)	0	100	100
7	G	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
7	J	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
7	N	40/46 (87%)	39 (98%)	1 (2%)	0	100	100
7	R	42/46 (91%)	42 (100%)	0	0	100	100
7	T	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
7	V	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
7	X	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
7	Z	40/46 (87%)	39 (98%)	1 (2%)	0	100	100
8	Q	76/81 (94%)	73 (96%)	3 (4%)	0	100	100
9	1	70/77 (91%)	69 (99%)	1 (1%)	0	100	100
9	3	71/77 (92%)	70 (99%)	1 (1%)	0	100	100
9	5	72/77 (94%)	72 (100%)	0	0	100	100
9	7	71/77 (92%)	71 (100%)	0	0	100	100
9	S	70/77 (91%)	68 (97%)	2 (3%)	0	100	100
9	U	70/77 (91%)	68 (97%)	2 (3%)	0	100	100
9	W	71/77 (92%)	71 (100%)	0	0	100	100
9	Y	71/77 (92%)	71 (100%)	0	0	100	100
10	9	82/86 (95%)	76 (93%)	6 (7%)	0	100	100
All	All	2937/3208 (92%)	2819 (96%)	114 (4%)	4 (0%)	50	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	86	ASP
7	8	6	THR

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Mol	Chain	Res	Type
4	H	257	VAL
4	H	256	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	266/314 (85%)	265 (100%)	1 (0%)	89 96
2	L	217/218 (100%)	216 (100%)	1 (0%)	86 95
3	M	256/260 (98%)	253 (99%)	3 (1%)	67 89
4	H	211/212 (100%)	209 (99%)	2 (1%)	75 92
5	A	62/65 (95%)	62 (100%)	0	100 100
5	D	64/65 (98%)	64 (100%)	0	100 100
5	F	64/65 (98%)	64 (100%)	0	100 100
5	I	65/65 (100%)	65 (100%)	0	100 100
5	K	64/65 (98%)	64 (100%)	0	100 100
5	O	65/65 (100%)	65 (100%)	0	100 100
6	4	38/39 (97%)	38 (100%)	0	100 100
6	B	37/39 (95%)	36 (97%)	1 (3%)	40 72
6	P	36/39 (92%)	36 (100%)	0	100 100
7	0	35/39 (90%)	35 (100%)	0	100 100
7	2	35/39 (90%)	35 (100%)	0	100 100
7	6	37/39 (95%)	37 (100%)	0	100 100
7	8	36/39 (92%)	36 (100%)	0	100 100
7	E	36/39 (92%)	36 (100%)	0	100 100
7	G	35/39 (90%)	35 (100%)	0	100 100
7	J	35/39 (90%)	35 (100%)	0	100 100
7	N	36/39 (92%)	36 (100%)	0	100 100
7	R	38/39 (97%)	38 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	T	37/39 (95%)	37 (100%)	0	100 100
7	V	37/39 (95%)	37 (100%)	0	100 100
7	X	35/39 (90%)	35 (100%)	0	100 100
7	Z	36/39 (92%)	36 (100%)	0	100 100
8	Q	67/70 (96%)	66 (98%)	1 (2%)	60 85
9	1	63/68 (93%)	63 (100%)	0	100 100
9	3	64/68 (94%)	64 (100%)	0	100 100
9	5	64/68 (94%)	64 (100%)	0	100 100
9	7	64/68 (94%)	64 (100%)	0	100 100
9	S	64/68 (94%)	64 (100%)	0	100 100
9	U	63/68 (93%)	63 (100%)	0	100 100
9	W	64/68 (94%)	63 (98%)	1 (2%)	58 84
9	Y	64/68 (94%)	64 (100%)	0	100 100
10	9	72/74 (97%)	72 (100%)	0	100 100
All	All	2562/2706 (95%)	2552 (100%)	10 (0%)	88 96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	226	ILE
2	L	258	ARG
3	M	160	LEU
3	M	192	ARG
3	M	216	PHE
4	H	211	ARG
4	H	216	ILE
6	B	20	LEU
8	Q	69	MET
9	W	58	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	42	GLN
1	C	50	GLN
1	C	189	ASN

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Mol	Chain	Res	Type
1	C	215	ASN
1	C	238	HIS
1	C	275	ASN
2	L	88	GLN
2	L	240	ASN
3	M	259	ASN
4	H	46	GLN
5	A	29	GLN
5	I	29	GLN
5	K	29	GLN
9	S	2	ASN
9	W	59	GLN
9	Y	29	GLN
9	3	29	GLN
9	7	59	GLN
10	9	29	GLN
10	9	86	ASN

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 124 ligands modelled in this entry, 19 are monoatomic - leaving 105 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BPH	M	404	-	51,70,70	0.78	2 (3%)	52,101,101	1.04	3 (5%)
15	PGV	K	106	-	42,42,50	1.06	2 (4%)	46,47,56	1.03	3 (6%)
16	BCL	T	101	-	64,74,74	1.94	16 (25%)	78,115,115	1.91	23 (29%)
23	H4X	O	106	-	43,43,43	2.44	17 (39%)	50,54,54	2.05	18 (36%)
23	H4X	5	105	-	43,43,43	2.24	12 (27%)	50,54,54	2.10	14 (28%)
16	BCL	K	108	-	64,74,74	1.93	14 (21%)	78,115,115	2.07	24 (30%)
24	LMT	X	102	-	36,36,36	0.75	1 (2%)	47,47,47	1.36	5 (10%)
16	BCL	Y	104	-	64,74,74	1.78	10 (15%)	78,115,115	1.92	22 (28%)
17	BPH	L	302	-	51,70,70	0.75	2 (3%)	52,101,101	0.97	1 (1%)
23	H4X	7	104	-	43,43,43	2.34	12 (27%)	50,54,54	2.18	14 (28%)
18	UQ8	L	306	-	33,33,53	1.67	2 (6%)	40,43,67	1.86	11 (27%)
24	LMT	T	102	-	36,36,36	0.91	2 (5%)	47,47,47	1.49	9 (19%)
24	LMT	R	101	-	36,36,36	0.85	2 (5%)	47,47,47	1.36	8 (17%)
15	PGV	I	103	-	40,40,50	1.01	2 (5%)	44,45,56	1.17	7 (15%)
16	BCL	1	102	-	64,74,74	1.82	13 (20%)	78,115,115	2.12	19 (24%)
24	LMT	B	102	-	36,36,36	0.53	0	47,47,47	1.16	3 (6%)
23	H4X	V	101	-	43,43,43	2.32	13 (30%)	50,54,54	2.67	17 (34%)
23	H4X	B	101	-	43,43,43	2.22	13 (30%)	50,54,54	2.06	19 (38%)
16	BCL	3	104	-	64,74,74	2.02	14 (21%)	78,115,115	2.02	25 (32%)
15	PGV	5	101	-	46,46,50	1.05	2 (4%)	49,52,56	1.03	3 (6%)
15	PGV	3	101	-	46,46,50	1.05	2 (4%)	48,52,56	1.40	8 (16%)
11	HEM	C	402	1	41,50,50	1.61	8 (19%)	45,82,82	2.15	15 (33%)
16	BCL	A	102	-	64,74,74	1.78	15 (23%)	78,115,115	2.26	16 (20%)
16	BCL	B	103	-	64,74,74	2.07	16 (25%)	78,115,115	2.02	26 (33%)
15	PGV	C	408	-	15,15,50	1.45	3 (20%)	18,19,56	2.34	5 (27%)
15	PGV	A	101	-	22,22,50	1.50	4 (18%)	23,27,56	1.55	6 (26%)
23	H4X	U	104	-	43,43,43	2.35	14 (32%)	50,54,54	2.05	14 (28%)
24	LMT	8	101	-	36,36,36	0.56	0	47,47,47	0.78	0
16	BCL	L	301	-	64,74,74	1.89	14 (21%)	78,115,115	2.25	28 (35%)
23	H4X	E	101	-	43,43,43	2.49	13 (30%)	50,54,54	2.18	15 (30%)
11	HEM	C	403	1	41,50,50	1.41	5 (12%)	45,82,82	2.51	19 (42%)
16	BCL	U	103	-	64,74,74	2.15	13 (20%)	78,115,115	1.92	19 (24%)
15	PGV	Q	101	-	37,37,50	1.09	3 (8%)	40,43,56	1.47	6 (15%)
16	BCL	W	102	-	64,74,74	1.72	14 (21%)	78,115,115	2.05	18 (23%)
23	H4X	Z	101	-	43,43,43	2.28	11 (25%)	50,54,54	1.87	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCL	D	103	-	64,74,74	1.70	14 (21%)	78,115,115	2.18	14 (17%)
16	BCL	L	304	-	64,74,74	1.91	14 (21%)	78,115,115	3.14	23 (29%)
24	LMT	V	102	-	36,36,36	0.90	0	47,47,47	1.72	7 (14%)
22	CDL	H	302	-	72,72,99	0.45	0	78,84,111	1.01	5 (6%)
16	BCL	7	103	-	64,74,74	2.00	13 (20%)	78,115,115	1.88	17 (21%)
11	HEM	C	404	1	41,50,50	1.44	6 (14%)	45,82,82	2.24	13 (28%)
23	H4X	Q	105	-	43,43,43	2.25	12 (27%)	50,54,54	2.30	22 (44%)
24	LMT	Z	102	-	36,36,36	0.83	1 (2%)	47,47,47	1.62	10 (21%)
16	BCL	9	104	-	64,74,74	2.03	12 (18%)	78,115,115	1.83	22 (28%)
16	BCL	F	103	-	64,74,74	1.65	11 (17%)	78,115,115	2.13	20 (25%)
24	LMT	6	102	-	36,36,36	0.94	3 (8%)	47,47,47	1.68	8 (17%)
16	BCL	I	102	-	64,74,74	1.60	13 (20%)	78,115,115	2.15	21 (26%)
16	BCL	5	104	-	64,74,74	1.86	13 (20%)	78,115,115	1.99	22 (28%)
14	DGA	C	407	1	31,31,43	0.61	0	33,33,45	0.77	1 (3%)
16	BCL	9	103	-	64,74,74	1.76	13 (20%)	78,115,115	2.13	20 (25%)
23	H4X	K	103	-	43,43,43	2.18	11 (25%)	50,54,54	2.00	21 (42%)
15	PGV	9	101	-	46,46,50	0.95	2 (4%)	48,52,56	1.12	4 (8%)
24	LMT	G	102	-	36,36,36	0.85	2 (5%)	47,47,47	1.69	8 (17%)
16	BCL	7	102	-	59,69,74	1.80	13 (22%)	72,109,115	2.13	19 (26%)
16	BCL	K	105	-	64,74,74	1.83	13 (20%)	78,115,115	1.89	20 (25%)
23	H4X	2	101	-	43,43,43	2.25	10 (23%)	50,54,54	1.90	16 (32%)
16	BCL	Q	103	-	64,74,74	1.70	12 (18%)	78,115,115	1.93	14 (17%)
15	PGV	O	102	-	43,43,50	0.93	2 (4%)	46,49,56	1.23	3 (6%)
16	BCL	5	103	-	64,74,74	1.79	13 (20%)	78,115,115	2.03	18 (23%)
24	LMT	B	104	-	36,36,36	1.13	3 (8%)	47,47,47	1.38	8 (17%)
24	LMT	P	102	-	36,36,36	0.92	1 (2%)	47,47,47	1.36	6 (12%)
16	BCL	Q	104	-	64,74,74	2.18	18 (28%)	78,115,115	2.20	29 (37%)
16	BCL	O	105	-	64,74,74	1.87	14 (21%)	78,115,115	2.08	24 (30%)
18	UQ8	L	303	-	33,33,53	1.70	4 (12%)	40,43,67	2.02	13 (32%)
15	PGV	K	102	-	18,18,50	1.27	1 (5%)	20,22,56	1.10	1 (5%)
23	H4X	K	107	-	43,43,43	2.20	11 (25%)	50,54,54	1.95	13 (26%)
24	LMT	4	102	-	36,36,36	0.96	3 (8%)	47,47,47	1.76	9 (19%)
15	PGV	F	101	-	33,33,50	1.34	2 (6%)	36,38,56	1.65	10 (27%)
23	H4X	4	101	-	43,43,43	2.13	12 (27%)	50,54,54	1.90	16 (32%)
16	BCL	U	102	-	64,74,74	1.71	12 (18%)	78,115,115	2.25	20 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	8K6	5	106	-	14,14,17	0.29	0	13,13,16	0.11	0
22	CDL	S	101	-	73,73,99	0.48	0	79,85,111	0.81	3 (3%)
24	LMT	0	101	-	36,36,36	0.83	2 (5%)	47,47,47	1.37	7 (14%)
23	H4X	G	101	-	43,43,43	2.29	14 (32%)	50,54,54	2.16	18 (36%)
16	BCL	3	103	-	64,74,74	1.79	15 (23%)	78,115,115	1.95	20 (25%)
15	PGV	1	103	-	25,25,50	1.37	2 (8%)	29,30,56	1.57	3 (10%)
22	CDL	Y	103	-	29,29,99	0.59	0	33,38,111	0.84	1 (3%)
11	HEM	C	401	1	41,50,50	1.50	11 (26%)	45,82,82	2.18	18 (40%)
24	LMT	N	101	-	36,36,36	0.83	1 (2%)	47,47,47	1.53	6 (12%)
15	PGV	F	104	-	36,36,50	1.11	2 (5%)	39,42,56	1.49	6 (15%)
21	MQ8	M	405	-	54,54,54	0.80	3 (5%)	66,69,69	0.85	1 (1%)
23	H4X	6	101	-	43,43,43	2.29	12 (27%)	50,54,54	2.19	19 (38%)
16	BCL	D	104	-	64,74,74	1.95	16 (25%)	78,115,115	1.83	16 (20%)
15	PGV	M	406	-	38,38,50	1.15	2 (5%)	41,44,56	1.19	3 (7%)
15	PGV	H	301	-	35,35,50	1.27	3 (8%)	38,41,56	1.92	5 (13%)
16	BCL	S	103	-	64,74,74	1.62	12 (18%)	78,115,115	2.00	16 (20%)
16	BCL	F	105	-	64,74,74	1.87	15 (23%)	78,115,115	1.90	17 (21%)
16	BCL	M	402	-	64,74,74	1.77	11 (17%)	78,115,115	2.35	18 (23%)
16	BCL	J	101	-	64,74,74	1.86	13 (20%)	78,115,115	1.97	23 (29%)
24	LMT	2	103	-	36,36,36	0.92	3 (8%)	47,47,47	1.91	13 (27%)
24	LMT	8	102	-	36,36,36	0.74	0	47,47,47	1.32	6 (12%)
16	BCL	M	403	-	64,74,74	1.71	11 (17%)	78,115,115	2.27	25 (32%)
16	BCL	Y	102	-	64,74,74	1.72	12 (18%)	78,115,115	2.15	19 (24%)
19	8K6	L	307	-	17,17,17	0.45	0	16,16,16	0.17	0
23	H4X	P	101	-	43,43,43	2.34	14 (32%)	50,54,54	1.92	17 (34%)
15	PGV	L	305	-	46,46,50	1.05	2 (4%)	49,52,56	1.45	6 (12%)
23	H4X	O	101	-	43,43,43	2.25	15 (34%)	50,54,54	2.50	19 (38%)
16	BCL	X	101	-	64,74,74	1.98	14 (21%)	78,115,115	1.99	20 (25%)
24	LMT	E	102	-	36,36,36	0.92	2 (5%)	47,47,47	1.53	9 (19%)
15	PGV	D	101	-	42,42,50	0.95	2 (4%)	45,48,56	1.52	7 (15%)
24	LMT	J	102	-	36,36,36	0.90	2 (5%)	47,47,47	1.75	11 (23%)
15	PGV	Y	105	-	26,26,50	1.37	2 (7%)	30,31,56	1.28	5 (16%)
16	BCL	2	102	-	64,74,74	1.57	9 (14%)	78,115,115	2.07	22 (28%)
15	PGV	K	101	-	35,35,50	1.20	2 (5%)	38,41,56	1.14	5 (13%)
16	BCL	O	104	-	64,74,74	1.84	15 (23%)	78,115,115	1.97	19 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BPH	M	404	-	-	19/37/105/105	0/5/6/6
15	PGV	K	106	-	-	17/44/44/55	-
16	BCL	T	101	-	-	16/37/137/137	-
23	H4X	O	106	-	-	8/51/51/51	-
23	H4X	5	105	-	-	10/51/51/51	-
16	BCL	K	108	-	-	19/37/137/137	-
24	LMT	X	102	-	-	11/21/61/61	0/2/2/2
16	BCL	Y	104	-	-	18/37/137/137	-
17	BPH	L	302	-	-	17/37/105/105	0/5/6/6
23	H4X	7	104	-	-	7/51/51/51	-
18	UQ8	L	306	-	-	7/27/51/75	0/1/1/1
24	LMT	T	102	-	-	11/21/61/61	0/2/2/2
24	LMT	R	101	-	-	9/21/61/61	0/2/2/2
15	PGV	I	103	-	-	19/42/42/55	-
16	BCL	1	102	-	-	9/37/137/137	-
24	LMT	B	102	-	-	13/21/61/61	0/2/2/2
23	H4X	V	101	-	-	11/51/51/51	-
23	H4X	B	101	-	-	3/51/51/51	-
16	BCL	3	104	-	-	17/37/137/137	-
15	PGV	5	101	-	-	23/51/51/55	-
15	PGV	3	101	-	-	24/51/51/55	-
11	HEM	C	402	1	-	5/12/54/54	-
16	BCL	A	102	-	-	14/37/137/137	-
16	BCL	B	103	-	-	14/37/137/137	-
15	PGV	C	408	-	-	10/15/15/55	-
15	PGV	A	101	-	-	10/26/26/55	-
23	H4X	U	104	-	-	5/51/51/51	-
24	LMT	8	101	-	-	8/21/61/61	0/2/2/2
16	BCL	L	301	-	-	8/37/137/137	-
23	H4X	E	101	-	-	5/51/51/51	-
11	HEM	C	403	1	-	4/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCL	U	103	-	-	15/37/137/137	-
15	PGV	Q	101	-	-	21/42/42/55	-
16	BCL	W	102	-	-	6/37/137/137	-
23	H4X	Z	101	-	-	8/51/51/51	-
16	BCL	D	103	-	-	6/37/137/137	-
16	BCL	L	304	-	-	7/37/137/137	-
24	LMT	V	102	-	-	10/21/61/61	0/2/2/2
22	CDL	H	302	-	-	29/83/83/110	-
16	BCL	7	103	-	-	14/37/137/137	-
11	HEM	C	404	1	-	5/12/54/54	-
23	H4X	Q	105	-	-	11/51/51/51	-
24	LMT	Z	102	-	-	11/21/61/61	0/2/2/2
16	BCL	9	104	-	-	14/37/137/137	-
16	BCL	F	103	-	-	13/37/137/137	-
24	LMT	6	102	-	-	10/21/61/61	0/2/2/2
16	BCL	I	102	-	-	13/37/137/137	-
16	BCL	5	104	-	-	18/37/137/137	-
14	DGA	C	407	1	-	20/32/32/45	-
16	BCL	9	103	-	-	21/37/137/137	-
23	H4X	K	103	-	-	10/51/51/51	-
15	PGV	9	101	-	-	23/51/51/55	-
24	LMT	G	102	-	-	12/21/61/61	0/2/2/2
16	BCL	7	102	-	-	8/31/131/137	-
16	BCL	K	105	-	-	22/37/137/137	-
23	H4X	2	101	-	-	10/51/51/51	-
16	BCL	Q	103	-	-	17/37/137/137	-
15	PGV	O	102	-	-	23/48/48/55	-
16	BCL	5	103	-	-	14/37/137/137	-
24	LMT	B	104	-	-	12/21/61/61	0/2/2/2
24	LMT	P	102	-	-	12/21/61/61	0/2/2/2
16	BCL	Q	104	-	-	14/37/137/137	-
16	BCL	O	105	-	-	17/37/137/137	-
18	UQ8	L	303	-	-	6/27/51/75	0/1/1/1
15	PGV	K	102	-	-	5/20/20/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	H4X	K	107	-	-	9/51/51/51	-
24	LMT	4	102	-	-	11/21/61/61	0/2/2/2
15	PGV	F	101	-	-	13/35/35/55	-
23	H4X	4	101	-	-	10/51/51/51	-
16	BCL	U	102	-	-	14/37/137/137	-
19	8K6	5	106	-	-	4/12/12/15	-
22	CDL	S	101	-	-	35/84/84/110	-
24	LMT	0	101	-	-	11/21/61/61	0/2/2/2
23	H4X	G	101	-	-	7/51/51/51	-
16	BCL	3	103	-	-	17/37/137/137	-
15	PGV	1	103	-	-	11/27/27/55	-
22	CDL	Y	103	-	-	13/35/35/110	-
11	HEM	C	401	1	-	7/12/54/54	-
24	LMT	N	101	-	-	11/21/61/61	0/2/2/2
15	PGV	F	104	-	-	23/41/41/55	-
21	MQ8	M	405	-	-	10/47/67/67	0/2/2/2
23	H4X	6	101	-	-	5/51/51/51	-
16	BCL	D	104	-	-	16/37/137/137	-
15	PGV	M	406	-	-	21/43/43/55	-
15	PGV	H	301	-	-	17/40/40/55	-
16	BCL	S	103	-	-	5/37/137/137	-
16	BCL	F	105	-	-	14/37/137/137	-
16	BCL	M	402	-	-	15/37/137/137	-
16	BCL	J	101	-	-	15/37/137/137	-
24	LMT	2	103	-	-	10/21/61/61	0/2/2/2
24	LMT	8	102	-	-	11/21/61/61	0/2/2/2
16	BCL	M	403	-	-	13/37/137/137	-
16	BCL	Y	102	-	-	10/37/137/137	-
19	8K6	L	307	-	-	11/15/15/15	-
23	H4X	P	101	-	-	6/51/51/51	-
15	PGV	L	305	-	-	14/51/51/55	-
23	H4X	O	101	-	-	14/51/51/51	-
16	BCL	X	101	-	-	16/37/137/137	-
24	LMT	E	102	-	-	12/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PGV	D	101	-	-	14/47/47/55	-
24	LMT	J	102	-	-	10/21/61/61	0/2/2/2
15	PGV	Y	105	-	-	9/28/28/55	-
16	BCL	2	102	-	-	15/37/137/137	-
15	PGV	K	101	-	-	18/40/40/55	-
16	BCL	O	104	-	-	13/37/137/137	-

All (809) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	306	UQ8	C6-C1	8.07	1.49	1.35
18	L	303	UQ8	C6-C1	7.22	1.48	1.35
16	U	103	BCL	C3D-C4D	-6.72	1.29	1.44
16	L	301	BCL	O2D-CGD	6.54	1.49	1.33
16	B	103	BCL	C3D-C4D	-6.29	1.30	1.44
16	3	104	BCL	C3D-C4D	-6.24	1.30	1.44
16	U	103	BCL	C1D-ND	-6.10	1.30	1.37
16	U	103	BCL	OBD-CAD	6.07	1.33	1.22
16	M	402	BCL	C3D-C4D	-5.95	1.30	1.44
16	D	104	BCL	C3D-C4D	-5.94	1.30	1.44
16	5	104	BCL	C3D-C4D	-5.93	1.30	1.44
16	7	103	BCL	C3D-C4D	-5.80	1.31	1.44
16	B	103	BCL	CHD-C1D	5.80	1.49	1.38
16	Q	104	BCL	OBD-CAD	5.79	1.32	1.22
16	J	101	BCL	OBD-CAD	5.78	1.32	1.22
23	O	106	H4X	C25-C23	5.74	1.58	1.45
16	X	101	BCL	C3D-C4D	-5.71	1.31	1.44
23	6	101	H4X	C25-C23	5.68	1.58	1.45
16	F	105	BCL	C3D-C4D	-5.66	1.31	1.44
16	K	108	BCL	C3D-C4D	-5.66	1.31	1.44
16	K	105	BCL	C3D-C4D	-5.65	1.31	1.44
16	Q	104	BCL	C3B-C2B	5.63	1.49	1.39
16	M	403	BCL	O2A-CGA	5.61	1.49	1.33
16	L	301	BCL	C3D-C4D	-5.60	1.31	1.44
16	9	103	BCL	C3D-C4D	-5.58	1.31	1.44
16	7	103	BCL	O2A-CGA	5.58	1.49	1.33
23	7	104	H4X	C25-C23	5.57	1.57	1.45
16	B	103	BCL	OBD-CAD	5.56	1.32	1.22
16	7	103	BCL	OBD-CAD	5.53	1.32	1.22
16	Y	102	BCL	C3D-C4D	-5.49	1.31	1.44
16	K	108	BCL	O2D-CGD	5.48	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	101	BCL	C3D-C4D	-5.47	1.31	1.44
16	T	101	BCL	C3B-C2B	5.46	1.49	1.39
16	9	104	BCL	CHD-C1D	5.44	1.48	1.38
16	L	304	BCL	C1B-NB	5.42	1.40	1.35
16	Y	104	BCL	C3D-C4D	-5.40	1.32	1.44
16	Q	103	BCL	C3D-C4D	-5.38	1.32	1.44
16	U	103	BCL	O2A-CGA	5.37	1.49	1.33
16	F	105	BCL	C1D-ND	-5.33	1.31	1.37
16	7	103	BCL	C1D-ND	-5.31	1.31	1.37
23	O	101	H4X	C16-C17	5.30	1.57	1.45
16	9	104	BCL	O2A-CGA	5.30	1.48	1.33
16	Q	104	BCL	C3D-C4D	-5.29	1.32	1.44
16	3	104	BCL	OBD-CAD	5.29	1.31	1.22
16	L	304	BCL	C3B-C2B	5.28	1.48	1.39
16	Q	104	BCL	CHD-C1D	5.27	1.48	1.38
16	B	103	BCL	C3C-C4C	-5.26	1.45	1.51
16	7	102	BCL	C3D-C4D	-5.25	1.32	1.44
16	M	402	BCL	C3B-C2B	5.22	1.48	1.39
23	U	104	H4X	C11-C12	5.21	1.57	1.45
23	V	101	H4X	C25-C23	5.19	1.57	1.45
16	5	104	BCL	O2A-CGA	5.17	1.48	1.33
23	K	107	H4X	C16-C17	5.16	1.57	1.45
16	2	102	BCL	O2A-CGA	5.15	1.48	1.33
16	Y	102	BCL	O2D-CGD	5.15	1.45	1.33
16	A	102	BCL	C3D-C4D	-5.15	1.32	1.44
16	O	105	BCL	C3D-C4D	-5.14	1.32	1.44
16	5	103	BCL	O2A-CGA	5.11	1.48	1.33
16	9	104	BCL	C3D-C4D	-5.11	1.32	1.44
23	2	101	H4X	C11-C12	5.10	1.56	1.45
16	O	104	BCL	O2A-CGA	5.09	1.48	1.33
16	D	103	BCL	C3D-C4D	-5.09	1.32	1.44
16	U	102	BCL	CHD-C1D	5.09	1.48	1.38
23	E	101	H4X	C25-C23	5.08	1.56	1.45
16	U	102	BCL	C3C-C4C	-5.07	1.45	1.51
16	L	304	BCL	O2A-CGA	5.07	1.48	1.33
16	3	104	BCL	O2A-CGA	5.06	1.48	1.33
16	9	104	BCL	C1D-ND	-5.06	1.31	1.37
16	1	102	BCL	C3D-C4D	-5.06	1.32	1.44
16	B	103	BCL	O2A-CGA	5.05	1.48	1.33
16	D	104	BCL	O2A-CGA	5.04	1.48	1.33
23	O	101	H4X	C25-C23	5.04	1.56	1.45
16	T	101	BCL	O2A-CGA	5.04	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	101	H4X	C25-C23	5.04	1.56	1.45
23	P	101	H4X	C16-C17	5.02	1.56	1.45
16	3	103	BCL	C3D-C4D	-5.02	1.32	1.44
16	J	101	BCL	O2A-CGA	5.01	1.48	1.33
23	Z	101	H4X	C25-C23	5.00	1.56	1.45
23	E	101	H4X	C16-C17	4.98	1.56	1.45
15	K	102	PGV	O01-C1	4.98	1.47	1.33
23	G	101	H4X	C21-C22	4.97	1.58	1.43
16	S	103	BCL	O2A-CGA	4.97	1.47	1.33
16	3	104	BCL	CHD-C1D	4.96	1.48	1.38
16	O	105	BCL	CHD-C1D	4.95	1.48	1.38
23	Z	101	H4X	C26-C27	4.94	1.58	1.43
16	F	103	BCL	C3D-C4D	-4.94	1.33	1.44
23	Q	105	H4X	C16-C17	4.94	1.56	1.45
23	V	101	H4X	C21-C22	4.91	1.58	1.43
16	K	108	BCL	O2A-CGA	4.91	1.47	1.33
15	5	101	PGV	O01-C1	4.91	1.48	1.34
23	Q	105	H4X	C26-C27	4.90	1.58	1.43
16	O	105	BCL	O2D-CGD	4.90	1.45	1.33
23	K	103	H4X	C16-C17	4.90	1.56	1.45
23	B	101	H4X	C20-C19	4.90	1.58	1.43
16	3	104	BCL	C3B-C2B	4.88	1.48	1.39
23	E	101	H4X	C21-C22	4.88	1.58	1.43
23	5	105	H4X	C21-C22	4.88	1.58	1.43
16	Q	104	BCL	O2A-CGA	4.87	1.47	1.33
16	K	108	BCL	OBD-CAD	4.85	1.30	1.22
16	T	101	BCL	OBD-CAD	4.85	1.30	1.22
16	X	101	BCL	C3C-C4C	-4.84	1.45	1.51
16	3	103	BCL	C3B-C2B	4.84	1.48	1.39
16	Q	103	BCL	CHD-C1D	4.84	1.47	1.38
16	Y	104	BCL	O2A-CGA	4.83	1.47	1.33
23	P	101	H4X	C26-C27	4.82	1.58	1.43
16	9	103	BCL	O2A-CGA	4.82	1.47	1.33
23	K	103	H4X	C25-C23	4.82	1.56	1.45
16	X	101	BCL	CHD-C1D	4.81	1.47	1.38
15	F	101	PGV	O03-C19	4.81	1.47	1.33
16	O	105	BCL	O2A-CGA	4.81	1.47	1.33
23	6	101	H4X	C21-C22	4.80	1.58	1.43
23	P	101	H4X	C21-C22	4.78	1.58	1.43
16	K	105	BCL	CHD-C1D	4.78	1.47	1.38
23	Z	101	H4X	C21-C22	4.78	1.58	1.43
23	O	106	H4X	C16-C17	4.77	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	101	BCL	C3D-C4D	-4.77	1.33	1.44
16	F	105	BCL	O2A-CGA	4.77	1.47	1.33
16	M	403	BCL	O2D-CGD	4.77	1.44	1.33
23	E	101	H4X	C11-C12	4.76	1.56	1.45
16	D	104	BCL	O2D-CGD	4.76	1.44	1.33
16	O	104	BCL	O2D-CGD	4.75	1.44	1.33
16	X	101	BCL	OBD-CAD	4.75	1.30	1.22
15	K	101	PGV	O03-C19	4.74	1.47	1.33
15	3	101	PGV	O03-C19	4.74	1.47	1.33
23	O	101	H4X	C11-C12	4.73	1.56	1.45
23	K	107	H4X	C26-C27	4.73	1.58	1.43
15	H	301	PGV	O03-C19	4.73	1.47	1.33
23	4	101	H4X	C21-C22	4.72	1.58	1.43
23	P	101	H4X	C25-C23	4.72	1.56	1.45
16	U	103	BCL	O2D-CGD	4.71	1.44	1.33
16	7	102	BCL	O2D-CGD	4.70	1.44	1.33
23	K	103	H4X	C26-C27	4.70	1.58	1.43
23	B	101	H4X	C26-C27	4.69	1.58	1.43
15	K	106	PGV	O03-C19	4.68	1.47	1.33
16	A	102	BCL	O2A-CGA	4.68	1.47	1.33
16	1	102	BCL	CHD-C1D	4.67	1.47	1.38
23	7	104	H4X	C26-C27	4.67	1.57	1.43
16	5	104	BCL	C3B-C2B	4.66	1.47	1.39
16	1	102	BCL	O2A-CGA	4.66	1.47	1.33
23	5	105	H4X	C15-C14	4.66	1.57	1.43
15	L	305	PGV	O01-C1	4.66	1.47	1.34
15	M	406	PGV	O01-C1	4.64	1.47	1.34
23	E	101	H4X	C26-C27	4.64	1.57	1.43
15	1	103	PGV	O01-C1	4.63	1.47	1.34
16	5	104	BCL	C1D-ND	-4.63	1.32	1.37
23	7	104	H4X	C11-C12	4.62	1.55	1.45
16	F	105	BCL	O2D-CGD	4.62	1.44	1.33
16	5	104	BCL	O2D-CGD	4.61	1.44	1.33
23	K	107	H4X	C25-C23	4.61	1.55	1.45
23	2	101	H4X	C21-C22	4.61	1.57	1.43
23	O	106	H4X	C26-C27	4.60	1.57	1.43
16	9	104	BCL	OBD-CAD	4.60	1.30	1.22
23	V	101	H4X	C26-C27	4.60	1.57	1.43
23	G	101	H4X	C11-C12	4.58	1.55	1.45
23	E	101	H4X	C31-C32	4.57	1.57	1.43
16	2	102	BCL	C3D-C4D	-4.57	1.33	1.44
15	Y	105	PGV	O03-C19	4.56	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	101	H4X	C11-C12	4.56	1.55	1.45
23	K	107	H4X	C31-C32	4.55	1.57	1.43
16	F	105	BCL	OBD-CAD	4.55	1.30	1.22
16	W	102	BCL	C3D-C4D	-4.54	1.33	1.44
23	U	104	H4X	C21-C22	4.54	1.57	1.43
23	6	101	H4X	C20-C19	4.54	1.57	1.43
16	T	101	BCL	CHD-C1D	4.53	1.47	1.38
16	3	104	BCL	O2D-CGD	4.53	1.44	1.33
16	L	304	BCL	C3D-C4D	-4.53	1.34	1.44
23	6	101	H4X	C16-C17	4.53	1.55	1.45
16	X	101	BCL	O2A-CGA	4.53	1.46	1.33
16	K	108	BCL	C3B-C2B	4.53	1.47	1.39
23	7	104	H4X	C21-C22	4.52	1.57	1.43
16	D	104	BCL	C3C-C4C	-4.52	1.45	1.51
16	M	403	BCL	C3B-C2B	4.52	1.47	1.39
23	7	104	H4X	C20-C19	4.51	1.57	1.43
16	D	104	BCL	CHD-C1D	4.51	1.47	1.38
16	Y	104	BCL	OBD-CAD	4.50	1.30	1.22
23	U	104	H4X	C16-C17	4.50	1.55	1.45
23	Q	105	H4X	C20-C19	4.49	1.57	1.43
16	A	102	BCL	C1D-ND	-4.49	1.32	1.37
16	3	103	BCL	CHD-C1D	4.49	1.47	1.38
23	E	101	H4X	C15-C14	4.48	1.57	1.43
23	K	103	H4X	C21-C22	4.48	1.57	1.43
23	O	106	H4X	C20-C19	4.48	1.57	1.43
16	T	101	BCL	C3C-C4C	-4.48	1.46	1.51
16	W	102	BCL	CHD-C1D	4.48	1.47	1.38
23	Z	101	H4X	C11-C12	4.48	1.55	1.45
23	Q	105	H4X	C10-C9	4.48	1.57	1.43
23	E	101	H4X	C20-C19	4.46	1.57	1.43
16	K	105	BCL	O2A-CGA	4.45	1.46	1.33
23	B	101	H4X	C21-C22	4.45	1.57	1.43
15	F	101	PGV	O01-C1	4.44	1.46	1.34
23	U	104	H4X	C26-C27	4.43	1.57	1.43
16	D	103	BCL	O2A-CGA	4.43	1.46	1.33
16	L	301	BCL	OBD-CAD	4.43	1.30	1.22
16	5	103	BCL	CHD-C1D	4.43	1.47	1.38
15	L	305	PGV	O03-C19	4.43	1.46	1.33
23	V	101	H4X	C20-C19	4.42	1.57	1.43
16	U	103	BCL	C3B-C2B	4.42	1.47	1.39
16	Q	104	BCL	C3C-C4C	-4.42	1.46	1.51
16	1	102	BCL	O2D-CGD	4.41	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	101	BCL	O2D-CGD	4.40	1.43	1.33
16	W	102	BCL	O2A-CGA	4.40	1.46	1.33
23	G	101	H4X	C16-C17	4.39	1.55	1.45
23	5	105	H4X	C25-C23	4.39	1.55	1.45
23	5	105	H4X	C26-C27	4.39	1.57	1.43
23	Z	101	H4X	C20-C19	4.39	1.57	1.43
23	5	105	H4X	C16-C17	4.38	1.55	1.45
23	U	104	H4X	C25-C23	4.38	1.55	1.45
16	F	103	BCL	O2A-CGA	4.38	1.46	1.33
16	I	102	BCL	O2D-CGD	4.37	1.43	1.33
23	2	101	H4X	C20-C19	4.37	1.57	1.43
16	Q	104	BCL	C1B-NB	4.37	1.39	1.35
23	G	101	H4X	C30-C28	4.37	1.55	1.45
23	Z	101	H4X	C31-C32	4.37	1.57	1.43
23	U	104	H4X	C20-C19	4.36	1.57	1.43
23	2	101	H4X	C26-C27	4.36	1.57	1.43
23	Z	101	H4X	C16-C17	4.36	1.55	1.45
16	F	103	BCL	O2D-CGD	4.36	1.43	1.33
16	3	103	BCL	O2A-CGA	4.36	1.46	1.33
23	4	101	H4X	C26-C27	4.35	1.56	1.43
16	M	402	BCL	CHD-C1D	4.35	1.46	1.38
16	5	103	BCL	C3C-C4C	-4.34	1.46	1.51
23	K	107	H4X	C20-C19	4.34	1.56	1.43
23	P	101	H4X	C20-C19	4.34	1.56	1.43
16	9	104	BCL	C3B-C2B	4.33	1.47	1.39
23	G	101	H4X	C25-C23	4.33	1.55	1.45
23	5	105	H4X	C30-C28	4.33	1.55	1.45
16	U	102	BCL	C3D-C4D	-4.32	1.34	1.44
16	X	101	BCL	O2D-CGD	4.32	1.43	1.33
16	L	304	BCL	CHD-C1D	4.32	1.46	1.38
16	M	403	BCL	C3D-C4D	-4.31	1.34	1.44
15	3	101	PGV	O01-C1	4.31	1.46	1.34
16	3	103	BCL	O2D-CGD	4.29	1.43	1.33
23	O	101	H4X	C26-C27	4.29	1.56	1.43
16	K	105	BCL	O2D-CGD	4.28	1.43	1.33
16	O	104	BCL	C1D-ND	-4.27	1.32	1.37
23	4	101	H4X	C25-C23	4.27	1.55	1.45
23	Q	105	H4X	C25-C23	4.27	1.55	1.45
23	2	101	H4X	C16-C17	4.26	1.55	1.45
15	Q	101	PGV	O03-C19	4.25	1.45	1.33
23	O	106	H4X	C15-C14	4.25	1.56	1.43
16	D	103	BCL	CHD-C1D	4.25	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	103	BCL	O2D-CGD	4.25	1.43	1.33
16	S	103	BCL	C3D-C4D	-4.24	1.34	1.44
23	6	101	H4X	C30-C28	4.24	1.55	1.45
23	V	101	H4X	C16-C17	4.24	1.55	1.45
16	I	102	BCL	C3D-C4D	-4.24	1.34	1.44
16	O	105	BCL	C1D-ND	-4.24	1.32	1.37
16	9	103	BCL	O2D-CGD	4.24	1.43	1.33
16	1	102	BCL	C3B-C2B	4.24	1.47	1.39
23	O	106	H4X	C11-C12	4.24	1.55	1.45
23	Q	105	H4X	C21-C22	4.23	1.56	1.43
16	O	104	BCL	C3D-C4D	-4.23	1.34	1.44
16	D	104	BCL	OBD-CAD	4.22	1.29	1.22
16	X	101	BCL	C3B-C2B	4.22	1.47	1.39
15	F	104	PGV	O03-C19	4.21	1.45	1.33
23	4	101	H4X	C11-C12	4.21	1.55	1.45
23	K	107	H4X	C21-C22	4.21	1.56	1.43
23	6	101	H4X	C15-C14	4.21	1.56	1.43
23	E	101	H4X	C10-C9	4.20	1.56	1.43
23	4	101	H4X	C20-C19	4.20	1.56	1.43
23	O	106	H4X	C21-C22	4.19	1.56	1.43
15	D	101	PGV	O01-C1	4.19	1.46	1.34
23	O	106	H4X	C31-C32	4.18	1.56	1.43
23	K	107	H4X	C10-C9	4.18	1.56	1.43
16	Y	104	BCL	C3B-C2B	4.18	1.46	1.39
15	9	101	PGV	O03-C19	4.15	1.45	1.33
23	4	101	H4X	C15-C14	4.15	1.56	1.43
23	G	101	H4X	C26-C27	4.15	1.56	1.43
16	Q	103	BCL	O2A-CGA	4.15	1.45	1.33
16	Y	102	BCL	CHD-C1D	4.15	1.46	1.38
16	9	103	BCL	C3B-C2B	4.15	1.46	1.39
23	V	101	H4X	C11-C12	4.14	1.54	1.45
15	K	101	PGV	O01-C1	4.13	1.46	1.34
15	1	103	PGV	O03-C19	4.13	1.45	1.33
23	B	101	H4X	C25-C23	4.13	1.54	1.45
23	P	101	H4X	C15-C14	4.12	1.56	1.43
16	F	103	BCL	CHD-C1D	4.12	1.46	1.38
23	5	105	H4X	C20-C19	4.11	1.56	1.43
23	7	104	H4X	C31-C32	4.11	1.56	1.43
23	B	101	H4X	C11-C12	4.11	1.54	1.45
23	Q	105	H4X	C31-C32	4.10	1.56	1.43
23	5	105	H4X	C11-C12	4.10	1.54	1.45
16	M	402	BCL	O2A-CGA	4.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	102	BCL	O2A-CGA	4.09	1.45	1.33
23	K	103	H4X	C20-C19	4.08	1.56	1.43
16	U	103	BCL	CHD-C1D	4.08	1.46	1.38
15	Y	105	PGV	O01-C1	4.07	1.45	1.34
16	J	101	BCL	CHD-C1D	4.06	1.46	1.38
15	A	101	PGV	O03-C19	4.06	1.49	1.33
15	M	406	PGV	O03-C19	4.05	1.45	1.33
23	5	105	H4X	C31-C32	4.05	1.56	1.43
23	6	101	H4X	C31-C32	4.05	1.56	1.43
16	Q	104	BCL	O2D-CGD	4.05	1.43	1.33
16	O	104	BCL	CHD-C1D	4.04	1.46	1.38
23	E	101	H4X	C30-C28	4.03	1.54	1.45
16	9	104	BCL	O2D-CGD	4.03	1.43	1.33
16	7	102	BCL	CHD-C1D	4.03	1.46	1.38
16	B	103	BCL	C1D-ND	-4.03	1.32	1.37
16	9	103	BCL	CHD-C1D	4.02	1.46	1.38
15	I	103	PGV	O03-C19	4.01	1.45	1.33
23	5	105	H4X	C10-C9	4.01	1.55	1.43
23	2	101	H4X	C31-C32	4.00	1.55	1.43
16	W	102	BCL	O2D-CGD	4.00	1.42	1.33
23	6	101	H4X	C10-C9	3.99	1.55	1.43
16	M	402	BCL	OBD-CAD	3.98	1.29	1.22
23	B	101	H4X	C10-C9	3.97	1.55	1.43
16	M	402	BCL	O2D-CGD	3.97	1.42	1.33
15	C	408	PGV	O01-C1	3.96	1.45	1.34
16	7	103	BCL	C3C-C4C	-3.96	1.46	1.51
16	T	101	BCL	O2D-CGD	3.96	1.42	1.33
23	Z	101	H4X	C15-C14	3.94	1.55	1.43
23	K	103	H4X	C31-C32	3.93	1.55	1.43
16	7	102	BCL	O2A-CGA	3.93	1.44	1.33
16	3	104	BCL	C3C-C4C	-3.93	1.46	1.51
16	K	105	BCL	OBD-CAD	3.91	1.29	1.22
16	U	102	BCL	C3B-C2B	3.91	1.46	1.39
16	A	102	BCL	CHD-C1D	3.91	1.46	1.38
23	K	107	H4X	C15-C14	3.91	1.55	1.43
16	U	102	BCL	O2A-CGA	3.90	1.44	1.33
23	U	104	H4X	C30-C28	3.90	1.54	1.45
16	Q	104	BCL	MG-ND	-3.90	1.98	2.05
23	Z	101	H4X	C10-C9	3.89	1.55	1.43
23	V	101	H4X	C30-C28	3.89	1.54	1.45
16	5	103	BCL	C3D-C4D	-3.88	1.35	1.44
16	S	103	BCL	CMA-C3A	-3.88	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	101	H4X	C31-C32	3.88	1.55	1.43
23	Q	105	H4X	C11-C12	3.86	1.54	1.45
23	B	101	H4X	C15-C14	3.86	1.55	1.43
23	G	101	H4X	C20-C19	3.86	1.55	1.43
23	P	101	H4X	C31-C32	3.84	1.55	1.43
16	7	102	BCL	C3B-C2B	3.84	1.46	1.39
16	U	102	BCL	O2D-CGD	3.84	1.42	1.33
16	Q	104	BCL	C1D-ND	-3.83	1.33	1.37
23	7	104	H4X	C16-C17	3.83	1.54	1.45
23	B	101	H4X	C30-C28	3.82	1.54	1.45
23	P	101	H4X	C30-C28	3.82	1.54	1.45
16	A	102	BCL	O2D-CGD	3.81	1.42	1.33
23	4	101	H4X	C10-C9	3.81	1.55	1.43
23	O	106	H4X	C30-C28	3.80	1.54	1.45
23	2	101	H4X	C15-C14	3.80	1.55	1.43
23	6	101	H4X	C26-C27	3.79	1.55	1.43
16	1	102	BCL	C3C-C4C	-3.79	1.46	1.51
16	7	103	BCL	C3B-C2B	3.78	1.46	1.39
23	O	101	H4X	C21-C22	3.78	1.55	1.43
16	B	103	BCL	O2D-CGD	3.77	1.42	1.33
16	Y	104	BCL	O2D-CGD	3.76	1.42	1.33
16	2	102	BCL	C3B-C2B	3.76	1.46	1.39
23	B	101	H4X	C16-C17	3.76	1.54	1.45
23	K	103	H4X	C10-C9	3.76	1.55	1.43
16	F	105	BCL	C3B-C2B	3.76	1.46	1.39
23	V	101	H4X	C10-C9	3.75	1.55	1.43
23	K	103	H4X	C11-C12	3.74	1.54	1.45
23	2	101	H4X	C10-C9	3.74	1.55	1.43
23	P	101	H4X	C10-C9	3.74	1.55	1.43
16	Q	103	BCL	O2D-CGD	3.74	1.42	1.33
23	Q	105	H4X	C30-C28	3.74	1.54	1.45
16	7	102	BCL	CAA-C2A	-3.73	1.47	1.54
16	L	301	BCL	C3D-C2D	3.73	1.49	1.39
23	Q	105	H4X	C15-C14	3.73	1.55	1.43
23	V	101	H4X	C15-C14	3.72	1.55	1.43
16	K	105	BCL	C3C-C4C	-3.72	1.46	1.51
23	E	101	H4X	C18-C17	3.71	1.58	1.50
16	D	103	BCL	C3C-C4C	-3.71	1.46	1.51
16	X	101	BCL	C1D-ND	-3.70	1.33	1.37
23	2	101	H4X	C30-C28	3.70	1.53	1.45
15	I	103	PGV	O01-C1	3.69	1.44	1.34
16	F	105	BCL	CHD-C1D	3.68	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	102	PGV	O03-C19	3.68	1.44	1.33
16	K	105	BCL	C3B-C2B	3.68	1.46	1.39
16	1	102	BCL	OBD-CAD	3.67	1.28	1.22
23	6	101	H4X	C11-C12	3.66	1.53	1.45
11	C	402	HEM	C1B-NB	-3.65	1.34	1.40
16	D	103	BCL	C3B-C2B	3.65	1.46	1.39
23	K	107	H4X	C11-C12	3.64	1.53	1.45
23	G	101	H4X	C10-C9	3.64	1.54	1.43
23	U	104	H4X	C31-C32	3.64	1.54	1.43
16	7	103	BCL	CHD-C1D	3.64	1.45	1.38
16	2	102	BCL	O2D-CGD	3.63	1.42	1.33
16	5	103	BCL	C3B-C2B	3.63	1.45	1.39
23	7	104	H4X	C30-C28	3.63	1.53	1.45
23	V	101	H4X	C24-C23	3.63	1.58	1.50
16	K	108	BCL	CHD-C1D	3.62	1.45	1.38
23	V	101	H4X	C31-C32	3.62	1.54	1.43
11	C	402	HEM	C4D-ND	-3.62	1.34	1.40
23	4	101	H4X	C16-C17	3.62	1.53	1.45
15	O	102	PGV	O01-C1	3.62	1.44	1.34
15	5	101	PGV	O03-C19	3.60	1.43	1.33
23	O	101	H4X	C10-C9	3.60	1.54	1.43
23	U	104	H4X	C18-C17	3.60	1.58	1.50
16	Y	104	BCL	CHD-C1D	3.60	1.45	1.38
23	U	104	H4X	C10-C9	3.59	1.54	1.43
23	K	103	H4X	C15-C14	3.59	1.54	1.43
16	7	103	BCL	O2D-CGD	3.58	1.41	1.33
15	H	301	PGV	O01-C1	3.58	1.44	1.34
23	G	101	H4X	C31-C32	3.57	1.54	1.43
11	C	401	HEM	C1B-NB	-3.57	1.34	1.40
16	9	104	BCL	C3C-C4C	-3.57	1.47	1.51
16	I	102	BCL	CHD-C1D	3.57	1.45	1.38
23	4	101	H4X	C31-C32	3.55	1.54	1.43
16	L	304	BCL	CAA-C2A	-3.55	1.47	1.54
16	D	104	BCL	C3B-C2B	3.54	1.45	1.39
23	U	104	H4X	C15-C14	3.54	1.54	1.43
15	K	106	PGV	O01-C1	3.53	1.44	1.34
16	Y	104	BCL	C3D-C2D	3.52	1.48	1.39
16	O	105	BCL	OBD-CAD	3.51	1.28	1.22
16	K	108	BCL	C1B-NB	3.49	1.38	1.35
23	4	101	H4X	C30-C28	3.48	1.53	1.45
16	Q	103	BCL	CAC-C3C	-3.48	1.47	1.54
16	J	101	BCL	C1D-ND	-3.48	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	102	BCL	C3D-C2D	3.47	1.48	1.39
23	G	101	H4X	C15-C14	3.46	1.54	1.43
16	7	103	BCL	C3D-C2D	3.46	1.48	1.39
16	Y	102	BCL	O2A-CGA	3.46	1.43	1.33
23	O	101	H4X	C15-C14	3.45	1.54	1.43
16	5	104	BCL	CHD-C1D	3.44	1.45	1.38
16	Y	102	BCL	C1D-ND	-3.42	1.33	1.37
23	7	104	H4X	C15-C14	3.41	1.54	1.43
16	Q	103	BCL	C1D-ND	-3.40	1.33	1.37
23	O	101	H4X	C30-C28	3.39	1.53	1.45
16	Q	103	BCL	C3C-C4C	-3.38	1.47	1.51
16	5	103	BCL	C3D-C2D	3.38	1.48	1.39
16	D	104	BCL	C3D-C2D	3.38	1.48	1.39
16	L	301	BCL	O2A-CGA	3.38	1.43	1.33
23	O	106	H4X	C10-C9	3.38	1.53	1.43
16	M	403	BCL	C3D-C2D	3.38	1.48	1.39
23	7	104	H4X	C10-C9	3.37	1.53	1.43
16	5	103	BCL	MG-ND	-3.36	1.99	2.05
15	F	104	PGV	O01-C1	3.36	1.43	1.34
23	O	101	H4X	C31-C32	3.35	1.53	1.43
16	L	304	BCL	O2D-CED	3.35	1.53	1.45
16	U	103	BCL	CAA-C2A	-3.34	1.47	1.54
16	O	104	BCL	MG-ND	-3.34	1.99	2.05
16	O	105	BCL	C3C-C4C	-3.33	1.47	1.51
16	L	304	BCL	C3D-C2D	3.32	1.48	1.39
16	Y	104	BCL	CAC-C3C	-3.32	1.47	1.54
16	3	104	BCL	C1D-ND	-3.32	1.33	1.37
16	9	104	BCL	MG-ND	-3.31	1.99	2.05
16	L	301	BCL	CHD-C1D	3.31	1.44	1.38
16	A	102	BCL	OBD-CAD	3.30	1.28	1.22
21	M	405	MQ8	C3-C2	3.30	1.41	1.35
17	M	404	BPH	CBD-CGD	-3.28	1.48	1.52
16	O	105	BCL	C3B-C2B	3.28	1.45	1.39
16	B	103	BCL	C1B-NB	3.27	1.38	1.35
16	S	103	BCL	CHD-C1D	3.26	1.44	1.38
16	B	103	BCL	C3B-C2B	3.26	1.45	1.39
16	A	102	BCL	C3B-C2B	3.25	1.45	1.39
16	J	101	BCL	MG-ND	-3.25	1.99	2.05
15	Q	101	PGV	O01-C1	3.25	1.43	1.34
16	5	104	BCL	CAA-C2A	-3.21	1.48	1.54
15	9	101	PGV	O01-C1	3.20	1.43	1.34
16	O	104	BCL	C3B-C2B	3.20	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	7	102	BCL	C1B-NB	3.18	1.38	1.35
16	7	102	BCL	OBD-CAD	3.18	1.28	1.22
16	2	102	BCL	CMC-C2C	-3.18	1.46	1.53
16	L	301	BCL	C1B-NB	3.18	1.38	1.35
16	L	301	BCL	C1B-CHB	3.17	1.49	1.41
23	7	104	H4X	C24-C23	3.17	1.57	1.50
16	U	103	BCL	C3C-C4C	-3.16	1.47	1.51
16	X	101	BCL	CAA-C2A	-3.16	1.48	1.54
23	K	103	H4X	C30-C28	3.14	1.52	1.45
16	3	103	BCL	C1B-NB	3.13	1.38	1.35
16	O	104	BCL	C3D-C2D	3.12	1.47	1.39
16	J	101	BCL	C3C-C4C	-3.12	1.47	1.51
16	3	103	BCL	OBD-CAD	3.11	1.27	1.22
16	Y	102	BCL	C3B-C2B	3.09	1.45	1.39
16	I	102	BCL	C3C-C4C	-3.08	1.47	1.51
16	M	403	BCL	MG-ND	-3.07	1.99	2.05
16	9	103	BCL	C4B-NB	3.07	1.37	1.35
23	Z	101	H4X	C30-C28	3.06	1.52	1.45
16	K	105	BCL	C1B-NB	3.06	1.37	1.35
16	O	104	BCL	CAC-C3C	-3.05	1.48	1.54
16	I	102	BCL	C3B-C2B	3.04	1.44	1.39
16	7	103	BCL	CAA-C2A	-3.04	1.48	1.54
16	Y	102	BCL	OBD-CAD	3.02	1.27	1.22
16	S	103	BCL	O2D-CGD	3.02	1.40	1.33
23	O	106	H4X	C39-C38	3.00	1.59	1.52
16	U	102	BCL	CAA-C2A	-3.00	1.48	1.54
23	K	107	H4X	C30-C28	2.99	1.52	1.45
16	O	104	BCL	C4D-CHA	2.98	1.49	1.38
23	7	104	H4X	C32-C33	-2.97	1.31	1.34
16	W	102	BCL	CMB-C2B	-2.97	1.45	1.51
16	M	403	BCL	CHD-C1D	2.97	1.44	1.38
16	O	104	BCL	C4B-CHC	2.96	1.49	1.41
23	E	101	H4X	C39-C38	2.96	1.59	1.52
16	S	103	BCL	C3D-C2D	2.95	1.47	1.39
24	P	102	LMT	C12-C11	2.95	1.74	1.49
16	W	102	BCL	CAA-C2A	-2.94	1.48	1.54
16	5	104	BCL	C1B-NB	2.93	1.37	1.35
16	A	102	BCL	C3C-C4C	-2.93	1.47	1.51
16	7	102	BCL	C3D-C2D	2.91	1.47	1.39
11	C	403	HEM	CAA-C2A	-2.91	1.47	1.52
16	Y	102	BCL	C4D-CHA	2.90	1.48	1.38
11	C	402	HEM	C1B-C2B	-2.90	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	102	BCL	C3D-C2D	2.89	1.47	1.39
16	S	103	BCL	C3C-C4C	-2.88	1.48	1.51
16	5	104	BCL	OBD-CAD	2.88	1.27	1.22
16	9	103	BCL	CMC-C2C	-2.88	1.47	1.53
24	T	102	LMT	C12-C11	2.88	1.73	1.49
16	D	103	BCL	O2D-CGD	2.87	1.40	1.33
16	L	301	BCL	C4D-CHA	2.85	1.48	1.38
16	D	103	BCL	C1D-ND	-2.85	1.34	1.37
16	U	103	BCL	C3D-C2D	2.85	1.46	1.39
16	M	402	BCL	C1B-CHB	2.85	1.48	1.41
16	3	104	BCL	C3D-C2D	2.84	1.46	1.39
15	D	101	PGV	O03-C19	2.84	1.41	1.33
23	O	106	H4X	C18-C17	2.84	1.56	1.50
16	F	103	BCL	C3B-C2B	2.84	1.44	1.39
16	3	103	BCL	MG-ND	-2.83	2.00	2.05
15	Q	101	PGV	O01-C02	-2.83	1.39	1.46
15	A	101	PGV	O01-C1	2.82	1.42	1.34
16	I	102	BCL	C4B-CHC	2.81	1.48	1.41
16	O	105	BCL	C1B-CHB	2.80	1.48	1.41
16	U	103	BCL	C1B-NB	2.80	1.37	1.35
16	B	103	BCL	C4D-CHA	2.79	1.48	1.38
16	M	403	BCL	CMD-C2D	-2.79	1.44	1.50
16	D	104	BCL	C1D-ND	-2.79	1.34	1.37
23	6	101	H4X	C32-C33	-2.78	1.31	1.34
11	C	402	HEM	C2C-C1C	-2.78	1.36	1.42
16	5	104	BCL	C3D-C2D	2.77	1.46	1.39
16	O	104	BCL	C3C-C4C	-2.77	1.48	1.51
16	K	105	BCL	C4D-CHA	2.77	1.48	1.38
18	L	303	UQ8	C4-C3	2.77	1.47	1.36
16	Q	103	BCL	C4D-CHA	2.76	1.48	1.38
16	9	103	BCL	C4D-CHA	2.76	1.48	1.38
23	P	101	H4X	C18-C17	2.76	1.56	1.50
16	X	101	BCL	C3D-C2D	2.76	1.46	1.39
16	A	102	BCL	C4D-CHA	2.76	1.48	1.38
16	9	104	BCL	C1B-NB	2.76	1.37	1.35
11	C	401	HEM	FE-NB	2.75	2.10	1.96
16	D	103	BCL	C4B-CHC	2.75	1.48	1.41
16	I	102	BCL	C1B-CHB	2.74	1.48	1.41
16	F	105	BCL	C1B-CHB	2.74	1.48	1.41
23	O	106	H4X	C32-C33	-2.74	1.31	1.34
16	X	101	BCL	CHD-C4C	2.73	1.46	1.39
16	Q	104	BCL	CMB-C2B	-2.72	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	9	104	BCL	C4D-CHA	2.72	1.48	1.38
16	A	102	BCL	CAA-C2A	-2.71	1.49	1.54
16	5	103	BCL	C1D-ND	-2.70	1.34	1.37
16	L	304	BCL	CBD-CGD	-2.68	1.44	1.52
16	L	304	BCL	OBD-CAD	2.68	1.27	1.22
16	M	402	BCL	CHD-C4C	2.68	1.46	1.39
16	2	102	BCL	CHD-C4C	2.66	1.46	1.39
15	C	408	PGV	O01-C02	-2.66	1.42	1.47
16	5	103	BCL	CMC-C2C	-2.65	1.47	1.53
23	P	101	H4X	C13-C12	2.65	1.56	1.50
16	Q	103	BCL	C4B-CHC	2.64	1.48	1.41
24	T	102	LMT	O1'-C1'	2.64	1.44	1.40
16	3	103	BCL	C3D-C2D	2.64	1.46	1.39
24	R	101	LMT	O1'-C1'	2.64	1.44	1.40
16	O	104	BCL	C1B-CHB	2.64	1.48	1.41
16	L	301	BCL	CHD-C4C	2.63	1.46	1.39
16	K	108	BCL	C1D-ND	-2.63	1.34	1.37
23	O	101	H4X	C14-C12	-2.63	1.32	1.35
16	F	103	BCL	CMA-C3A	-2.63	1.47	1.53
16	Q	104	BCL	CAC-C3C	-2.62	1.48	1.54
16	Y	102	BCL	C1B-CHB	2.62	1.48	1.41
11	C	403	HEM	C1A-NA	2.62	1.41	1.36
16	M	402	BCL	C3D-C2D	2.61	1.46	1.39
16	W	102	BCL	C4D-CHA	2.61	1.47	1.38
16	O	105	BCL	C4B-CHC	2.61	1.48	1.41
11	C	403	HEM	C1B-C2B	-2.61	1.39	1.44
16	3	103	BCL	CAA-C2A	-2.60	1.49	1.54
16	W	102	BCL	C3D-C2D	2.60	1.46	1.39
16	L	301	BCL	C3B-C2B	2.59	1.44	1.39
16	K	105	BCL	CAA-C2A	-2.59	1.49	1.54
23	K	103	H4X	C32-C33	-2.59	1.31	1.34
16	9	103	BCL	C3D-C2D	2.58	1.46	1.39
16	1	102	BCL	C4B-CHC	2.58	1.48	1.41
16	3	104	BCL	CAA-C2A	-2.58	1.49	1.54
16	7	103	BCL	C1B-NB	2.57	1.37	1.35
23	U	104	H4X	C35-C33	2.57	1.56	1.51
16	B	103	BCL	CMB-C2B	-2.57	1.46	1.51
16	9	103	BCL	OBD-CAD	2.57	1.26	1.22
16	J	101	BCL	C3D-C2D	2.57	1.46	1.39
16	1	102	BCL	CAC-C3C	-2.57	1.48	1.54
16	D	103	BCL	OBD-CAD	2.57	1.26	1.22
16	W	102	BCL	C3B-C2B	2.56	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	304	BCL	CAC-C3C	-2.56	1.48	1.54
24	6	102	LMT	O1'-C1'	2.56	1.44	1.40
16	7	102	BCL	CHD-C4C	2.56	1.46	1.39
16	L	304	BCL	MG-ND	-2.56	2.00	2.05
23	E	101	H4X	C29-C28	2.56	1.56	1.50
11	C	404	HEM	CMC-C2C	-2.56	1.45	1.51
23	O	101	H4X	C31-C30	-2.55	1.28	1.34
16	3	103	BCL	C4B-CHC	2.55	1.48	1.41
16	D	104	BCL	C1B-CHB	2.54	1.48	1.41
16	J	101	BCL	C3B-C2B	2.53	1.44	1.39
24	B	104	LMT	O5B-C1B	2.53	1.48	1.41
18	L	303	UQ8	O3-C3M	-2.53	1.39	1.45
16	D	103	BCL	C3D-C2D	2.52	1.46	1.39
16	F	103	BCL	CHD-C4C	2.52	1.46	1.39
23	4	101	H4X	C27-C28	-2.52	1.32	1.35
24	4	102	LMT	O1'-C1'	2.52	1.44	1.40
11	C	404	HEM	CAB-C3B	2.52	1.54	1.47
16	U	102	BCL	C4D-CHA	2.52	1.47	1.38
16	O	105	BCL	C3D-C2D	2.51	1.46	1.39
16	L	301	BCL	C2A-C1A	-2.51	1.46	1.52
16	W	102	BCL	OBD-CAD	2.51	1.26	1.22
16	U	102	BCL	C3D-C2D	2.50	1.46	1.39
16	O	105	BCL	C4D-CHA	2.50	1.47	1.38
24	J	102	LMT	C1'-C2'	2.50	1.59	1.52
24	2	103	LMT	C1'-C2'	2.50	1.59	1.52
16	A	102	BCL	C1B-CHB	2.49	1.47	1.41
23	O	106	H4X	C27-C28	-2.49	1.32	1.35
24	E	102	LMT	O1'-C1'	2.49	1.44	1.40
16	I	102	BCL	CAA-C2A	-2.49	1.49	1.54
23	O	101	H4X	C6-C7	2.49	1.56	1.51
23	K	107	H4X	C18-C17	2.48	1.56	1.50
16	M	402	BCL	C4D-CHA	2.48	1.47	1.38
16	Q	104	BCL	C4D-CHA	2.48	1.47	1.38
16	F	103	BCL	OBD-CAD	2.48	1.26	1.22
16	L	304	BCL	C1B-CHB	2.47	1.47	1.41
16	T	101	BCL	C1D-ND	-2.47	1.34	1.37
16	Q	103	BCL	C1B-CHB	2.47	1.47	1.41
16	K	108	BCL	C3D-C2D	2.47	1.45	1.39
16	O	105	BCL	C1B-NB	2.47	1.37	1.35
16	O	105	BCL	CHD-C4C	2.47	1.46	1.39
16	Q	103	BCL	CAA-C2A	-2.46	1.49	1.54
16	K	108	BCL	C3C-C4C	-2.46	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	3	103	BCL	C1D-ND	-2.46	1.34	1.37
16	F	103	BCL	C2C-C3C	-2.46	1.47	1.54
16	3	103	BCL	C3C-C4C	-2.46	1.48	1.51
24	4	102	LMT	C1'-C2'	2.45	1.59	1.52
16	W	102	BCL	CHD-C4C	2.45	1.46	1.39
16	Y	102	BCL	CAA-C2A	-2.45	1.49	1.54
21	M	405	MQ8	C8-C7	2.45	1.44	1.38
16	U	103	BCL	O1D-CGD	2.45	1.27	1.21
16	F	105	BCL	CAA-C2A	-2.45	1.49	1.54
16	D	103	BCL	C4D-CHA	2.45	1.47	1.38
16	D	104	BCL	CHD-C4C	2.44	1.46	1.39
16	F	103	BCL	C4B-CHC	2.44	1.47	1.41
16	Y	102	BCL	C4B-CHC	2.44	1.47	1.41
18	L	306	UQ8	C4-C3	2.44	1.46	1.36
16	K	105	BCL	C1B-CHB	2.43	1.47	1.41
16	K	108	BCL	CMA-C3A	-2.43	1.47	1.53
16	1	102	BCL	CMA-C3A	-2.43	1.48	1.53
16	Q	104	BCL	C3D-C2D	2.43	1.45	1.39
23	Q	105	H4X	C18-C17	2.43	1.55	1.50
11	C	402	HEM	FE-NB	2.43	2.08	1.96
24	4	102	LMT	C12-C11	2.42	1.69	1.49
16	L	304	BCL	C1D-C2D	2.42	1.50	1.45
16	7	102	BCL	C4D-CHA	2.42	1.47	1.38
16	3	104	BCL	CMC-C2C	-2.41	1.48	1.53
23	6	101	H4X	C18-C17	2.41	1.55	1.50
16	T	101	BCL	C4B-NB	2.41	1.37	1.35
24	G	102	LMT	C1'-C2'	2.41	1.59	1.52
11	C	404	HEM	C1B-C2B	-2.41	1.39	1.44
16	Y	102	BCL	O2A-C1	-2.40	1.39	1.46
16	T	101	BCL	CMD-C2D	-2.40	1.45	1.50
16	Y	104	BCL	C1D-ND	-2.40	1.34	1.37
11	C	404	HEM	FE-NB	2.40	2.08	1.96
16	3	104	BCL	C4D-CHA	2.40	1.46	1.38
16	Q	104	BCL	CHD-C4C	2.40	1.46	1.39
16	D	104	BCL	C1B-NB	2.39	1.37	1.35
16	U	102	BCL	C1D-ND	-2.39	1.34	1.37
16	D	104	BCL	MG-ND	-2.39	2.01	2.05
16	5	103	BCL	C4D-CHA	2.39	1.46	1.38
24	E	102	LMT	C12-C11	2.39	1.69	1.49
18	L	303	UQ8	C7-C8	-2.38	1.47	1.50
23	U	104	H4X	C14-C12	-2.38	1.32	1.35
23	P	101	H4X	C27-C28	-2.37	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	103	BCL	C1B-CHB	2.37	1.47	1.41
24	J	102	LMT	O1'-C1'	2.37	1.44	1.40
15	H	301	PGV	O03-C01	-2.36	1.39	1.45
16	F	105	BCL	C4B-CHC	2.36	1.47	1.41
16	A	102	BCL	C1B-NB	2.36	1.37	1.35
16	S	103	BCL	MG-ND	-2.36	2.01	2.05
16	F	105	BCL	O1D-CGD	2.35	1.27	1.21
16	S	103	BCL	OBD-CAD	2.35	1.26	1.22
16	7	102	BCL	O2A-C1	-2.35	1.39	1.46
24	N	101	LMT	O1'-C1'	2.34	1.44	1.40
16	B	103	BCL	C1B-CHB	2.33	1.47	1.41
23	5	105	H4X	C18-C17	2.33	1.55	1.50
16	L	301	BCL	C2-C3	2.33	1.38	1.33
16	F	105	BCL	C4D-CHA	2.33	1.46	1.38
23	B	101	H4X	C24-C23	2.33	1.55	1.50
16	J	101	BCL	CMA-C3A	-2.33	1.48	1.53
16	T	101	BCL	MG-ND	-2.32	2.01	2.05
23	B	101	H4X	C2-C1	2.32	1.57	1.52
16	9	103	BCL	C3C-C4C	-2.32	1.48	1.51
16	5	104	BCL	C4D-CHA	2.31	1.46	1.38
15	C	408	PGV	P-O12	2.31	1.63	1.54
11	C	401	HEM	CBD-CGD	2.31	1.55	1.50
16	I	102	BCL	CHD-C4C	2.31	1.45	1.39
16	O	104	BCL	CAA-C2A	-2.31	1.49	1.54
23	4	101	H4X	C14-C12	-2.31	1.32	1.35
23	P	101	H4X	C39-C38	2.31	1.57	1.52
24	0	101	LMT	O1'-C1'	2.30	1.44	1.40
16	T	101	BCL	C1B-NB	2.30	1.37	1.35
16	M	403	BCL	CMB-C2B	-2.30	1.46	1.51
16	L	301	BCL	C4B-CHC	2.30	1.47	1.41
24	B	104	LMT	O1'-C1'	2.30	1.44	1.40
16	Q	104	BCL	CAA-C2A	-2.30	1.49	1.54
24	0	101	LMT	C12-C11	2.30	1.68	1.49
24	6	102	LMT	C12-C11	2.30	1.68	1.49
16	W	102	BCL	C4B-CHC	2.29	1.47	1.41
16	3	104	BCL	CMA-C3A	-2.29	1.48	1.53
16	5	104	BCL	MG-NC	-2.29	2.00	2.06
16	1	102	BCL	C4D-CHA	2.29	1.46	1.38
16	1	102	BCL	CBD-CGD	-2.28	1.45	1.52
24	2	103	LMT	C12-C11	2.28	1.68	1.49
16	9	103	BCL	C1D-ND	-2.28	1.35	1.37
16	3	103	BCL	C4D-CHA	2.27	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	103	BCL	C3D-C2D	2.27	1.45	1.39
17	L	302	BPH	CHA-CBD	-2.27	1.49	1.52
16	B	103	BCL	C4D-ND	-2.27	1.34	1.37
16	T	101	BCL	C3D-C2D	2.26	1.45	1.39
16	W	102	BCL	C3C-C4C	-2.26	1.48	1.51
16	U	102	BCL	CAC-C3C	-2.26	1.49	1.54
16	T	101	BCL	CAA-C2A	-2.26	1.49	1.54
16	3	104	BCL	CHD-C4C	2.25	1.45	1.39
16	7	102	BCL	C1B-CHB	2.25	1.47	1.41
23	O	101	H4X	C24-C23	2.25	1.55	1.50
16	Y	104	BCL	MG-ND	-2.24	2.01	2.05
11	C	401	HEM	C1D-ND	-2.24	1.34	1.38
11	C	401	HEM	C4B-NB	-2.24	1.34	1.38
23	U	104	H4X	C37-C38	2.24	1.56	1.53
16	9	103	BCL	CAA-C2A	-2.24	1.50	1.54
16	I	102	BCL	OBD-CAD	2.23	1.26	1.22
11	C	401	HEM	CHA-C4D	2.23	1.40	1.35
16	7	103	BCL	MG-ND	-2.23	2.01	2.05
16	2	102	BCL	CHD-C1D	2.23	1.42	1.38
16	S	103	BCL	C4B-CHC	2.22	1.47	1.41
16	3	103	BCL	CHD-C4C	2.22	1.45	1.39
16	D	103	BCL	CMA-C3A	-2.22	1.48	1.53
23	B	101	H4X	C27-C28	-2.22	1.32	1.35
24	R	101	LMT	C12-C11	2.22	1.68	1.49
23	G	101	H4X	C24-C23	2.22	1.55	1.50
23	Q	105	H4X	C32-C33	-2.21	1.31	1.34
16	K	108	BCL	CHD-C4C	2.21	1.45	1.39
16	D	104	BCL	C4D-ND	-2.21	1.34	1.37
11	C	402	HEM	C4B-NB	-2.21	1.34	1.38
16	M	403	BCL	C4D-CHA	2.20	1.46	1.38
24	2	103	LMT	O1'-C1'	2.20	1.43	1.40
16	F	105	BCL	C3C-C4C	-2.20	1.48	1.51
16	J	101	BCL	C1D-C2D	2.19	1.49	1.45
16	D	104	BCL	C4B-CHC	2.19	1.47	1.41
21	M	405	MQ8	C15-C16	-2.19	1.46	1.53
16	X	101	BCL	C3A-C2A	-2.19	1.48	1.54
11	C	404	HEM	C4A-NA	2.18	1.40	1.36
15	A	101	PGV	O05-C05	-2.18	1.36	1.43
16	M	402	BCL	C3C-C4C	-2.18	1.48	1.51
16	K	108	BCL	CMC-C2C	-2.18	1.48	1.53
17	L	302	BPH	C3B-C2B	2.18	1.43	1.39
11	C	403	HEM	FE-NB	2.17	2.07	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	104	BCL	CHD-C4C	2.17	1.45	1.39
16	A	102	BCL	C4B-NB	-2.17	1.33	1.35
11	C	401	HEM	C4D-ND	-2.16	1.36	1.40
16	Q	104	BCL	CBD-CGD	-2.16	1.45	1.52
16	B	103	BCL	CAA-C2A	-2.16	1.50	1.54
11	C	404	HEM	CMD-C2D	-2.15	1.46	1.50
16	U	103	BCL	C4D-CHA	2.15	1.46	1.38
16	F	103	BCL	C3D-C2D	2.15	1.45	1.39
16	J	101	BCL	C4B-NB	2.15	1.37	1.35
16	1	102	BCL	O2A-C1	-2.14	1.40	1.46
23	V	101	H4X	C2-C1	2.14	1.57	1.52
11	C	401	HEM	C3B-C2B	-2.14	1.32	1.37
16	A	102	BCL	C3D-C2D	2.14	1.45	1.39
11	C	402	HEM	CAB-C3B	2.14	1.53	1.47
24	6	102	LMT	C1'-C2'	2.14	1.58	1.52
16	D	104	BCL	CAA-C2A	-2.14	1.50	1.54
16	2	102	BCL	MG-ND	-2.13	2.01	2.05
16	F	105	BCL	O2D-CED	-2.13	1.40	1.45
16	D	103	BCL	CMD-C2D	-2.13	1.46	1.50
23	Z	101	H4X	C18-C17	2.12	1.55	1.50
16	Q	104	BCL	C3A-C2A	-2.12	1.48	1.54
16	A	102	BCL	O2A-C1	-2.12	1.40	1.46
16	S	103	BCL	C1B-CHB	2.12	1.46	1.41
16	W	102	BCL	O2A-C1	-2.12	1.40	1.46
11	C	401	HEM	FE-ND	-2.12	1.86	1.96
23	O	106	H4X	C6-C7	2.11	1.55	1.51
11	C	403	HEM	C1B-NB	-2.11	1.36	1.40
15	A	101	PGV	P-O12	2.11	1.67	1.59
24	X	102	LMT	O1'-C1'	2.11	1.43	1.40
24	Z	102	LMT	C12-C11	2.10	1.67	1.49
16	K	105	BCL	CMA-C3A	-2.10	1.48	1.53
24	B	104	LMT	C12-C11	2.10	1.67	1.49
16	F	105	BCL	C3D-C2D	2.10	1.44	1.39
23	V	101	H4X	C18-C17	2.10	1.55	1.50
16	K	105	BCL	C3D-C2D	2.10	1.44	1.39
23	5	105	H4X	C8-C7	2.10	1.56	1.50
16	K	108	BCL	MG-ND	-2.09	2.01	2.05
16	5	103	BCL	CAA-C2A	-2.09	1.50	1.54
11	C	401	HEM	CHB-C1B	2.09	1.40	1.35
16	B	103	BCL	C4B-CHC	2.09	1.46	1.41
16	U	102	BCL	C1B-CHB	2.09	1.46	1.41
16	X	101	BCL	C4B-CHC	2.09	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	403	BCL	CAC-C3C	-2.08	1.49	1.54
16	I	102	BCL	C4D-CHA	2.07	1.45	1.38
16	T	101	BCL	C4D-CHA	2.07	1.45	1.38
16	O	104	BCL	CMC-C2C	-2.07	1.48	1.53
16	X	101	BCL	C4D-CHA	2.07	1.45	1.38
23	O	101	H4X	C37-C38	2.06	1.56	1.53
23	O	106	H4X	C4-C1	2.06	1.56	1.53
16	B	103	BCL	CBD-CGD	-2.05	1.46	1.52
16	7	103	BCL	O2D-CED	-2.05	1.40	1.45
16	T	101	BCL	C1B-CHB	2.05	1.46	1.41
24	G	102	LMT	O1'-C1'	2.05	1.43	1.40
23	G	101	H4X	C6-C7	2.03	1.55	1.51
11	C	402	HEM	CBD-CGD	-2.03	1.45	1.50
23	O	101	H4X	C4-C1	2.02	1.56	1.53
23	G	101	H4X	C18-C17	2.02	1.55	1.50
23	O	106	H4X	C29-C28	2.02	1.55	1.50
16	S	103	BCL	CHD-C4C	2.02	1.44	1.39
16	5	103	BCL	CHD-C4C	2.01	1.44	1.39
16	9	104	BCL	C1B-CHB	2.01	1.46	1.41
17	M	404	BPH	C3B-C2B	2.01	1.43	1.39
11	C	401	HEM	C3D-C2D	-2.00	1.32	1.36
23	G	101	H4X	C3-C1	2.00	1.57	1.52

All (1354) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	L	304	BCL	O2D-CGD-CBD	15.70	139.16	111.27
16	L	304	BCL	O2D-CGD-O1D	-13.24	97.96	123.84
23	V	101	H4X	C21-C22-C23	-9.25	114.11	127.31
16	M	402	BCL	CHD-C1D-ND	-9.00	116.19	124.45
16	F	103	BCL	CHD-C1D-ND	-8.72	116.44	124.45
16	D	103	BCL	O2D-CGD-CBD	8.49	126.36	111.27
16	A	102	BCL	O2D-CGD-CBD	8.26	125.94	111.27
16	S	103	BCL	O2D-CGD-CBD	7.92	125.34	111.27
16	I	102	BCL	CHD-C1D-ND	-7.88	117.21	124.45
15	H	301	PGV	O01-C1-C2	7.88	128.49	111.50
16	M	403	BCL	C1C-NC-C4C	-7.86	103.17	106.71
16	I	102	BCL	O2D-CGD-CBD	7.78	125.10	111.27
16	1	102	BCL	CHD-C1D-ND	-7.71	117.37	124.45
16	U	102	BCL	O2D-CGD-CBD	7.70	124.95	111.27
23	5	105	H4X	C21-C22-C23	-7.50	116.60	127.31
16	9	103	BCL	O2D-CGD-CBD	7.44	124.49	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	3	103	BCL	O2D-CGD-CBD	7.43	124.47	111.27
16	L	301	BCL	C1C-NC-C4C	-7.26	103.44	106.71
18	L	303	UQ8	C15-C14-C16	7.24	127.45	115.27
16	M	402	BCL	O2D-CGD-CBD	7.19	124.05	111.27
23	V	101	H4X	C20-C19-C17	-7.13	117.13	127.31
16	Y	102	BCL	CHD-C1D-ND	-7.09	117.93	124.45
11	C	403	HEM	CHC-C4B-NB	7.03	132.07	124.43
16	Q	103	BCL	O2D-CGD-CBD	6.94	123.60	111.27
16	U	102	BCL	CHD-C1D-ND	-6.94	118.08	124.45
16	A	102	BCL	O2D-CGD-O1D	-6.92	110.31	123.84
16	D	103	BCL	CHD-C1D-ND	-6.83	118.17	124.45
16	M	403	BCL	O2D-CGD-CBD	6.81	123.37	111.27
23	7	104	H4X	C21-C22-C23	-6.75	117.68	127.31
16	K	108	BCL	C6-C5-C3	-6.74	95.79	113.45
16	M	402	BCL	O2D-CGD-O1D	-6.71	110.73	123.84
16	W	102	BCL	CHD-C1D-ND	-6.65	118.34	124.45
23	Z	101	H4X	C21-C22-C23	-6.64	117.83	127.31
16	7	102	BCL	CHD-C1D-ND	-6.62	118.37	124.45
16	1	102	BCL	O2D-CGD-CBD	6.58	122.96	111.27
16	2	102	BCL	C4-C3-C5	6.46	126.14	115.27
16	A	102	BCL	CHD-C1D-ND	-6.43	118.54	124.45
15	D	101	PGV	O01-C1-C2	6.41	125.32	111.50
16	O	104	BCL	CHD-C1D-ND	-6.38	118.59	124.45
16	F	103	BCL	CMD-C2D-C1D	6.35	135.90	124.71
16	F	103	BCL	O2D-CGD-CBD	6.31	122.48	111.27
16	L	304	BCL	CHD-C1D-ND	-6.28	118.68	124.45
16	7	102	BCL	O2D-CGD-CBD	6.27	122.41	111.27
16	K	105	BCL	CHD-C1D-ND	-6.23	118.73	124.45
23	E	101	H4X	C36-C35-C33	6.22	129.77	113.45
18	L	306	UQ8	C15-C14-C16	6.22	125.73	115.27
16	Y	102	BCL	O2D-CGD-CBD	6.21	122.30	111.27
16	U	103	BCL	CMD-C2D-C1D	6.19	135.63	124.71
23	G	101	H4X	C8-C7-C6	6.18	125.67	115.27
16	M	402	BCL	CHD-C4C-NC	6.10	131.85	125.08
16	5	103	BCL	CHD-C1D-ND	-6.09	118.86	124.45
23	V	101	H4X	C39-C38-C37	-6.02	100.20	111.14
23	Q	105	H4X	C21-C22-C23	-6.02	118.72	127.31
16	F	105	BCL	CMD-C2D-C1D	5.96	135.22	124.71
11	C	404	HEM	CHC-C4B-NB	5.94	130.89	124.43
16	S	103	BCL	O2D-CGD-O1D	-5.92	112.26	123.84
16	1	102	BCL	CMD-C2D-C1D	5.91	135.13	124.71
23	U	104	H4X	C34-C33-C35	5.90	125.20	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	O	101	H4X	C20-C21-C22	5.88	135.52	123.47
16	5	103	BCL	CMD-C2D-C1D	5.86	135.04	124.71
15	C	408	PGV	O01-C1-C2	5.85	124.11	111.50
16	K	105	BCL	O2D-CGD-CBD	5.78	121.54	111.27
16	W	102	BCL	O2D-CGD-CBD	5.74	121.47	111.27
16	O	104	BCL	O2D-CGD-CBD	5.74	121.47	111.27
23	G	101	H4X	C21-C22-C23	-5.74	119.12	127.31
16	S	103	BCL	CHD-C1D-ND	-5.74	119.18	124.45
16	5	103	BCL	O2D-CGD-CBD	5.71	121.41	111.27
23	E	101	H4X	C21-C22-C23	-5.67	119.22	127.31
16	I	102	BCL	O2D-CGD-O1D	-5.65	112.79	123.84
16	A	102	BCL	CMD-C2D-C1D	5.65	134.68	124.71
16	7	103	BCL	CMD-C2D-C1D	5.65	134.67	124.71
23	6	101	H4X	C20-C19-C17	-5.58	119.35	127.31
11	C	403	HEM	CBA-CAA-C2A	-5.55	103.14	112.62
24	V	102	LMT	O5B-C5B-C6B	5.55	120.23	106.44
16	5	104	BCL	CMD-C2D-C1D	5.53	134.47	124.71
16	D	103	BCL	O2D-CGD-O1D	-5.53	113.03	123.84
16	L	304	BCL	C1-O2A-CGA	5.53	130.94	116.44
16	U	102	BCL	O2D-CGD-O1D	-5.52	113.04	123.84
11	C	403	HEM	C1B-NB-C4B	5.49	110.74	105.07
11	C	404	HEM	CBA-CAA-C2A	-5.48	103.27	112.62
16	S	103	BCL	CMD-C2D-C1D	5.45	134.32	124.71
16	A	102	BCL	C4-C3-C5	5.38	124.31	115.27
16	3	103	BCL	CHD-C1D-ND	-5.35	119.53	124.45
24	2	103	LMT	O5B-C5B-C6B	5.34	119.72	106.44
16	Q	103	BCL	CHD-C1D-ND	-5.34	119.54	124.45
24	Z	102	LMT	O5B-C5B-C6B	5.27	119.54	106.44
23	O	101	H4X	C4-C5-C6	5.27	125.00	112.33
16	1	102	BCL	CHD-C4C-NC	5.27	130.93	125.08
16	D	104	BCL	CED-O2D-CGD	5.25	127.81	115.94
16	U	102	BCL	CMD-C2D-C1D	5.24	133.96	124.71
11	C	403	HEM	O2D-CGD-O1D	-5.24	110.23	123.30
16	L	304	BCL	CMD-C2D-C1D	5.24	133.95	124.71
23	6	101	H4X	C24-C23-C22	-5.23	115.59	122.92
16	3	103	BCL	O2D-CGD-O1D	-5.22	113.64	123.84
23	O	101	H4X	C8-C7-C6	5.21	124.04	115.27
16	O	105	BCL	C6-C5-C3	-5.21	99.79	113.45
16	K	105	BCL	CMD-C2D-C1D	5.20	133.88	124.71
16	O	104	BCL	CMD-C2D-C1D	5.18	133.84	124.71
16	L	304	BCL	C3D-C2D-C1D	-5.18	98.76	105.83
22	H	302	CDL	OA6-CA5-C11	5.18	122.66	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	L	305	PGV	O01-C1-C2	5.16	122.63	111.50
23	7	104	H4X	C26-C27-C28	-5.16	119.95	127.31
11	C	401	HEM	CHC-C4B-NB	5.16	130.03	124.43
23	O	101	H4X	C13-C12-C11	5.15	126.19	118.08
23	6	101	H4X	C21-C22-C23	-5.14	119.97	127.31
24	6	102	LMT	C1'-C2'-C3'	5.14	120.70	110.00
16	7	103	BCL	C1-C2-C3	-5.13	117.17	126.04
16	9	103	BCL	CMD-C2D-C1D	5.13	133.75	124.71
16	9	104	BCL	C6-C5-C3	-5.10	100.08	113.45
16	Q	104	BCL	C1C-NC-C4C	-5.10	104.41	106.71
11	C	402	HEM	C1B-NB-C4B	5.10	110.34	105.07
16	L	304	BCL	CED-O2D-CGD	-5.09	104.42	115.94
15	H	301	PGV	O01-C1-O02	-5.08	111.43	123.70
16	3	104	BCL	CMD-C2D-C1D	5.07	133.66	124.71
16	Q	104	BCL	C6-C5-C3	-5.06	100.20	113.45
16	Q	103	BCL	O2D-CGD-O1D	-5.06	113.95	123.84
16	O	105	BCL	C3C-C4C-CHD	-5.06	112.59	123.39
16	J	101	BCL	CMD-C2D-C1D	5.05	133.61	124.71
24	4	102	LMT	O5B-C5B-C6B	5.05	118.99	106.44
16	7	102	BCL	C3C-C4C-CHD	-5.04	112.61	123.39
23	U	104	H4X	C21-C22-C23	-5.03	120.14	127.31
16	Y	102	BCL	CMD-C2D-C1D	5.02	133.56	124.71
23	4	101	H4X	C21-C22-C23	-4.99	120.18	127.31
16	D	103	BCL	C4A-NA-C1A	-4.99	104.46	106.71
24	G	102	LMT	O5B-C5B-C6B	4.99	118.85	106.44
16	L	301	BCL	C3D-C2D-C1D	-4.97	99.04	105.83
16	9	103	BCL	CHD-C1D-ND	-4.97	119.89	124.45
23	V	101	H4X	C8-C7-C6	4.96	123.61	115.27
16	5	104	BCL	CHD-C1D-ND	-4.94	119.91	124.45
23	2	101	H4X	C21-C22-C23	-4.93	120.27	127.31
16	M	402	BCL	CMD-C2D-C1D	4.92	133.39	124.71
23	E	101	H4X	C20-C19-C17	-4.92	120.29	127.31
16	U	103	BCL	C1-C2-C3	-4.91	117.56	126.04
16	L	301	BCL	O2D-CGD-CBD	4.90	119.98	111.27
16	I	102	BCL	CMD-C2D-C1D	4.90	133.35	124.71
24	2	103	LMT	C1'-C2'-C3'	4.89	120.17	110.00
23	B	101	H4X	C39-C38-C37	-4.87	102.29	111.14
16	5	104	BCL	C3C-C4C-CHD	-4.86	113.00	123.39
16	T	101	BCL	C3C-C4C-CHD	-4.86	113.00	123.39
23	O	101	H4X	C21-C22-C23	-4.86	120.38	127.31
16	O	104	BCL	C2D-C1D-ND	4.85	113.68	110.10
24	4	102	LMT	C1'-C2'-C3'	4.85	120.09	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	K	108	BCL	C3C-C4C-CHD	-4.85	113.04	123.39
16	9	103	BCL	O2D-CGD-O1D	-4.84	114.37	123.84
16	W	102	BCL	CMD-C2D-C1D	4.83	133.22	124.71
24	J	102	LMT	C1'-C2'-C3'	4.81	120.02	110.00
23	U	104	H4X	C20-C19-C17	-4.81	120.44	127.31
16	Q	104	BCL	C4A-NA-C1A	-4.81	104.54	106.71
16	M	403	BCL	CMD-C2D-C1D	4.80	133.18	124.71
16	O	105	BCL	CMD-C2D-C1D	4.79	133.16	124.71
16	M	402	BCL	C3C-C4C-CHD	-4.78	113.17	123.39
23	7	104	H4X	C20-C19-C17	-4.77	120.50	127.31
16	K	108	BCL	CMD-C2D-C1D	4.75	133.09	124.71
16	Y	104	BCL	O2D-CGD-CBD	4.72	119.66	111.27
15	C	408	PGV	C02-O01-C1	-4.72	111.81	117.88
16	1	102	BCL	C3C-C4C-CHD	-4.72	113.31	123.39
16	L	304	BCL	C3C-C4C-CHD	-4.70	113.36	123.39
16	D	103	BCL	C2D-C1D-ND	4.68	113.55	110.10
16	B	103	BCL	CED-O2D-CGD	4.68	126.52	115.94
16	U	103	BCL	C6-C5-C3	-4.68	101.19	113.45
11	C	404	HEM	C1B-NB-C4B	4.67	109.89	105.07
16	B	103	BCL	CMD-C2D-C1D	4.67	132.94	124.71
16	U	103	BCL	C3D-C2D-C1D	-4.66	99.47	105.83
16	Y	102	BCL	C4-C3-C5	4.66	123.11	115.27
15	L	305	PGV	O03-C19-C20	4.66	126.53	111.91
15	3	101	PGV	O03-C19-C20	4.65	126.50	111.91
16	2	102	BCL	C3C-C4C-CHD	-4.63	113.49	123.39
16	2	102	BCL	CMD-C2D-C1D	4.63	132.87	124.71
11	C	403	HEM	CHB-C1B-NB	4.62	130.09	124.38
16	9	104	BCL	CMD-C2D-C1D	4.62	132.86	124.71
23	5	105	H4X	C20-C19-C17	-4.62	120.72	127.31
16	L	301	BCL	C3C-C4C-CHD	-4.62	113.52	123.39
24	V	102	LMT	C1'-C2'-C3'	4.61	119.60	110.00
16	X	101	BCL	O2D-CGD-CBD	4.61	119.45	111.27
23	V	101	H4X	C2-C1-C3	-4.60	101.71	110.37
16	9	103	BCL	CMB-C2B-C1B	4.60	135.54	128.46
16	Q	103	BCL	CMD-C2D-C1D	4.60	132.81	124.71
16	D	104	BCL	CMD-C2D-C1D	4.59	132.80	124.71
16	M	403	BCL	C3C-C4C-CHD	-4.59	113.59	123.39
16	T	101	BCL	CHD-C1D-ND	-4.58	120.24	124.45
16	M	403	BCL	CHD-C1D-ND	-4.58	120.25	124.45
23	O	106	H4X	C4-C5-C6	4.57	123.33	112.33
16	B	103	BCL	C3D-C2D-C1D	-4.57	99.60	105.83
16	J	101	BCL	CHD-C1D-ND	-4.56	120.27	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	X	101	BCL	C3C-C4C-CHD	-4.55	113.66	123.39
23	2	101	H4X	C26-C27-C28	-4.54	120.83	127.31
11	C	402	HEM	CHC-C4B-NB	4.53	129.35	124.43
16	B	103	BCL	C3C-C4C-CHD	-4.53	113.71	123.39
24	E	102	LMT	O5B-C5B-C6B	4.53	117.70	106.44
16	Q	104	BCL	C3C-C4C-CHD	-4.52	113.72	123.39
23	Z	101	H4X	C2-C1-C3	-4.52	101.86	110.37
15	F	104	PGV	O01-C1-C2	4.52	121.25	111.50
11	C	402	HEM	CHB-C1B-NB	4.52	129.97	124.38
16	W	102	BCL	O2D-CGD-O1D	-4.52	115.00	123.84
16	3	104	BCL	C4A-NA-C1A	-4.52	104.67	106.71
16	2	102	BCL	O2D-CGD-CBD	4.51	119.29	111.27
16	O	104	BCL	O2D-CGD-O1D	-4.51	115.02	123.84
16	Y	102	BCL	OBB-CAB-CBB	-4.51	110.03	120.17
15	O	102	PGV	O01-C1-C2	4.50	121.21	111.50
16	X	101	BCL	CMD-C2D-C1D	4.50	132.64	124.71
24	J	102	LMT	O5B-C5B-C6B	4.49	117.59	106.44
16	X	101	BCL	C1-C2-C3	-4.48	118.30	126.04
16	X	101	BCL	CHD-C1D-ND	-4.47	120.35	124.45
16	7	102	BCL	CHD-C4C-NC	4.46	130.03	125.08
16	Y	104	BCL	C3C-C4C-CHD	-4.45	113.88	123.39
24	G	102	LMT	C1'-C2'-C3'	4.45	119.26	110.00
16	L	301	BCL	CMD-C2D-C1D	4.45	132.55	124.71
16	9	104	BCL	C1-C2-C3	-4.44	118.36	126.04
23	E	101	H4X	C26-C27-C28	-4.44	120.98	127.31
16	F	105	BCL	CHD-C1D-ND	-4.44	120.38	124.45
24	J	102	LMT	O5'-C5'-C6'	-4.44	95.40	106.44
16	X	101	BCL	CMB-C2B-C3B	4.43	132.97	124.68
16	U	102	BCL	C3C-C4C-CHD	-4.43	113.92	123.39
23	P	101	H4X	C21-C22-C23	-4.43	120.99	127.31
24	2	103	LMT	O5'-C5'-C6'	-4.42	95.44	106.44
24	N	101	LMT	O5B-C5B-C6B	4.41	117.41	106.44
16	D	103	BCL	C3C-C4C-CHD	-4.40	113.98	123.39
15	1	103	PGV	O01-C1-C2	4.40	120.98	111.50
23	O	101	H4X	C39-C38-C37	-4.38	103.18	111.14
16	7	103	BCL	CED-O2D-CGD	4.37	125.83	115.94
16	U	103	BCL	CHD-C1D-ND	-4.37	120.44	124.45
16	7	103	BCL	C6-C5-C3	-4.37	102.00	113.45
16	Y	104	BCL	CMD-C2D-C1D	4.35	132.39	124.71
16	3	104	BCL	C3C-C4C-CHD	-4.34	114.12	123.39
15	K	101	PGV	O01-C1-C2	4.33	120.83	111.50
23	K	107	H4X	C21-C22-C23	-4.32	121.14	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	K	108	BCL	C3D-C2D-C1D	-4.31	99.95	105.83
24	6	102	LMT	O5B-C5B-C6B	4.30	117.13	106.44
16	7	103	BCL	C1-O2A-CGA	4.30	127.72	116.44
16	A	102	BCL	C1C-NC-C4C	-4.28	104.78	106.71
16	J	101	BCL	C3C-C4C-CHD	-4.27	114.27	123.39
16	2	102	BCL	C4-C3-C2	-4.27	112.72	123.68
16	M	403	BCL	O2D-CGD-O1D	-4.27	115.50	123.84
16	F	105	BCL	C1-C2-C3	-4.26	118.68	126.04
16	Y	102	BCL	C3C-C4C-CHD	-4.25	114.32	123.39
16	O	105	BCL	CED-O2D-CGD	4.24	125.53	115.94
17	M	404	BPH	CAC-C3C-C2C	-4.23	103.69	114.26
16	T	101	BCL	CMD-C2D-C1D	4.23	132.16	124.71
16	J	101	BCL	O2D-CGD-CBD	4.23	118.78	111.27
23	4	101	H4X	C20-C19-C17	-4.23	121.28	127.31
16	D	103	BCL	CMD-C2D-C1D	4.21	132.14	124.71
24	P	102	LMT	C1B-O5B-C5B	4.21	121.96	113.69
16	Y	102	BCL	C1C-NC-C4C	-4.21	104.81	106.71
16	Q	104	BCL	C1-C2-C3	-4.21	118.77	126.04
15	F	104	PGV	O01-C1-O02	-4.20	113.56	123.70
23	B	101	H4X	C34-C33-C35	4.20	122.33	115.27
16	7	102	BCL	CMD-C2D-C1D	4.19	132.10	124.71
16	7	103	BCL	C3D-C2D-C1D	-4.18	100.12	105.83
16	T	101	BCL	C3D-C2D-C1D	-4.18	100.13	105.83
16	O	105	BCL	CHD-C1D-ND	-4.17	120.62	124.45
23	K	103	H4X	C21-C22-C23	-4.17	121.36	127.31
15	C	408	PGV	O01-C1-O02	-4.17	113.63	123.70
16	J	101	BCL	C3D-C2D-C1D	-4.17	100.14	105.83
16	D	103	BCL	C3D-C2D-C1D	-4.16	100.15	105.83
16	7	102	BCL	O2D-CGD-O1D	-4.16	115.71	123.84
24	T	102	LMT	C1'-C2'-C3'	4.15	118.64	110.00
16	U	102	BCL	CAA-C2A-C3A	-4.15	101.42	112.78
16	A	102	BCL	C2D-C1D-ND	4.15	113.16	110.10
23	O	101	H4X	C13-C12-C14	-4.14	117.12	122.92
16	5	104	BCL	C1-C2-C3	-4.14	118.88	126.04
15	H	301	PGV	O03-C19-C20	4.13	124.88	111.91
16	W	102	BCL	C1C-NC-C4C	-4.12	104.85	106.71
16	L	304	BCL	C2D-C1D-ND	4.12	113.14	110.10
16	I	102	BCL	C4-C3-C5	4.12	122.21	115.27
15	Q	101	PGV	O03-C19-C20	4.12	124.84	111.91
16	L	301	BCL	CMB-C2B-C1B	4.12	134.80	128.46
16	3	103	BCL	C3C-C4C-CHD	-4.11	114.60	123.39
16	F	103	BCL	O2D-CGD-O1D	-4.11	115.80	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	O	105	BCL	C4-C3-C5	4.11	122.18	115.27
23	Q	105	H4X	C34-C33-C35	4.09	122.16	115.27
23	Z	101	H4X	C20-C19-C17	-4.09	121.47	127.31
23	O	101	H4X	C5-C6-C7	4.08	124.15	113.45
11	C	401	HEM	C1B-NB-C4B	4.08	109.28	105.07
11	C	404	HEM	CMA-C3A-C4A	-4.08	122.20	128.46
23	E	101	H4X	C5-C6-C7	4.07	124.12	113.45
16	U	102	BCL	C2D-C1D-ND	4.06	113.09	110.10
16	W	102	BCL	C4A-NA-C1A	-4.05	104.89	106.71
15	F	101	PGV	O01-C1-C2	4.05	120.23	111.50
16	M	402	BCL	C4-C3-C5	4.05	122.08	115.27
16	L	304	BCL	CHD-C4C-NC	4.03	129.56	125.08
23	2	101	H4X	C20-C19-C17	-4.03	121.56	127.31
24	T	102	LMT	O5B-C5B-C6B	4.02	116.44	106.44
16	B	103	BCL	O2D-CGD-CBD	4.01	118.39	111.27
16	A	102	BCL	C3D-C2D-C1D	-4.00	100.37	105.83
16	F	103	BCL	CHD-C4C-NC	4.00	129.52	125.08
22	H	302	CDL	OB6-CB5-C51	4.00	120.13	111.50
23	5	105	H4X	C4-C5-C6	4.00	121.95	112.33
16	7	102	BCL	C3D-C2D-C1D	-3.99	100.38	105.83
16	Q	103	BCL	C3C-C4C-CHD	-3.97	114.90	123.39
16	K	108	BCL	CHD-C4C-NC	3.97	129.49	125.08
16	3	104	BCL	C1C-NC-C4C	-3.97	104.92	106.71
16	B	103	BCL	C6-C5-C3	-3.96	103.06	113.45
16	Y	104	BCL	C3D-C2D-C1D	-3.96	100.43	105.83
16	D	104	BCL	C1-C2-C3	-3.95	119.20	126.04
16	J	101	BCL	C1-C2-C3	-3.95	119.20	126.04
16	Q	104	BCL	C4-C3-C5	3.95	121.91	115.27
23	7	104	H4X	C2-C1-C3	-3.94	102.96	110.37
16	S	103	BCL	C3C-C4C-CHD	-3.94	114.97	123.39
16	5	103	BCL	O2D-CGD-O1D	-3.94	116.14	123.84
23	Q	105	H4X	C39-C38-C37	-3.94	103.99	111.14
24	R	101	LMT	C1'-C2'-C3'	3.93	118.19	110.00
16	U	102	BCL	C3D-C2D-C1D	-3.93	100.46	105.83
16	D	104	BCL	C3D-C2D-C1D	-3.93	100.46	105.83
18	L	306	UQ8	C10-C9-C11	3.93	121.89	115.27
24	N	101	LMT	C1'-C2'-C3'	3.93	118.18	110.00
23	O	106	H4X	C20-C19-C17	-3.93	121.70	127.31
16	B	103	BCL	C1-C2-C3	-3.93	119.25	126.04
11	C	401	HEM	CHA-C4D-ND	3.92	129.22	124.38
16	3	104	BCL	C4-C3-C5	3.92	121.86	115.27
23	K	107	H4X	C24-C23-C22	-3.92	117.44	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	101	H4X	C26-C27-C28	-3.92	121.72	127.31
24	0	101	LMT	C1B-O5B-C5B	3.91	121.37	113.69
16	7	103	BCL	C3C-C4C-CHD	-3.91	115.03	123.39
23	4	101	H4X	C15-C14-C12	-3.91	121.73	127.31
16	Q	104	BCL	C1-O2A-CGA	3.90	126.67	116.44
16	Q	104	BCL	CMD-C2D-C1D	3.89	131.57	124.71
16	D	104	BCL	C3C-C4C-CHD	-3.88	115.09	123.39
16	O	105	BCL	O2D-CGD-CBD	3.88	118.17	111.27
16	Y	104	BCL	C6-C5-C3	-3.88	103.27	113.45
16	B	103	BCL	CHD-C4C-NC	3.88	129.39	125.08
16	9	103	BCL	C3C-C4C-CHD	-3.88	115.10	123.39
23	Z	101	H4X	C5-C6-C7	3.88	123.63	113.45
16	K	108	BCL	CED-O2D-CGD	3.88	124.71	115.94
16	W	102	BCL	C3D-C2D-C1D	-3.88	100.54	105.83
23	Q	105	H4X	C36-C35-C33	3.87	123.61	113.45
16	Q	104	BCL	O2D-CGD-CBD	3.87	118.14	111.27
16	O	104	BCL	C3D-C2D-C1D	-3.86	100.57	105.83
16	F	105	BCL	C4-C3-C5	3.85	121.75	115.27
16	L	301	BCL	C4-C3-C5	3.85	121.75	115.27
16	Q	104	BCL	C3D-C2D-C1D	-3.85	100.57	105.83
16	Q	103	BCL	C3D-C2D-C1D	-3.85	100.58	105.83
23	Q	105	H4X	C5-C6-C7	3.85	123.54	113.45
23	V	101	H4X	C3-C1-C4	-3.84	104.16	111.14
16	K	105	BCL	O2D-CGD-O1D	-3.84	116.33	123.84
23	O	101	H4X	C2-C1-C3	-3.83	103.17	110.37
16	O	105	BCL	C1-C2-C3	-3.83	119.43	126.04
16	F	103	BCL	C3C-C4C-CHD	-3.82	115.22	123.39
23	K	103	H4X	C24-C23-C22	-3.82	117.57	122.92
16	Y	104	BCL	O2D-CGD-O1D	-3.82	116.37	123.84
16	X	101	BCL	C3D-C2D-C1D	-3.82	100.62	105.83
16	3	104	BCL	CED-O2D-CGD	3.82	124.57	115.94
11	C	402	HEM	CHD-C1D-ND	3.80	128.56	124.43
23	5	105	H4X	C39-C38-C37	-3.80	104.24	111.14
23	7	104	H4X	C34-C33-C35	3.79	121.64	115.27
16	M	403	BCL	C3D-C2D-C1D	-3.78	100.68	105.83
16	1	102	BCL	O2D-CGD-O1D	-3.77	116.46	123.84
16	U	103	BCL	C3C-C4C-CHD	-3.77	115.33	123.39
16	W	102	BCL	C3C-C4C-CHD	-3.76	115.36	123.39
23	6	101	H4X	C34-C33-C35	3.76	121.60	115.27
16	D	103	BCL	CHD-C4C-NC	3.76	129.25	125.08
23	K	107	H4X	C26-C27-C28	-3.76	121.95	127.31
16	5	103	BCL	CAC-C3C-C2C	-3.75	104.88	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	103	BCL	CHD-C4C-NC	3.75	129.24	125.08
16	K	108	BCL	CHD-C1D-ND	-3.75	121.01	124.45
16	L	304	BCL	C4A-NA-C1A	-3.75	105.02	106.71
11	C	402	HEM	CAD-CBD-CGD	-3.75	105.54	113.60
24	4	102	LMT	O5'-C5'-C6'	-3.74	97.12	106.44
16	Q	104	BCL	O2D-CGD-O1D	-3.74	116.53	123.84
11	C	404	HEM	CHB-C1B-NB	3.74	129.00	124.38
23	G	101	H4X	C20-C19-C17	-3.74	121.98	127.31
15	F	101	PGV	O01-C02-C01	3.73	121.92	108.40
23	K	107	H4X	C20-C19-C17	-3.73	121.98	127.31
16	U	103	BCL	O2D-CGD-CBD	3.72	117.88	111.27
15	3	101	PGV	O01-C1-C2	3.71	119.50	111.50
23	G	101	H4X	C4-C5-C6	3.71	121.24	112.33
16	5	104	BCL	O2D-CGD-CBD	3.70	117.85	111.27
24	G	102	LMT	O5'-C5'-C6'	-3.70	97.24	106.44
23	O	101	H4X	C36-C35-C33	3.69	123.14	113.45
16	5	103	BCL	C3D-C2D-C1D	-3.69	100.80	105.83
16	U	102	BCL	CHD-C4C-NC	3.69	129.17	125.08
16	F	105	BCL	C3C-C4C-CHD	-3.69	115.52	123.39
16	9	103	BCL	CAA-C2A-C3A	-3.69	102.69	112.78
11	C	401	HEM	O2D-CGD-O1D	-3.68	114.12	123.30
16	F	105	BCL	C1-O2A-CGA	3.68	126.10	116.44
16	X	101	BCL	O2D-CGD-O1D	-3.68	116.65	123.84
16	O	104	BCL	C3C-C4C-CHD	-3.67	115.54	123.39
23	P	101	H4X	C40-C38-C39	3.67	117.27	110.37
16	L	301	BCL	CHD-C1D-ND	-3.66	121.09	124.45
16	5	104	BCL	CHD-C4C-NC	3.65	129.13	125.08
23	P	101	H4X	C5-C6-C7	3.65	123.03	113.45
16	3	104	BCL	C3D-C2D-C1D	-3.63	100.88	105.83
16	J	101	BCL	CHD-C4C-NC	3.63	129.11	125.08
15	M	406	PGV	O01-C1-C2	3.63	119.31	111.50
16	3	103	BCL	CMD-C2D-C1D	3.63	131.10	124.71
24	B	102	LMT	C1B-O5B-C5B	3.62	120.80	113.69
23	Q	105	H4X	C13-C12-C14	3.61	127.98	122.92
16	9	104	BCL	O2D-CGD-CBD	3.61	117.68	111.27
16	K	105	BCL	C3C-C4C-CHD	-3.61	115.68	123.39
16	Y	104	BCL	CAC-C3C-C2C	-3.60	105.25	114.26
16	5	104	BCL	C3D-C2D-C1D	-3.60	100.92	105.83
24	X	102	LMT	O5B-C5B-C6B	3.60	115.39	106.44
16	L	301	BCL	C2D-C1D-ND	3.60	112.76	110.10
16	T	101	BCL	CHD-C4C-NC	3.60	129.07	125.08
23	K	107	H4X	C36-C35-C33	3.60	122.89	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	W	102	BCL	CAA-C2A-C3A	-3.60	102.92	112.78
16	Y	104	BCL	C1-C2-C3	-3.60	119.82	126.04
16	Q	104	BCL	C2D-C1D-ND	3.59	112.75	110.10
16	5	103	BCL	C2D-C1D-ND	3.58	112.74	110.10
24	V	102	LMT	O5'-C5'-C6'	-3.57	97.55	106.44
23	K	107	H4X	C4-C5-C6	3.57	120.91	112.33
16	2	102	BCL	O2D-CGD-O1D	-3.57	116.86	123.84
16	T	101	BCL	O2D-CGD-CBD	3.57	117.61	111.27
11	C	403	HEM	CMA-C3A-C4A	-3.57	122.98	128.46
16	3	104	BCL	C1-O2A-CGA	3.57	125.80	116.44
23	O	106	H4X	C34-C33-C35	3.56	121.27	115.27
23	O	106	H4X	C21-C22-C23	-3.56	122.22	127.31
16	T	101	BCL	C2D-C1D-ND	3.56	112.73	110.10
16	9	103	BCL	O2A-CGA-CBA	3.56	123.08	111.91
16	O	105	BCL	C3D-C2D-C1D	-3.56	100.98	105.83
16	I	102	BCL	C3C-C4C-CHD	-3.55	115.80	123.39
16	2	102	BCL	C7-C6-C5	3.55	123.00	113.36
23	Z	101	H4X	C26-C27-C28	-3.55	122.25	127.31
24	E	102	LMT	O5'-C5'-C6'	-3.55	97.62	106.44
16	3	104	BCL	O2D-CGD-CBD	3.54	117.56	111.27
15	9	101	PGV	O01-C1-C2	3.54	119.13	111.50
23	O	106	H4X	C24-C23-C25	3.54	123.65	118.08
24	E	102	LMT	C1'-C2'-C3'	3.54	117.36	110.00
16	2	102	BCL	CMB-C2B-C3B	3.54	131.29	124.68
16	7	102	BCL	C2D-C1D-ND	3.53	112.71	110.10
23	6	101	H4X	C24-C23-C25	3.53	123.64	118.08
16	S	103	BCL	C3D-C2D-C1D	-3.53	101.01	105.83
23	K	103	H4X	C39-C38-C37	-3.53	104.73	111.14
23	Q	105	H4X	C20-C19-C17	-3.52	122.28	127.31
23	G	101	H4X	C14-C15-C16	-3.52	112.24	123.22
16	9	103	BCL	C3D-C2D-C1D	-3.52	101.03	105.83
23	2	101	H4X	C40-C38-C37	-3.51	104.76	111.14
16	L	301	BCL	CMC-C2C-C3C	-3.50	99.72	113.83
16	2	102	BCL	CHD-C1D-ND	-3.50	121.24	124.45
11	C	401	HEM	CHD-C1D-ND	3.49	128.23	124.43
23	Q	105	H4X	C26-C27-C28	-3.49	122.33	127.31
23	O	106	H4X	C26-C27-C28	-3.49	122.33	127.31
16	W	102	BCL	C2D-C1D-ND	3.49	112.67	110.10
15	5	101	PGV	O03-C19-O04	-3.48	114.80	123.59
23	6	101	H4X	C9-C10-C11	-3.48	112.35	123.22
16	D	104	BCL	CMB-C2B-C3B	3.48	131.19	124.68
16	3	104	BCL	CAA-C2A-C3A	-3.47	103.26	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	9	104	BCL	C3D-C2D-C1D	-3.47	101.10	105.83
23	B	101	H4X	C13-C12-C14	3.45	127.76	122.92
11	C	401	HEM	CMD-C2D-C1D	3.45	130.29	125.04
16	M	402	BCL	C1D-ND-C4D	-3.44	103.89	106.33
23	K	103	H4X	C32-C31-C30	-3.44	112.48	123.22
23	U	104	H4X	C36-C35-C33	3.44	122.47	113.45
16	Y	104	BCL	CHD-C4C-NC	3.43	128.89	125.08
15	Q	101	PGV	O01-C1-C2	3.43	118.89	111.50
16	M	403	BCL	CMB-C2B-C1B	3.43	133.73	128.46
16	5	103	BCL	CED-O2D-CGD	3.42	123.68	115.94
16	K	105	BCL	C3D-C2D-C1D	-3.42	101.16	105.83
16	M	402	BCL	C3D-C2D-C1D	-3.42	101.17	105.83
23	E	101	H4X	C2-C1-C3	-3.42	103.95	110.37
16	3	103	BCL	C3D-C2D-C1D	-3.42	101.17	105.83
18	L	303	UQ8	C16-C14-C13	-3.42	114.21	121.12
16	U	103	BCL	C1-O2A-CGA	3.41	125.40	116.44
16	T	101	BCL	C4-C3-C2	-3.41	114.94	123.68
16	S	103	BCL	CAC-C3C-C4C	-3.41	105.02	112.58
23	Q	105	H4X	C9-C10-C11	-3.41	112.58	123.22
16	Q	103	BCL	CAA-C2A-C3A	-3.41	103.45	112.78
11	C	402	HEM	C2C-C3C-C4C	-3.39	104.53	106.90
16	7	102	BCL	C1C-NC-C4C	-3.39	105.18	106.71
23	U	104	H4X	C26-C27-C28	-3.39	122.47	127.31
24	X	102	LMT	C1'-C2'-C3'	3.39	117.06	110.00
24	B	104	LMT	C1'-C2'-C3'	3.38	117.04	110.00
16	M	403	BCL	CAA-C2A-C3A	-3.38	103.52	112.78
11	C	404	HEM	CMA-C3A-C2A	3.38	131.31	124.94
16	Y	102	BCL	C1D-ND-C4D	-3.38	103.94	106.33
23	O	106	H4X	C32-C31-C30	-3.37	112.71	123.22
15	A	101	PGV	O01-C1-C2	3.37	118.75	111.50
16	K	108	BCL	CAA-C2A-C3A	-3.36	103.57	112.78
24	Z	102	LMT	C1'-C2'-C3'	3.35	116.97	110.00
23	2	101	H4X	C24-C23-C22	-3.35	118.23	122.92
16	B	103	BCL	O2D-CGD-O1D	-3.34	117.31	123.84
11	C	402	HEM	CHA-C4D-ND	3.34	128.51	124.38
16	L	304	BCL	CMB-C2B-C3B	3.34	130.93	124.68
16	1	102	BCL	C3D-C2D-C1D	-3.34	101.28	105.83
11	C	404	HEM	C4B-C3B-C2B	3.34	109.76	107.11
16	Y	104	BCL	C1D-CHD-C4C	-3.33	118.58	126.62
23	V	101	H4X	C2-C1-C4	3.33	117.19	111.14
16	5	104	BCL	C4-C3-C5	3.33	120.87	115.27
16	X	101	BCL	C1-O2A-CGA	3.33	125.18	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	4	101	H4X	C4-C5-C6	3.33	120.33	112.33
16	9	103	BCL	C4-C3-C5	3.32	120.86	115.27
16	9	103	BCL	C1C-NC-C4C	-3.32	105.22	106.71
16	3	104	BCL	C4-C3-C2	-3.32	115.17	123.68
23	O	106	H4X	C21-C20-C19	-3.31	116.69	123.47
16	X	101	BCL	C6-C5-C3	-3.31	104.77	113.45
23	5	105	H4X	C9-C10-C11	-3.31	112.88	123.22
16	B	103	BCL	C1D-CHD-C4C	-3.31	118.63	126.62
16	U	102	BCL	C1D-ND-C4D	-3.31	103.98	106.33
16	5	104	BCL	CAA-C2A-C3A	-3.31	103.72	112.78
16	U	103	BCL	CHD-C4C-NC	3.31	128.75	125.08
15	F	101	PGV	O03-C19-C20	3.30	122.28	111.91
16	W	102	BCL	O2A-CGA-CBA	3.30	122.27	111.91
22	S	101	CDL	OB6-CB5-C51	3.30	118.62	111.50
23	Q	105	H4X	C29-C28-C27	-3.30	118.30	122.92
23	O	106	H4X	C24-C23-C22	-3.29	118.32	122.92
16	5	103	BCL	C3C-C4C-CHD	-3.28	116.38	123.39
23	K	103	H4X	C5-C6-C7	3.28	122.06	113.45
16	F	105	BCL	C4-C3-C2	-3.28	115.27	123.68
16	F	103	BCL	C3D-C2D-C1D	-3.28	101.36	105.83
16	K	105	BCL	O2A-C1-C2	3.28	117.24	108.64
15	A	101	PGV	O01-C1-O02	-3.27	115.80	123.70
16	Y	104	BCL	C1-O2A-CGA	3.27	125.02	116.44
16	M	403	BCL	OBB-CAB-CBB	3.27	127.53	120.17
23	E	101	H4X	C20-C21-C22	-3.27	116.78	123.47
16	2	102	BCL	C3D-C2D-C1D	-3.27	101.38	105.83
16	T	101	BCL	C1-C2-C3	-3.26	120.40	126.04
16	D	104	BCL	O2D-CGD-CBD	3.26	117.05	111.27
11	C	404	HEM	CHD-C1D-ND	3.25	127.97	124.43
16	F	105	BCL	C3D-C2D-C1D	-3.25	101.40	105.83
16	5	103	BCL	C1-C2-C3	-3.25	120.42	126.04
16	7	103	BCL	O2D-CGD-CBD	3.25	117.04	111.27
23	P	101	H4X	C36-C35-C33	3.25	121.97	113.45
16	5	104	BCL	C4-C3-C2	-3.24	115.36	123.68
16	U	102	BCL	C4-C3-C5	3.24	120.73	115.27
16	L	301	BCL	C1B-CHB-C4A	-3.24	123.69	130.12
16	2	102	BCL	CAA-C2A-C3A	-3.24	103.91	112.78
16	M	403	BCL	C1D-CHD-C4C	-3.24	118.81	126.62
16	T	101	BCL	C4-C3-C5	3.24	120.71	115.27
24	G	102	LMT	C4B-C3B-C2B	-3.23	105.18	110.82
16	F	105	BCL	O2D-CGD-CBD	3.23	117.01	111.27
16	F	103	BCL	C4A-NA-C1A	-3.23	105.25	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	M	403	BCL	C4A-NA-C1A	3.23	108.16	106.71
16	B	103	BCL	C2D-C1D-ND	3.22	112.48	110.10
24	8	102	LMT	C1B-O5B-C5B	3.22	120.01	113.69
15	F	104	PGV	O03-C19-O04	-3.22	115.47	123.59
16	K	108	BCL	C4-C3-C5	3.21	120.68	115.27
16	B	103	BCL	CHD-C1D-ND	-3.21	121.51	124.45
16	D	104	BCL	C1-O2A-CGA	3.21	124.86	116.44
24	P	102	LMT	C1'-C2'-C3'	3.21	116.67	110.00
16	Q	104	BCL	C4-C3-C2	-3.20	115.46	123.68
11	C	403	HEM	CAD-C3D-C4D	3.20	130.25	124.66
16	3	104	BCL	O2D-CGD-O1D	-3.19	117.59	123.84
24	8	102	LMT	O5B-C5B-C6B	3.19	114.38	106.44
16	Y	102	BCL	C2D-C1D-ND	3.19	112.46	110.10
16	A	102	BCL	C3C-C4C-CHD	-3.19	116.57	123.39
16	9	104	BCL	C3C-C4C-CHD	-3.19	116.58	123.39
23	P	101	H4X	C32-C31-C30	-3.19	113.27	123.22
16	Y	102	BCL	O2A-CGA-O1A	-3.18	115.57	123.59
23	G	101	H4X	C36-C35-C33	3.18	121.79	113.45
16	J	101	BCL	O2D-CGD-O1D	-3.17	117.63	123.84
16	L	301	BCL	O2A-CGA-CBA	3.17	121.87	111.91
23	V	101	H4X	C14-C15-C16	-3.17	113.33	123.22
23	O	101	H4X	C14-C15-C16	-3.16	113.34	123.22
11	C	401	HEM	CBD-CAD-C3D	-3.16	103.84	112.63
11	C	403	HEM	C2C-C3C-C4C	3.15	109.10	106.90
16	T	101	BCL	O2D-CGD-O1D	-3.15	117.67	123.84
16	X	101	BCL	OBB-CAB-CBB	3.15	127.26	120.17
16	L	301	BCL	CAC-C3C-C4C	-3.15	105.59	112.58
18	L	303	UQ8	C1M-C1-C6	-3.15	119.26	124.40
23	K	107	H4X	C18-C17-C16	3.15	123.04	118.08
23	7	104	H4X	C36-C35-C33	3.14	121.70	113.45
16	L	301	BCL	C1D-CHD-C4C	-3.14	119.05	126.62
16	L	301	BCL	CHD-C4C-NC	3.14	128.56	125.08
23	V	101	H4X	C34-C33-C35	3.13	120.54	115.27
23	K	103	H4X	C24-C23-C25	3.13	123.01	118.08
23	O	106	H4X	C2-C1-C4	3.13	116.82	111.14
16	U	102	BCL	C4A-NA-C1A	-3.13	105.30	106.71
18	L	306	UQ8	C1M-C1-C6	-3.12	119.30	124.40
16	S	103	BCL	C2D-C1D-ND	3.12	112.40	110.10
16	D	103	BCL	C1D-ND-C4D	-3.12	104.12	106.33
16	Y	104	BCL	CAC-C3C-C4C	-3.11	105.68	112.58
23	G	101	H4X	C29-C28-C30	3.11	122.98	118.08
15	I	103	PGV	O01-C1-C2	3.10	118.19	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	O	102	PGV	C03-C02-C01	-3.10	104.46	111.79
15	5	101	PGV	O01-C1-C2	3.10	118.18	111.50
16	5	103	BCL	CHD-C4C-NC	3.10	128.52	125.08
23	Q	105	H4X	C3-C1-C4	-3.09	105.52	111.14
15	Q	101	PGV	C22-C21-C20	3.09	124.28	113.19
23	G	101	H4X	C20-C21-C22	-3.08	117.16	123.47
16	X	101	BCL	C2D-C1D-ND	3.08	112.38	110.10
23	P	101	H4X	C20-C19-C17	-3.07	122.92	127.31
16	Q	104	BCL	CMB-C2B-C3B	3.07	130.43	124.68
23	7	104	H4X	C39-C38-C37	-3.07	105.56	111.14
23	2	101	H4X	C32-C31-C30	-3.07	113.63	123.22
23	5	105	H4X	C2-C1-C4	-3.07	105.56	111.14
24	0	101	LMT	C1'-C2'-C3'	3.07	116.39	110.00
23	B	101	H4X	C21-C22-C23	-3.07	122.93	127.31
15	5	101	PGV	O03-C19-C20	3.07	121.54	111.91
15	9	101	PGV	O03-C19-C20	3.07	121.53	111.91
23	K	103	H4X	C9-C10-C11	-3.06	113.65	123.22
16	O	105	BCL	CHD-C4C-NC	3.06	128.48	125.08
16	9	104	BCL	C1-O2A-CGA	3.06	124.47	116.44
16	3	103	BCL	C1C-NC-C4C	-3.06	105.33	106.71
15	1	103	PGV	O12-P-O11	-3.05	98.60	106.73
23	E	101	H4X	C9-C10-C11	-3.05	113.69	123.22
16	Y	102	BCL	CHD-C4C-NC	3.05	128.47	125.08
23	B	101	H4X	C9-C10-C11	-3.05	113.70	123.22
16	F	103	BCL	CHD-C1D-C2D	3.05	131.87	125.48
23	K	107	H4X	C13-C12-C14	3.05	127.19	122.92
23	B	101	H4X	C13-C12-C11	-3.05	113.28	118.08
15	Q	101	PGV	C21-C20-C19	-3.04	102.56	113.62
16	F	103	BCL	CBA-CAA-C2A	-3.04	104.89	113.86
15	F	101	PGV	C02-O01-C1	-3.04	110.31	117.79
11	C	401	HEM	CHB-C1B-NB	3.03	128.12	124.38
16	9	104	BCL	O2D-CGD-O1D	-3.03	117.91	123.84
16	J	101	BCL	CHC-C1C-NC	3.02	128.69	124.51
15	H	301	PGV	C02-O01-C1	-3.02	110.36	117.79
16	T	101	BCL	C1-O2A-CGA	3.02	124.36	116.44
18	L	306	UQ8	C20-C19-C21	3.02	120.35	115.27
16	U	102	BCL	C1-C2-C3	-3.01	120.83	126.04
18	L	303	UQ8	C3M-O3-C3	3.01	127.15	116.47
16	2	102	BCL	CHD-C4C-NC	3.01	128.42	125.08
16	5	103	BCL	CAA-C2A-C3A	-3.01	104.53	112.78
16	5	103	BCL	C1C-NC-C4C	-3.01	105.35	106.71
15	1	103	PGV	O03-C19-C20	3.01	121.34	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	9	103	BCL	C1-C2-C3	-3.01	120.84	126.04
16	A	102	BCL	C5-C3-C2	-3.00	115.05	121.12
16	Y	102	BCL	C3D-C2D-C1D	-3.00	101.74	105.83
16	5	104	BCL	C6-C5-C3	-3.00	105.60	113.45
23	E	101	H4X	C18-C17-C16	2.99	122.79	118.08
16	L	301	BCL	C5-C3-C2	-2.99	115.06	121.12
18	L	303	UQ8	C7-C8-C9	-2.99	121.81	126.79
23	2	101	H4X	C34-C33-C35	2.99	120.30	115.27
16	A	102	BCL	C1D-ND-C4D	-2.99	104.21	106.33
16	9	103	BCL	C3D-C4D-ND	2.99	115.07	110.24
16	L	301	BCL	CHB-C4A-NA	2.99	128.64	124.51
16	Q	104	BCL	CAC-C3C-C4C	-2.99	105.96	112.58
16	L	304	BCL	C3D-C4D-ND	2.98	115.06	110.24
24	2	103	LMT	C4B-C3B-C2B	-2.98	105.62	110.82
24	4	102	LMT	C4B-C3B-C2B	-2.98	105.62	110.82
16	F	105	BCL	CAA-C2A-C3A	-2.98	104.62	112.78
22	Y	103	CDL	OA6-CA5-C11	2.98	119.18	111.38
24	N	101	LMT	O5'-C5'-C6'	-2.97	99.04	106.44
23	O	101	H4X	C16-C17-C19	-2.97	114.38	118.94
24	B	104	LMT	O5B-C5B-C6B	2.97	113.82	106.44
16	I	102	BCL	C3D-C2D-C1D	-2.97	101.78	105.83
16	K	108	BCL	C1C-NC-C4C	-2.97	105.37	106.71
23	6	101	H4X	C29-C28-C27	2.97	127.08	122.92
16	K	108	BCL	C1D-CHD-C4C	-2.97	119.47	126.62
23	B	101	H4X	C8-C7-C6	2.97	120.26	115.27
15	Y	105	PGV	O01-C1-C2	2.97	117.89	111.50
23	7	104	H4X	C14-C15-C16	-2.96	113.98	123.22
23	O	101	H4X	C2-C1-C4	-2.96	105.76	111.14
16	K	108	BCL	CAC-C3C-C4C	-2.96	106.02	112.58
24	B	102	LMT	O5B-C5B-C4B	2.95	115.06	109.69
16	L	304	BCL	CMA-C3A-C4A	-2.95	103.84	111.77
16	O	105	BCL	CMB-C2B-C3B	2.95	130.20	124.68
11	C	401	HEM	CMA-C3A-C4A	-2.95	123.93	128.46
16	J	101	BCL	C4-C3-C5	2.95	120.23	115.27
16	7	102	BCL	C5-C3-C2	-2.95	115.16	121.12
16	3	104	BCL	C1D-CHD-C4C	-2.94	119.52	126.62
16	K	108	BCL	C1-C2-C3	-2.94	120.96	126.04
16	B	103	BCL	CMB-C2B-C3B	2.94	130.18	124.68
18	L	306	UQ8	C11-C9-C8	-2.94	115.17	121.12
24	6	102	LMT	C4B-C3B-C2B	-2.94	105.70	110.82
16	I	102	BCL	CHD-C4C-NC	2.93	128.33	125.08
16	2	102	BCL	OBB-CAB-CBB	2.92	126.75	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	O	105	BCL	O2D-CGD-O1D	-2.92	118.12	123.84
11	C	403	HEM	CHD-C1D-ND	2.92	127.60	124.43
16	O	104	BCL	C3D-C4D-ND	2.92	114.96	110.24
23	G	101	H4X	C9-C10-C11	-2.92	114.11	123.22
23	K	107	H4X	C32-C31-C30	-2.92	114.11	123.22
16	J	101	BCL	C6-C5-C3	-2.91	105.82	113.45
16	O	105	BCL	C2D-C1D-ND	2.91	112.25	110.10
16	Y	102	BCL	C5-C3-C2	-2.91	115.23	121.12
16	K	105	BCL	O2A-CGA-CBA	2.91	121.04	111.91
16	L	301	BCL	CAA-C2A-C3A	-2.91	104.81	112.78
16	D	104	BCL	C1D-CHD-C4C	-2.91	119.61	126.62
23	B	101	H4X	C14-C15-C16	-2.91	114.15	123.22
15	A	101	PGV	O11-P-O13	2.90	120.41	109.07
23	2	101	H4X	C4-C5-C6	2.90	119.30	112.33
16	K	105	BCL	CHD-C4C-NC	2.90	128.30	125.08
16	M	403	BCL	CHD-C4C-NC	2.90	128.29	125.08
23	5	105	H4X	C15-C14-C12	-2.89	123.18	127.31
16	O	105	BCL	C2A-C1A-CHA	-2.89	118.80	123.86
16	Q	103	BCL	O2A-CGA-CBA	2.89	120.98	111.91
23	P	101	H4X	C39-C38-C37	-2.89	105.90	111.14
16	K	105	BCL	CAA-C2A-C3A	-2.88	104.88	112.78
16	K	108	BCL	O2D-CGD-CBD	2.88	116.39	111.27
16	J	101	BCL	CAA-C2A-C3A	-2.88	104.89	112.78
24	6	102	LMT	O5'-C5'-C6'	-2.88	99.28	106.44
16	T	101	BCL	C1D-CHD-C4C	-2.88	119.68	126.62
16	A	102	BCL	O2A-CGA-CBA	2.88	120.94	111.91
16	L	304	BCL	C1D-ND-C4D	-2.87	104.29	106.33
24	J	102	LMT	C4B-C3B-C2B	-2.87	105.81	110.82
23	B	101	H4X	C24-C23-C22	-2.87	118.90	122.92
16	J	101	BCL	C1-O2A-CGA	2.87	123.97	116.44
23	G	101	H4X	C26-C27-C28	-2.87	123.22	127.31
16	K	108	BCL	C2A-C1A-CHA	-2.86	118.85	123.86
24	Z	102	LMT	C4B-C3B-C2B	-2.86	105.83	110.82
16	7	103	BCL	CAA-C2A-C3A	-2.86	104.94	112.78
16	U	102	BCL	C3D-C4D-ND	2.86	114.87	110.24
11	C	401	HEM	CAD-CBD-CGD	-2.86	107.45	113.60
16	Q	104	BCL	CED-O2D-CGD	2.86	122.41	115.94
23	O	101	H4X	C27-C26-C25	-2.85	114.33	123.22
16	3	103	BCL	C6-C5-C3	-2.85	105.99	113.45
16	3	103	BCL	CAC-C3C-C4C	-2.85	106.26	112.58
16	T	101	BCL	CMB-C2B-C3B	2.85	130.00	124.68
23	G	101	H4X	C6-C7-C9	-2.84	113.37	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	101	LMT	C1'-O5'-C5'	2.84	119.27	113.69
16	M	402	BCL	CHD-C1D-C2D	2.84	131.44	125.48
15	K	102	PGV	O01-C1-C2	2.84	120.83	111.91
16	K	105	BCL	C11-C12-C13	-2.83	106.76	115.92
24	X	102	LMT	C1B-O5B-C5B	2.83	119.24	113.69
23	V	101	H4X	C36-C35-C33	2.83	120.87	113.45
16	Y	102	BCL	O2D-CGD-O1D	-2.83	118.31	123.84
16	O	105	BCL	C1D-CHD-C4C	-2.83	119.81	126.62
15	O	102	PGV	C02-O01-C1	-2.82	110.84	117.79
23	Q	105	H4X	C29-C28-C30	2.82	122.53	118.08
16	M	403	BCL	C3A-C2A-C1A	2.82	105.56	101.34
16	2	102	BCL	C1D-CHD-C4C	-2.82	119.82	126.62
16	O	105	BCL	C4-C3-C2	-2.81	116.46	123.68
14	C	407	DGA	OG2-CG2-CG3	2.81	114.35	107.93
16	7	102	BCL	OBB-CAB-CBB	-2.81	113.85	120.17
23	4	101	H4X	C8-C7-C6	2.81	119.99	115.27
16	F	105	BCL	C6-C7-C8	-2.80	106.86	115.92
16	M	403	BCL	C1-O2A-CGA	2.80	123.80	116.44
16	1	102	BCL	C4-C3-C5	2.80	119.99	115.27
16	F	105	BCL	CHC-C1C-NC	2.80	128.39	124.51
16	I	102	BCL	CBA-CAA-C2A	-2.80	105.60	113.86
16	9	103	BCL	CHD-C4C-NC	2.79	128.18	125.08
23	B	101	H4X	C40-C38-C37	2.79	116.20	111.14
23	7	104	H4X	C24-C23-C25	2.79	122.47	118.08
11	C	401	HEM	CBA-CAA-C2A	-2.79	107.86	112.62
16	I	102	BCL	C5-C3-C2	-2.79	115.47	121.12
16	3	103	BCL	CHD-C4C-NC	2.79	128.18	125.08
15	F	104	PGV	O03-C19-C20	2.79	120.66	111.91
11	C	402	HEM	CMD-C2D-C1D	2.79	129.29	125.04
16	O	105	BCL	C1-O2A-CGA	2.79	123.75	116.44
23	4	101	H4X	C36-C35-C33	2.78	120.75	113.45
16	9	104	BCL	C1D-CHD-C4C	-2.78	119.91	126.62
23	6	101	H4X	C3-C1-C4	-2.78	106.08	111.14
23	B	101	H4X	C2-C1-C4	2.78	116.18	111.14
16	M	403	BCL	O2A-CGA-CBA	2.78	120.63	111.91
16	W	102	BCL	CMB-C2B-C1B	2.78	132.73	128.46
16	7	103	BCL	CHD-C1D-ND	-2.77	121.91	124.45
16	K	108	BCL	C4-C3-C2	-2.77	116.56	123.68
16	J	101	BCL	C2D-C1D-ND	2.77	112.15	110.10
15	M	406	PGV	O03-C19-C20	2.77	120.60	111.91
18	L	303	UQ8	C20-C19-C21	2.77	119.93	115.27
23	B	101	H4X	C2-C1-C3	-2.77	105.17	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	5	104	BCL	CHC-C1C-NC	2.76	128.34	124.51
24	8	102	LMT	C1'-C2'-C3'	2.76	115.75	110.00
16	5	104	BCL	C1-O2A-CGA	2.76	123.69	116.44
16	2	102	BCL	CHC-C1C-NC	2.76	128.33	124.51
16	M	402	BCL	C2D-C1D-ND	2.76	112.14	110.10
16	D	103	BCL	CBA-CAA-C2A	-2.76	105.72	113.86
16	A	102	BCL	C3D-C4D-ND	2.75	114.69	110.24
23	4	101	H4X	C14-C15-C16	-2.75	114.63	123.22
16	Y	102	BCL	O2A-CGA-CBA	2.75	120.55	111.91
16	J	101	BCL	C4-C3-C2	-2.75	116.62	123.68
23	V	101	H4X	C9-C10-C11	-2.75	114.63	123.22
24	2	103	LMT	C12-C11-C10	2.75	134.31	113.42
23	Z	101	H4X	C36-C35-C33	2.75	120.66	113.45
23	Q	105	H4X	C40-C38-C39	-2.75	105.20	110.37
16	3	104	BCL	CAC-C3C-C4C	-2.75	106.49	112.58
24	6	102	LMT	C1B-O1B-C4'	2.74	124.76	117.96
16	9	104	BCL	CAA-C2A-C3A	-2.74	105.26	112.78
11	C	404	HEM	CHA-C4D-ND	2.74	127.77	124.38
23	E	101	H4X	C24-C23-C22	-2.74	119.09	122.92
16	Q	104	BCL	C4D-CHA-C1A	-2.73	117.92	121.25
16	7	103	BCL	O2D-CGD-O1D	-2.73	118.49	123.84
16	O	104	BCL	C2A-C3A-C4A	-2.73	97.45	101.87
16	T	101	BCL	CED-O2D-CGD	2.73	122.12	115.94
16	9	103	BCL	C11-C12-C13	-2.73	107.10	115.92
16	D	104	BCL	C4-C3-C5	2.73	119.86	115.27
16	3	103	BCL	CMC-C2C-C3C	-2.72	102.84	113.83
23	K	103	H4X	C20-C21-C22	-2.72	117.89	123.47
16	3	103	BCL	C3D-C4D-ND	2.72	114.64	110.24
15	K	106	PGV	O01-C1-C2	2.72	117.37	111.50
16	7	102	BCL	C1D-ND-C4D	-2.72	104.40	106.33
16	L	301	BCL	O2A-CGA-O1A	-2.72	116.72	123.59
23	O	106	H4X	C2-C1-C3	-2.72	105.26	110.37
16	Q	104	BCL	OBD-CAD-C3D	-2.71	121.99	128.52
23	K	103	H4X	C26-C27-C28	-2.71	123.44	127.31
16	Y	102	BCL	C3D-C4D-ND	2.71	114.62	110.24
23	U	104	H4X	C29-C28-C30	2.71	122.34	118.08
24	X	102	LMT	C6B-C5B-C4B	-2.71	106.66	113.00
11	C	404	HEM	C3B-C2B-C1B	-2.71	104.48	106.49
16	Q	104	BCL	CHD-C1D-ND	-2.71	121.97	124.45
16	3	104	BCL	CAC-C3C-C2C	-2.70	107.50	114.26
24	6	102	LMT	O1B-C1B-C2B	2.70	115.10	108.10
23	4	101	H4X	C34-C33-C35	2.70	119.81	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	101	H4X	C4-C5-C6	2.70	118.82	112.33
16	O	104	BCL	CHD-C4C-NC	2.70	128.07	125.08
15	I	103	PGV	O12-P-O11	-2.70	99.55	106.73
16	D	104	BCL	CAA-C2A-C3A	-2.70	105.39	112.78
16	F	105	BCL	C6-C5-C3	-2.70	106.38	113.45
16	3	103	BCL	CMB-C2B-C3B	2.69	129.72	124.68
23	Q	105	H4X	C21-C20-C19	-2.69	117.95	123.47
16	M	403	BCL	C16-C15-C13	-2.69	107.21	115.92
16	Q	103	BCL	CMC-C2C-C1C	2.69	119.01	111.77
23	V	101	H4X	C13-C12-C14	2.69	126.69	122.92
23	2	101	H4X	C5-C6-C7	2.69	120.51	113.45
23	2	101	H4X	C9-C10-C11	-2.69	114.83	123.22
24	P	102	LMT	C6B-C5B-C4B	-2.69	106.71	113.00
24	Z	102	LMT	O5'-C5'-C6'	-2.69	99.75	106.44
16	F	105	BCL	CMB-C2B-C3B	2.69	129.70	124.68
23	2	101	H4X	C13-C12-C11	2.69	122.31	118.08
18	L	303	UQ8	O3-C3-C2	2.68	125.63	116.56
16	S	103	BCL	C1C-NC-C4C	-2.68	105.50	106.71
16	9	104	BCL	C1C-NC-C4C	-2.68	105.50	106.71
11	C	402	HEM	C4D-ND-C1D	2.68	107.84	105.07
16	M	402	BCL	OBB-CAB-CBB	2.68	126.19	120.17
16	X	101	BCL	CHD-C4C-NC	2.68	128.05	125.08
15	I	103	PGV	O03-C19-C20	2.68	120.31	111.91
16	B	103	BCL	C7-C6-C5	2.68	120.62	113.36
11	C	401	HEM	O2D-CGD-CBD	2.67	122.61	114.03
16	Q	104	BCL	C1D-CHD-C4C	-2.67	120.18	126.62
16	X	101	BCL	C1D-CHD-C4C	-2.67	120.18	126.62
16	3	103	BCL	C2D-C1D-ND	2.67	112.07	110.10
16	3	104	BCL	CMC-C2C-C3C	-2.66	103.08	113.83
16	T	101	BCL	CHC-C1C-NC	2.66	128.19	124.51
16	D	104	BCL	C4-C3-C2	-2.66	116.85	123.68
16	5	103	BCL	C3D-C4D-ND	2.66	114.55	110.24
16	M	402	BCL	C4B-CHC-C1C	-2.66	124.85	130.12
23	K	103	H4X	C18-C17-C16	2.66	122.27	118.08
23	4	101	H4X	C2-C1-C4	-2.66	106.31	111.14
23	O	106	H4X	C14-C15-C16	-2.66	114.93	123.22
23	B	101	H4X	C5-C6-C7	2.65	120.41	113.45
16	J	101	BCL	C1D-CHD-C4C	-2.65	120.22	126.62
23	7	104	H4X	C24-C23-C22	-2.65	119.21	122.92
16	U	103	BCL	CMB-C2B-C3B	2.65	129.64	124.68
16	5	104	BCL	C2A-C1A-CHA	-2.65	119.22	123.86
24	2	103	LMT	O3B-C3B-C4B	-2.65	104.22	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	5	104	BCL	CHB-C4A-NA	2.65	128.17	124.51
11	C	403	HEM	O2D-CGD-CBD	2.64	122.53	114.03
15	L	305	PGV	O04-C19-C20	-2.64	113.42	123.73
18	L	306	UQ8	C21-C19-C18	-2.64	115.77	121.12
23	U	104	H4X	C5-C6-C7	2.64	120.38	113.45
18	L	306	UQ8	C12-C13-C14	-2.64	121.30	127.66
15	Y	105	PGV	O03-C19-C20	2.64	120.19	111.91
15	F	104	PGV	C02-O01-C1	-2.64	111.30	117.79
16	Y	104	BCL	CMB-C2B-C3B	2.63	129.61	124.68
23	5	105	H4X	C14-C15-C16	-2.63	114.99	123.22
16	O	104	BCL	CBA-CAA-C2A	-2.63	106.10	113.86
23	P	101	H4X	C2-C1-C4	-2.63	106.36	111.14
16	I	102	BCL	CMC-C2C-C3C	-2.63	103.22	113.83
15	3	101	PGV	O04-C19-C20	-2.63	113.49	123.73
15	C	408	PGV	O01-C02-C03	2.63	112.21	106.13
23	7	104	H4X	C5-C6-C7	2.62	120.34	113.45
16	B	103	BCL	C3D-C4D-ND	2.62	114.48	110.24
16	B	103	BCL	CAA-C2A-C3A	-2.62	105.60	112.78
24	T	102	LMT	C6B-C5B-C4B	-2.62	106.88	113.00
15	L	305	PGV	C21-C20-C19	-2.62	104.11	113.62
23	O	106	H4X	C9-C10-C11	-2.61	115.06	123.22
16	J	101	BCL	C2A-C1A-CHA	-2.61	119.29	123.86
16	L	301	BCL	CED-O2D-CGD	2.61	121.84	115.94
16	5	103	BCL	C6-C5-C3	-2.61	106.61	113.45
16	Q	104	BCL	C2A-C1A-CHA	-2.61	119.30	123.86
23	B	101	H4X	C26-C25-C23	-2.61	119.09	126.42
16	M	403	BCL	CGD-CBD-CAD	-2.61	102.28	110.73
16	M	402	BCL	CHC-C1C-NC	2.61	128.12	124.51
16	7	102	BCL	C4-C3-C5	2.61	119.66	115.27
16	Q	104	BCL	CAA-C2A-C3A	-2.61	105.64	112.78
16	9	104	BCL	CMB-C2B-C3B	2.61	129.55	124.68
24	Z	102	LMT	O5'-C1'-O1'	-2.60	103.81	109.97
23	O	106	H4X	C18-C17-C16	2.60	122.18	118.08
16	B	103	BCL	C1D-ND-C4D	-2.60	104.49	106.33
16	5	104	BCL	C1D-CHD-C4C	-2.60	120.34	126.62
22	H	302	CDL	OA6-CA5-OA7	-2.60	117.42	123.70
23	B	101	H4X	C36-C35-C33	2.60	120.27	113.45
24	8	102	LMT	C6B-C5B-C4B	-2.59	106.93	113.00
16	3	104	BCL	CMB-C2B-C3B	2.59	129.53	124.68
23	B	101	H4X	C20-C19-C17	-2.59	123.61	127.31
24	2	103	LMT	C3B-C4B-C5B	-2.59	105.62	110.24
15	3	101	PGV	C03-C02-C01	-2.59	105.66	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	I	103	PGV	O14-P-O13	2.59	120.82	110.68
15	F	101	PGV	C21-C20-C19	-2.59	104.21	113.62
18	L	306	UQ8	C16-C14-C13	-2.58	115.89	121.12
16	B	103	BCL	O2A-CGA-CBA	2.58	120.01	111.91
16	7	102	BCL	C1D-CHD-C4C	-2.58	120.40	126.62
16	Q	104	BCL	C3D-C4D-ND	2.58	114.41	110.24
16	1	102	BCL	CBA-CAA-C2A	-2.58	106.25	113.86
23	K	103	H4X	C15-C14-C12	-2.58	123.63	127.31
16	3	104	BCL	C1-C2-C3	-2.58	121.59	126.04
16	D	104	BCL	C4A-NA-C1A	-2.58	105.55	106.71
24	V	102	LMT	C6B-C5B-C4B	-2.58	106.97	113.00
16	O	105	BCL	CHC-C1C-NC	2.58	128.07	124.51
16	L	304	BCL	C1D-CHD-C4C	-2.57	120.41	126.62
23	K	103	H4X	C2-C1-C4	-2.57	106.46	111.14
23	O	101	H4X	C15-C14-C12	-2.57	123.64	127.31
24	E	102	LMT	C4B-C3B-C2B	-2.57	106.33	110.82
16	3	103	BCL	CBA-CAA-C2A	-2.57	106.27	113.86
24	B	104	LMT	C3B-C4B-C5B	-2.57	105.65	110.24
16	D	104	BCL	CHC-C1C-NC	2.57	128.07	124.51
24	P	102	LMT	O5B-C5B-C6B	2.57	112.83	106.44
23	V	101	H4X	C40-C38-C37	2.56	115.79	111.14
23	Q	105	H4X	C18-C17-C16	2.56	122.12	118.08
23	6	101	H4X	C36-C35-C33	2.56	120.18	113.45
24	T	102	LMT	O5B-C5B-C4B	2.56	114.35	109.69
16	U	102	BCL	O2A-CGA-CBA	2.56	119.95	111.91
23	E	101	H4X	C32-C31-C30	-2.56	115.23	123.22
16	B	103	BCL	C4-C3-C5	2.56	119.58	115.27
16	W	102	BCL	OBB-CAB-C3B	-2.56	115.45	119.99
23	O	101	H4X	C18-C17-C19	2.56	126.51	122.92
23	V	101	H4X	C27-C26-C25	-2.56	115.24	123.22
16	5	104	BCL	C2D-C1D-ND	2.56	111.99	110.10
16	F	103	BCL	C1C-NC-C4C	-2.55	105.56	106.71
16	T	101	BCL	C2A-C1A-CHA	-2.55	119.39	123.86
23	6	101	H4X	C14-C15-C16	-2.55	115.27	123.22
16	I	102	BCL	CHD-C1D-C2D	2.55	130.82	125.48
23	Q	105	H4X	C24-C23-C22	-2.55	119.36	122.92
23	V	101	H4X	C5-C6-C7	2.55	120.13	113.45
16	F	105	BCL	C2A-C1A-CHA	-2.54	119.41	123.86
16	O	105	BCL	C7-C6-C5	2.54	120.26	113.36
16	3	103	BCL	CAC-C3C-C2C	-2.54	107.91	114.26
15	3	101	PGV	C02-O01-C1	-2.54	111.53	117.79
22	S	101	CDL	OA6-CA5-C11	2.54	116.97	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	X	101	BCL	C4A-NA-C1A	-2.54	105.56	106.71
16	T	101	BCL	CAA-C2A-C3A	-2.54	105.83	112.78
15	Y	105	PGV	C02-O01-C1	-2.53	111.55	117.79
23	K	103	H4X	C29-C28-C27	2.53	126.47	122.92
23	P	101	H4X	C18-C17-C16	2.53	122.06	118.08
16	I	102	BCL	CAA-C2A-C3A	-2.53	105.85	112.78
16	K	108	BCL	O2A-CGA-CBA	2.53	119.84	111.91
16	X	101	BCL	O2A-CGA-CBA	2.53	119.83	111.91
15	F	101	PGV	P-O11-C03	-2.52	111.35	118.30
16	K	105	BCL	C6-C5-C3	-2.52	106.85	113.45
16	O	104	BCL	C1D-ND-C4D	-2.52	104.55	106.33
16	Y	104	BCL	CMC-C2C-C3C	-2.52	103.68	113.83
16	7	103	BCL	C2D-C1D-ND	2.52	111.96	110.10
16	X	101	BCL	CAA-C2A-C3A	-2.51	105.89	112.78
16	5	104	BCL	CMC-C2C-C3C	-2.51	103.69	113.83
16	S	103	BCL	CBA-CAA-C2A	-2.51	106.45	113.86
11	C	403	HEM	CAD-C3D-C2D	-2.51	123.20	127.88
15	D	101	PGV	C02-O01-C1	-2.51	111.61	117.79
23	B	101	H4X	C32-C31-C30	-2.51	115.38	123.22
16	9	103	BCL	C1D-CHD-C4C	-2.51	120.57	126.62
15	3	101	PGV	O01-C1-O02	-2.51	117.64	123.70
16	B	103	BCL	C2A-C1A-CHA	-2.51	119.47	123.86
16	1	102	BCL	C1D-ND-C4D	-2.51	104.56	106.33
16	L	304	BCL	O2A-CGA-O1A	-2.50	117.27	123.59
23	6	101	H4X	C8-C7-C6	2.50	119.48	115.27
16	L	304	BCL	CHC-C1C-NC	2.50	127.97	124.51
16	9	104	BCL	C4A-NA-C1A	-2.50	105.58	106.71
16	I	102	BCL	C2D-C1D-ND	2.50	111.95	110.10
23	K	103	H4X	C14-C15-C16	-2.50	115.42	123.22
23	O	106	H4X	C36-C35-C33	2.49	119.99	113.45
23	Q	105	H4X	C24-C23-C25	2.49	122.00	118.08
23	U	104	H4X	C14-C15-C16	-2.49	115.45	123.22
16	F	103	BCL	CMA-C3A-C2A	-2.49	103.79	113.83
23	5	105	H4X	C27-C26-C25	-2.49	115.45	123.22
24	Z	102	LMT	C1B-O5B-C5B	2.49	118.57	113.69
16	Y	102	BCL	O1D-CGD-CBD	-2.49	119.39	124.48
16	L	301	BCL	C1-O2A-CGA	2.49	122.97	116.44
16	1	102	BCL	C2D-C1D-ND	2.48	111.94	110.10
24	J	102	LMT	O5'-C1'-O1'	-2.48	104.09	109.97
24	B	104	LMT	O5'-C5'-C6'	-2.48	100.26	106.44
16	F	105	BCL	C7-C6-C5	2.48	120.09	113.36
23	K	103	H4X	C16-C17-C19	-2.48	115.14	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	1	102	BCL	CHD-C1D-C2D	2.48	130.67	125.48
23	6	101	H4X	C13-C12-C14	2.48	126.39	122.92
24	R	101	LMT	C3B-C4B-C5B	-2.48	105.82	110.24
16	J	101	BCL	C6-C7-C8	-2.47	107.93	115.92
16	9	104	BCL	C2D-C1D-ND	2.47	111.92	110.10
16	M	402	BCL	C3D-C4D-ND	2.47	114.23	110.24
11	C	403	HEM	CHB-C1B-C2B	-2.47	119.89	126.72
16	U	102	BCL	CBA-CAA-C2A	-2.47	106.58	113.86
16	J	101	BCL	CMB-C2B-C3B	2.47	129.29	124.68
11	C	402	HEM	C4B-C3B-C2B	-2.46	105.16	107.11
11	C	403	HEM	C3B-C2B-C1B	-2.46	104.66	106.49
16	A	102	BCL	O2A-C1-C2	-2.46	102.16	108.64
16	S	103	BCL	CMB-C2B-C1B	2.46	132.25	128.46
16	Y	104	BCL	O2A-CGA-CBA	2.46	119.63	111.91
16	I	102	BCL	CAC-C3C-C2C	-2.46	108.12	114.26
16	5	104	BCL	C3D-C4D-ND	2.46	114.21	110.24
23	B	101	H4X	C21-C20-C19	-2.46	118.44	123.47
16	9	103	BCL	OBB-CAB-C3B	-2.46	115.63	119.99
11	C	404	HEM	C3C-C4C-NC	-2.46	106.31	110.94
24	R	101	LMT	O5B-C5B-C6B	2.45	112.53	106.44
15	A	101	PGV	O05-C05-C04	-2.45	100.96	109.56
16	A	102	BCL	C4A-NA-C1A	-2.45	105.61	106.71
11	C	402	HEM	CHB-C1B-C2B	-2.45	119.95	126.72
16	9	104	BCL	CHC-C1C-NC	2.45	127.89	124.51
16	7	102	BCL	CAA-C2A-C3A	-2.45	106.08	112.78
24	T	102	LMT	C1B-O5B-C5B	2.44	118.49	113.69
23	7	104	H4X	C2-C1-C4	2.44	115.57	111.14
16	U	103	BCL	C1D-CHD-C4C	-2.44	120.73	126.62
16	K	108	BCL	C1-O2A-CGA	2.44	122.83	116.44
24	R	101	LMT	C4B-C3B-C2B	-2.44	106.57	110.82
24	R	101	LMT	C1B-O5B-C5B	2.43	118.47	113.69
16	L	301	BCL	CMA-C3A-C4A	-2.43	105.23	111.77
16	K	108	BCL	C2D-C1D-ND	2.43	111.89	110.10
16	Q	104	BCL	OBB-CAB-CBB	2.42	125.62	120.17
16	1	102	BCL	C3A-C2A-C1A	2.42	104.96	101.34
16	2	102	BCL	C1-O2A-CGA	2.42	122.79	116.44
15	F	101	PGV	C01-O03-C19	2.42	126.07	117.12
16	D	103	BCL	OBB-CAB-C3B	-2.42	115.70	119.99
11	C	403	HEM	CMA-C3A-C2A	2.42	129.50	124.94
21	M	405	MQ8	C36-C35-C33	2.41	120.92	112.98
23	Z	101	H4X	C14-C15-C16	-2.41	115.69	123.22
16	2	102	BCL	C19-C18-C17	2.41	126.44	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	U	104	H4X	C8-C7-C9	2.41	128.82	122.59
11	C	402	HEM	CAA-C2A-C3A	-2.41	120.32	127.25
16	Q	103	BCL	C3D-C4D-ND	2.41	114.13	110.24
23	K	107	H4X	C9-C10-C11	-2.41	115.70	123.22
16	Y	102	BCL	CMA-C3A-C2A	-2.41	104.12	113.83
16	D	103	BCL	C3A-C2A-C1A	2.40	104.94	101.34
16	U	103	BCL	C3D-C4D-ND	2.40	114.12	110.24
11	C	403	HEM	C4B-C3B-C2B	2.40	109.02	107.11
16	J	101	BCL	C3D-C4D-ND	2.40	114.12	110.24
23	U	104	H4X	C16-C17-C19	-2.40	115.27	118.94
16	2	102	BCL	C1-C2-C3	-2.39	121.90	126.04
16	M	403	BCL	CMC-C2C-C1C	-2.39	105.34	111.77
16	F	103	BCL	C4B-CHC-C1C	-2.39	125.38	130.12
16	B	103	BCL	CHC-C1C-NC	2.39	127.82	124.51
23	7	104	H4X	C32-C31-C30	-2.39	115.76	123.22
23	6	101	H4X	C40-C38-C37	-2.39	106.80	111.14
16	I	102	BCL	CMB-C2B-C1B	2.39	132.13	128.46
23	E	101	H4X	C14-C15-C16	-2.39	115.77	123.22
16	U	103	BCL	C2A-C1A-CHA	-2.38	119.69	123.86
15	L	305	PGV	O14-P-O13	2.38	124.02	112.24
15	I	103	PGV	P-O11-C03	2.38	124.85	118.30
16	2	102	BCL	CAC-C3C-C4C	-2.38	107.30	112.58
23	E	101	H4X	C2-C1-C4	-2.37	106.83	111.14
16	L	301	BCL	C7-C6-C5	-2.37	106.92	113.36
23	O	101	H4X	C9-C10-C11	-2.37	115.83	123.22
23	5	105	H4X	C32-C31-C30	-2.37	115.83	123.22
16	W	102	BCL	C5-C3-C2	-2.37	116.33	121.12
11	C	404	HEM	CHB-C1B-C2B	-2.36	120.18	126.72
16	O	104	BCL	C3A-C2A-C1A	2.36	104.88	101.34
16	I	102	BCL	C4B-CHC-C1C	-2.36	125.44	130.12
16	L	301	BCL	CAA-CBA-CGA	-2.36	106.35	113.25
24	4	102	LMT	O5'-C1'-O1'	-2.36	104.38	109.97
16	S	103	BCL	C3D-C4D-ND	2.36	114.05	110.24
23	G	101	H4X	C26-C25-C23	-2.36	119.80	126.42
23	U	104	H4X	C9-C10-C11	-2.36	115.86	123.22
16	L	301	BCL	C11-C10-C8	-2.35	108.31	115.92
23	U	104	H4X	C26-C25-C23	-2.35	119.80	126.42
16	M	403	BCL	O2A-CGA-O1A	-2.35	117.65	123.59
16	M	403	BCL	C7-C6-C5	-2.35	106.97	113.36
24	2	103	LMT	O3'-C3'-C2'	-2.35	104.91	110.35
16	7	102	BCL	C4A-NA-C1A	-2.35	105.65	106.71
23	6	101	H4X	C40-C38-C39	2.35	114.79	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	101	PGV	C03-C02-C01	-2.35	106.23	111.79
11	C	401	HEM	CMB-C2B-C1B	2.35	128.61	125.04
23	K	107	H4X	C14-C15-C16	-2.35	115.90	123.22
23	O	106	H4X	C35-C33-C32	-2.34	114.89	121.98
24	2	103	LMT	O5B-C5B-C4B	2.34	113.95	109.69
24	V	102	LMT	C4B-C3B-C2B	-2.34	106.73	110.82
16	L	301	BCL	O1D-CGD-CBD	-2.34	119.69	124.48
23	Z	101	H4X	C27-C26-C25	-2.34	115.91	123.22
15	D	101	PGV	O03-C19-O04	-2.34	117.69	123.59
18	L	303	UQ8	C6-C1-C2	2.34	121.03	119.18
24	J	102	LMT	O1B-C4'-C5'	2.34	115.86	109.45
16	M	403	BCL	CMC-C2C-C3C	-2.34	104.41	113.83
16	Y	102	BCL	C4A-NA-C1A	-2.34	105.66	106.71
11	C	401	HEM	CHD-C1D-C2D	-2.33	121.33	124.98
16	D	104	BCL	O2D-CGD-O1D	-2.33	119.27	123.84
24	2	103	LMT	O5'-C1'-C2'	2.33	115.29	110.35
16	3	104	BCL	O2A-CGA-CBA	2.33	119.23	111.91
16	M	402	BCL	C1-O2A-CGA	2.33	122.56	116.44
24	6	102	LMT	O5'-C1'-O1'	-2.33	104.46	109.97
16	1	102	BCL	C16-C15-C13	-2.33	108.40	115.92
16	3	103	BCL	C1D-CHD-C4C	-2.33	121.01	126.62
23	O	101	H4X	C24-C23-C22	2.33	126.18	122.92
16	3	104	BCL	CHD-C1D-ND	-2.33	122.32	124.45
15	H	301	PGV	O04-C19-C20	-2.32	114.66	123.73
16	K	105	BCL	C3A-C2A-C1A	2.32	104.81	101.34
16	O	105	BCL	C3D-C4D-ND	2.32	113.99	110.24
16	1	102	BCL	C1D-CHD-C4C	-2.32	121.02	126.62
16	Y	104	BCL	C4-C3-C5	2.32	119.17	115.27
16	5	104	BCL	CAC-C3C-C4C	-2.32	107.44	112.58
16	W	102	BCL	C4-C3-C5	2.32	119.17	115.27
23	P	101	H4X	C4-C5-C6	2.32	117.90	112.33
23	K	103	H4X	C36-C35-C33	2.32	119.53	113.45
24	B	104	LMT	C4-C3-C2	2.32	126.18	114.42
16	B	103	BCL	C1-O2A-CGA	2.32	122.52	116.44
23	5	105	H4X	C18-C17-C16	2.31	121.72	118.08
16	M	403	BCL	C3D-C4D-ND	2.31	113.98	110.24
23	4	101	H4X	C5-C6-C7	2.31	119.52	113.45
23	5	105	H4X	C6-C7-C9	-2.31	114.98	121.98
16	U	103	BCL	O2D-CGD-O1D	-2.31	119.32	123.84
16	Q	104	BCL	C1D-ND-C4D	-2.31	104.69	106.33
23	4	101	H4X	C13-C12-C14	-2.31	119.69	122.92
16	5	103	BCL	CBA-CAA-C2A	-2.31	107.05	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2	101	H4X	C3-C1-C4	-2.31	106.94	111.14
16	Q	103	BCL	C2D-C1D-ND	2.31	111.81	110.10
16	5	103	BCL	C1D-CHD-C4C	-2.31	121.05	126.62
23	P	101	H4X	C9-C10-C11	-2.31	116.02	123.22
24	N	101	LMT	O3B-C3B-C4B	-2.31	105.02	110.35
16	B	103	BCL	C4-C3-C2	-2.30	117.77	123.68
23	Z	101	H4X	C32-C31-C30	-2.30	116.02	123.22
11	C	403	HEM	C3C-C4C-NC	-2.30	106.60	110.94
16	1	102	BCL	C1C-NC-C4C	2.30	107.74	106.71
15	D	101	PGV	C25-C24-C23	-2.30	102.75	114.42
16	M	402	BCL	C1D-CHD-C4C	-2.29	121.09	126.62
11	C	401	HEM	C3B-C2B-C1B	2.29	108.19	106.49
23	6	101	H4X	C29-C28-C30	-2.29	114.47	118.08
16	K	108	BCL	C7-C6-C5	2.29	119.57	113.36
16	L	304	BCL	C1C-NC-C4C	-2.29	105.68	106.71
22	H	302	CDL	OA4-PA1-OA3	2.29	123.56	112.24
16	J	101	BCL	O2A-CGA-CBA	2.29	119.09	111.91
16	J	101	BCL	CHB-C4A-NA	2.29	127.67	124.51
23	O	106	H4X	C39-C38-C37	-2.29	106.99	111.14
23	V	101	H4X	C26-C27-C28	-2.28	124.05	127.31
18	L	306	UQ8	C12-C11-C9	-2.28	105.46	112.98
15	3	101	PGV	O01-C02-C03	2.28	116.67	108.40
16	5	103	BCL	C1-O2A-CGA	2.28	122.43	116.44
16	L	301	BCL	C17-C16-C15	-2.28	102.78	113.24
16	L	304	BCL	O2A-CGA-CBA	2.28	119.05	111.91
16	F	103	BCL	C3D-C4D-ND	2.27	113.92	110.24
24	J	102	LMT	O1B-C1B-C2B	2.27	113.99	108.10
23	O	106	H4X	C3-C1-C4	-2.27	107.01	111.14
23	G	101	H4X	C13-C12-C11	2.27	121.66	118.08
24	G	102	LMT	O5'-C1'-O1'	-2.27	104.60	109.97
24	E	102	LMT	C6B-C5B-C4B	-2.27	107.69	113.00
24	0	101	LMT	C12-C11-C10	2.27	130.65	113.42
17	M	404	BPH	C1C-C2C-C3C	2.27	105.00	102.84
24	N	101	LMT	O1B-C1B-C2B	2.27	113.98	108.10
16	Q	103	BCL	C1D-CHD-C4C	-2.27	121.15	126.62
16	K	108	BCL	CHB-C4A-NA	2.27	127.65	124.51
15	F	101	PGV	O04-C19-C20	-2.27	114.89	123.73
16	7	103	BCL	CMA-C3A-C2A	-2.26	104.70	113.83
16	3	103	BCL	CMC-C2C-C1C	2.26	117.85	111.77
24	R	101	LMT	C1'-O5'-C5'	2.26	118.12	113.69
24	T	102	LMT	C1'-O5'-C5'	2.26	118.12	113.69
15	F	104	PGV	C01-O03-C19	2.26	125.47	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	103	BCL	CHB-C4A-NA	2.25	127.63	124.51
16	Q	104	BCL	C7-C6-C5	2.25	119.48	113.36
16	U	102	BCL	C11-C12-C13	-2.25	108.64	115.92
24	Z	102	LMT	C6B-C5B-C4B	-2.25	107.73	113.00
23	5	105	H4X	C34-C33-C35	2.25	119.06	115.27
18	L	303	UQ8	C20-C19-C18	-2.25	117.91	123.68
24	2	103	LMT	C1B-O1B-C4'	2.25	123.53	117.96
23	P	101	H4X	C20-C21-C22	-2.25	118.87	123.47
16	5	104	BCL	CMB-C2B-C3B	2.25	128.88	124.68
23	5	105	H4X	C26-C27-C28	-2.24	124.11	127.31
16	9	104	BCL	C3D-C4D-ND	2.24	113.86	110.24
24	8	102	LMT	C1-O1'-C1'	-2.24	110.12	113.84
16	B	103	BCL	C6-C7-C8	-2.24	108.67	115.92
15	A	101	PGV	O05-C05-C06	-2.24	99.25	109.12
16	F	103	BCL	C2A-C1A-CHA	-2.24	119.94	123.86
16	3	104	BCL	CMA-C3A-C2A	-2.24	104.79	113.83
16	O	105	BCL	OBD-CAD-C3D	-2.24	123.13	128.52
11	C	403	HEM	O2A-CGA-CBA	2.24	121.22	114.03
16	I	102	BCL	CAC-C3C-C4C	-2.23	107.62	112.58
16	O	105	BCL	CAA-C2A-C3A	-2.23	106.66	112.78
24	0	101	LMT	O1B-C1B-C2B	2.23	113.89	108.10
16	Q	104	BCL	C1B-CHB-C4A	-2.23	125.70	130.12
16	Y	104	BCL	CHC-C1C-NC	2.23	127.60	124.51
16	5	104	BCL	O2D-CGD-O1D	-2.23	119.48	123.84
16	W	102	BCL	CAC-C3C-C4C	-2.22	107.65	112.58
24	4	102	LMT	C1B-O1B-C4'	2.22	123.45	117.96
16	3	104	BCL	C7-C6-C5	2.22	119.38	113.36
16	3	104	BCL	C2A-C1A-CHA	-2.22	119.98	123.86
18	L	303	UQ8	C10-C9-C11	2.21	118.99	115.27
16	T	101	BCL	OBD-CAD-C3D	-2.21	123.19	128.52
16	D	103	BCL	C3D-C4D-ND	2.21	113.82	110.24
16	K	105	BCL	CGD-CBD-CAD	-2.21	103.57	110.73
16	3	103	BCL	C1D-ND-C4D	-2.21	104.77	106.33
24	V	102	LMT	O1B-C4'-C5'	2.21	115.50	109.45
16	U	103	BCL	C2D-C1D-ND	2.21	111.73	110.10
23	Z	101	H4X	C34-C33-C35	2.21	118.98	115.27
24	P	102	LMT	O5B-C5B-C4B	2.21	113.70	109.69
23	U	104	H4X	C39-C38-C37	-2.21	107.13	111.14
16	Q	104	BCL	CMA-C3A-C2A	-2.20	104.94	113.83
16	U	103	BCL	CED-O2D-CGD	2.20	120.92	115.94
16	W	102	BCL	CAC-C3C-C2C	-2.20	108.75	114.26
23	6	101	H4X	C15-C14-C12	-2.20	124.17	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	U	103	BCL	C5-C3-C2	2.20	125.57	121.12
15	A	101	PGV	O14-P-O11	-2.20	97.52	107.75
16	Y	104	BCL	CHD-C1D-ND	-2.20	122.43	124.45
16	9	104	BCL	CHD-C1D-ND	-2.20	122.43	124.45
24	6	102	LMT	O5B-C5B-C4B	2.20	113.69	109.69
16	D	104	BCL	CHD-C1D-ND	-2.20	122.43	124.45
16	T	101	BCL	CHB-C4A-NA	2.20	127.55	124.51
23	Q	105	H4X	C32-C31-C30	-2.20	116.36	123.22
24	4	102	LMT	O1B-C1B-C2B	2.19	113.79	108.10
24	4	102	LMT	O5B-C5B-C4B	2.19	113.68	109.69
16	K	105	BCL	C1D-CHD-C4C	-2.19	121.33	126.62
24	R	101	LMT	C1B-O1B-C4'	2.19	123.39	117.96
23	Z	101	H4X	C24-C23-C22	-2.19	119.85	122.92
23	E	101	H4X	C8-C7-C6	2.19	118.96	115.27
16	U	102	BCL	C1D-CHD-C4C	-2.19	121.34	126.62
16	M	402	BCL	CED-O2D-CGD	-2.19	110.98	115.94
23	4	101	H4X	C20-C21-C22	-2.19	118.99	123.47
16	9	104	BCL	C4D-CHA-C1A	-2.19	118.59	121.25
16	L	301	BCL	OBB-CAB-C3B	-2.19	116.11	119.99
16	7	102	BCL	C3D-C4D-ND	2.19	113.77	110.24
24	T	102	LMT	O1B-C1B-C2B	2.19	113.76	108.10
15	9	101	PGV	C02-O01-C1	-2.19	112.41	117.79
16	T	101	BCL	C6-C5-C3	-2.18	107.73	113.45
23	Q	105	H4X	O2-C38-C39	2.18	123.99	108.97
24	X	102	LMT	O3B-C3B-C4B	-2.18	105.30	110.35
16	I	102	BCL	O2A-CGA-CBA	2.18	118.76	111.91
23	U	104	H4X	C30-C28-C27	-2.18	115.60	118.94
11	C	402	HEM	CBA-CAA-C2A	-2.18	108.90	112.62
23	2	101	H4X	C36-C35-C33	2.18	119.16	113.45
16	9	103	BCL	C1D-ND-C4D	-2.17	104.79	106.33
23	G	101	H4X	C11-C12-C14	-2.17	115.60	118.94
16	X	101	BCL	CAA-CBA-CGA	-2.17	106.91	113.25
18	L	303	UQ8	C17-C18-C19	-2.17	122.44	127.66
15	Y	105	PGV	O14-P-O13	2.17	119.17	110.68
24	G	102	LMT	O3'-C3'-C2'	-2.17	105.34	110.35
16	9	104	BCL	O2A-CGA-CBA	2.17	118.70	111.91
24	Z	102	LMT	O1B-C1B-C2B	2.16	113.71	108.10
16	S	103	BCL	CHD-C4C-NC	2.16	127.48	125.08
24	J	102	LMT	O3B-C3B-C4B	-2.16	105.35	110.35
16	F	103	BCL	C1D-ND-C4D	-2.16	104.80	106.33
23	4	101	H4X	C9-C10-C11	-2.16	116.48	123.22
16	J	101	BCL	O1A-CGA-CBA	-2.16	115.32	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	104	BCL	CHC-C1C-NC	2.16	127.50	124.51
15	F	101	PGV	O14-P-O11	2.16	112.47	106.73
15	Q	101	PGV	O01-C1-O02	-2.16	118.49	123.70
23	G	101	H4X	C18-C17-C19	2.16	125.94	122.92
16	7	103	BCL	CAC-C3C-C4C	-2.15	107.80	112.58
23	K	103	H4X	C40-C38-C39	-2.15	106.32	110.37
22	S	101	CDL	O1-C1-CB2	2.15	117.09	109.56
16	I	102	BCL	C1C-NC-C4C	-2.15	105.74	106.71
17	M	404	BPH	O2D-CGD-CBD	2.15	113.72	111.00
16	I	102	BCL	C1B-CHB-C4A	-2.15	125.86	130.12
24	E	102	LMT	C12-C11-C10	2.15	129.72	113.42
16	7	102	BCL	O2A-CGA-O1A	-2.14	118.18	123.59
23	Q	105	H4X	C27-C26-C25	-2.14	116.52	123.22
24	2	103	LMT	O1B-C1B-C2B	2.14	113.66	108.10
24	B	104	LMT	O5'-C1'-O1'	-2.14	104.90	109.97
17	L	302	BPH	CAC-C3C-C2C	-2.14	108.91	114.26
18	L	306	UQ8	C8-C7-C6	-2.14	106.27	112.05
16	F	103	BCL	C2D-C1D-ND	2.14	111.68	110.10
24	P	102	LMT	C12-C11-C10	2.14	129.66	113.42
16	K	108	BCL	CMC-C2C-C3C	-2.14	105.20	113.83
16	9	104	BCL	C2A-C1A-CHA	-2.14	120.12	123.86
16	2	102	BCL	C6-C7-C8	-2.14	109.01	115.92
16	W	102	BCL	CHD-C4C-NC	2.14	127.45	125.08
15	K	101	PGV	O03-C19-O04	-2.14	118.20	123.59
24	J	102	LMT	O3'-C3'-C2'	-2.14	105.41	110.35
16	F	103	BCL	CMD-C2D-C3D	-2.13	122.70	127.61
16	1	102	BCL	C3D-C4D-ND	2.13	113.69	110.24
15	I	103	PGV	O03-C19-O04	-2.13	118.21	123.59
15	Y	105	PGV	O12-P-O11	-2.13	101.06	106.73
23	6	101	H4X	C4-C5-C6	2.13	117.45	112.33
16	K	105	BCL	CHC-C1C-NC	2.13	127.45	124.51
15	K	106	PGV	C01-O03-C19	2.13	125.00	117.12
16	7	102	BCL	CBC-CAC-C3C	-2.13	108.73	113.47
16	7	103	BCL	C2A-C1A-CHA	-2.12	120.15	123.86
16	K	108	BCL	C3D-C4D-ND	2.12	113.66	110.24
16	O	104	BCL	C4A-NA-C1A	-2.12	105.75	106.71
23	4	101	H4X	C34-C33-C32	-2.12	117.14	122.59
16	S	103	BCL	O2A-CGA-CBA	2.12	118.55	111.91
16	O	104	BCL	CBB-CAB-C3B	2.12	126.62	120.34
16	M	403	BCL	C2D-C1D-ND	2.11	111.66	110.10
16	X	101	BCL	CHC-C1C-NC	2.11	127.44	124.51
24	N	101	LMT	C6B-C5B-C4B	-2.11	108.05	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	X	101	BCL	CMA-C3A-C2A	-2.11	105.31	113.83
16	F	103	BCL	CED-O2D-CGD	2.11	120.71	115.94
16	T	101	BCL	OBB-CAB-C3B	-2.11	116.25	119.99
24	T	102	LMT	C12-C11-C10	2.11	129.43	113.42
24	T	102	LMT	C1B-O1B-C4'	2.11	123.18	117.96
23	7	104	H4X	C20-C21-C22	-2.11	119.16	123.47
16	K	105	BCL	CHD-C1D-C2D	2.10	129.89	125.48
23	2	101	H4X	C2-C1-C4	-2.10	107.32	111.14
16	K	105	BCL	CAC-C3C-C2C	-2.10	109.01	114.26
11	C	403	HEM	CHA-C4D-ND	2.10	126.98	124.38
24	E	102	LMT	O5'-C1'-O1'	-2.10	105.00	109.97
23	P	101	H4X	C27-C26-C25	-2.10	116.66	123.22
23	K	107	H4X	C39-C38-C37	-2.10	107.33	111.14
24	0	101	LMT	C3'-C4'-C5'	-2.10	106.12	110.93
16	2	102	BCL	C2A-C1A-CHA	-2.10	120.19	123.86
23	K	103	H4X	C34-C33-C35	2.10	118.80	115.27
11	C	402	HEM	CBD-CAD-C3D	-2.10	106.81	112.63
23	P	101	H4X	C21-C20-C19	-2.09	119.18	123.47
24	Z	102	LMT	O5B-C5B-C4B	2.09	113.50	109.69
24	G	102	LMT	O3B-C3B-C4B	-2.09	105.52	110.35
16	3	104	BCL	OBB-CAB-CBB	2.09	124.87	120.17
23	P	101	H4X	C2-C1-C3	-2.09	106.44	110.37
16	Y	104	BCL	C7-C6-C5	2.09	119.03	113.36
16	7	103	BCL	OBD-CAD-C3D	-2.09	123.49	128.52
24	2	103	LMT	O1B-C1B-O5B	2.09	116.51	110.67
15	D	101	PGV	O01-C1-O02	-2.09	118.66	123.70
11	C	402	HEM	CMB-C2B-C1B	2.09	128.22	125.04
15	K	106	PGV	O12-P-O11	-2.09	101.18	106.73
18	L	303	UQ8	C15-C14-C13	-2.09	118.33	123.68
11	C	401	HEM	CMB-C2B-C3B	-2.08	123.20	128.30
16	Q	103	BCL	OBD-CAD-C3D	-2.08	123.51	128.52
16	K	105	BCL	CED-O2D-CGD	2.08	120.64	115.94
16	9	104	BCL	C4-C3-C2	-2.08	118.34	123.68
24	4	102	LMT	C1-O1'-C1'	2.08	117.29	113.84
16	3	103	BCL	O2A-CGA-CBA	2.08	118.42	111.91
16	K	105	BCL	C3D-C4D-ND	2.08	113.60	110.24
16	Y	104	BCL	C3D-C4D-ND	2.08	113.60	110.24
16	O	104	BCL	CMB-C2B-C3B	2.08	128.56	124.68
16	U	103	BCL	CHC-C1C-NC	2.08	127.38	124.51
11	C	401	HEM	CMC-C2C-C3C	2.08	128.56	124.68
16	7	103	BCL	CHA-C4D-ND	2.07	136.83	132.50
16	Y	104	BCL	CAA-C2A-C3A	-2.07	107.11	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	404	HEM	C4C-CHD-C1D	-2.07	119.83	122.56
23	O	101	H4X	C26-C25-C23	-2.07	120.61	126.42
16	K	108	BCL	CAA-CBA-CGA	-2.07	107.21	113.25
16	O	104	BCL	C1C-NC-C4C	-2.07	105.78	106.71
16	O	105	BCL	C1C-NC-C4C	-2.06	105.78	106.71
23	P	101	H4X	C24-C23-C22	-2.06	120.03	122.92
23	K	103	H4X	C26-C25-C23	-2.06	120.62	126.42
15	3	101	PGV	O03-C01-C02	2.06	114.44	108.43
24	Z	102	LMT	O4'-C4B-C5B	2.06	114.42	109.30
18	L	306	UQ8	C15-C14-C13	-2.06	118.39	123.68
24	B	104	LMT	C3'-C4'-C5'	-2.06	106.20	110.93
16	U	102	BCL	C6-C5-C3	-2.06	108.05	113.45
15	L	305	PGV	C02-O01-C1	-2.06	112.72	117.79
16	3	104	BCL	CAA-CBA-CGA	-2.06	107.23	113.25
23	6	101	H4X	C39-C38-C37	-2.06	107.40	111.14
16	U	102	BCL	CMC-C2C-C3C	-2.06	105.52	113.83
23	G	101	H4X	C5-C6-C7	2.05	118.84	113.45
16	1	102	BCL	CED-O2D-CGD	2.05	120.58	115.94
22	H	302	CDL	OB4-PB2-OB5	2.05	117.28	107.75
23	K	107	H4X	C13-C12-C11	-2.05	114.84	118.08
23	Q	105	H4X	C40-C38-C37	2.05	114.86	111.14
16	L	304	BCL	C1-C2-C3	-2.05	122.50	126.04
23	E	101	H4X	C16-C17-C19	-2.05	115.79	118.94
16	O	105	BCL	CHB-C4A-NA	2.05	127.34	124.51
15	D	101	PGV	C04-C05-C06	-2.05	104.38	111.67
15	Q	101	PGV	O04-C19-C20	-2.05	115.75	123.73
16	L	304	BCL	CMC-C2C-C3C	-2.05	105.57	113.83
16	S	103	BCL	CMA-C3A-C2A	-2.04	105.58	113.83
16	T	101	BCL	C4D-CHA-C1A	-2.04	118.76	121.25
23	G	101	H4X	C24-C23-C22	-2.04	120.06	122.92
15	C	408	PGV	O12-P-O11	-2.04	101.30	106.73
18	L	303	UQ8	O3-C3-C4	-2.04	115.95	123.64
15	K	101	PGV	O03-C19-C20	2.04	118.31	111.91
16	1	102	BCL	C2A-C3A-C4A	-2.04	98.57	101.87
24	E	102	LMT	O3B-C3B-C4B	-2.04	105.63	110.35
16	O	104	BCL	OBB-CAB-C3B	-2.04	116.37	119.99
16	B	103	BCL	OBD-CAD-C3D	-2.04	123.61	128.52
24	0	101	LMT	O5B-C5B-C6B	2.04	111.50	106.44
23	K	103	H4X	C2M-O2-C38	-2.04	104.36	117.25
16	9	103	BCL	C1-O2A-CGA	2.04	121.79	116.44
16	L	304	BCL	CHA-C1A-NA	-2.04	121.73	126.40
23	Q	105	H4X	C13-C12-C11	-2.04	114.87	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	E	102	LMT	O5B-C5B-C4B	2.03	113.39	109.69
24	J	102	LMT	O6'-C6'-C5'	2.03	118.27	111.29
15	9	101	PGV	O01-C1-O02	-2.03	118.79	123.70
24	V	102	LMT	O1B-C1B-C2B	2.03	113.36	108.10
23	2	101	H4X	C24-C23-C25	2.03	121.28	118.08
16	M	403	BCL	CBB-CAB-C3B	-2.03	114.31	120.34
23	4	101	H4X	C26-C27-C28	-2.03	124.41	127.31
15	K	101	PGV	O01-C1-O02	-2.03	118.80	123.70
24	8	102	LMT	O3B-C3B-C4B	-2.03	105.66	110.35
24	J	102	LMT	O1B-C1B-O5B	2.03	116.34	110.67
16	9	104	BCL	C4-C3-C5	2.03	118.68	115.27
16	S	103	BCL	C1-O2A-CGA	2.03	121.76	116.44
24	B	102	LMT	C1B-C2B-C3B	2.03	114.22	110.00
15	I	103	PGV	O01-C1-O02	-2.03	118.81	123.70
16	F	103	BCL	CHC-C1C-NC	2.02	127.31	124.51
16	Y	104	BCL	C4-C3-C2	-2.02	118.48	123.68
11	C	403	HEM	CMB-C2B-C1B	2.02	128.12	125.04
15	K	101	PGV	C02-O01-C1	-2.02	112.81	117.79
24	R	101	LMT	C3'-C4'-C5'	-2.02	106.29	110.93
16	9	103	BCL	C2D-C1D-ND	2.02	111.59	110.10
23	2	101	H4X	C14-C15-C16	-2.02	116.91	123.22
23	6	101	H4X	C5-C6-C7	2.02	118.75	113.45
23	V	101	H4X	C6-C7-C9	-2.02	115.86	121.98
16	O	104	BCL	C1D-CHD-C4C	-2.02	121.75	126.62
23	4	101	H4X	C26-C25-C23	-2.02	120.75	126.42
24	B	104	LMT	C1B-C2B-C3B	-2.02	105.79	110.00
16	A	102	BCL	CMB-C2B-C1B	2.02	131.57	128.46
23	K	103	H4X	C21-C20-C19	-2.02	119.34	123.47
15	M	406	PGV	C7-C6-C5	2.01	124.64	114.42
16	U	103	BCL	C4-C3-C2	-2.01	118.53	123.68
24	G	102	LMT	O4'-C4B-C5B	2.01	114.28	109.30
15	F	101	PGV	O14-P-O12	-2.01	99.97	107.64
16	F	105	BCL	CHB-C4A-NA	2.01	127.29	124.51
11	C	401	HEM	C4D-ND-C1D	2.00	107.14	105.07
16	2	102	BCL	O2A-CGA-CBA	2.00	118.19	111.91
23	G	101	H4X	C27-C26-C25	-2.00	116.97	123.22

There are no chirality outliers.

All (1338) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	401	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	C	401	HEM	C4B-C3B-CAB-CBB
11	C	404	HEM	C2B-C3B-CAB-CBB
14	C	407	DGA	CA2-CA1-OG1-CG1
14	C	407	DGA	OA1-CA1-OG1-CG1
14	C	407	DGA	CB2-CB1-OG2-CG2
15	C	408	PGV	C03-O11-P-O12
15	C	408	PGV	C03-O11-P-O14
15	C	408	PGV	C01-C02-C03-O11
15	C	408	PGV	C2-C1-O01-C02
15	L	305	PGV	C03-O11-P-O14
15	M	406	PGV	C03-O11-P-O13
15	M	406	PGV	C04-O12-P-O13
15	M	406	PGV	C04-O12-P-O14
15	H	301	PGV	C03-O11-P-O14
15	H	301	PGV	C04-O12-P-O11
15	H	301	PGV	C04-O12-P-O13
15	H	301	PGV	C04-O12-P-O14
15	H	301	PGV	O12-C04-C05-C06
15	H	301	PGV	O12-C04-C05-O05
15	F	101	PGV	C03-O11-P-O12
15	F	104	PGV	C03-O11-P-O14
15	F	104	PGV	C05-C04-O12-P
15	F	104	PGV	O02-C1-O01-C02
15	I	103	PGV	C03-O11-P-O14
15	K	101	PGV	O12-C04-C05-C06
15	K	101	PGV	O02-C1-O01-C02
15	K	102	PGV	C03-O11-P-O12
15	K	102	PGV	C03-O11-P-O13
15	K	102	PGV	O01-C02-C03-O11
15	K	106	PGV	C03-O11-P-O12
15	O	102	PGV	C03-O11-P-O13
15	O	102	PGV	C04-O12-P-O14
15	Q	101	PGV	C03-O11-P-O13
15	Q	101	PGV	C03-O11-P-O14
15	Q	101	PGV	O03-C01-C02-O01
15	Q	101	PGV	C04-C05-C06-O06
15	Y	105	PGV	O02-C1-O01-C02
15	Y	105	PGV	C2-C1-O01-C02
15	1	103	PGV	C03-O11-P-O12
15	1	103	PGV	C03-O11-P-O14
15	3	101	PGV	C11-C12-C13-C14
15	5	101	PGV	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
15	9	101	PGV	C03-O11-P-O14
15	9	101	PGV	C04-O12-P-O13
15	9	101	PGV	C04-O12-P-O14
15	9	101	PGV	O01-C02-C03-O11
15	9	101	PGV	O12-C04-C05-O05
15	9	101	PGV	C11-C12-C13-C14
16	L	304	BCL	C11-C10-C8-C9
16	M	402	BCL	C6-C7-C8-C9
16	M	403	BCL	CHA-CBD-CGD-O1D
16	M	403	BCL	CAD-CBD-CGD-O1D
16	A	102	BCL	C2-C3-C5-C6
16	A	102	BCL	C4-C3-C5-C6
16	B	103	BCL	C1A-C2A-CAA-CBA
16	F	105	BCL	C1A-C2A-CAA-CBA
16	J	101	BCL	C1A-C2A-CAA-CBA
16	K	105	BCL	C2-C3-C5-C6
16	K	105	BCL	C4-C3-C5-C6
16	K	108	BCL	C1A-C2A-CAA-CBA
16	O	104	BCL	C2-C3-C5-C6
16	O	104	BCL	C4-C3-C5-C6
16	O	105	BCL	C1A-C2A-CAA-CBA
16	Q	103	BCL	C11-C10-C8-C7
16	T	101	BCL	C1A-C2A-CAA-CBA
16	2	102	BCL	C1A-C2A-CAA-CBA
16	3	104	BCL	C1A-C2A-CAA-CBA
16	5	103	BCL	C2C-C3C-CAC-CBC
16	5	104	BCL	C1A-C2A-CAA-CBA
16	9	104	BCL	C1A-C2A-CAA-CBA
17	L	302	BPH	C4C-C3C-CAC-CBC
17	L	302	BPH	O2A-C1-C2-C3
17	M	404	BPH	C1-C2-C3-C4
17	M	404	BPH	C1-C2-C3-C5
18	L	303	UQ8	C19-C21-C22-C23
18	L	303	UQ8	C15-C14-C16-C17
18	L	303	UQ8	C13-C14-C16-C17
18	L	306	UQ8	C14-C16-C17-C18
18	L	306	UQ8	C12-C11-C9-C10
21	M	405	MQ8	C33-C35-C36-C37
21	M	405	MQ8	C38-C40-C41-C42
21	M	405	MQ8	C43-C44-C46-C47
22	H	302	CDL	CA2-OA2-PA1-OA4
22	H	302	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
22	H	302	CDL	CA3-OA5-PA1-OA3
22	H	302	CDL	CB2-OB2-PB2-OB3
22	H	302	CDL	CB3-OB5-PB2-OB3
22	S	101	CDL	CA2-C1-CB2-OB2
22	S	101	CDL	CB2-OB2-PB2-OB3
22	S	101	CDL	CB2-OB2-PB2-OB4
22	Y	103	CDL	CA3-OA5-PA1-OA3
22	Y	103	CDL	CB3-OB5-PB2-OB2
22	Y	103	CDL	CB3-OB5-PB2-OB3
22	Y	103	CDL	CB3-OB5-PB2-OB4
22	Y	103	CDL	OB5-CB3-CB4-OB6
23	B	101	H4X	C36-C37-C38-O2
23	B	101	H4X	C36-C37-C38-C39
23	B	101	H4X	C36-C37-C38-C40
23	E	101	H4X	C4-C1-O1-C1M
23	G	101	H4X	C29-C28-C30-C31
23	G	101	H4X	C27-C28-C30-C31
23	G	101	H4X	C2-C1-O1-C1M
23	K	103	H4X	C37-C38-O2-C2M
23	K	103	H4X	C36-C37-C38-O2
23	K	103	H4X	C36-C37-C38-C39
23	K	103	H4X	C36-C37-C38-C40
23	K	103	H4X	C3-C1-C4-C5
23	K	103	H4X	O1-C1-C4-C5
23	K	107	H4X	C27-C28-C30-C31
23	K	107	H4X	C3-C1-C4-C5
23	K	107	H4X	C2-C1-C4-C5
23	K	107	H4X	O1-C1-C4-C5
23	K	107	H4X	C2-C1-O1-C1M
23	O	101	H4X	C36-C37-C38-C39
23	O	101	H4X	C15-C16-C17-C19
23	O	101	H4X	C15-C16-C17-C18
23	O	101	H4X	C5-C6-C7-C9
23	O	101	H4X	C5-C6-C7-C8
23	O	101	H4X	C3-C1-C4-C5
23	O	101	H4X	C2-C1-C4-C5
23	O	101	H4X	O1-C1-C4-C5
23	O	106	H4X	C15-C16-C17-C19
23	O	106	H4X	C15-C16-C17-C18
23	O	106	H4X	C4-C1-O1-C1M
23	P	101	H4X	C3-C1-C4-C5
23	P	101	H4X	C2-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
23	P	101	H4X	O1-C1-C4-C5
23	Q	105	H4X	C40-C38-O2-C2M
23	Q	105	H4X	C36-C37-C38-O2
23	Q	105	H4X	C36-C37-C38-C40
23	Q	105	H4X	C29-C28-C30-C31
23	Q	105	H4X	C27-C28-C30-C31
23	U	104	H4X	C29-C28-C30-C31
23	U	104	H4X	C27-C28-C30-C31
23	U	104	H4X	C15-C16-C17-C18
23	V	101	H4X	C36-C37-C38-C39
23	V	101	H4X	C36-C37-C38-C40
23	V	101	H4X	C29-C28-C30-C31
23	V	101	H4X	C27-C28-C30-C31
23	V	101	H4X	C4-C1-O1-C1M
23	Z	101	H4X	C29-C28-C30-C31
23	Z	101	H4X	C27-C28-C30-C31
23	2	101	H4X	C29-C28-C30-C31
23	2	101	H4X	C27-C28-C30-C31
23	2	101	H4X	C3-C1-C4-C5
23	2	101	H4X	C2-C1-C4-C5
23	4	101	H4X	C15-C16-C17-C19
23	4	101	H4X	C15-C16-C17-C18
23	4	101	H4X	C5-C6-C7-C8
23	4	101	H4X	C3-C1-C4-C5
23	4	101	H4X	C2-C1-C4-C5
23	5	105	H4X	C3-C1-C4-C5
23	5	105	H4X	O1-C1-C4-C5
23	5	105	H4X	C4-C1-O1-C1M
23	5	105	H4X	C3-C1-O1-C1M
23	6	101	H4X	C29-C28-C30-C31
23	6	101	H4X	C27-C28-C30-C31
23	7	104	H4X	C29-C28-C30-C31
23	7	104	H4X	C27-C28-C30-C31
23	7	104	H4X	C3-C1-C4-C5
24	E	102	LMT	O5'-C1'-O1'-C1
24	G	102	LMT	O5'-C1'-O1'-C1
24	J	102	LMT	O5'-C1'-O1'-C1
24	N	101	LMT	O5'-C1'-O1'-C1
24	R	101	LMT	O5'-C1'-O1'-C1
24	2	103	LMT	O5'-C1'-O1'-C1
24	4	102	LMT	O5'-C1'-O1'-C1
24	6	102	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
24	0	101	LMT	O5'-C1'-O1'-C1
24	E	102	LMT	O5B-C1B-O1B-C4'
24	G	102	LMT	O5B-C1B-O1B-C4'
24	R	101	LMT	O5B-C1B-O1B-C4'
24	V	102	LMT	O5B-C1B-O1B-C4'
24	B	104	LMT	O5B-C1B-O1B-C4'
24	J	102	LMT	O5B-C1B-O1B-C4'
24	N	101	LMT	O5B-C1B-O1B-C4'
24	P	102	LMT	O5B-C1B-O1B-C4'
24	T	102	LMT	O5B-C1B-O1B-C4'
24	X	102	LMT	O5B-C1B-O1B-C4'
24	2	103	LMT	O5B-C1B-O1B-C4'
24	4	102	LMT	O5B-C1B-O1B-C4'
24	8	102	LMT	O5B-C1B-O1B-C4'
24	0	101	LMT	O5B-C1B-O1B-C4'
24	Z	102	LMT	O5B-C1B-O1B-C4'
24	6	102	LMT	O5B-C1B-O1B-C4'
16	A	102	BCL	C5-C6-C7-C8
14	C	407	DGA	OB1-CB1-OG2-CG2
15	C	408	PGV	O02-C1-O01-C02
16	O	105	BCL	C3-C5-C6-C7
16	Q	104	BCL	C3-C5-C6-C7
16	U	103	BCL	C3-C5-C6-C7
16	7	103	BCL	C3-C5-C6-C7
16	9	104	BCL	C3-C5-C6-C7
17	L	302	BPH	C3-C5-C6-C7
15	F	104	PGV	C2-C1-O01-C02
15	K	101	PGV	C2-C1-O01-C02
16	U	102	BCL	C4-C3-C5-C6
18	L	306	UQ8	C20-C19-C21-C22
23	5	105	H4X	C5-C6-C7-C8
18	L	306	UQ8	C12-C11-C9-C8
23	4	101	H4X	C5-C6-C7-C9
16	9	103	BCL	CBD-CGD-O2D-CED
16	M	402	BCL	C2A-CAA-CBA-CGA
16	K	108	BCL	C3-C5-C6-C7
21	M	405	MQ8	C41-C42-C43-C45
21	M	405	MQ8	C41-C42-C43-C44
16	Q	103	BCL	O1A-CGA-O2A-C1
14	C	407	DGA	CG1-CG2-OG2-CB1
16	A	102	BCL	CBD-CGD-O2D-CED
16	F	103	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	K	105	BCL	CBD-CGD-O2D-CED
17	M	404	BPH	CBD-CGD-O2D-CED
15	5	101	PGV	O12-C04-C05-O05
22	H	302	CDL	O1-C1-CA2-OA2
16	A	102	BCL	C3-C5-C6-C7
16	U	102	BCL	C3-C5-C6-C7
15	F	104	PGV	C20-C19-O03-C01
16	Q	103	BCL	CBA-CGA-O2A-C1
15	K	106	PGV	C2-C1-O01-C02
16	I	102	BCL	CBD-CGD-O2D-CED
16	U	102	BCL	CBD-CGD-O2D-CED
24	B	102	LMT	O5B-C5B-C6B-O6B
24	G	102	LMT	O5B-C5B-C6B-O6B
24	T	102	LMT	O5'-C5'-C6'-O6'
24	2	103	LMT	O5B-C5B-C6B-O6B
24	8	101	LMT	O5B-C5B-C6B-O6B
16	X	101	BCL	C3-C5-C6-C7
16	Y	104	BCL	C3-C5-C6-C7
24	J	102	LMT	O5B-C5B-C6B-O6B
24	R	101	LMT	O5'-C5'-C6'-O6'
24	X	102	LMT	O5'-C5'-C6'-O6'
24	4	102	LMT	O5B-C5B-C6B-O6B
24	4	102	LMT	O5'-C5'-C6'-O6'
15	K	106	PGV	O02-C1-O01-C02
24	8	101	LMT	C4'-C5'-C6'-O6'
11	C	402	HEM	C3D-CAD-CBD-CGD
16	M	402	BCL	C4-C3-C5-C6
17	M	404	BPH	C4-C3-C5-C6
21	M	405	MQ8	C29-C28-C30-C31
16	M	402	BCL	C2-C3-C5-C6
16	U	102	BCL	C2-C3-C5-C6
17	M	404	BPH	C2-C3-C5-C6
18	L	306	UQ8	C18-C19-C21-C22
21	M	405	MQ8	C27-C28-C30-C31
24	B	104	LMT	O5'-C1'-O1'-C1
24	T	102	LMT	O5'-C1'-O1'-C1
24	X	102	LMT	O5'-C1'-O1'-C1
24	Z	102	LMT	O5'-C1'-O1'-C1
18	L	303	UQ8	C14-C16-C17-C18
21	M	405	MQ8	C28-C30-C31-C32
15	9	101	PGV	C29-C30-C31-C32
16	9	103	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	K	107	H4X	C1-C4-C5-C6
23	O	101	H4X	C1-C4-C5-C6
23	4	101	H4X	C1-C4-C5-C6
24	N	101	LMT	O5'-C5'-C6'-O6'
24	2	103	LMT	O5'-C5'-C6'-O6'
15	F	104	PGV	O04-C19-O03-C01
24	4	102	LMT	C4'-C5'-C6'-O6'
16	M	402	BCL	C8-C10-C11-C12
15	A	101	PGV	O12-C04-C05-C06
15	3	101	PGV	O12-C04-C05-C06
15	9	101	PGV	O12-C04-C05-C06
22	H	302	CDL	CB2-C1-CA2-OA2
24	V	102	LMT	O5'-C5'-C6'-O6'
24	G	102	LMT	C4'-C5'-C6'-O6'
16	B	103	BCL	C3-C5-C6-C7
15	Q	101	PGV	C20-C19-O03-C01
15	3	101	PGV	C20-C19-O03-C01
24	E	102	LMT	O5B-C5B-C6B-O6B
24	G	102	LMT	O5'-C5'-C6'-O6'
24	8	102	LMT	O5'-C5'-C6'-O6'
24	V	102	LMT	C4'-C5'-C6'-O6'
14	C	407	DGA	CA1-CA2-CA3-CA4
24	R	101	LMT	O5B-C5B-C6B-O6B
24	6	102	LMT	O5'-C5'-C6'-O6'
24	0	101	LMT	O5'-C5'-C6'-O6'
22	Y	103	CDL	CB3-CB4-CB6-OB8
24	J	102	LMT	O5'-C5'-C6'-O6'
24	X	102	LMT	C4'-C5'-C6'-O6'
16	Q	103	BCL	C8-C10-C11-C12
16	5	104	BCL	C15-C16-C17-C18
16	9	104	BCL	C15-C16-C17-C18
17	L	302	BPH	C10-C11-C12-C13
15	K	101	PGV	O12-C04-C05-O05
22	S	101	CDL	O1-C1-CB2-OB2
24	8	101	LMT	O5'-C5'-C6'-O6'
24	2	103	LMT	C4'-C5'-C6'-O6'
16	M	403	BCL	C11-C10-C8-C9
16	M	403	BCL	C11-C12-C13-C14
16	B	103	BCL	C11-C10-C8-C9
16	D	104	BCL	C11-C10-C8-C9
16	F	105	BCL	C11-C10-C8-C9
16	J	101	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
16	K	108	BCL	C11-C10-C8-C9
16	O	105	BCL	C14-C13-C15-C16
16	T	101	BCL	C11-C10-C8-C9
16	U	102	BCL	C6-C7-C8-C9
16	U	103	BCL	C11-C10-C8-C9
16	X	101	BCL	C11-C10-C8-C9
16	Y	104	BCL	C11-C10-C8-C9
16	2	102	BCL	C11-C10-C8-C9
16	3	103	BCL	C6-C7-C8-C9
16	3	104	BCL	C11-C10-C8-C9
16	5	104	BCL	C11-C10-C8-C9
16	7	103	BCL	C11-C10-C8-C9
16	9	103	BCL	C11-C10-C8-C9
16	9	104	BCL	C11-C10-C8-C9
17	L	302	BPH	C6-C7-C8-C9
17	L	302	BPH	C11-C10-C8-C9
17	M	404	BPH	C11-C12-C13-C14
17	M	404	BPH	C14-C13-C15-C16
16	2	102	BCL	C15-C16-C17-C18
23	K	107	H4X	C29-C28-C30-C31
23	Q	105	H4X	C10-C11-C12-C13
22	Y	103	CDL	OB6-CB4-CB6-OB8
24	Z	102	LMT	O5B-C5B-C6B-O6B
14	C	407	DGA	CB2-CB3-CB4-CB5
24	R	101	LMT	C4'-C5'-C6'-O6'
24	T	102	LMT	C4'-C5'-C6'-O6'
24	8	102	LMT	C4'-C5'-C6'-O6'
15	M	406	PGV	C1-C2-C3-C4
16	L	304	BCL	C13-C15-C16-C17
24	6	102	LMT	C2B-C1B-O1B-C4'
24	Z	102	LMT	O5'-C5'-C6'-O6'
24	J	102	LMT	C4'-C5'-C6'-O6'
24	N	101	LMT	C4'-C5'-C6'-O6'
19	L	307	8K6	C12-C13-C14-C15
24	Z	102	LMT	C2B-C1B-O1B-C4'
16	B	103	BCL	C15-C16-C17-C18
16	D	104	BCL	C15-C16-C17-C18
16	K	108	BCL	C15-C16-C17-C18
16	T	101	BCL	C15-C16-C17-C18
16	U	103	BCL	C15-C16-C17-C18
16	1	102	BCL	C10-C11-C12-C13
16	7	103	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
17	L	302	BPH	C13-C15-C16-C17
17	M	404	BPH	C8-C10-C11-C12
24	V	102	LMT	O5B-C5B-C6B-O6B
15	O	102	PGV	C1-C2-C3-C4
15	1	103	PGV	C19-C20-C21-C22
22	H	302	CDL	CB7-C71-C72-C73
24	P	102	LMT	O5'-C5'-C6'-O6'
16	F	105	BCL	C15-C16-C17-C18
16	I	102	BCL	C10-C11-C12-C13
16	K	105	BCL	C13-C15-C16-C17
16	X	101	BCL	C15-C16-C17-C18
16	Y	104	BCL	C15-C16-C17-C18
16	3	104	BCL	C15-C16-C17-C18
15	I	103	PGV	C19-C20-C21-C22
15	K	101	PGV	C19-C20-C21-C22
15	K	106	PGV	C19-C20-C21-C22
15	3	101	PGV	C1-C2-C3-C4
24	6	102	LMT	O5B-C5B-C6B-O6B
16	O	104	BCL	C15-C16-C17-C18
16	Q	104	BCL	C15-C16-C17-C18
16	1	102	BCL	C8-C10-C11-C12
16	K	105	BCL	C3-C5-C6-C7
16	M	402	BCL	CBA-CGA-O2A-C1
24	B	102	LMT	O5'-C5'-C6'-O6'
16	J	101	BCL	C15-C16-C17-C18
15	M	406	PGV	C19-C20-C21-C22
15	F	101	PGV	C1-C2-C3-C4
16	L	301	BCL	C11-C10-C8-C7
16	B	103	BCL	C11-C12-C13-C15
16	D	103	BCL	C11-C10-C8-C7
16	D	104	BCL	C11-C12-C13-C15
16	F	103	BCL	C11-C10-C8-C7
16	F	105	BCL	C11-C10-C8-C7
16	I	102	BCL	C11-C10-C8-C7
16	J	101	BCL	C11-C12-C13-C15
16	K	105	BCL	C11-C10-C8-C7
16	K	108	BCL	C11-C12-C13-C15
16	O	104	BCL	C11-C10-C8-C7
16	T	101	BCL	C11-C10-C8-C7
16	T	101	BCL	C11-C12-C13-C15
16	W	102	BCL	C11-C10-C8-C7
16	X	101	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
16	Y	102	BCL	C11-C10-C8-C7
16	Y	104	BCL	C11-C12-C13-C15
16	1	102	BCL	C11-C10-C8-C7
16	3	103	BCL	C11-C10-C8-C7
16	3	104	BCL	C11-C12-C13-C15
16	7	102	BCL	C11-C10-C8-C7
16	7	103	BCL	C11-C12-C13-C15
17	M	404	BPH	C3-C5-C6-C7
15	Q	101	PGV	O04-C19-O03-C01
16	7	102	BCL	C8-C10-C11-C12
24	2	103	LMT	C2B-C1B-O1B-C4'
24	4	102	LMT	C2B-C1B-O1B-C4'
15	3	101	PGV	O04-C19-O03-C01
16	9	103	BCL	O1A-CGA-O2A-C1
24	B	104	LMT	C4'-C5'-C6'-O6'
24	6	102	LMT	C4'-C5'-C6'-O6'
24	P	102	LMT	O5'-C1'-O1'-C1
24	8	102	LMT	O5'-C1'-O1'-C1
16	M	403	BCL	C15-C16-C17-C18
18	L	306	UQ8	C9-C11-C12-C13
24	G	102	LMT	C2B-C1B-O1B-C4'
24	B	104	LMT	O5'-C5'-C6'-O6'
15	3	101	PGV	O12-C04-C05-O05
16	F	103	BCL	C8-C10-C11-C12
16	F	103	BCL	C10-C11-C12-C13
16	3	103	BCL	C8-C10-C11-C12
17	L	302	BPH	C5-C6-C7-C8
23	2	101	H4X	C1-C4-C5-C6
24	E	102	LMT	O5'-C5'-C6'-O6'
24	4	102	LMT	C9-C10-C11-C12
16	F	103	BCL	C15-C16-C17-C18
17	M	404	BPH	C13-C15-C16-C17
15	M	406	PGV	C2-C1-O01-C02
15	M	406	PGV	C21-C22-C23-C24
15	K	106	PGV	C6-C7-C8-C9
16	M	402	BCL	C15-C16-C17-C18
16	Q	103	BCL	C10-C11-C12-C13
15	L	305	PGV	C03-O11-P-O12
15	M	406	PGV	C04-O12-P-O11
15	O	102	PGV	C03-O11-P-O12
15	O	102	PGV	C04-O12-P-O11
15	Q	101	PGV	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
15	Q	101	PGV	C04-O12-P-O11
15	9	101	PGV	C03-O11-P-O12
15	9	101	PGV	C04-O12-P-O11
22	H	302	CDL	CA2-OA2-PA1-OA5
22	H	302	CDL	CB3-OB5-PB2-OB2
22	S	101	CDL	CA2-OA2-PA1-OA5
22	S	101	CDL	CB2-OB2-PB2-OB5
16	F	103	BCL	C13-C15-C16-C17
24	Z	102	LMT	C4'-C5'-C6'-O6'
24	0	101	LMT	C4'-C5'-C6'-O6'
24	V	102	LMT	C2B-C1B-O1B-C4'
15	5	101	PGV	O12-C04-C05-C06
22	Y	103	CDL	OB5-CB3-CB4-CB6
15	M	406	PGV	O02-C1-O01-C02
16	W	102	BCL	C10-C11-C12-C13
16	7	102	BCL	C10-C11-C12-C13
16	J	101	BCL	C3-C5-C6-C7
23	V	101	H4X	C33-C35-C36-C37
16	J	101	BCL	C10-C11-C12-C13
22	S	101	CDL	CA7-C31-C32-C33
16	5	103	BCL	C8-C10-C11-C12
23	O	101	H4X	C30-C31-C32-C33
15	Q	101	PGV	C19-C20-C21-C22
15	M	406	PGV	C3-C4-C5-C6
15	F	104	PGV	C3-C4-C5-C6
16	A	102	BCL	C16-C17-C18-C19
16	3	103	BCL	C16-C17-C18-C19
16	9	103	BCL	C16-C17-C18-C20
15	I	103	PGV	C24-C25-C26-C27
15	5	101	PGV	C7-C8-C9-C10
19	L	307	8K6	C7-C8-C9-C10
24	B	102	LMT	C5'-C4'-O1B-C1B
24	0	101	LMT	C2B-C1B-O1B-C4'
15	I	103	PGV	C26-C27-C28-C29
19	L	307	8K6	C10-C11-C12-C13
24	J	102	LMT	C2B-C1B-O1B-C4'
24	N	101	LMT	C2B-C1B-O1B-C4'
16	M	402	BCL	O1A-CGA-O2A-C1
19	L	307	8K6	C4-C5-C6-C7
15	M	406	PGV	C6-C7-C8-C9
15	3	101	PGV	C19-C20-C21-C22
16	7	103	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	I	103	PGV	C22-C23-C24-C25
15	9	101	PGV	C30-C31-C32-C33
24	B	104	LMT	C2-C3-C4-C5
21	M	405	MQ8	C39-C38-C40-C41
14	C	407	DGA	CA7-CA8-CA9-CAA
15	F	101	PGV	C3-C4-C5-C6
15	I	103	PGV	C27-C28-C29-C30
22	S	101	CDL	C73-C74-C75-C76
16	A	102	BCL	C11-C10-C8-C9
16	D	104	BCL	C11-C12-C13-C14
16	F	103	BCL	O1D-CGD-O2D-CED
17	M	404	BPH	O1D-CGD-O2D-CED
15	M	406	PGV	C4-C5-C6-C7
15	K	101	PGV	C22-C23-C24-C25
15	O	102	PGV	C4-C5-C6-C7
15	O	102	PGV	C24-C25-C26-C27
15	5	101	PGV	C23-C24-C25-C26
19	5	106	8K6	C6-C7-C8-C9
24	N	101	LMT	O5B-C5B-C6B-O6B
24	T	102	LMT	O5B-C5B-C6B-O6B
16	K	105	BCL	O1D-CGD-O2D-CED
23	Z	101	H4X	C10-C11-C12-C13
15	A	101	PGV	C04-C05-C06-O06
15	9	101	PGV	C04-C05-C06-O06
23	U	104	H4X	C15-C16-C17-C19
24	6	102	LMT	C1-C2-C3-C4
16	F	105	BCL	C3-C5-C6-C7
16	T	101	BCL	C3-C5-C6-C7
15	Q	101	PGV	C1-C2-C3-C4
15	Q	101	PGV	C22-C23-C24-C25
19	L	307	8K6	C11-C12-C13-C14
22	H	302	CDL	C11-C12-C13-C14
22	S	101	CDL	C18-C19-C20-C21
24	B	102	LMT	C1-C2-C3-C4
24	G	102	LMT	C1-C2-C3-C4
16	A	102	BCL	C16-C17-C18-C20
16	K	105	BCL	C16-C17-C18-C19
16	K	105	BCL	C16-C17-C18-C20
16	Q	103	BCL	C16-C17-C18-C19
16	1	102	BCL	C16-C17-C18-C19
16	1	102	BCL	C16-C17-C18-C20
16	Q	103	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	T	102	LMT	C2B-C1B-O1B-C4'
15	F	104	PGV	C25-C26-C27-C28
24	J	102	LMT	C1-C2-C3-C4
15	L	305	PGV	C29-C30-C31-C32
15	I	103	PGV	C4-C5-C6-C7
15	Q	101	PGV	C23-C24-C25-C26
24	E	102	LMT	C2B-C1B-O1B-C4'
24	R	101	LMT	C2B-C1B-O1B-C4'
16	O	105	BCL	C15-C16-C17-C18
16	S	103	BCL	C5-C6-C7-C8
15	D	101	PGV	C3-C4-C5-C6
16	Y	104	BCL	CBA-CGA-O2A-C1
15	Q	101	PGV	C21-C22-C23-C24
16	B	103	BCL	C3A-C2A-CAA-CBA
16	D	104	BCL	C3A-C2A-CAA-CBA
16	F	105	BCL	C3A-C2A-CAA-CBA
16	J	101	BCL	C3A-C2A-CAA-CBA
16	K	108	BCL	C3A-C2A-CAA-CBA
16	O	105	BCL	C3A-C2A-CAA-CBA
16	Q	103	BCL	C3A-C2A-CAA-CBA
16	Q	104	BCL	C3A-C2A-CAA-CBA
16	T	101	BCL	C3A-C2A-CAA-CBA
16	U	102	BCL	C3A-C2A-CAA-CBA
16	U	103	BCL	C3A-C2A-CAA-CBA
16	X	101	BCL	C3A-C2A-CAA-CBA
16	Y	104	BCL	C3A-C2A-CAA-CBA
16	2	102	BCL	C3A-C2A-CAA-CBA
16	3	104	BCL	C3A-C2A-CAA-CBA
16	5	104	BCL	C3A-C2A-CAA-CBA
16	7	103	BCL	C3A-C2A-CAA-CBA
16	9	103	BCL	C3A-C2A-CAA-CBA
16	9	104	BCL	C3A-C2A-CAA-CBA
16	Y	102	BCL	C13-C15-C16-C17
15	D	101	PGV	C28-C29-C30-C31
24	0	101	LMT	C2-C3-C4-C5
24	P	102	LMT	C4'-C5'-C6'-O6'
15	F	104	PGV	C5-C6-C7-C8
15	K	106	PGV	C25-C26-C27-C28
15	5	101	PGV	C25-C26-C27-C28
22	H	302	CDL	C12-C13-C14-C15
15	K	106	PGV	O03-C01-C02-C03
24	B	104	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
15	9	101	PGV	C23-C24-C25-C26
24	2	103	LMT	C1-C2-C3-C4
16	7	103	BCL	O1A-CGA-O2A-C1
22	H	302	CDL	C58-C59-C60-C61
24	T	102	LMT	C2-C3-C4-C5
24	V	102	LMT	C1-C2-C3-C4
24	Z	102	LMT	C1-C2-C3-C4
15	Q	101	PGV	O05-C05-C06-O06
15	3	101	PGV	C29-C30-C31-C32
22	S	101	CDL	C15-C16-C17-C18
16	L	304	BCL	C10-C11-C12-C13
16	K	108	BCL	C10-C11-C12-C13
16	5	104	BCL	C3-C5-C6-C7
24	4	102	LMT	C1-C2-C3-C4
16	Y	104	BCL	O1A-CGA-O2A-C1
24	8	101	LMT	C7-C8-C9-C10
15	9	101	PGV	C25-C26-C27-C28
16	D	104	BCL	C10-C11-C12-C13
15	Q	101	PGV	C2-C3-C4-C5
15	Y	105	PGV	C3-C4-C5-C6
16	F	103	BCL	C16-C17-C18-C19
23	G	101	H4X	C33-C35-C36-C37
16	B	103	BCL	CBA-CGA-O2A-C1
16	K	108	BCL	C5-C6-C7-C8
16	Q	103	BCL	C15-C16-C17-C18
24	T	102	LMT	C1-C2-C3-C4
16	Q	104	BCL	C10-C11-C12-C13
24	0	101	LMT	O5B-C5B-C6B-O6B
16	A	102	BCL	C11-C10-C8-C7
16	F	105	BCL	C11-C12-C13-C15
16	J	101	BCL	C11-C10-C8-C7
16	O	105	BCL	C11-C12-C13-C15
16	Q	104	BCL	C11-C10-C8-C7
16	U	103	BCL	C11-C10-C8-C7
16	U	103	BCL	C11-C12-C13-C15
16	X	101	BCL	C11-C12-C13-C15
16	5	104	BCL	C11-C10-C8-C7
16	9	103	BCL	C12-C13-C15-C16
16	9	104	BCL	C11-C10-C8-C7
16	9	104	BCL	C11-C12-C13-C15
21	M	405	MQ8	C37-C38-C40-C41
24	6	102	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
16	D	103	BCL	C8-C10-C11-C12
16	3	103	BCL	C16-C17-C18-C20
16	X	101	BCL	CBA-CGA-O2A-C1
24	N	101	LMT	C9-C10-C11-C12
24	2	103	LMT	C9-C10-C11-C12
16	B	103	BCL	C10-C11-C12-C13
16	F	105	BCL	C10-C11-C12-C13
16	Y	102	BCL	C15-C16-C17-C18
16	3	104	BCL	C10-C11-C12-C13
16	9	104	BCL	C10-C11-C12-C13
24	B	104	LMT	C9-C10-C11-C12
15	M	406	PGV	C2-C3-C4-C5
24	Z	102	LMT	C9-C10-C11-C12
15	K	106	PGV	C4-C5-C6-C7
11	C	403	HEM	C2B-C3B-CAB-CBB
15	Y	105	PGV	C2-C3-C4-C5
16	O	104	BCL	CBD-CGD-O2D-CED
16	M	402	BCL	C16-C17-C18-C19
16	A	102	BCL	O1D-CGD-O2D-CED
15	M	406	PGV	C7-C8-C9-C10
15	I	103	PGV	C7-C8-C9-C10
15	I	103	PGV	C2-C1-O01-C02
15	5	101	PGV	C2-C1-O01-C02
22	H	302	CDL	C51-CB5-OB6-CB4
22	S	101	CDL	C11-CA5-OA6-CA4
15	A	101	PGV	O01-C02-C03-O11
22	H	302	CDL	OA5-CA3-CA4-OA6
24	B	102	LMT	C3'-C4'-O1B-C1B
11	C	404	HEM	C4B-C3B-CAB-CBB
15	I	103	PGV	O02-C1-O01-C02
15	5	101	PGV	O02-C1-O01-C02
22	H	302	CDL	OB7-CB5-OB6-CB4
22	H	302	CDL	CA7-C31-C32-C33
16	U	103	BCL	C10-C11-C12-C13
15	K	106	PGV	O03-C01-C02-O01
24	P	102	LMT	O5B-C5B-C6B-O6B
16	K	105	BCL	C15-C16-C17-C18
15	5	101	PGV	C11-C10-C9-C8
15	Y	105	PGV	C19-C20-C21-C22
24	X	102	LMT	C2B-C1B-O1B-C4'
16	L	301	BCL	C11-C10-C8-C9
16	D	103	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
16	O	104	BCL	C11-C10-C8-C9
16	Q	104	BCL	C11-C10-C8-C9
16	Y	102	BCL	C14-C13-C15-C16
16	Y	104	BCL	C11-C12-C13-C14
16	9	103	BCL	C14-C13-C15-C16
16	B	103	BCL	O1A-CGA-O2A-C1
23	O	101	H4X	C4-C5-C6-C7
22	S	101	CDL	C81-C82-C83-C84
17	L	302	BPH	C2C-C3C-CAC-CBC
23	V	101	H4X	C15-C16-C17-C18
24	E	102	LMT	C4'-C5'-C6'-O6'
16	X	101	BCL	C8-C10-C11-C12
24	E	102	LMT	C1-C2-C3-C4
16	D	104	BCL	C1A-C2A-CAA-CBA
16	Q	104	BCL	C1A-C2A-CAA-CBA
16	U	103	BCL	C1A-C2A-CAA-CBA
16	X	101	BCL	C1A-C2A-CAA-CBA
16	Y	104	BCL	C1A-C2A-CAA-CBA
16	7	103	BCL	C1A-C2A-CAA-CBA
16	M	402	BCL	C16-C17-C18-C20
16	9	103	BCL	C16-C17-C18-C19
15	O	102	PGV	C2-C1-O01-C02
15	O	102	PGV	C2-C3-C4-C5
22	S	101	CDL	C72-C73-C74-C75
16	O	104	BCL	C10-C11-C12-C13
16	3	103	BCL	C15-C16-C17-C18
16	9	103	BCL	C10-C11-C12-C13
15	M	406	PGV	C03-O11-P-O12
24	J	102	LMT	C9-C10-C11-C12
16	3	103	BCL	C3-C5-C6-C7
22	H	302	CDL	C77-C78-C79-C80
22	H	302	CDL	OA5-CA3-CA4-CA6
22	S	101	CDL	C74-C75-C76-C77
24	V	102	LMT	C7-C8-C9-C10
15	5	101	PGV	C26-C27-C28-C29
16	I	102	BCL	C2C-C3C-CAC-CBC
16	Y	104	BCL	C2C-C3C-CAC-CBC
23	5	105	H4X	C5-C6-C7-C9
15	L	305	PGV	C5-C6-C7-C8
24	P	102	LMT	C9-C10-C11-C12
24	8	102	LMT	C9-C10-C11-C12
15	F	101	PGV	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
16	Q	104	BCL	O1A-CGA-O2A-C1
16	X	101	BCL	O1A-CGA-O2A-C1
16	L	301	BCL	C3-C5-C6-C7
15	H	301	PGV	O03-C01-C02-C03
15	F	104	PGV	O03-C01-C02-C03
19	L	307	8K6	C11-C10-C9-C8
24	T	102	LMT	C9-C10-C11-C12
16	J	101	BCL	CBA-CGA-O2A-C1
16	K	108	BCL	CBA-CGA-O2A-C1
16	U	102	BCL	C15-C16-C17-C18
15	H	301	PGV	C4-C5-C6-C7
24	X	102	LMT	O5B-C5B-C6B-O6B
15	H	301	PGV	C24-C25-C26-C27
15	I	103	PGV	C5-C6-C7-C8
22	S	101	CDL	C19-C20-C21-C22
24	X	102	LMT	C2-C3-C4-C5
24	V	102	LMT	O5'-C1'-O1'-C1
16	2	102	BCL	C10-C11-C12-C13
15	3	101	PGV	C27-C28-C29-C30
15	K	106	PGV	C3-C4-C5-C6
15	Y	105	PGV	C20-C21-C22-C23
24	B	102	LMT	C4B-C5B-C6B-O6B
14	C	407	DGA	CB3-CB4-CB5-CB6
14	C	407	DGA	CB5-CB6-CB7-CB8
17	L	302	BPH	C4-C3-C5-C6
16	L	304	BCL	C16-C17-C18-C19
16	D	104	BCL	CBA-CGA-O2A-C1
16	Q	104	BCL	CBA-CGA-O2A-C1
16	9	104	BCL	CBA-CGA-O2A-C1
24	8	102	LMT	O5B-C5B-C6B-O6B
16	M	402	BCL	C5-C6-C7-C8
24	T	102	LMT	C5-C6-C7-C8
24	B	104	LMT	O5B-C5B-C6B-O6B
16	1	102	BCL	C15-C16-C17-C18
14	C	407	DGA	CG3-CG2-OG2-CB1
15	L	305	PGV	C28-C29-C30-C31
19	5	106	8K6	C7-C8-C9-C10
22	H	302	CDL	C55-C56-C57-C58
24	P	102	LMT	C2-C3-C4-C5
24	B	102	LMT	C4'-C5'-C6'-O6'
15	9	101	PGV	C21-C22-C23-C24
24	V	102	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	O	104	BCL	O1D-CGD-O2D-CED
16	D	103	BCL	C5-C6-C7-C8
16	Y	104	BCL	C10-C11-C12-C13
15	C	408	PGV	C03-O11-P-O13
15	F	101	PGV	C03-O11-P-O13
15	K	106	PGV	C03-O11-P-O13
15	1	103	PGV	C03-O11-P-O13
22	S	101	CDL	C77-C78-C79-C80
24	6	102	LMT	C5-C6-C7-C8
15	L	305	PGV	C20-C19-O03-C01
15	M	406	PGV	O01-C02-C03-O11
16	F	103	BCL	C16-C17-C18-C20
22	H	302	CDL	C15-C16-C17-C18
22	S	101	CDL	C76-C77-C78-C79
24	E	102	LMT	C9-C10-C11-C12
16	9	104	BCL	O1A-CGA-O2A-C1
15	9	101	PGV	C31-C32-C33-C34
16	I	102	BCL	C8-C10-C11-C12
16	Y	102	BCL	C10-C11-C12-C13
16	9	103	BCL	C5-C6-C7-C8
23	E	101	H4X	C3-C1-O1-C1M
23	G	101	H4X	C3-C1-O1-C1M
23	K	103	H4X	C40-C38-O2-C2M
23	K	107	H4X	C3-C1-O1-C1M
23	O	106	H4X	C2-C1-O1-C1M
23	Q	105	H4X	C39-C38-O2-C2M
23	V	101	H4X	C2-C1-O1-C1M
23	Z	101	H4X	C2-C1-O1-C1M
23	2	101	H4X	C2-C1-O1-C1M
23	5	105	H4X	C2-C1-O1-C1M
23	7	104	H4X	C3-C1-O1-C1M
15	L	305	PGV	O03-C01-C02-O01
15	3	101	PGV	O03-C01-C02-O01
22	S	101	CDL	OA7-CA5-OA6-CA4
16	J	101	BCL	O1A-CGA-O2A-C1
16	3	104	BCL	O1A-CGA-O2A-C1
15	3	101	PGV	C28-C29-C30-C31
16	A	102	BCL	C6-C7-C8-C10
16	B	103	BCL	C11-C10-C8-C7
16	D	104	BCL	C11-C10-C8-C7
16	K	108	BCL	C11-C10-C8-C7
16	Y	102	BCL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
16	Y	104	BCL	C11-C10-C8-C7
16	2	102	BCL	C11-C10-C8-C7
16	3	103	BCL	C6-C7-C8-C10
16	3	103	BCL	C11-C12-C13-C15
16	3	104	BCL	C11-C10-C8-C7
16	5	103	BCL	C11-C10-C8-C7
16	7	103	BCL	C11-C10-C8-C7
17	L	302	BPH	C2-C3-C5-C6
17	L	302	BPH	C6-C7-C8-C10
15	Y	105	PGV	C21-C22-C23-C24
22	S	101	CDL	C11-C12-C13-C14
16	A	102	BCL	C6-C7-C8-C9
16	F	103	BCL	C11-C10-C8-C9
16	I	102	BCL	C11-C10-C8-C9
16	K	108	BCL	C11-C12-C13-C14
16	W	102	BCL	C11-C10-C8-C9
16	Y	102	BCL	C11-C10-C8-C9
16	7	102	BCL	C11-C10-C8-C9
15	D	101	PGV	C26-C27-C28-C29
16	U	103	BCL	CBA-CGA-O2A-C1
16	K	108	BCL	O1A-CGA-O2A-C1
23	P	101	H4X	C15-C16-C17-C18
16	9	103	BCL	O1D-CGD-O2D-CED
16	D	104	BCL	O1A-CGA-O2A-C1
16	7	103	BCL	C10-C11-C12-C13
24	R	101	LMT	C1-C2-C3-C4
24	E	102	LMT	C7-C8-C9-C10
16	2	102	BCL	C16-C17-C18-C20
15	A	101	PGV	C01-C02-C03-O11
15	9	101	PGV	C01-C02-C03-O11
22	S	101	CDL	OB5-CB3-CB4-CB6
16	5	103	BCL	C3-C5-C6-C7
15	D	101	PGV	C1-C2-C3-C4
14	C	407	DGA	CB7-CB8-CB9-CAB
16	U	103	BCL	O1A-CGA-O2A-C1
22	S	101	CDL	C34-C35-C36-C37
16	F	105	BCL	CBA-CGA-O2A-C1
16	2	102	BCL	CBA-CGA-O2A-C1
15	K	101	PGV	C6-C7-C8-C9
24	8	101	LMT	C6-C7-C8-C9
23	P	101	H4X	C1-C4-C5-C6
24	E	102	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
24	N	101	LMT	C2-C1-O1'-C1'
24	8	101	LMT	C2-C1-O1'-C1'
15	K	101	PGV	C4-C5-C6-C7
14	C	407	DGA	CBB-CAB-CB9-CB8
22	S	101	CDL	C80-C81-C82-C83
16	3	104	BCL	CBA-CGA-O2A-C1
16	I	102	BCL	C13-C15-C16-C17
16	U	102	BCL	C10-C11-C12-C13
17	L	302	BPH	C8-C10-C11-C12
15	L	305	PGV	O03-C01-C02-C03
15	O	102	PGV	O03-C01-C02-C03
15	3	101	PGV	O03-C01-C02-C03
23	E	101	H4X	C3-C1-C4-C5
23	K	103	H4X	C2-C1-C4-C5
23	O	101	H4X	C36-C37-C38-C40
23	5	105	H4X	C36-C37-C38-C40
23	5	105	H4X	C2-C1-C4-C5
23	6	101	H4X	C3-C1-C4-C5
23	6	101	H4X	C2-C1-C4-C5
23	7	104	H4X	C2-C1-C4-C5
15	K	101	PGV	C20-C21-C22-C23
15	Q	101	PGV	C24-C25-C26-C27
16	K	105	BCL	O2A-C1-C2-C3
16	D	104	BCL	C3-C5-C6-C7
16	I	102	BCL	C16-C17-C18-C20
24	N	101	LMT	C2-C3-C4-C5
15	A	101	PGV	C03-O11-P-O12
15	F	104	PGV	C03-O11-P-O12
15	5	101	PGV	C04-O12-P-O11
24	E	102	LMT	C5-C6-C7-C8
15	L	305	PGV	C4-C5-C6-C7
22	S	101	CDL	OB5-CB3-CB4-OB6
15	F	104	PGV	C20-C21-C22-C23
16	2	102	BCL	O1A-CGA-O2A-C1
15	9	101	PGV	C1-C2-C3-C4
24	G	102	LMT	C7-C8-C9-C10
15	C	408	PGV	O01-C02-C03-O11
24	B	104	LMT	C2B-C1B-O1B-C4'
24	8	102	LMT	C2B-C1B-O1B-C4'
15	F	104	PGV	O03-C01-C02-O01
19	L	307	8K6	C3-C4-C5-C6
15	H	301	PGV	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
16	Q	103	BCL	C16-C17-C18-C20
15	F	104	PGV	O12-C04-C05-C06
24	Z	102	LMT	C2-C3-C4-C5
15	O	102	PGV	O02-C1-O01-C02
16	D	104	BCL	C2-C1-O2A-CGA
16	J	101	BCL	C2-C1-O2A-CGA
16	K	105	BCL	C2-C1-O2A-CGA
16	K	108	BCL	C2-C1-O2A-CGA
16	2	102	BCL	C2-C1-O2A-CGA
16	3	103	BCL	C2-C1-O2A-CGA
16	3	104	BCL	C2-C1-O2A-CGA
16	9	104	BCL	C2-C1-O2A-CGA
16	M	402	BCL	C11-C10-C8-C9
16	F	105	BCL	C11-C12-C13-C14
16	Q	103	BCL	C11-C10-C8-C9
16	9	103	BCL	C11-C12-C13-C14
15	O	102	PGV	C7-C8-C9-C10
24	8	101	LMT	C5-C6-C7-C8
15	M	406	PGV	C22-C23-C24-C25
16	X	101	BCL	C10-C11-C12-C13
15	O	102	PGV	C20-C21-C22-C23
24	0	101	LMT	C7-C8-C9-C10
16	O	104	BCL	C16-C17-C18-C20
16	O	104	BCL	C5-C6-C7-C8
16	5	103	BCL	C4C-C3C-CAC-CBC
15	O	102	PGV	C11-C10-C9-C8
15	O	102	PGV	C30-C31-C32-C33
19	L	307	8K6	C15-C16-C17-C18
23	G	101	H4X	C1-C4-C5-C6
15	K	101	PGV	C23-C24-C25-C26
23	K	103	H4X	C4-C5-C6-C7
22	H	302	CDL	CB5-C51-C52-C53
15	L	305	PGV	O04-C19-O03-C01
15	O	102	PGV	C25-C26-C27-C28
22	H	302	CDL	OB5-CB3-CB4-CB6
15	L	305	PGV	C24-C25-C26-C27
16	M	402	BCL	C6-C7-C8-C10
16	M	402	BCL	C11-C10-C8-C7
16	K	105	BCL	C6-C7-C8-C10
16	Q	103	BCL	C6-C7-C8-C10
16	9	103	BCL	C6-C7-C8-C10
16	9	103	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
16	9	103	BCL	C11-C12-C13-C15
17	L	302	BPH	C11-C10-C8-C7
17	M	404	BPH	C6-C7-C8-C10
16	O	104	BCL	C3-C5-C6-C7
15	F	104	PGV	C24-C25-C26-C27
16	5	103	BCL	C15-C16-C17-C18
16	5	104	BCL	C10-C11-C12-C13
23	2	101	H4X	C30-C31-C32-C33
15	9	101	PGV	C24-C25-C26-C27
15	F	101	PGV	C22-C23-C24-C25
15	9	101	PGV	C28-C29-C30-C31
15	F	101	PGV	C03-O11-P-O14
15	I	103	PGV	C03-O11-P-O12
15	O	102	PGV	C19-C20-C21-C22
24	R	101	LMT	C9-C10-C11-C12
16	W	102	BCL	C13-C15-C16-C17
16	7	102	BCL	C5-C6-C7-C8
16	K	105	BCL	CBA-CGA-O2A-C1
15	K	101	PGV	C2-C3-C4-C5
24	E	102	LMT	C2-C3-C4-C5
11	C	401	HEM	C2A-CAA-CBA-CGA
16	T	101	BCL	C8-C10-C11-C12
15	F	101	PGV	O04-C19-O03-C01
11	C	402	HEM	C2B-C3B-CAB-CBB
16	M	403	BCL	CAD-CBD-CGD-O2D
16	S	103	BCL	CAD-CBD-CGD-O2D
16	3	103	BCL	CAD-CBD-CGD-O2D
15	H	301	PGV	C22-C23-C24-C25
24	B	102	LMT	C2-C3-C4-C5
14	C	407	DGA	CA6-CA7-CA8-CA9
24	2	103	LMT	C5-C6-C7-C8
15	Q	101	PGV	O03-C01-C02-C03
15	5	101	PGV	O03-C01-C02-C03
16	Q	103	BCL	C3-C5-C6-C7
15	L	305	PGV	C2-C3-C4-C5
16	M	403	BCL	CHA-CBD-CGD-O2D
16	Y	102	BCL	C8-C10-C11-C12
16	F	105	BCL	O1A-CGA-O2A-C1
16	5	104	BCL	O1A-CGA-O2A-C1
24	P	102	LMT	C1-C2-C3-C4
16	9	103	BCL	C15-C16-C17-C18
19	L	307	8K6	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
15	M	406	PGV	O03-C01-C02-O01
15	H	301	PGV	O03-C01-C02-O01
15	A	101	PGV	O03-C01-C02-O01
15	O	102	PGV	O03-C01-C02-O01
15	F	101	PGV	C20-C21-C22-C23
16	D	103	BCL	C13-C15-C16-C17
24	4	102	LMT	C11-C10-C9-C8
24	8	101	LMT	C4B-C5B-C6B-O6B
24	P	102	LMT	C2B-C1B-O1B-C4'
15	H	301	PGV	O02-C1-O01-C02
16	T	101	BCL	C11-C12-C13-C14
16	1	102	BCL	C11-C10-C8-C9
16	3	103	BCL	C11-C10-C8-C9
16	3	104	BCL	C11-C12-C13-C14
16	L	301	BCL	C2A-CAA-CBA-CGA
16	U	103	BCL	CAA-CBA-CGA-O2A
23	O	106	H4X	C24-C23-C25-C26
16	O	105	BCL	C10-C11-C12-C13
23	4	101	H4X	C27-C28-C30-C31
15	K	106	PGV	C27-C28-C29-C30
15	O	102	PGV	C5-C6-C7-C8
16	Q	103	BCL	C1A-C2A-CAA-CBA
16	L	304	BCL	C16-C17-C18-C20
16	I	102	BCL	C16-C17-C18-C19
16	5	104	BCL	C16-C17-C18-C19
16	3	104	BCL	C8-C10-C11-C12
16	B	103	BCL	C2-C1-O2A-CGA
16	U	103	BCL	C2-C1-O2A-CGA
15	F	101	PGV	C20-C19-O03-C01
16	O	105	BCL	CBA-CGA-O2A-C1
22	H	302	CDL	CB2-OB2-PB2-OB5
22	Y	103	CDL	CB2-OB2-PB2-OB5
15	5	101	PGV	C21-C22-C23-C24
24	Z	102	LMT	C5-C6-C7-C8
16	X	101	BCL	CAA-CBA-CGA-O2A
22	Y	103	CDL	CB4-CB3-OB5-PB2
15	M	406	PGV	C03-O11-P-O14
15	F	104	PGV	C03-O11-P-O13
15	O	102	PGV	C03-O11-P-O14
15	Q	101	PGV	C04-O12-P-O13
15	5	101	PGV	C03-O11-P-O14
22	S	101	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
16	5	104	BCL	C16-C17-C18-C20
16	M	403	BCL	CBD-CGD-O2D-CED
15	M	406	PGV	C01-C02-C03-O11
15	5	101	PGV	C01-C02-C03-O11
16	D	104	BCL	CAA-CBA-CGA-O2A
16	F	103	BCL	C5-C6-C7-C8
15	5	101	PGV	C14-C15-C16-C17
16	Y	102	BCL	C16-C17-C18-C20
16	O	105	BCL	CAA-CBA-CGA-O2A
16	T	101	BCL	CAA-CBA-CGA-O2A
16	5	103	BCL	C10-C11-C12-C13
16	K	105	BCL	O1A-CGA-O2A-C1
24	8	102	LMT	C2-C3-C4-C5
16	9	104	BCL	C5-C6-C7-C8
24	P	102	LMT	C7-C8-C9-C10
24	J	102	LMT	C5-C6-C7-C8
15	H	301	PGV	O01-C02-C03-O11
15	5	101	PGV	O01-C02-C03-O11
16	K	105	BCL	C3A-C2A-CAA-CBA
16	U	102	BCL	C6-C7-C8-C10
16	7	102	BCL	C6-C7-C8-C10
17	L	302	BPH	C12-C13-C15-C16
22	H	302	CDL	OB5-CB3-CB4-OB6
24	R	101	LMT	C7-C8-C9-C10
16	B	103	BCL	CAA-CBA-CGA-O2A
24	B	102	LMT	C9-C10-C11-C12
16	Y	104	BCL	C8-C10-C11-C12
15	F	104	PGV	C2-C3-C4-C5
16	M	403	BCL	C16-C17-C18-C19
15	H	301	PGV	O01-C1-C2-C3
16	5	104	BCL	CAA-CBA-CGA-O2A
16	7	103	BCL	CAA-CBA-CGA-O2A
15	3	101	PGV	C30-C31-C32-C33
23	O	101	H4X	C36-C37-C38-O2
15	3	101	PGV	C21-C22-C23-C24
16	J	101	BCL	CAA-CBA-CGA-O2A
16	3	104	BCL	CAA-CBA-CGA-O2A
16	L	301	BCL	O1D-CGD-O2D-CED
16	O	105	BCL	O1A-CGA-O2A-C1
16	K	108	BCL	CAA-CBA-CGA-O2A
16	2	102	BCL	CAA-CBA-CGA-O2A
16	9	104	BCL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	B	103	BCL	C11-C12-C13-C14
16	K	105	BCL	C6-C7-C8-C9
16	K	105	BCL	C11-C10-C8-C9
16	K	105	BCL	C14-C13-C15-C16
16	3	103	BCL	C11-C12-C13-C14
16	9	103	BCL	C6-C7-C8-C9
19	5	106	8K6	C5-C6-C7-C8
24	X	102	LMT	O1'-C1-C2-C3
16	Y	104	BCL	CAA-CBA-CGA-O2A
15	K	101	PGV	C5-C6-C7-C8
24	0	101	LMT	C9-C10-C11-C12
16	Q	104	BCL	CAA-CBA-CGA-O2A
16	T	101	BCL	O1A-CGA-O2A-C1
16	F	105	BCL	CAA-CBA-CGA-O2A
15	5	101	PGV	C03-C02-O01-C1
15	Q	101	PGV	C01-C02-C03-O11
15	I	103	PGV	C2-C3-C4-C5
16	F	103	BCL	C2-C1-O2A-CGA
16	F	105	BCL	C2-C1-O2A-CGA
16	O	105	BCL	C2-C1-O2A-CGA
16	Q	104	BCL	C2-C1-O2A-CGA
16	W	102	BCL	C2-C1-O2A-CGA
16	X	101	BCL	C2-C1-O2A-CGA
16	Y	104	BCL	C2-C1-O2A-CGA
16	5	103	BCL	C2-C1-O2A-CGA
16	5	104	BCL	C2-C1-O2A-CGA
16	9	103	BCL	C2-C1-O2A-CGA
15	F	104	PGV	C19-C20-C21-C22
17	M	404	BPH	O1A-CGA-O2A-C1
16	3	104	BCL	C3-C5-C6-C7
14	C	407	DGA	CB4-CB5-CB6-CB7
15	5	101	PGV	C15-C16-C17-C18
16	3	103	BCL	C10-C11-C12-C13
15	K	106	PGV	O01-C02-C03-O11
24	B	102	LMT	C6-C7-C8-C9
16	5	104	BCL	CBA-CGA-O2A-C1
22	H	302	CDL	C19-C20-C21-C22
16	5	103	BCL	C16-C17-C18-C19
23	E	101	H4X	C2-C1-O1-C1M
23	K	103	H4X	C39-C38-O2-C2M
23	O	106	H4X	C3-C1-O1-C1M
23	V	101	H4X	C3-C1-O1-C1M

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Mol	Chain	Res	Type	Atoms
23	2	101	H4X	C3-C1-O1-C1M
23	7	104	H4X	C2-C1-O1-C1M
24	B	104	LMT	C5-C6-C7-C8
24	J	102	LMT	C3-C4-C5-C6
15	L	305	PGV	C04-O12-P-O11
15	A	101	PGV	C04-O12-P-O11
15	D	101	PGV	C03-O11-P-O12
15	F	104	PGV	C04-O12-P-O11
15	K	101	PGV	C03-O11-P-O12
15	K	101	PGV	C04-O12-P-O11
15	K	102	PGV	C04-O12-P-O11
15	3	101	PGV	C03-O11-P-O12
22	S	101	CDL	CA3-OA5-PA1-OA2
22	S	101	CDL	CB3-OB5-PB2-OB2
22	Y	103	CDL	CA2-OA2-PA1-OA5
22	Y	103	CDL	CA3-OA5-PA1-OA2
15	5	101	PGV	C19-C20-C21-C22
16	A	102	BCL	C15-C16-C17-C18
19	L	307	8K6	C9-C10-C11-C12
16	I	102	BCL	O1D-CGD-O2D-CED
15	C	408	PGV	C2-C3-C4-C5
15	F	101	PGV	C21-C22-C23-C24
16	5	104	BCL	C11-C12-C13-C15
16	Q	103	BCL	C6-C7-C8-C9
23	O	101	H4X	C20-C21-C22-C23
16	Y	104	BCL	C16-C17-C18-C20
16	2	102	BCL	C16-C17-C18-C19
15	A	101	PGV	C1-C2-C3-C4
16	K	108	BCL	C16-C17-C18-C19
16	T	101	BCL	C10-C11-C12-C13
16	3	103	BCL	C13-C15-C16-C17
23	P	101	H4X	C15-C16-C17-C19
15	D	101	PGV	C2-C3-C4-C5
24	X	102	LMT	C7-C8-C9-C10
16	7	103	BCL	C8-C10-C11-C12
16	5	103	BCL	C4-C3-C5-C6
15	Y	105	PGV	C1-C2-C3-C4
16	3	104	BCL	C16-C17-C18-C20
17	M	404	BPH	CBA-CGA-O2A-C1
15	1	103	PGV	C4-C5-C6-C7
15	I	103	PGV	C11-C10-C9-C8
16	L	301	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	D	101	PGV	C27-C28-C29-C30
15	L	305	PGV	C23-C24-C25-C26
16	A	102	BCL	C10-C11-C12-C13
16	K	105	BCL	C8-C10-C11-C12
15	D	101	PGV	C4-C5-C6-C7
16	K	108	BCL	C16-C17-C18-C20
16	O	104	BCL	C16-C17-C18-C19
11	C	402	HEM	CAD-CBD-CGD-O1D
11	C	404	HEM	CAD-CBD-CGD-O1D
16	5	104	BCL	C8-C10-C11-C12
23	4	101	H4X	C11-C10-C9-C7
22	S	101	CDL	C79-C80-C81-C82
16	M	403	BCL	O1D-CGD-O2D-CED
15	Y	105	PGV	C22-C23-C24-C25
16	2	102	BCL	C8-C10-C11-C12
15	D	101	PGV	C7-C8-C9-C10
15	F	104	PGV	C6-C7-C8-C9
16	U	102	BCL	C13-C15-C16-C17
16	T	101	BCL	C2-C1-O2A-CGA
24	8	102	LMT	C7-C8-C9-C10
24	X	102	LMT	C9-C10-C11-C12
15	I	103	PGV	O03-C01-C02-O01
15	I	103	PGV	C02-C03-O11-P
24	Z	102	LMT	C7-C8-C9-C10
24	8	102	LMT	O1'-C1-C2-C3
24	B	102	LMT	C2-C1-O1'-C1'
16	7	102	BCL	C4-C3-C5-C6
15	5	101	PGV	C13-C14-C15-C16
22	S	101	CDL	C12-C13-C14-C15
16	J	101	BCL	C11-C12-C13-C14
16	O	105	BCL	C11-C10-C8-C9
16	5	103	BCL	C11-C10-C8-C9
11	C	401	HEM	CAA-CBA-CGA-O1A
11	C	401	HEM	CAA-CBA-CGA-O2A
24	N	101	LMT	C5-C6-C7-C8
15	D	101	PGV	C23-C24-C25-C26
24	B	104	LMT	C3-C4-C5-C6
19	L	307	8K6	C6-C7-C8-C9
15	A	101	PGV	O12-C04-C05-O05
23	Q	105	H4X	C15-C16-C17-C18
23	V	101	H4X	C24-C23-C25-C26
23	Z	101	H4X	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	4	101	H4X	C29-C28-C30-C31
23	Q	105	H4X	C10-C11-C12-C14
16	K	105	BCL	C1A-C2A-CAA-CBA
16	U	102	BCL	C1A-C2A-CAA-CBA
16	9	103	BCL	C1A-C2A-CAA-CBA
14	C	407	DGA	CB9-CAB-CBB-CCB
24	6	102	LMT	C2-C3-C4-C5
16	L	301	BCL	C12-C13-C15-C16
16	M	403	BCL	C11-C10-C8-C7
16	K	105	BCL	C12-C13-C15-C16
16	2	102	BCL	C11-C12-C13-C15
17	M	404	BPH	C11-C12-C13-C15
11	C	404	HEM	CAD-CBD-CGD-O2D
15	D	101	PGV	C20-C21-C22-C23
15	K	106	PGV	C28-C29-C30-C31
16	T	101	BCL	C2A-CAA-CBA-CGA
16	Q	104	BCL	C5-C6-C7-C8
15	F	104	PGV	C21-C22-C23-C24
24	G	102	LMT	C3-C4-C5-C6
11	C	402	HEM	CAD-CBD-CGD-O2D
16	Q	103	BCL	C4-C3-C5-C6
16	5	103	BCL	C13-C15-C16-C17
16	U	102	BCL	C16-C17-C18-C20
22	S	101	CDL	C14-C15-C16-C17
14	C	407	DGA	OG1-CG1-CG2-OG2
11	C	403	HEM	CAA-CBA-CGA-O2A
22	H	302	CDL	C74-C75-C76-C77
23	E	101	H4X	C17-C19-C20-C21
23	Q	105	H4X	C11-C10-C9-C7
24	B	104	LMT	C4-C5-C6-C7
16	7	103	BCL	C5-C6-C7-C8
15	K	101	PGV	O04-C19-O03-C01
16	9	103	BCL	C3-C5-C6-C7
16	3	103	BCL	C4-C3-C5-C6
16	7	103	BCL	C2-C1-O2A-CGA
16	S	103	BCL	C15-C16-C17-C18
11	C	403	HEM	CAA-CBA-CGA-O1A
17	M	404	BPH	C6-C7-C8-C9
24	B	102	LMT	O1'-C1-C2-C3
16	X	101	BCL	C2A-CAA-CBA-CGA
23	U	104	H4X	C30-C31-C32-C33
23	K	107	H4X	C15-C16-C17-C19

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Mol	Chain	Res	Type	Atoms
23	6	101	H4X	C15-C16-C17-C19
16	J	101	BCL	C16-C17-C18-C20
17	L	302	BPH	C15-C16-C17-C18
22	H	302	CDL	C71-C72-C73-C74
15	3	101	PGV	C23-C24-C25-C26
24	8	102	LMT	C1-C2-C3-C4
16	U	103	BCL	C5-C6-C7-C8
15	Q	101	PGV	C7-C8-C9-C10
15	9	101	PGV	C19-C20-C21-C22
23	O	106	H4X	C34-C33-C35-C36
23	2	101	H4X	C4-C1-O1-C1M
16	L	304	BCL	C6-C7-C8-C10
15	9	101	PGV	O05-C05-C06-O06
15	1	103	PGV	C21-C22-C23-C24
22	S	101	CDL	OB6-CB4-CB6-OB8
22	H	302	CDL	CA5-C11-C12-C13
16	X	101	BCL	C16-C17-C18-C20
15	C	408	PGV	C3-C4-C5-C6
15	K	106	PGV	C03-O11-P-O14
15	F	101	PGV	O03-C19-C20-C21
15	3	101	PGV	O01-C1-C2-C3
23	Z	101	H4X	C5-C6-C7-C8
15	1	103	PGV	O02-C1-O01-C02
15	I	103	PGV	O03-C19-C20-C21
16	K	108	BCL	C14-C13-C15-C16
16	Y	104	BCL	C14-C13-C15-C16
24	B	102	LMT	C11-C10-C9-C8
22	S	101	CDL	C83-C84-C85-C86
16	I	102	BCL	C3A-C2A-CAA-CBA
15	D	101	PGV	O03-C19-C20-C21
16	L	301	BCL	CAD-CBD-CGD-O2D
16	M	402	BCL	CAD-CBD-CGD-O2D
16	K	108	BCL	C2A-CAA-CBA-CGA
16	2	102	BCL	C2A-CAA-CBA-CGA
16	5	104	BCL	C2A-CAA-CBA-CGA
15	K	101	PGV	C21-C22-C23-C24
15	F	104	PGV	C4-C5-C6-C7
16	D	103	BCL	C4-C3-C5-C6
16	W	102	BCL	C4-C3-C5-C6
16	Q	103	BCL	C2-C3-C5-C6
23	V	101	H4X	C15-C16-C17-C19
18	L	303	UQ8	C5-C4-O4-C4M

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Mol	Chain	Res	Type	Atoms
16	S	103	BCL	C10-C11-C12-C13
15	1	103	PGV	O01-C1-C2-C3
15	O	102	PGV	C31-C32-C33-C34
16	3	103	BCL	O2A-C1-C2-C3
17	M	404	BPH	O2A-C1-C2-C3
15	3	101	PGV	C26-C27-C28-C29
11	C	403	HEM	C4B-C3B-CAB-CBB
16	F	105	BCL	C2A-CAA-CBA-CGA
16	O	105	BCL	C2A-CAA-CBA-CGA
19	5	106	8K6	C9-C10-C11-C12
15	3	101	PGV	C9-C10-C11-C12
16	Q	104	BCL	C16-C17-C18-C20
15	3	101	PGV	C25-C26-C27-C28
23	2	101	H4X	C5-C6-C7-C8
16	Y	104	BCL	C5-C6-C7-C8
23	5	105	H4X	C39-C38-O2-C2M
15	K	106	PGV	C7-C8-C9-C10
16	O	105	BCL	C5-C6-C7-C8
15	3	101	PGV	C3-C4-C5-C6
22	S	101	CDL	C82-C83-C84-C85
24	P	102	LMT	O1'-C1-C2-C3
17	L	302	BPH	CHA-CBD-CGD-O1D
17	M	404	BPH	CHA-CBD-CGD-O1D
14	C	407	DGA	CA3-CA4-CA5-CA6
24	2	103	LMT	C11-C10-C9-C8
16	L	304	BCL	C11-C10-C8-C7
17	M	404	BPH	C12-C13-C15-C16
14	C	407	DGA	OG1-CA1-CA2-CA3
15	1	103	PGV	O03-C19-C20-C21
24	G	102	LMT	C4-C5-C6-C7
16	O	105	BCL	C11-C12-C13-C14
16	S	103	BCL	C14-C13-C15-C16
16	1	102	BCL	C14-C13-C15-C16
16	7	102	BCL	C6-C7-C8-C9
16	9	104	BCL	C11-C12-C13-C14
15	O	102	PGV	C23-C24-C25-C26
16	T	101	BCL	CBA-CGA-O2A-C1
24	V	102	LMT	C2-C3-C4-C5
18	L	306	UQ8	C16-C17-C18-C19
15	O	102	PGV	C3-C4-C5-C6
16	Y	102	BCL	C16-C17-C18-C19
24	G	102	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
24	4	102	LMT	C7-C8-C9-C10
11	C	404	HEM	CAA-CBA-CGA-O1A
15	F	101	PGV	O04-C19-C20-C21
23	Z	101	H4X	C10-C11-C12-C14
15	Q	101	PGV	C6-C7-C8-C9
16	M	403	BCL	C1A-C2A-CAA-CBA
16	I	102	BCL	C1A-C2A-CAA-CBA
16	1	102	BCL	C1A-C2A-CAA-CBA
22	S	101	CDL	C75-C76-C77-C78
16	3	104	BCL	C16-C17-C18-C19
14	C	407	DGA	OA1-CA1-CA2-CA3
15	D	101	PGV	O04-C19-C20-C21
15	3	101	PGV	O02-C1-C2-C3
15	F	104	PGV	C02-C01-O03-C19
15	A	101	PGV	O03-C01-C02-C03
16	B	103	BCL	C2A-CAA-CBA-CGA
16	D	104	BCL	C2A-CAA-CBA-CGA
16	U	103	BCL	C2A-CAA-CBA-CGA
16	3	104	BCL	C2A-CAA-CBA-CGA
15	I	103	PGV	C12-C13-C14-C15
16	D	104	BCL	C16-C17-C18-C20
15	I	103	PGV	O04-C19-C20-C21
15	1	103	PGV	O04-C19-C20-C21
15	K	101	PGV	C25-C26-C27-C28
16	D	104	BCL	C4-C3-C5-C6
15	M	406	PGV	C02-C03-O11-P
15	H	301	PGV	C03-O11-P-O13
15	D	101	PGV	C03-O11-P-O13
15	K	101	PGV	C04-O12-P-O13
15	K	102	PGV	C04-O12-P-O13
15	3	101	PGV	C03-O11-P-O13
15	3	101	PGV	C04-O12-P-O13
15	5	101	PGV	C04-O12-P-O14
15	H	301	PGV	C01-C02-C03-O11
16	O	105	BCL	C8-C10-C11-C12
15	1	103	PGV	O02-C1-C2-C3
16	U	102	BCL	O1A-CGA-O2A-C1
24	0	101	LMT	C1-C2-C3-C4
24	T	102	LMT	C4-C5-C6-C7
18	L	303	UQ8	C12-C11-C9-C10
23	7	104	H4X	C5-C6-C7-C8
11	C	401	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	Y	103	CDL	O1-C1-CB2-OB2
24	N	101	LMT	O1'-C1-C2-C3
16	U	102	BCL	O1D-CGD-O2D-CED
11	C	402	HEM	CAA-CBA-CGA-O1A
22	S	101	CDL	C12-C11-CA5-OA7
16	M	403	BCL	C8-C10-C11-C12
15	9	101	PGV	C7-C8-C9-C10
24	G	102	LMT	C9-C10-C11-C12
16	5	103	BCL	C16-C17-C18-C20
16	J	101	BCL	C4-C3-C5-C6
16	X	101	BCL	C4-C3-C5-C6
16	5	104	BCL	C4-C3-C5-C6
23	G	101	H4X	C5-C6-C7-C8
16	U	103	BCL	C8-C10-C11-C12
16	F	103	BCL	C2C-C3C-CAC-CBC
16	I	102	BCL	C6-C7-C8-C10
16	K	108	BCL	C2C-C3C-CAC-CBC
16	O	104	BCL	C12-C13-C15-C16
16	O	105	BCL	C11-C10-C8-C7
16	Q	104	BCL	C11-C12-C13-C15
16	5	103	BCL	C2-C3-C5-C6
16	5	104	BCL	C2C-C3C-CAC-CBC
22	S	101	CDL	C12-C11-CA5-OA6
15	C	408	PGV	C1-C2-C3-C4
15	5	101	PGV	C1-C2-C3-C4
23	O	106	H4X	C22-C23-C25-C26
23	Q	105	H4X	C15-C16-C17-C19
11	C	401	HEM	CAD-CBD-CGD-O2D
23	Z	101	H4X	C30-C31-C32-C33
15	K	106	PGV	C22-C23-C24-C25
16	T	101	BCL	C16-C17-C18-C20
24	P	102	LMT	C2-C1-O1'-C1'
24	X	102	LMT	C2-C1-O1'-C1'
24	4	102	LMT	C2-C1-O1'-C1'
24	0	101	LMT	C2-C1-O1'-C1'

There are no ring outliers.

80 monomers are involved in 272 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	M	404	BPH	7	0
16	T	101	BCL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	O	106	H4X	1	0
16	K	108	BCL	4	0
24	X	102	LMT	2	0
16	Y	104	BCL	5	0
17	L	302	BPH	7	0
18	L	306	UQ8	8	0
24	T	102	LMT	2	0
24	R	101	LMT	2	0
16	1	102	BCL	6	0
24	B	102	LMT	1	0
16	3	104	BCL	6	0
15	5	101	PGV	4	0
15	3	101	PGV	4	0
11	C	402	HEM	5	0
16	A	102	BCL	9	0
16	B	103	BCL	4	0
24	8	101	LMT	2	0
16	L	301	BCL	2	0
23	E	101	H4X	1	0
11	C	403	HEM	10	0
16	U	103	BCL	3	0
15	Q	101	PGV	1	0
16	W	102	BCL	3	0
16	D	103	BCL	5	0
16	L	304	BCL	3	0
24	V	102	LMT	1	0
22	H	302	CDL	3	0
16	7	103	BCL	4	0
11	C	404	HEM	9	0
24	Z	102	LMT	1	0
16	9	104	BCL	3	0
16	F	103	BCL	6	0
24	6	102	LMT	2	0
16	I	102	BCL	4	0
16	5	104	BCL	3	0
14	C	407	DGA	6	0
16	9	103	BCL	6	0
23	K	103	H4X	1	0
15	9	101	PGV	2	0
24	G	102	LMT	1	0
16	7	102	BCL	5	0
16	K	105	BCL	7	0

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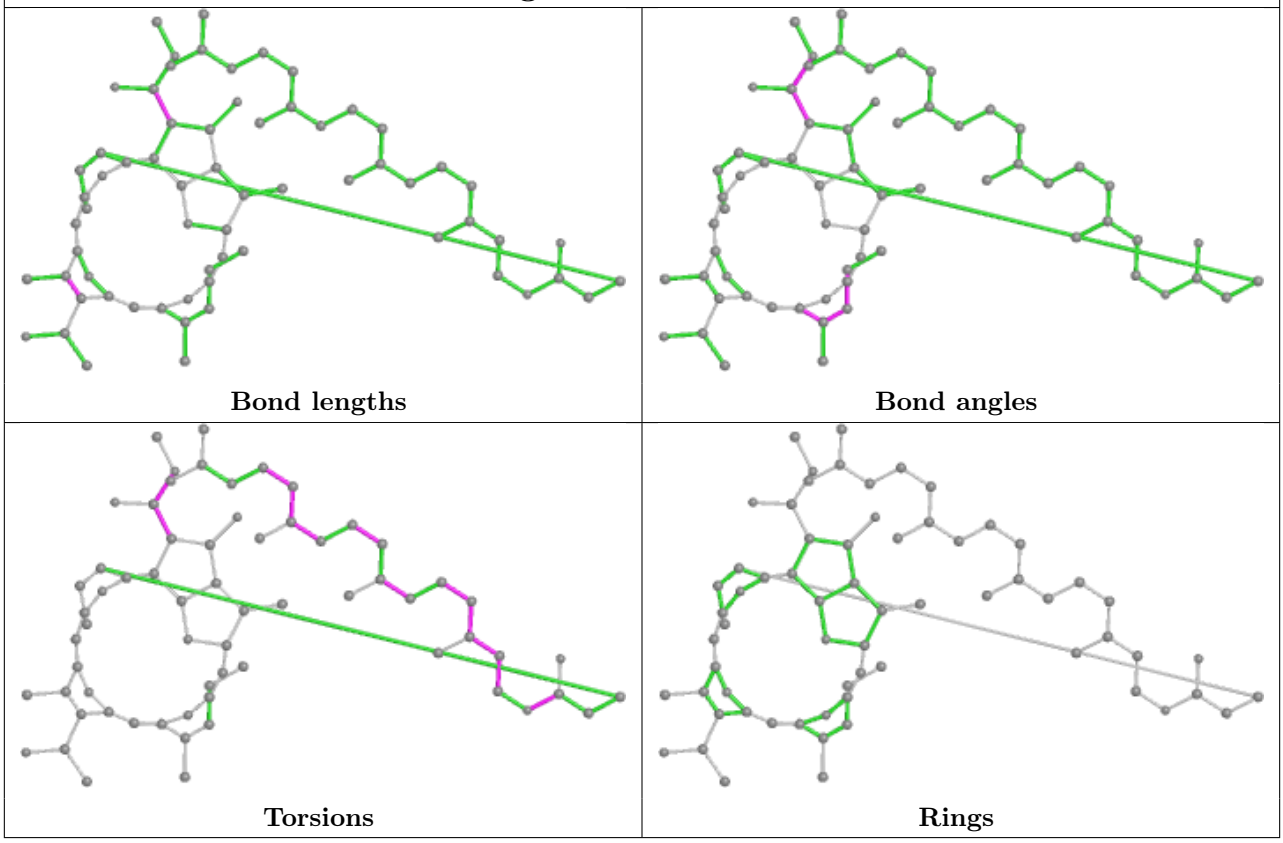
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Q	103	BCL	7	0
15	O	102	PGV	5	0
16	5	103	BCL	8	0
24	B	104	LMT	2	0
24	P	102	LMT	2	0
16	Q	104	BCL	5	0
16	O	105	BCL	4	0
24	4	102	LMT	3	0
16	U	102	BCL	6	0
22	S	101	CDL	1	0
24	0	101	LMT	1	0
16	3	103	BCL	8	0
11	C	401	HEM	6	0
24	N	101	LMT	3	0
15	F	104	PGV	2	0
21	M	405	MQ8	2	0
16	D	104	BCL	3	0
15	M	406	PGV	1	0
15	H	301	PGV	1	0
16	S	103	BCL	6	0
16	F	105	BCL	4	0
16	M	402	BCL	2	0
16	J	101	BCL	4	0
24	2	103	LMT	2	0
24	8	102	LMT	3	0
16	M	403	BCL	5	0
16	Y	102	BCL	3	0
19	L	307	8K6	1	0
15	L	305	PGV	3	0
16	X	101	BCL	4	0
24	E	102	LMT	2	0
24	J	102	LMT	2	0
15	Y	105	PGV	6	0
16	2	102	BCL	4	0
15	K	101	PGV	3	0
16	O	104	BCL	4	0

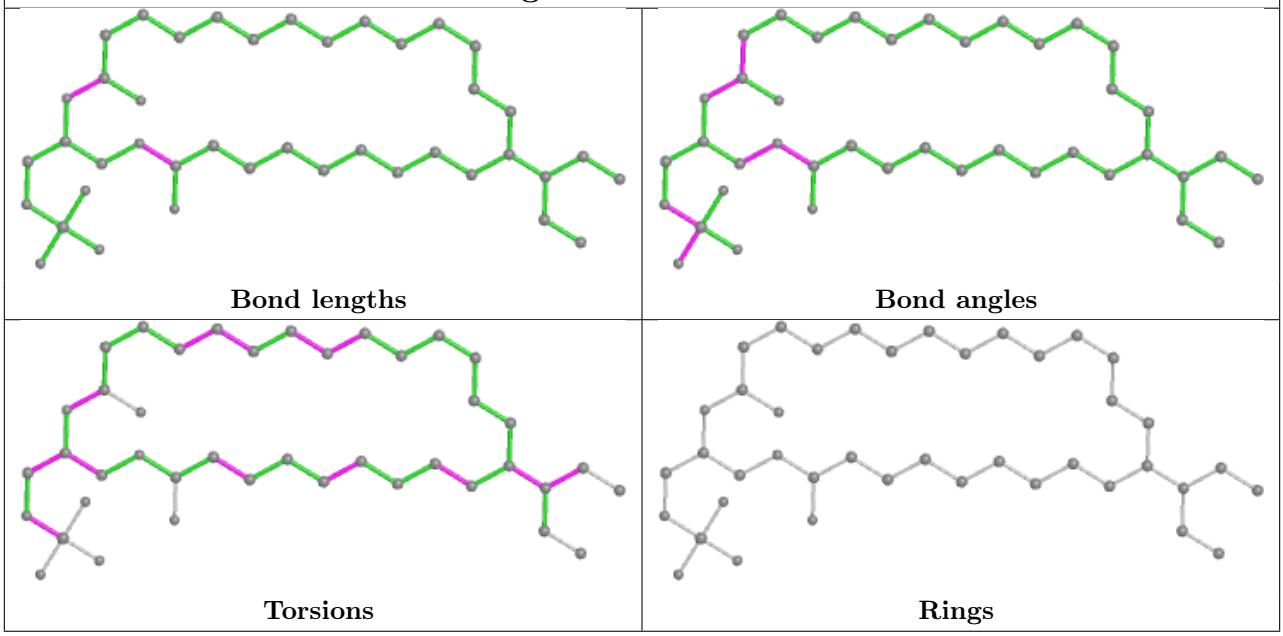
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

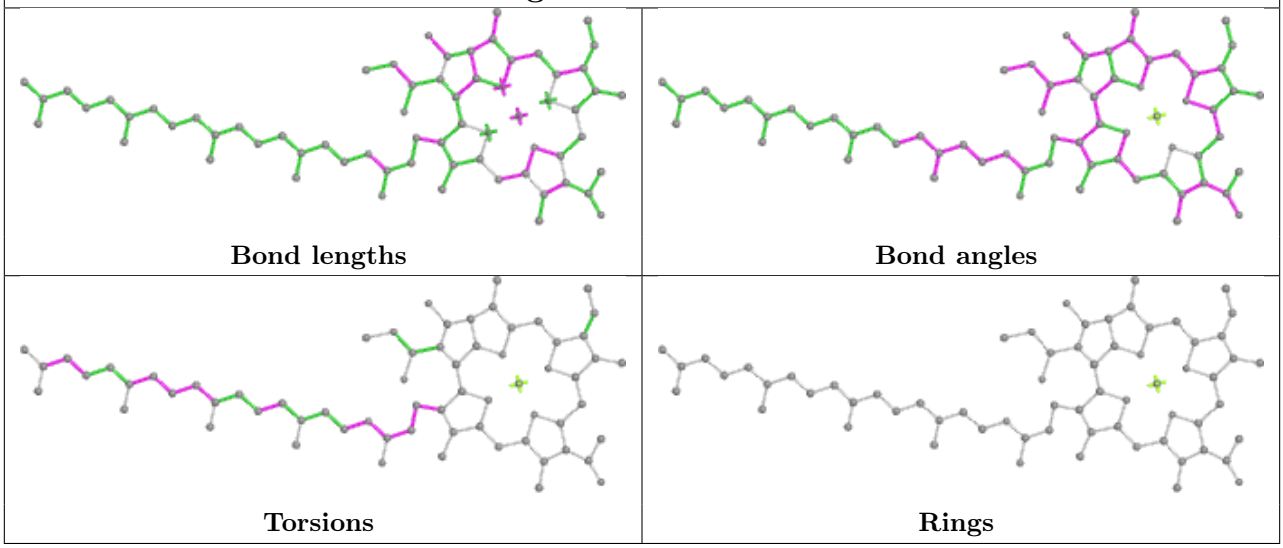
Ligand BPH M 404



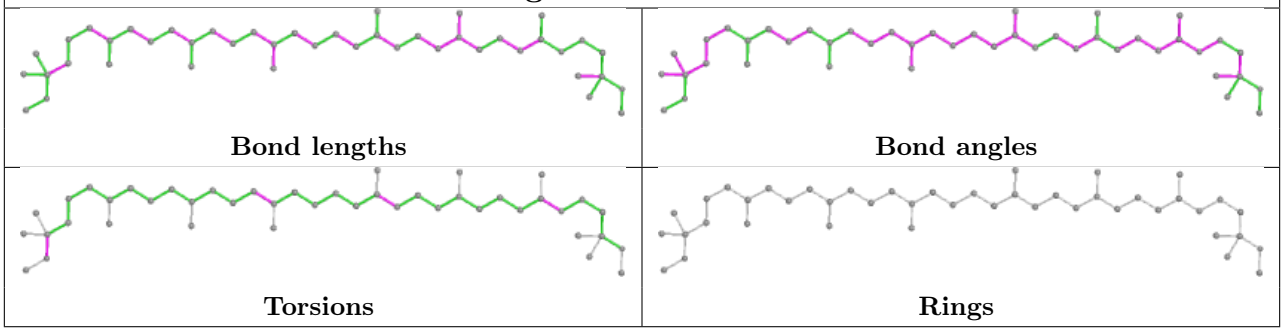
Ligand PGV K 106



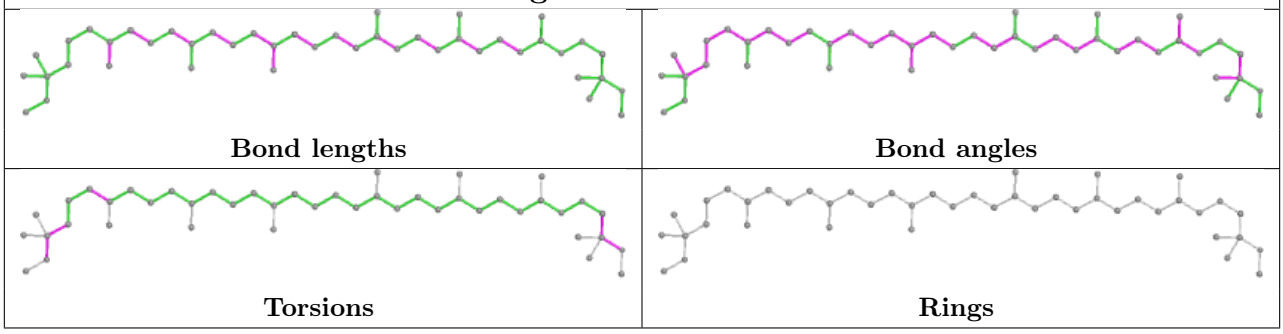
Ligand BCL T 101



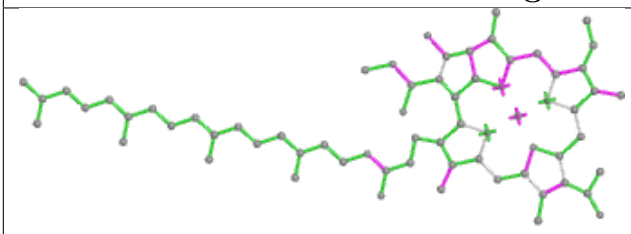
Ligand H4X O 106

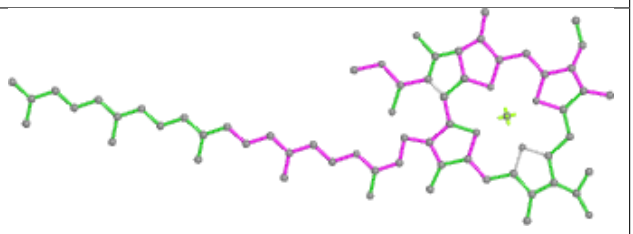


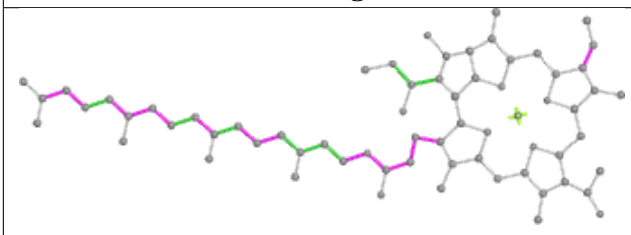
Ligand H4X 5 105

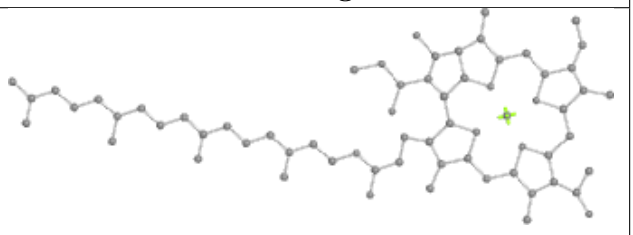


Ligand BCL K 108

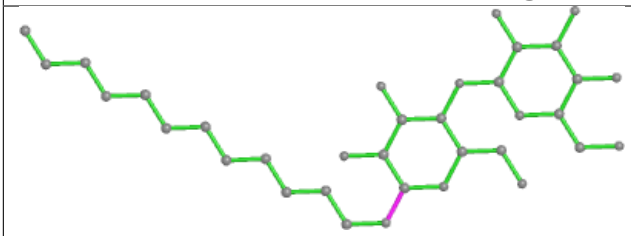

Bond lengths


Bond angles


Torsions


Rings

Ligand LMT X 102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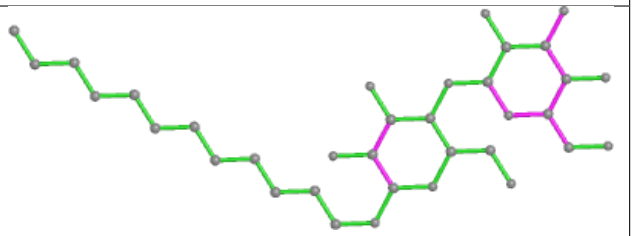
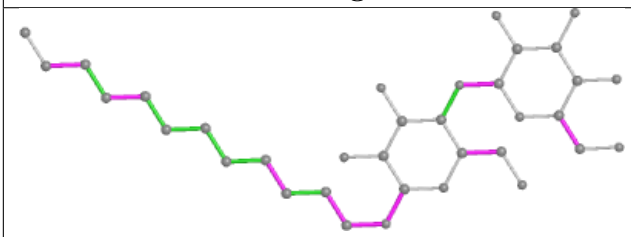
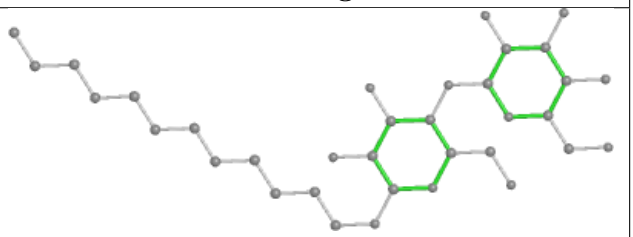
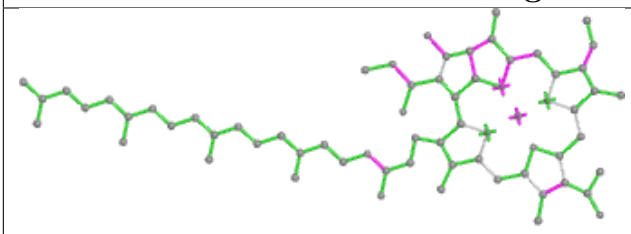
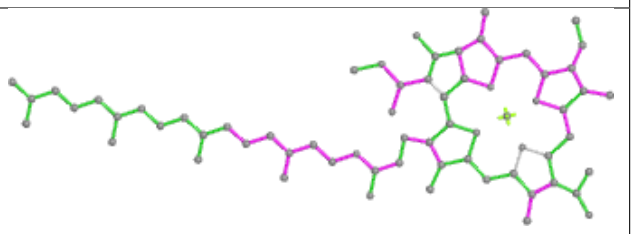

Bond angles

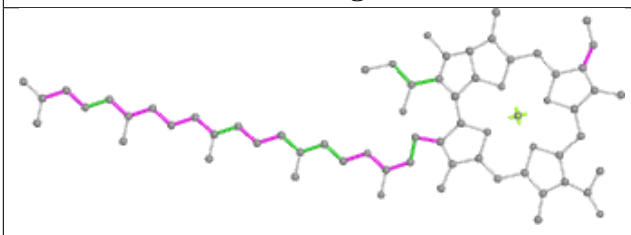

Torsions

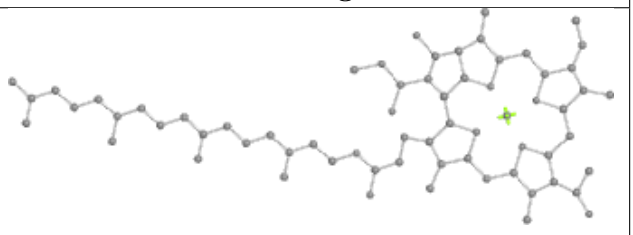

Rings

Ligand BCL Y 104

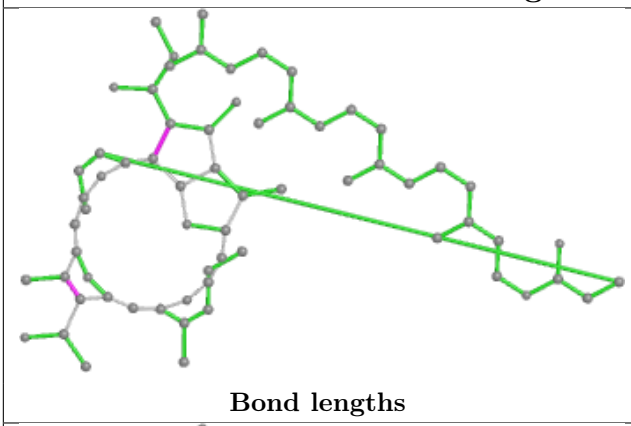

Bond lengths


Bond angles


Torsions


Rings

Ligand BPH L 302



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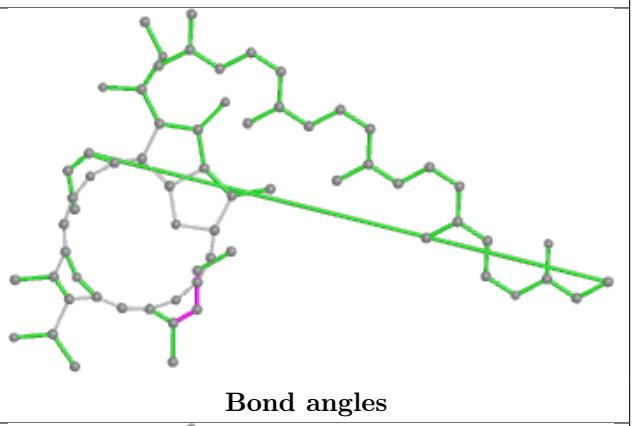
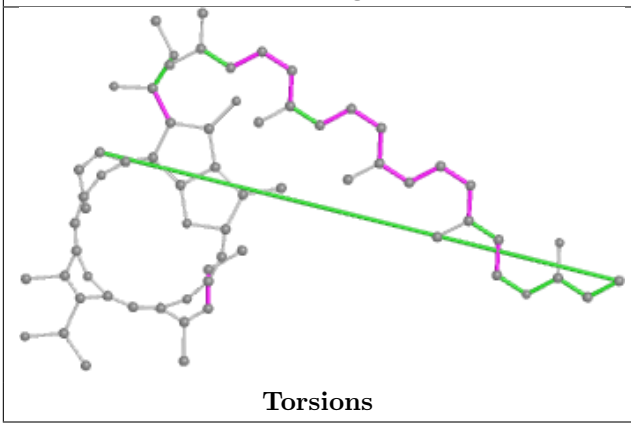
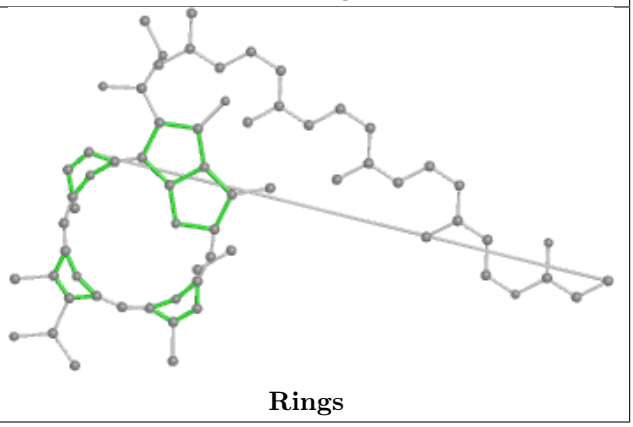


Bond angles

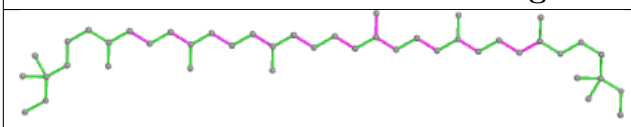


Torsions



Rings

Ligand H4X 7 104



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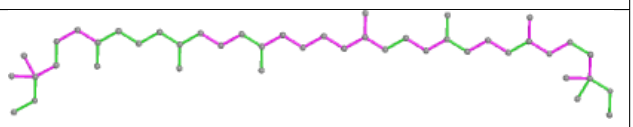
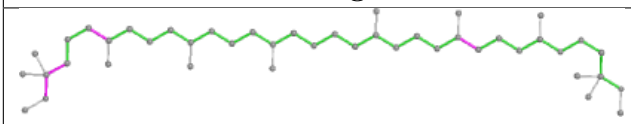


Bond angles



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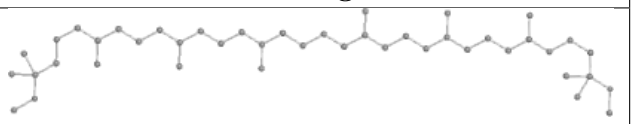
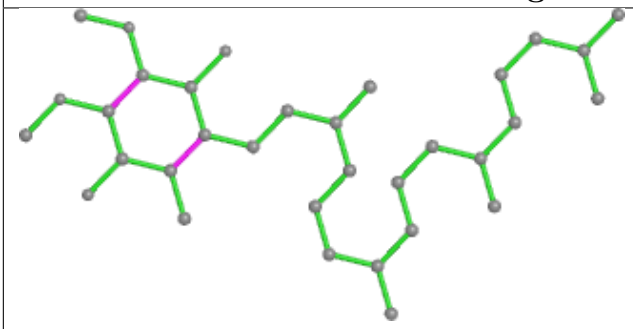


Rings

Ligand UQ8 L 306



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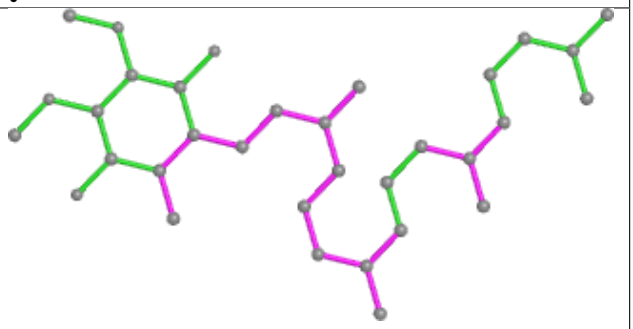
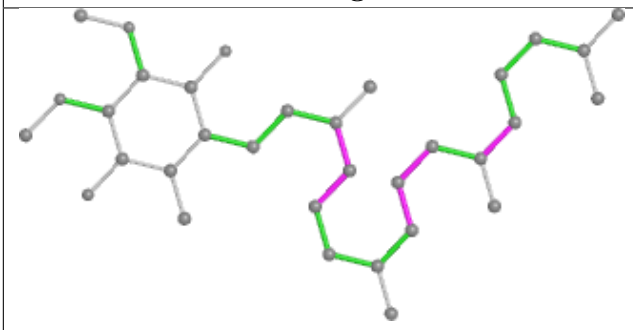


Bond angles



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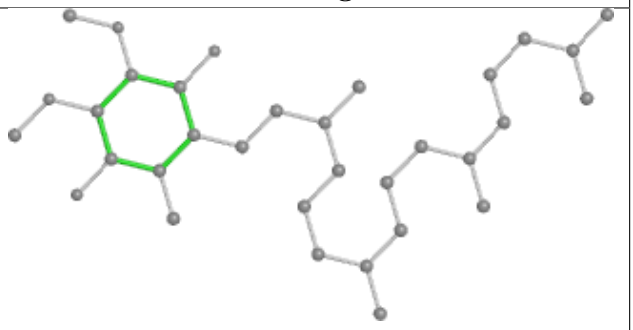
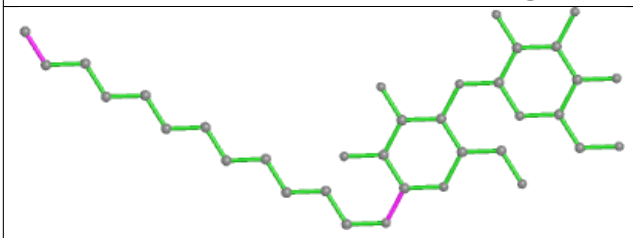


Rings

Ligand LMT T 102



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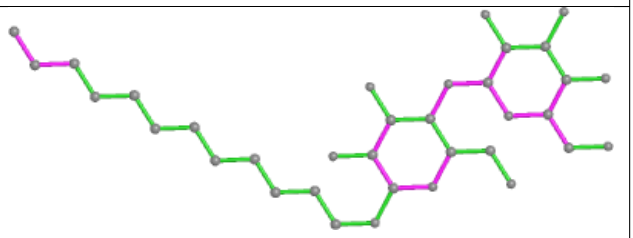
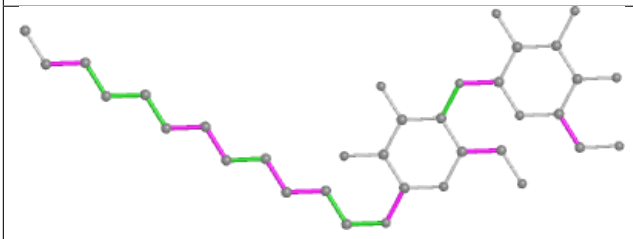


Bond angles



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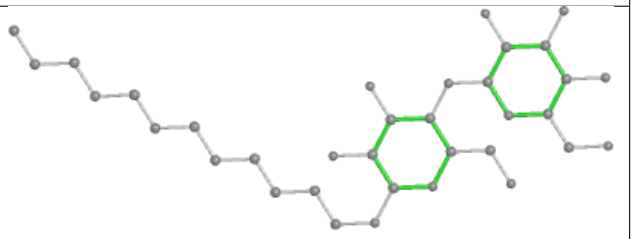
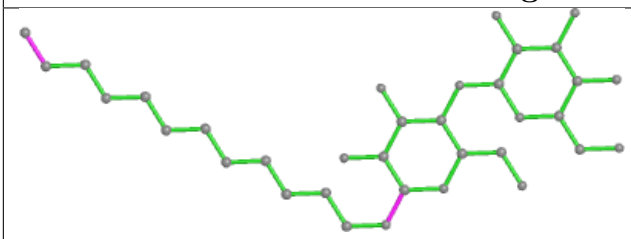


Rings

Ligand LMT R 101



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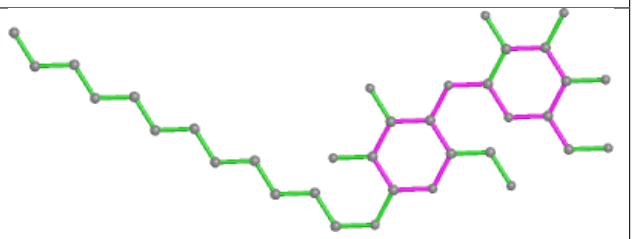
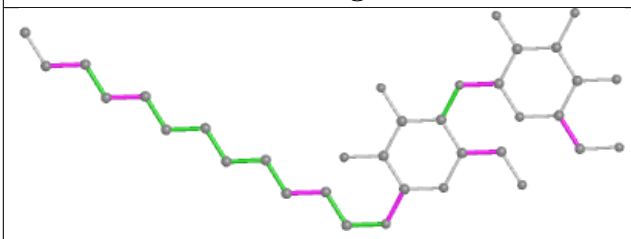


Bond angles



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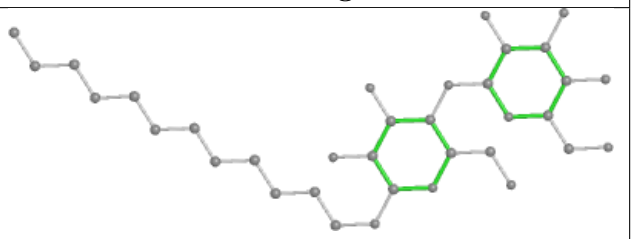
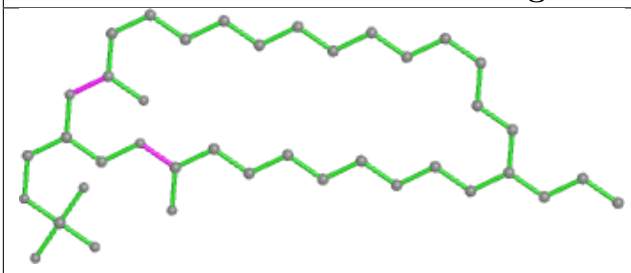


Rings

Ligand PGV I 103



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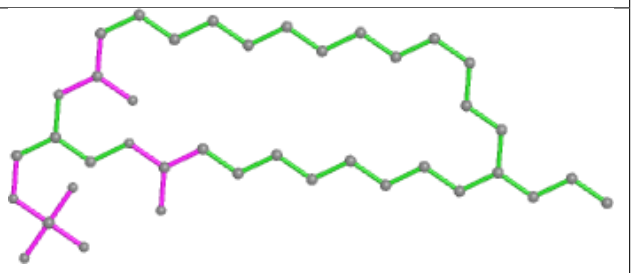
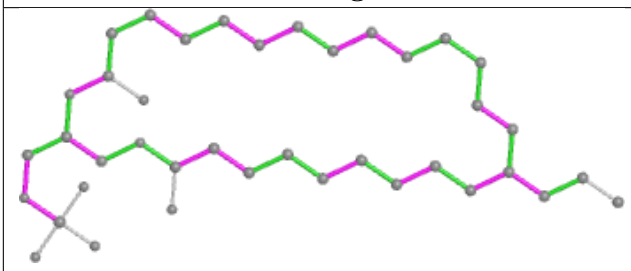
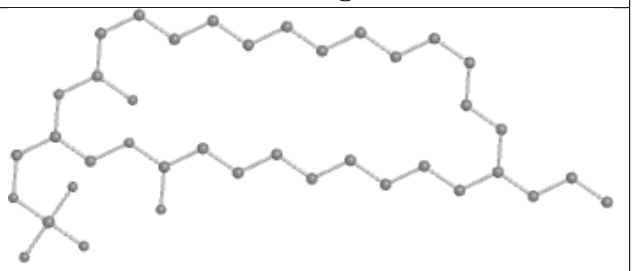


Bond angles

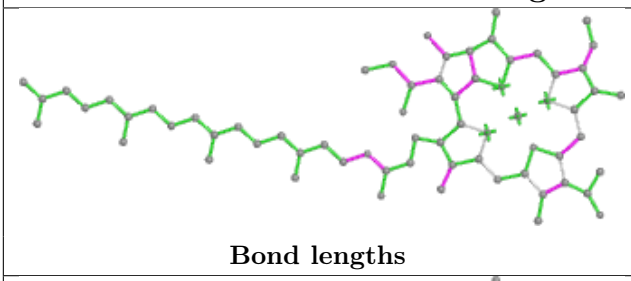


Torsions

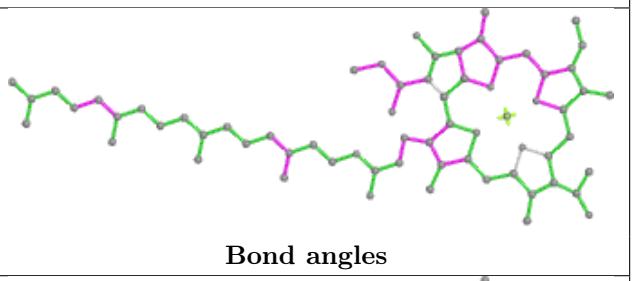


Rings

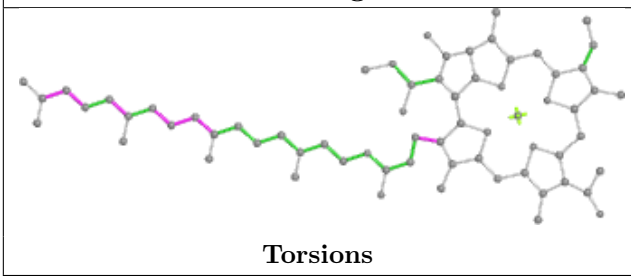
Ligand BCL 1 102



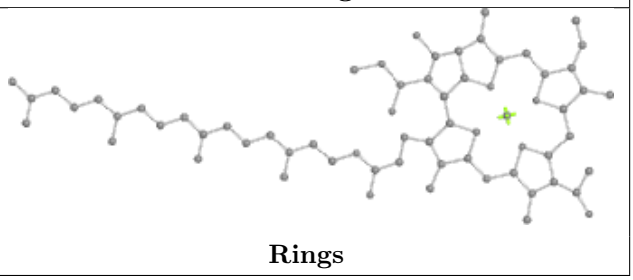
Bond lengths



Bond angles

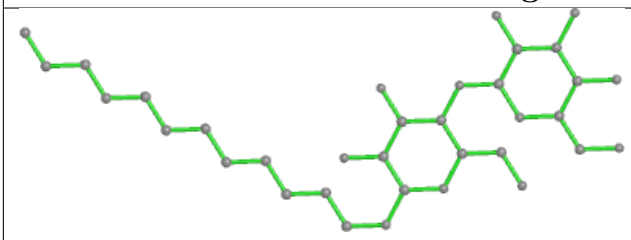


Torsions



Rings

Ligand LMT B 102



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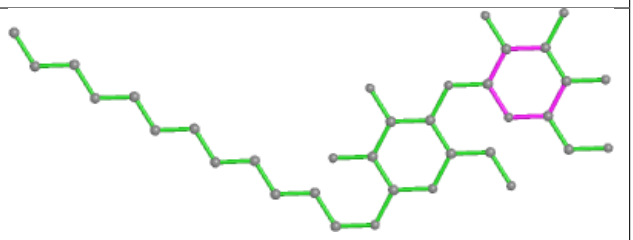
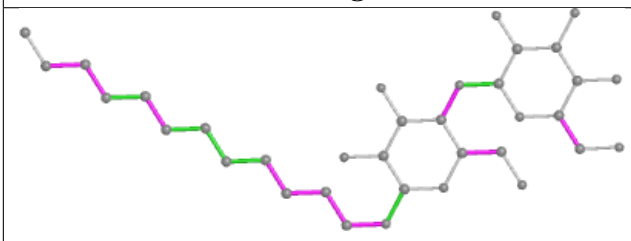


Bond angles



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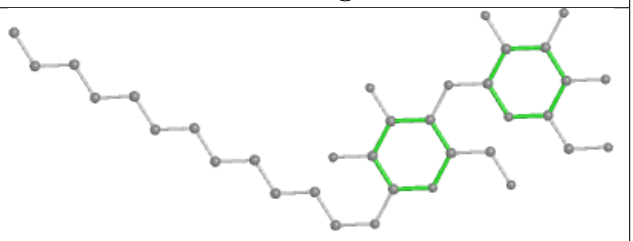
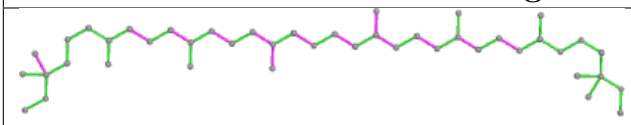


Rings

Ligand H4X V 101



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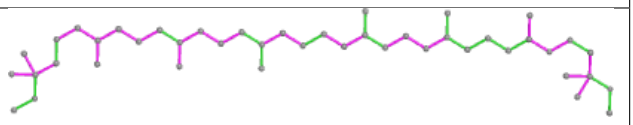
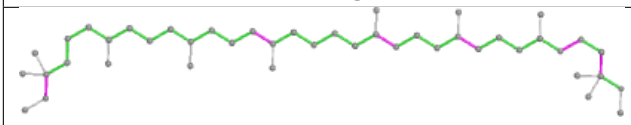
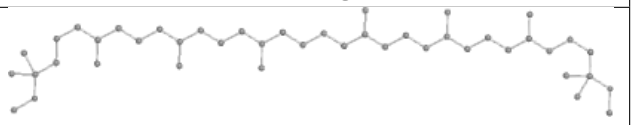


Bond angles

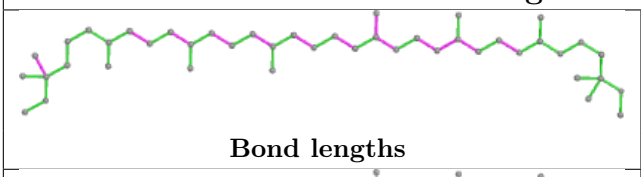


Torsions



Rings

Ligand H4X B 101



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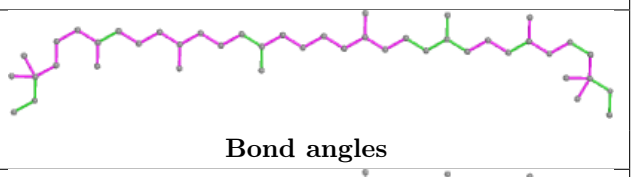
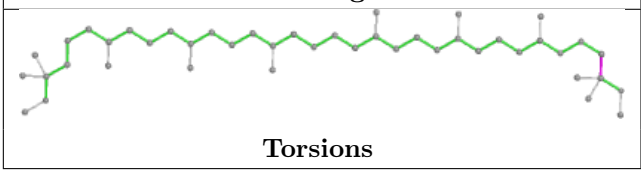
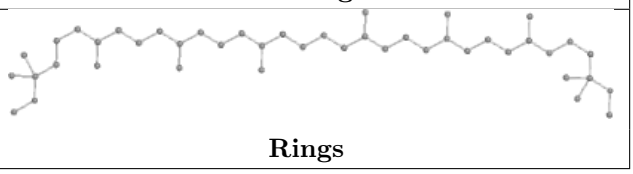


Bond angles

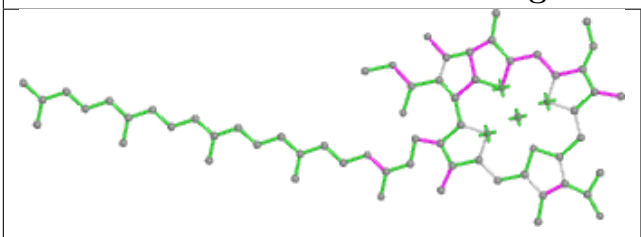


Torsions



Rings

Ligand BCL 3 104



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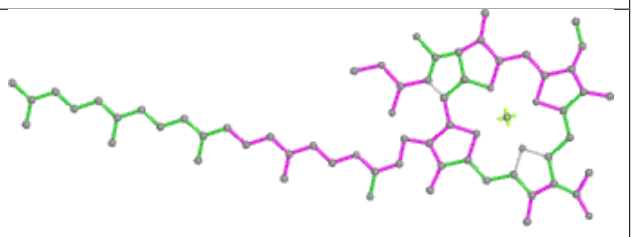
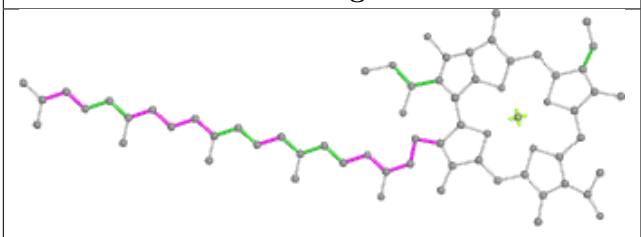
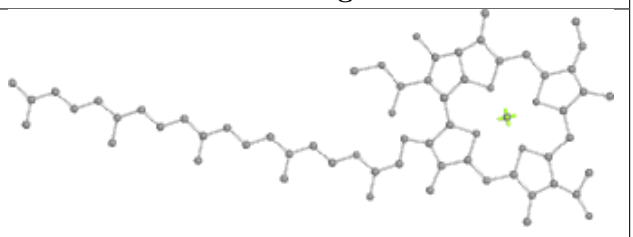


Bond angles

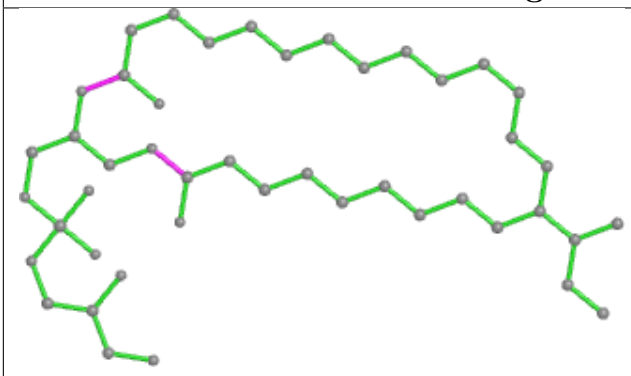


Torsions

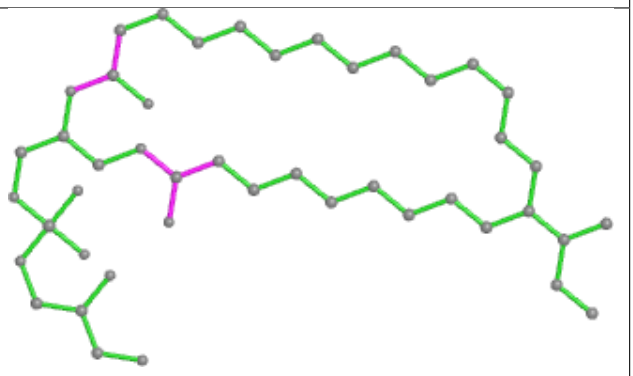


Rings

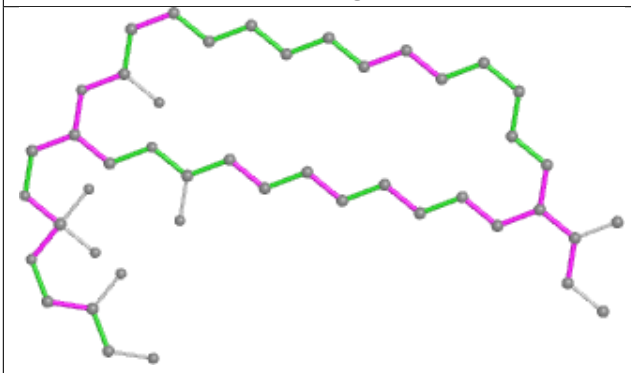
Ligand PGV 5 101



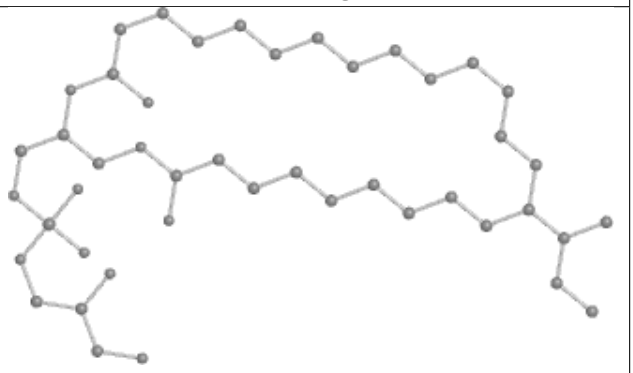
Bond lengths



Bond angles

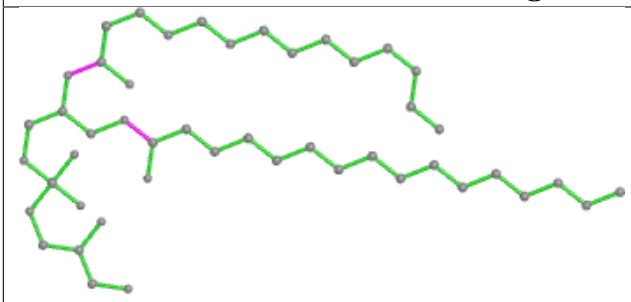


Torsions

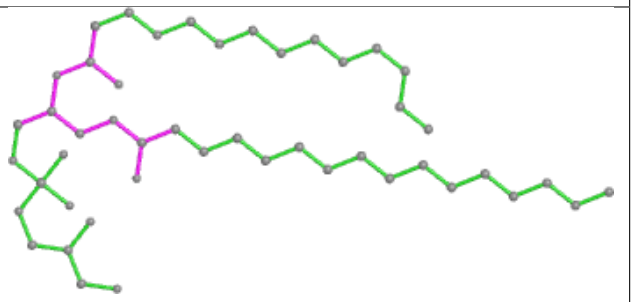


Rings

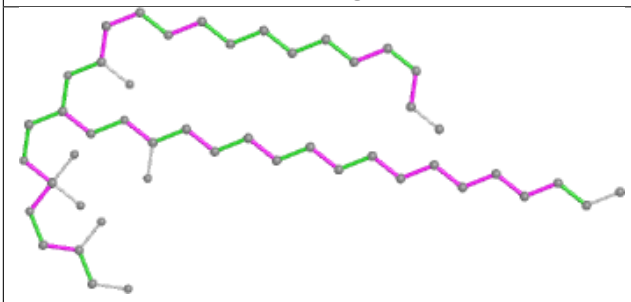
Ligand PGV 3 101



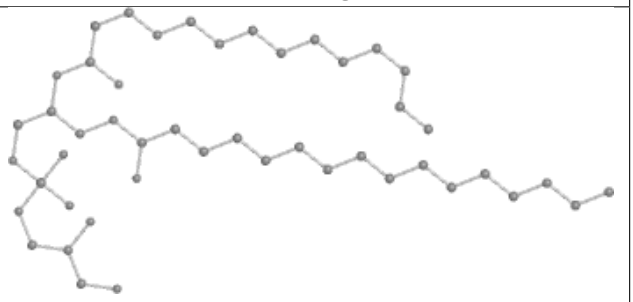
Bond lengths



Bond angles

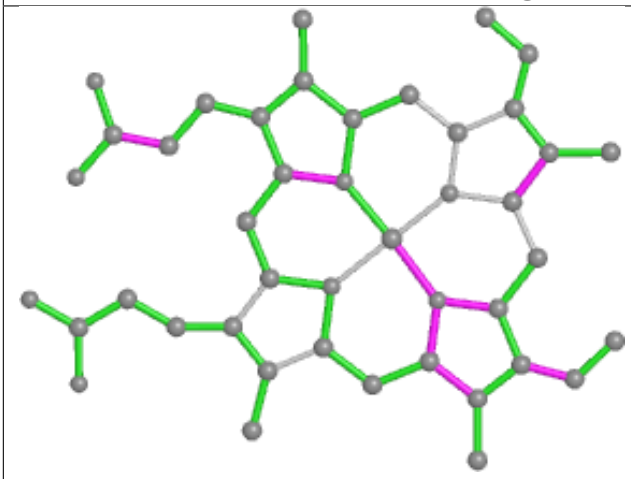


Torsions



Rings

Ligand HEM C 402



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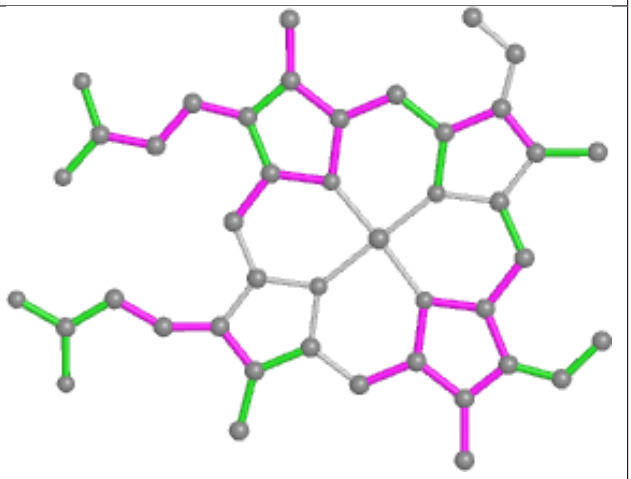
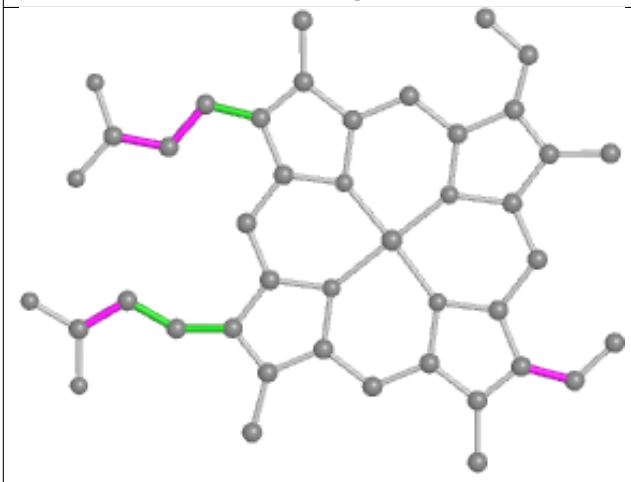
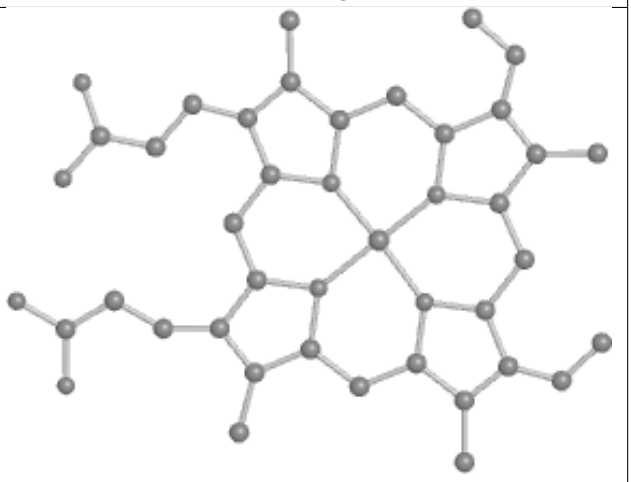


Bond angles

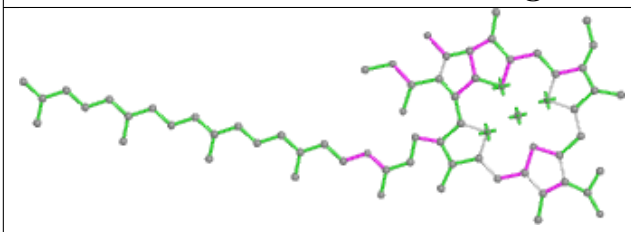


Torsions



Rings

Ligand BCL A 102



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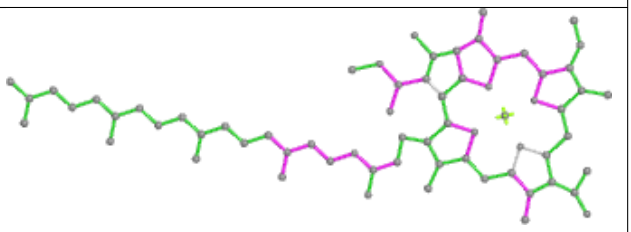
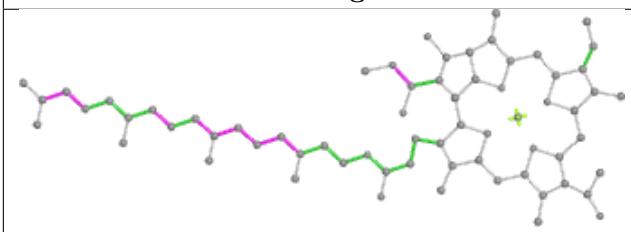
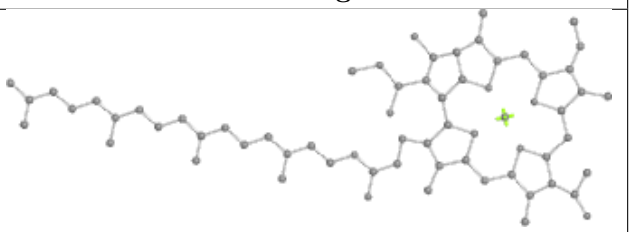


Bond angles

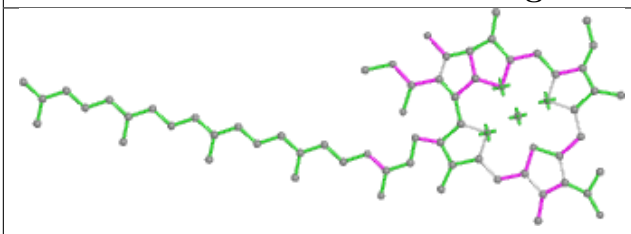


Torsions



Rings

Ligand BCL B 103



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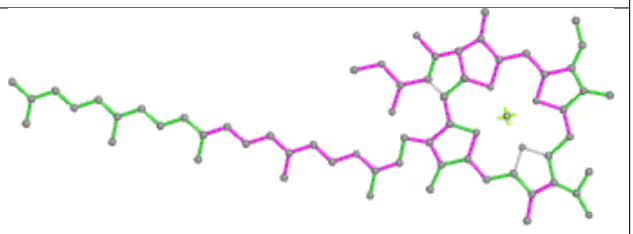
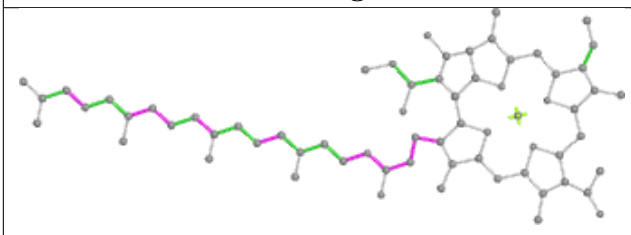


Bond angles



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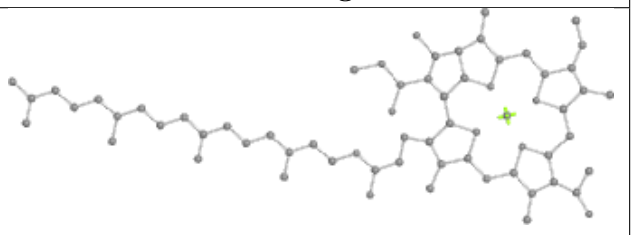
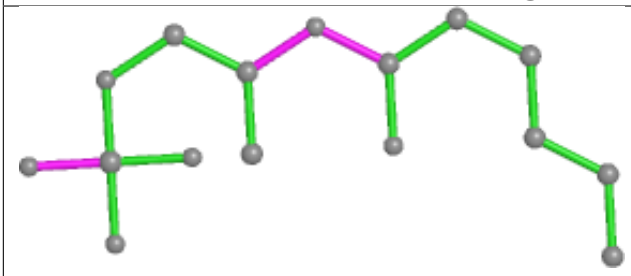
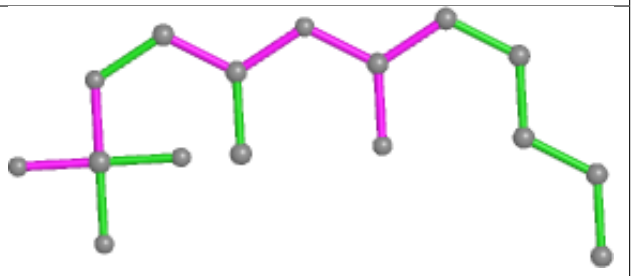


Rings

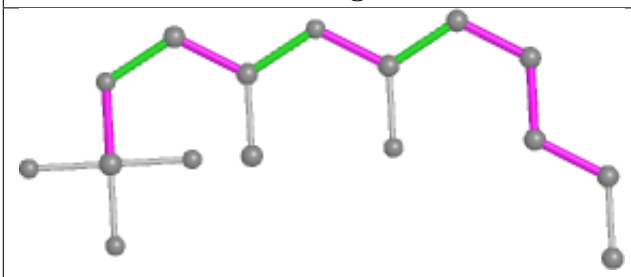
Ligand PGV C 408



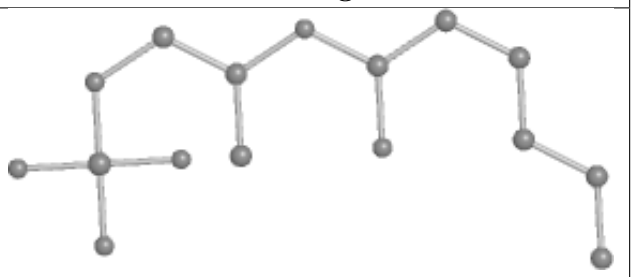
Bond lengths



Bond angles

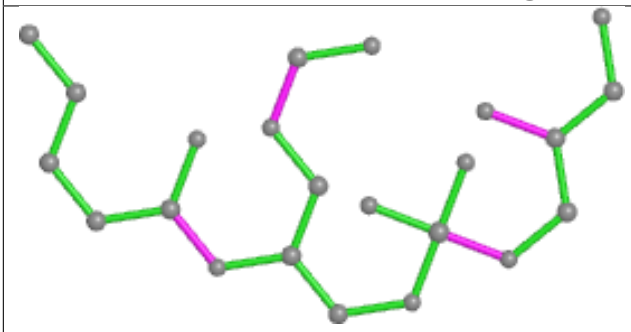


Torsions



Rings

Ligand PGV A 101



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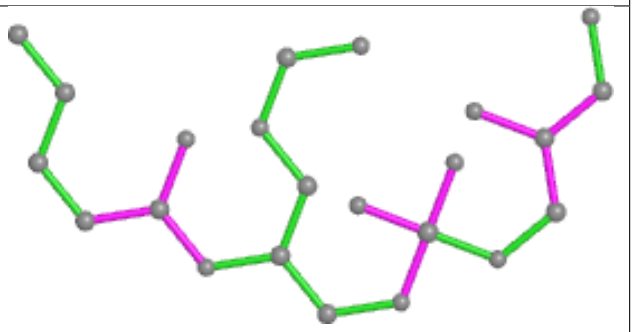
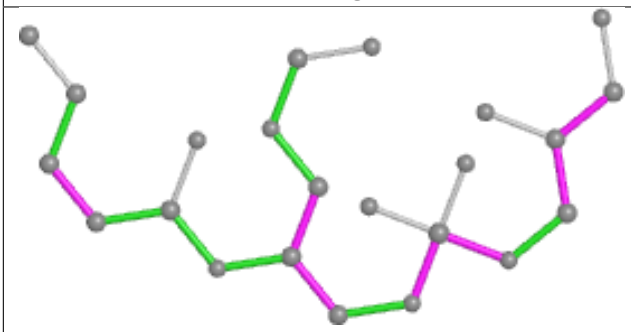
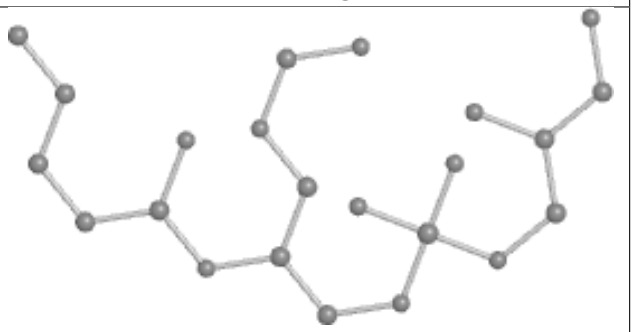


Bond angles

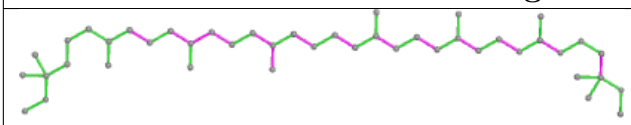


Torsions



Rings

Ligand H4X U 104



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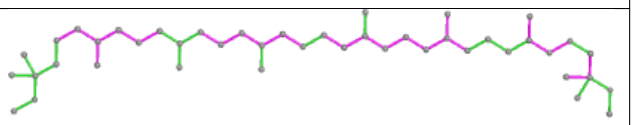
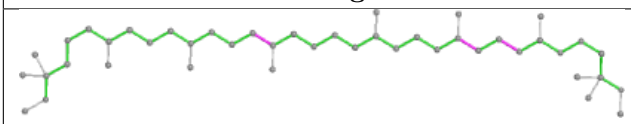
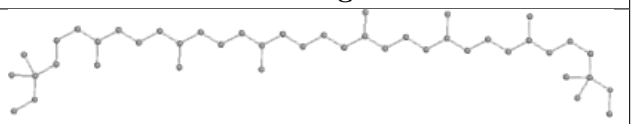


Bond angles

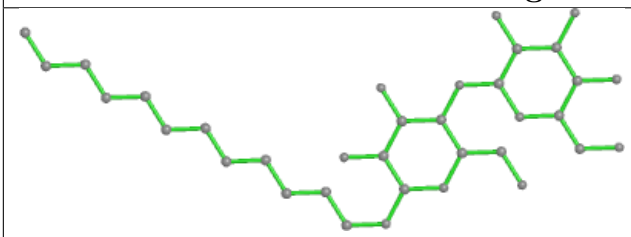


Torsions



Rings

Ligand LMT 8 101



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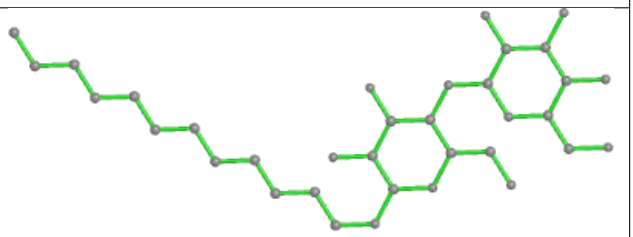
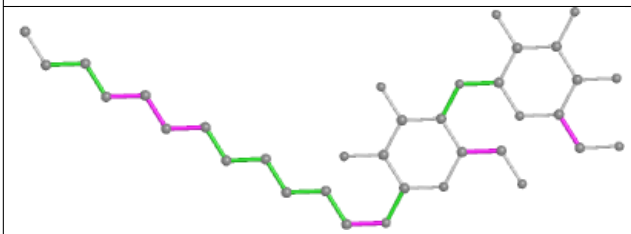
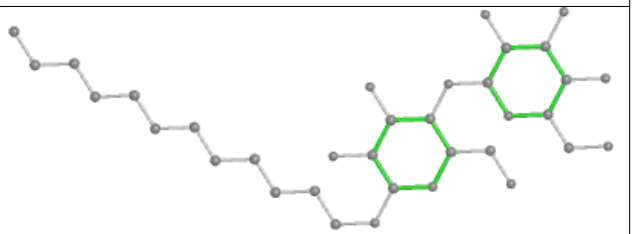


Bond angles

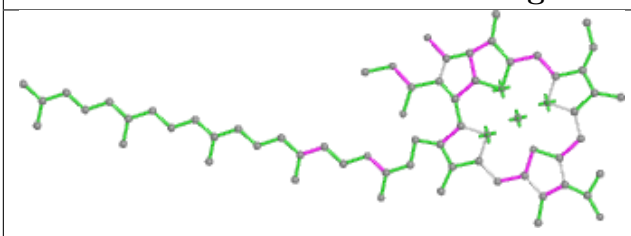


Torsions

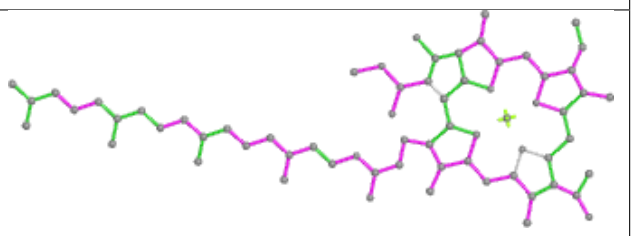


Rings

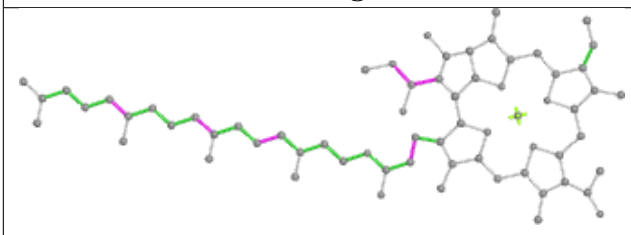
Ligand BCL L 301



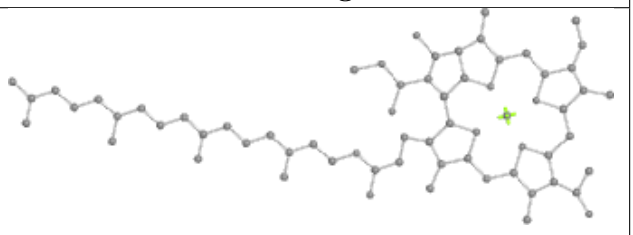
Bond lengths



Bond angles

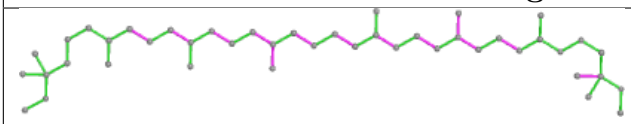


Torsions

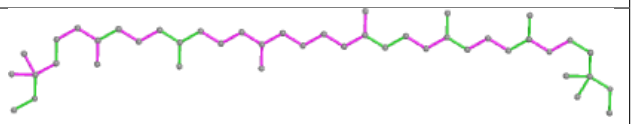


Rings

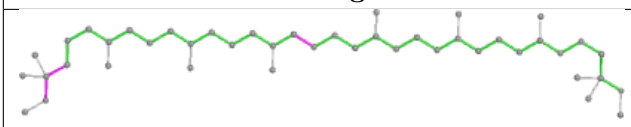
Ligand H4X E 101



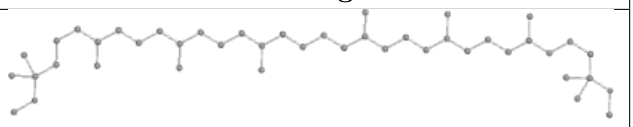
Bond lengths



Bond angles

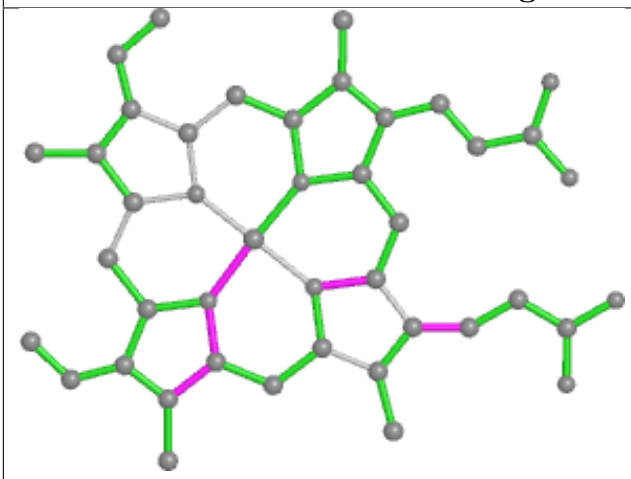


Torsions

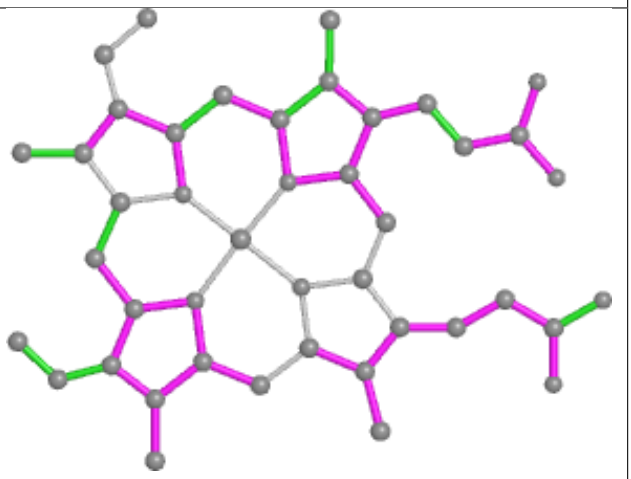


Rings

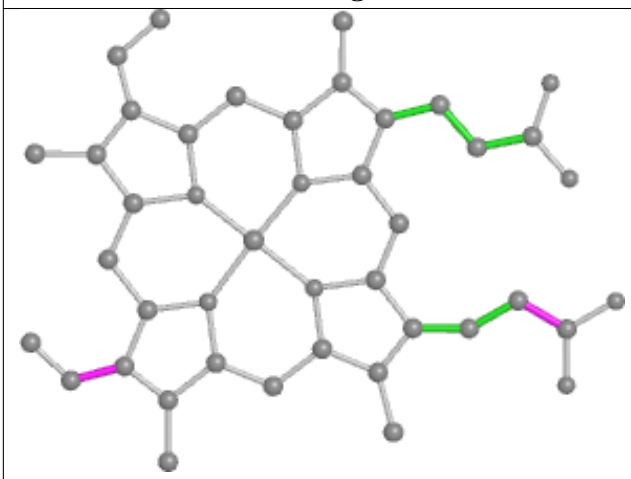
Ligand HEM C 403



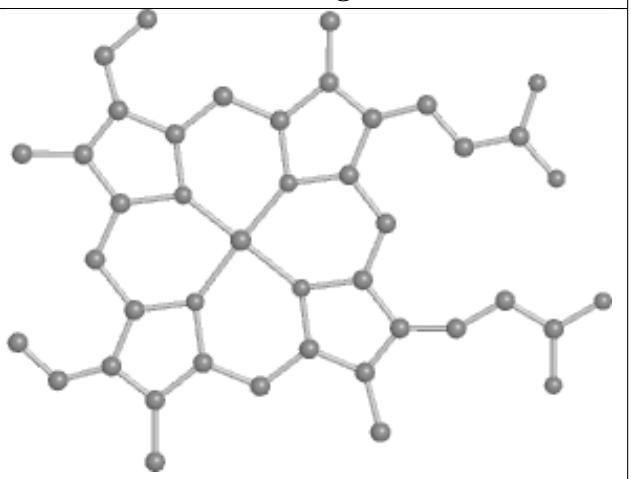
Bond lengths



Bond angles

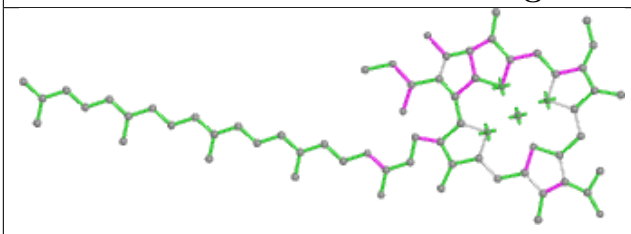


Torsions

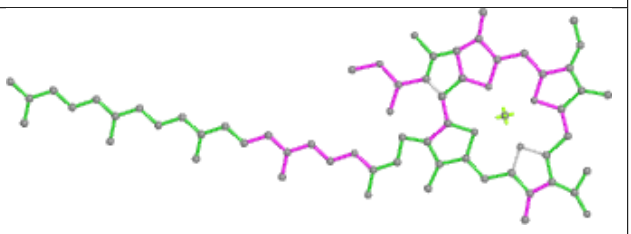


Rings

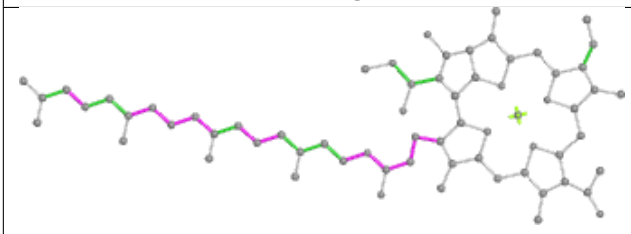
Ligand BCL U 103



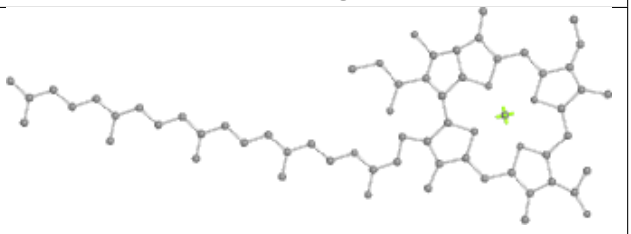
Bond lengths



Bond angles

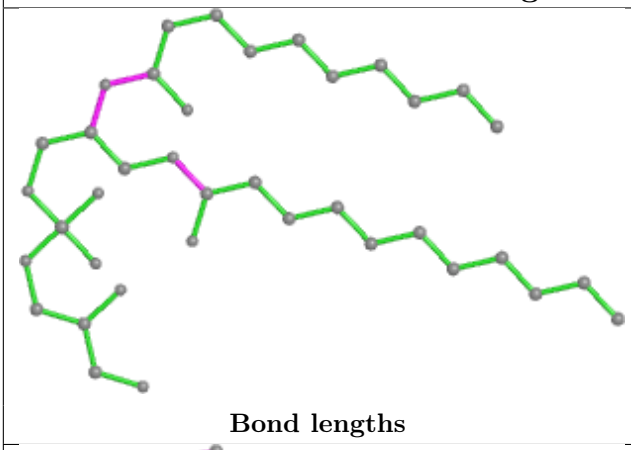


Torsions

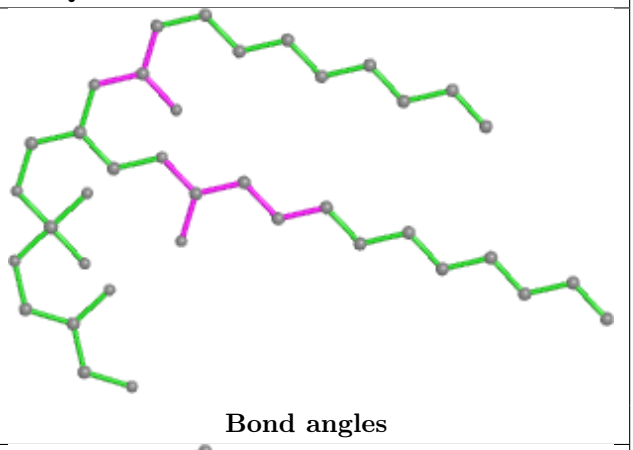


Rings

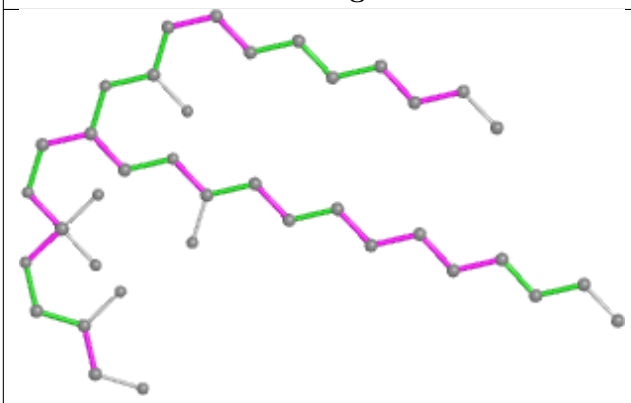
Ligand PGV Q 101



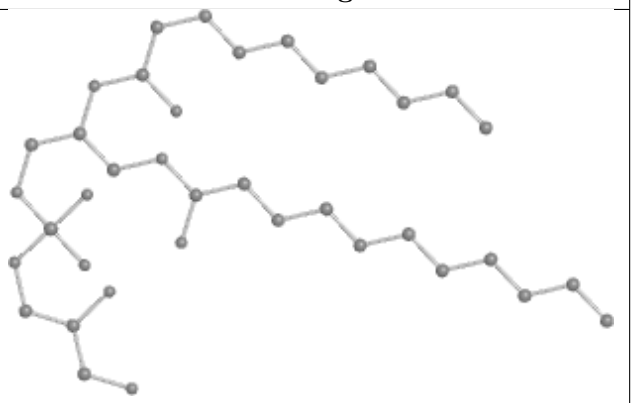
Bond lengths



Bond angles

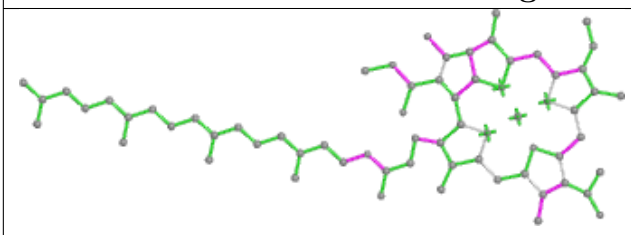


Torsions

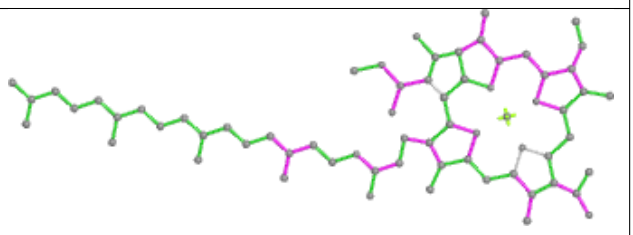


Rings

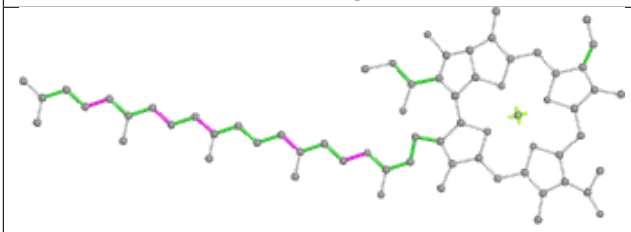
Ligand BCL W 102



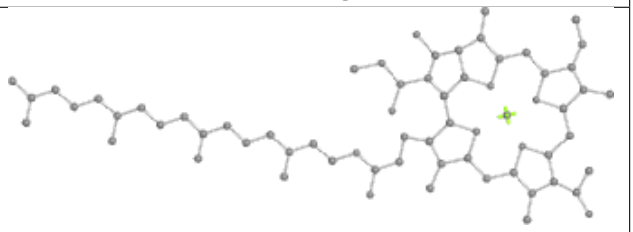
Bond lengths



Bond angles

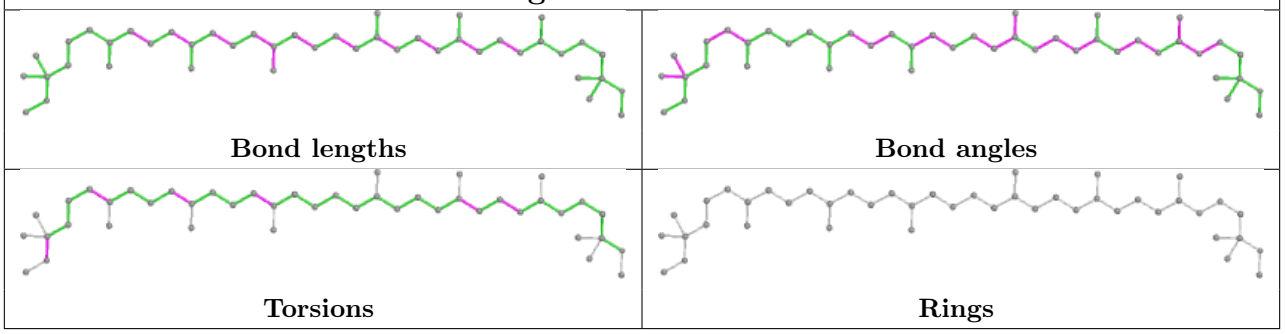


Torsions

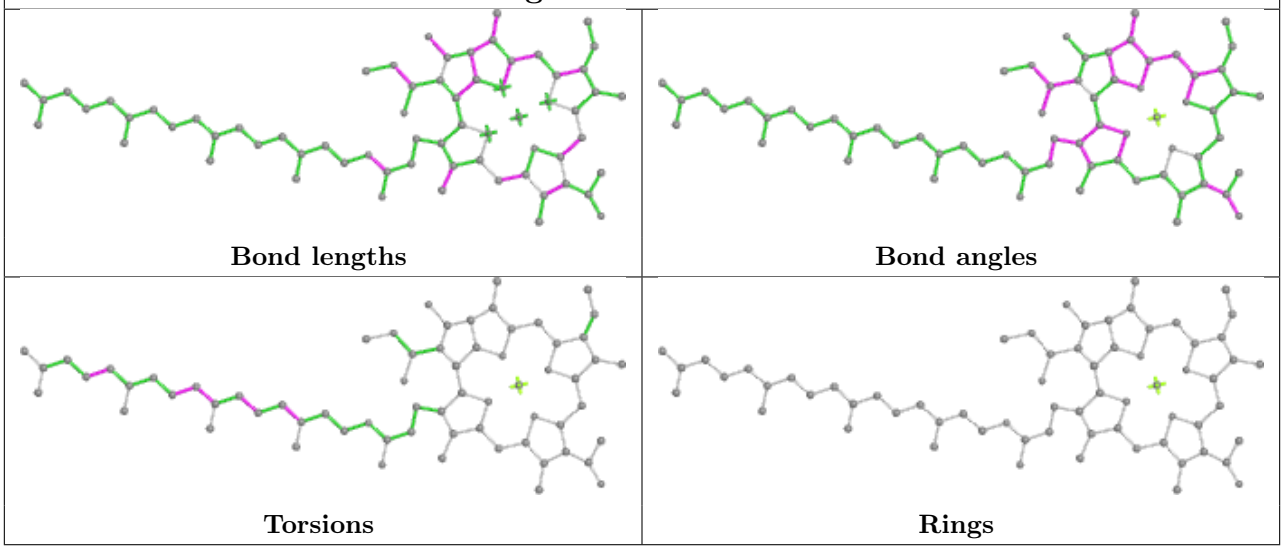


Rings

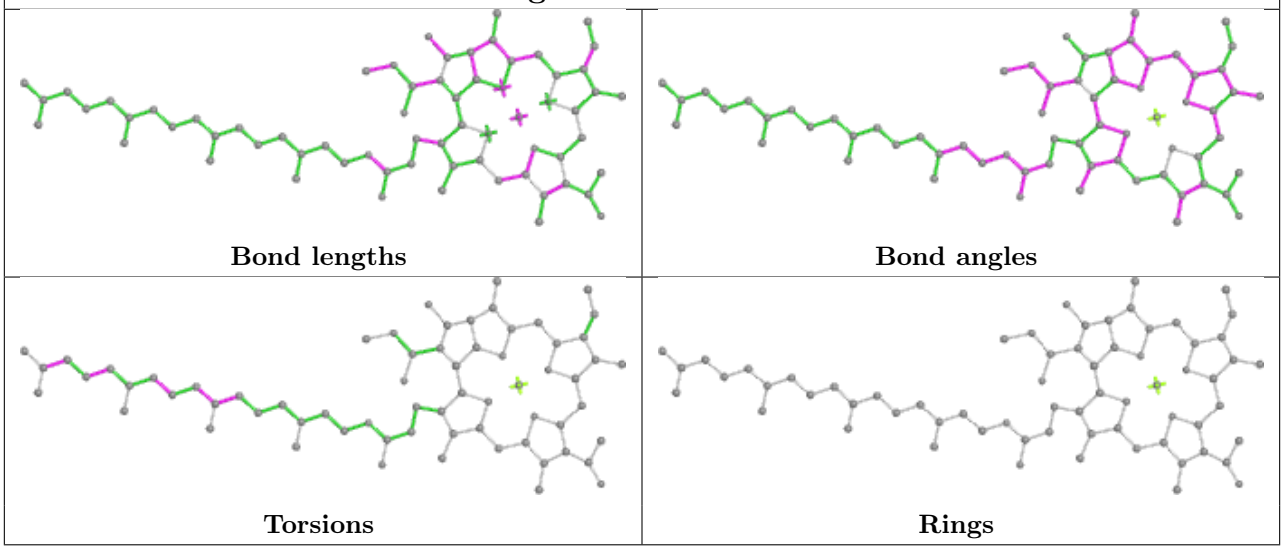
Ligand H4X Z 101



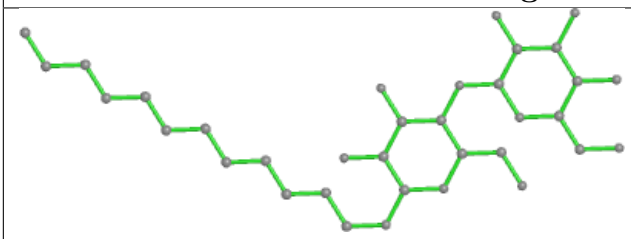
Ligand BCL D 103



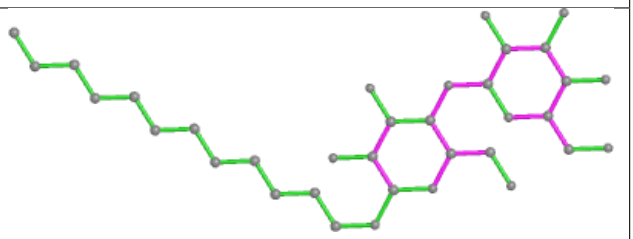
Ligand BCL L 304



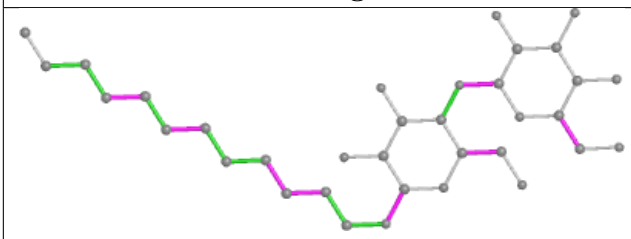
Ligand LMT V 102



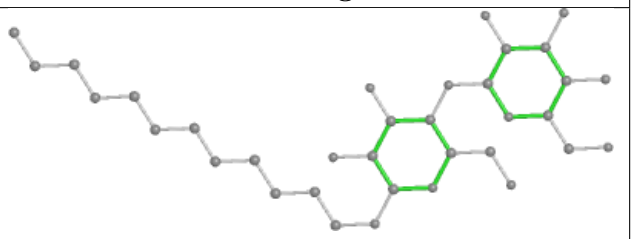
Bond lengths



Bond angles

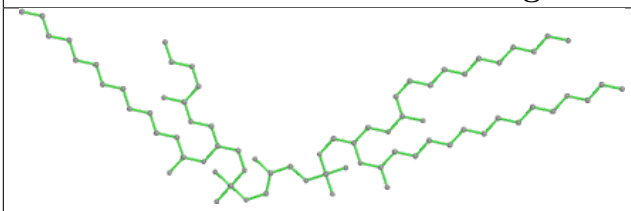


Torsions

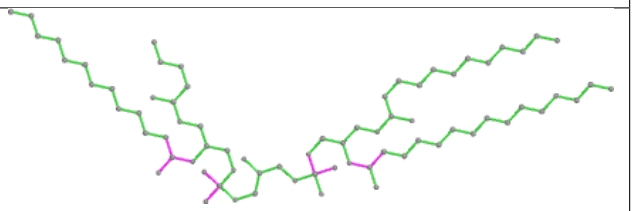


Rings

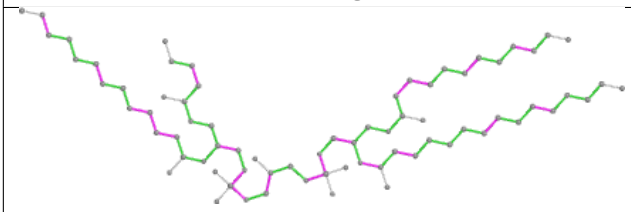
Ligand CDL H 302



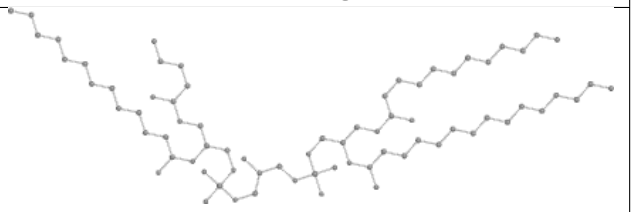
Bond lengths



Bond angles

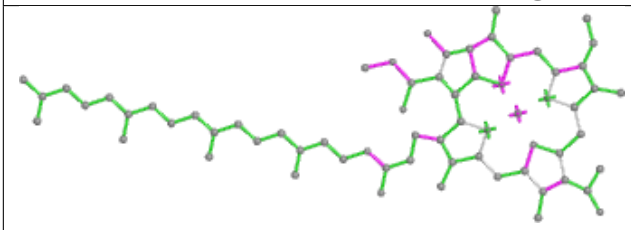


Torsions

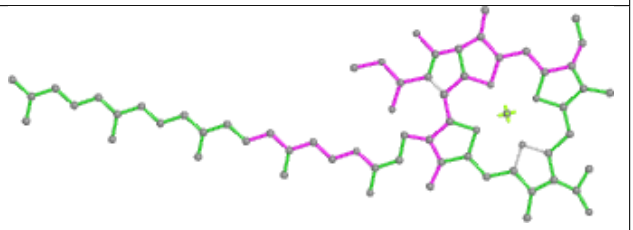


Rings

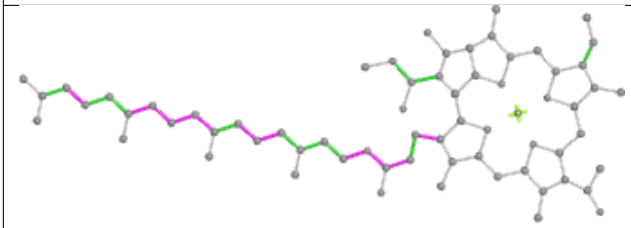
Ligand BCL 7 103



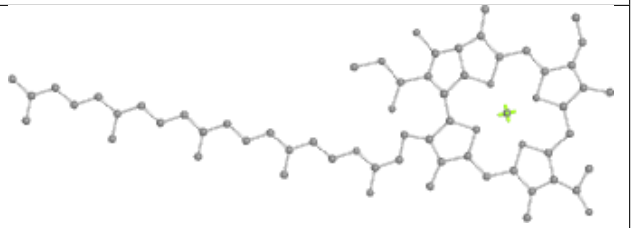
Bond lengths



Bond angles

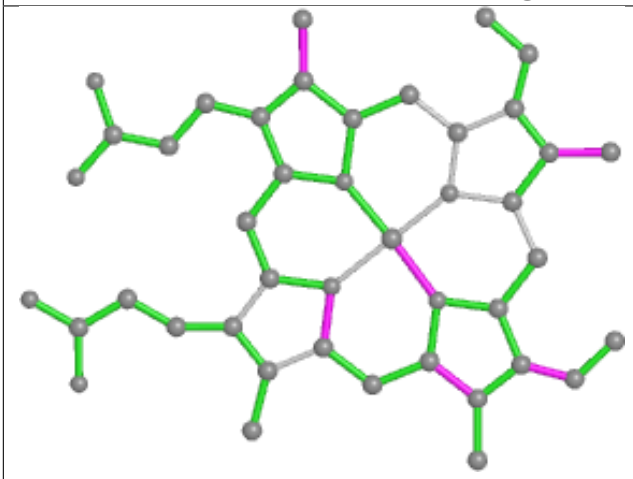


Torsions

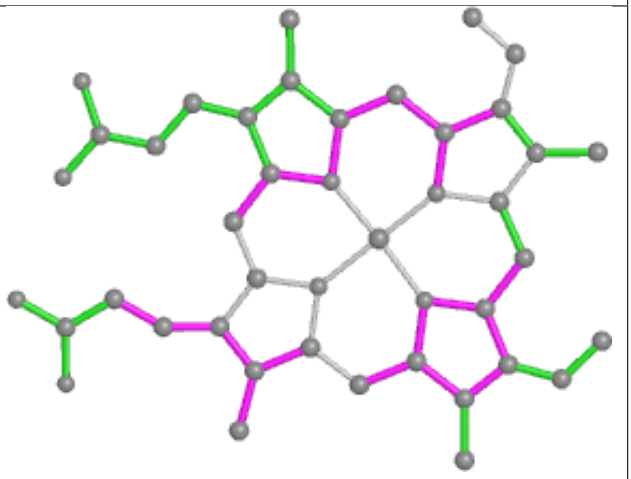


Rings

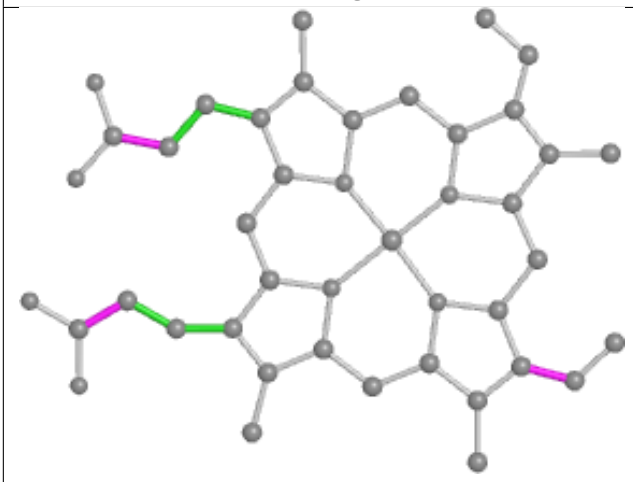
Ligand HEM C 404



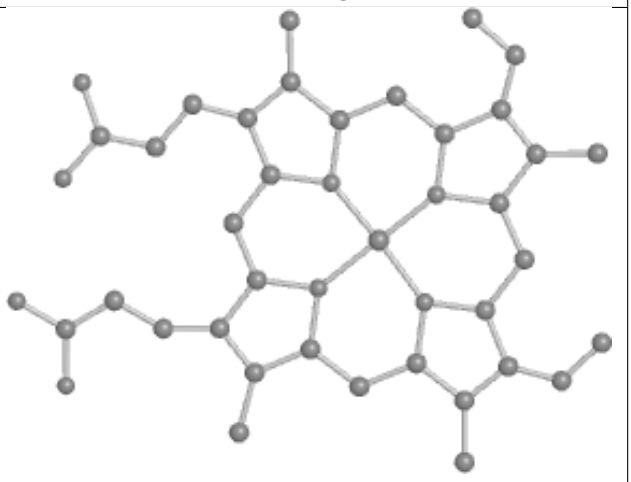
Bond lengths



Bond angles

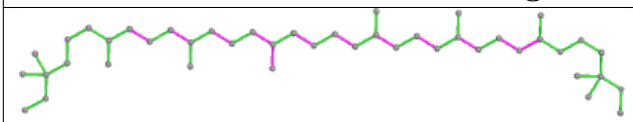


Torsions

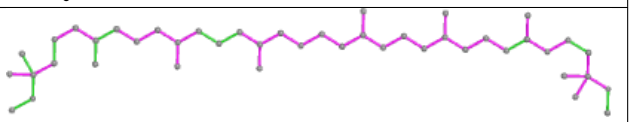


Rings

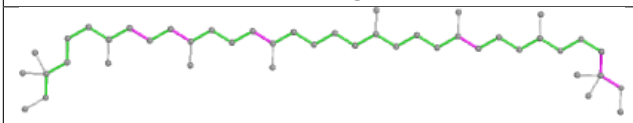
Ligand H4X Q 105



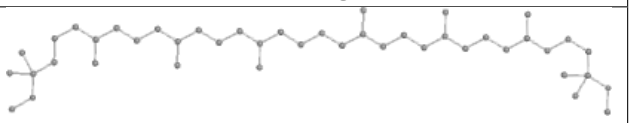
Bond lengths



Bond angles

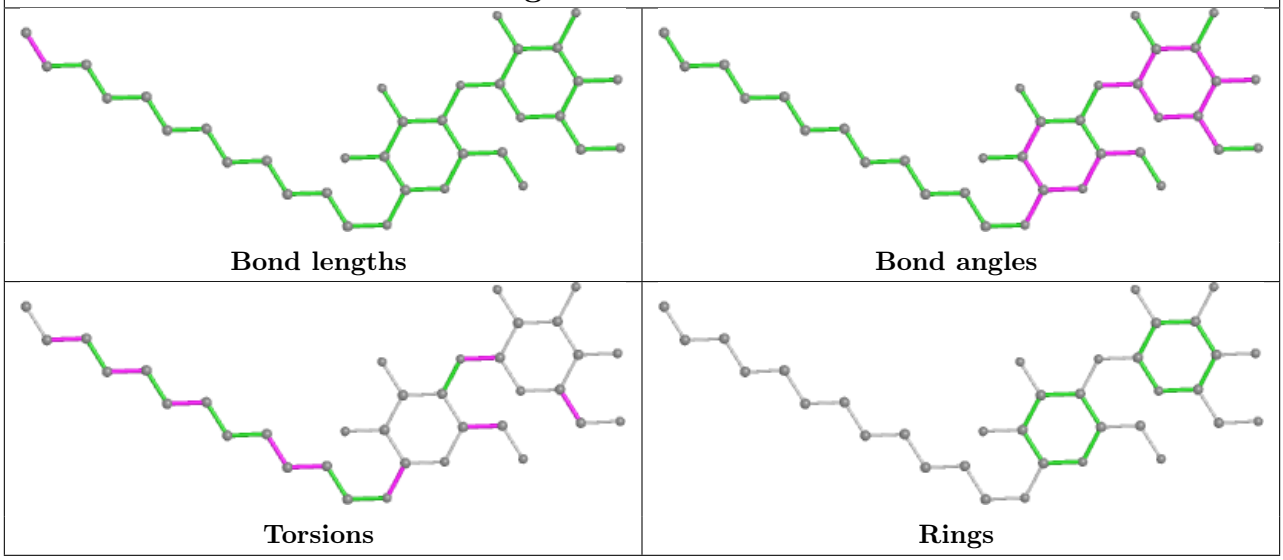


Torsions

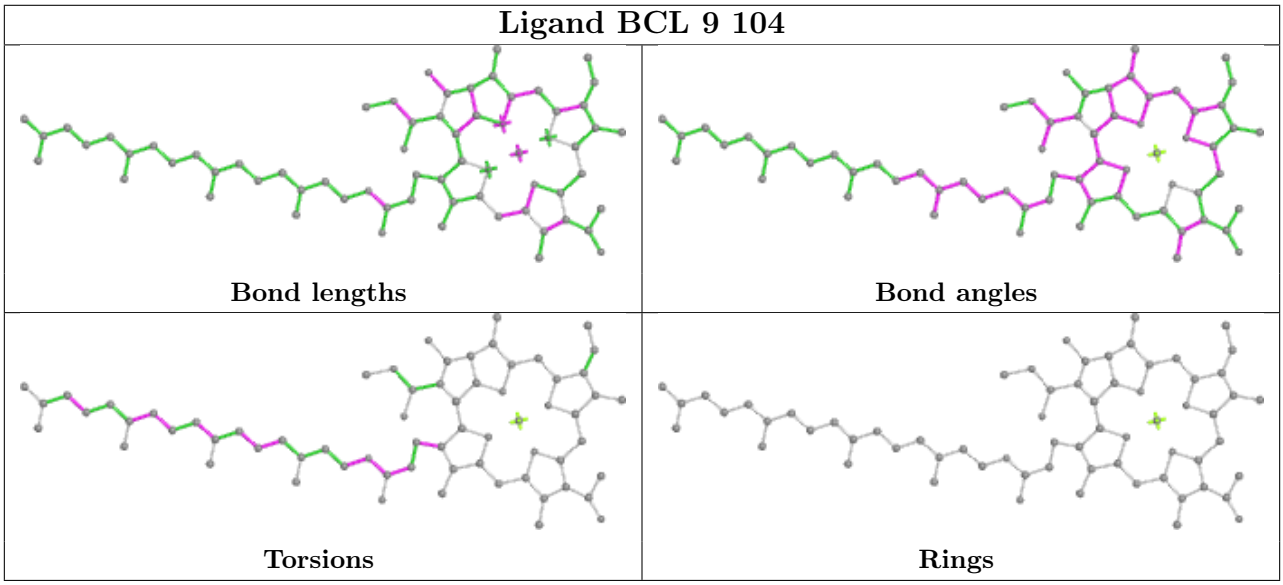


Rings

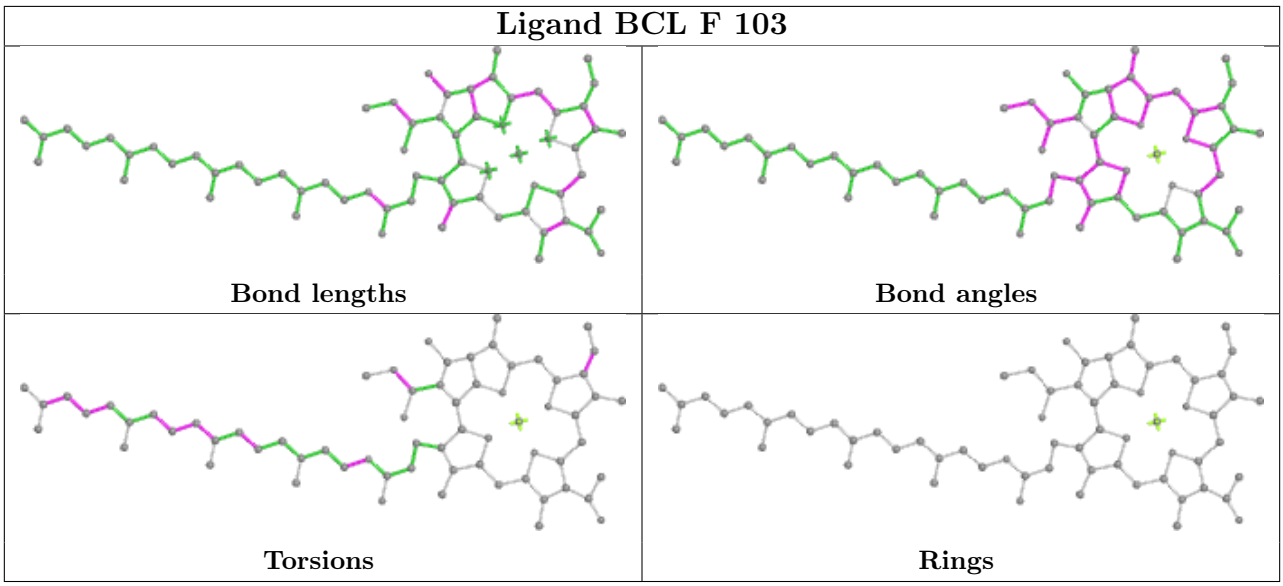
Ligand LMT Z 102



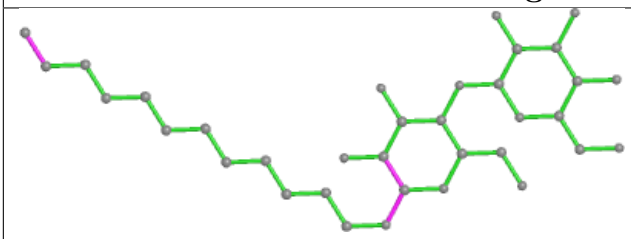
Ligand BCL 9 104



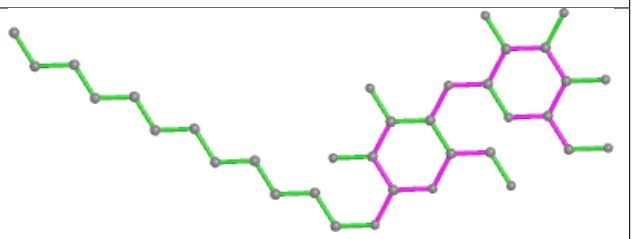
Ligand BCL F 103



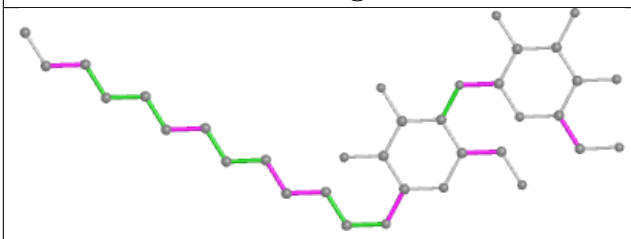
Ligand LMT 6 102



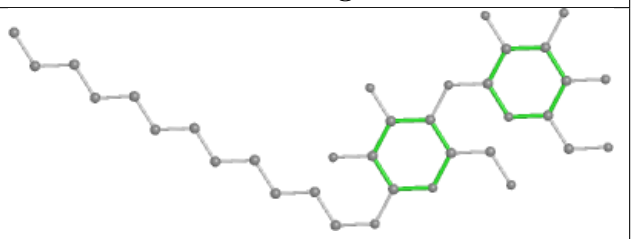
Bond lengths



Bond angles

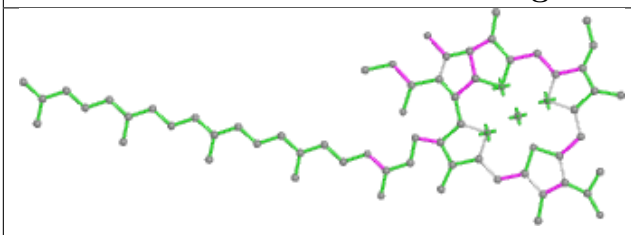


Torsions

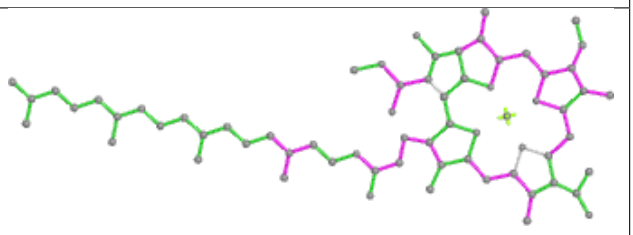


Rings

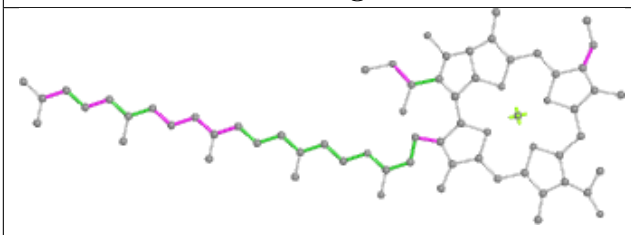
Ligand BCL I 102



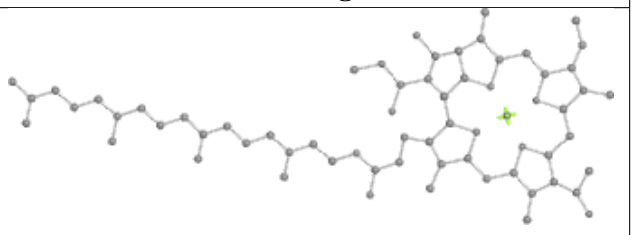
Bond lengths



Bond angles

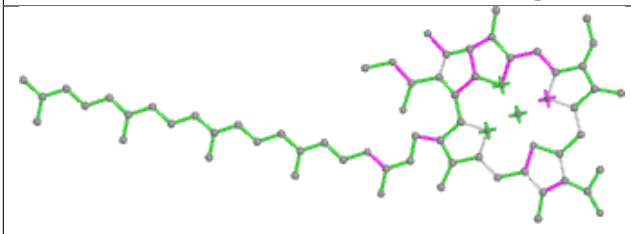


Torsions

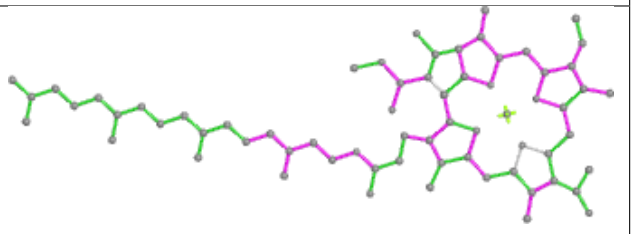


Rings

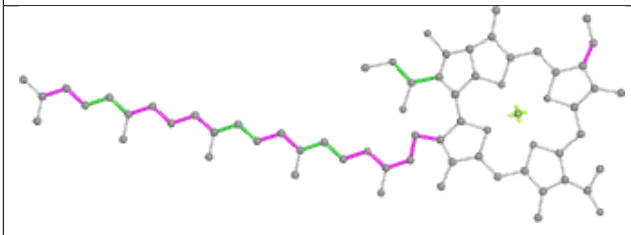
Ligand BCL 5 104



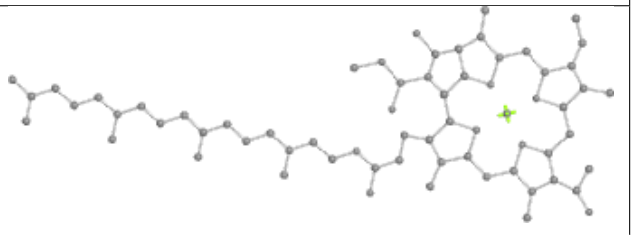
Bond lengths



Bond angles

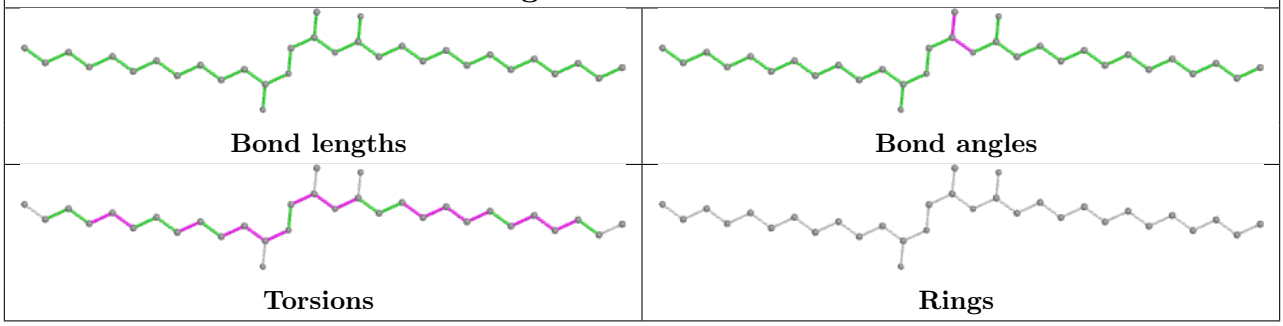


Torsions

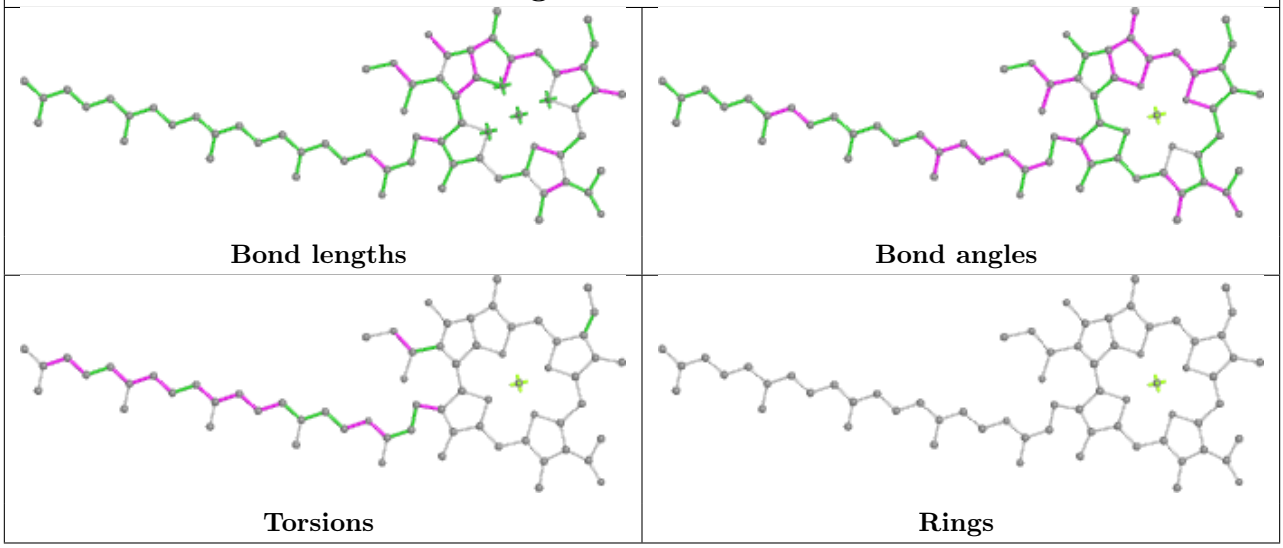


Rings

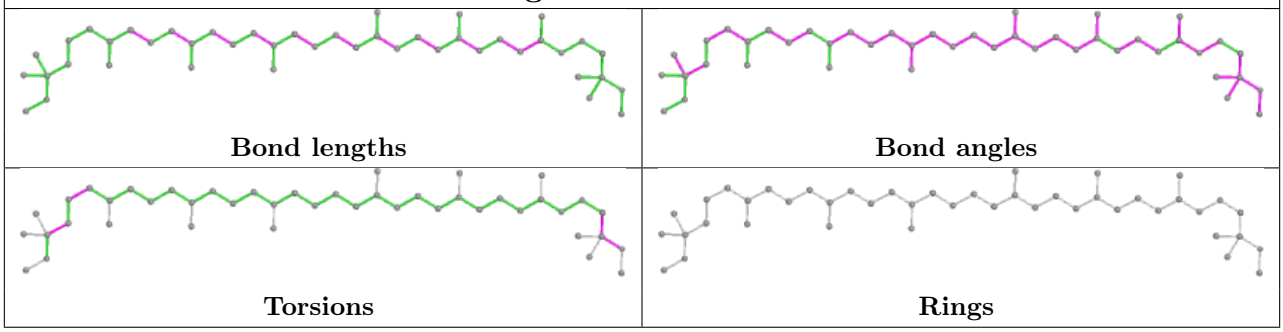
Ligand DGA C 407



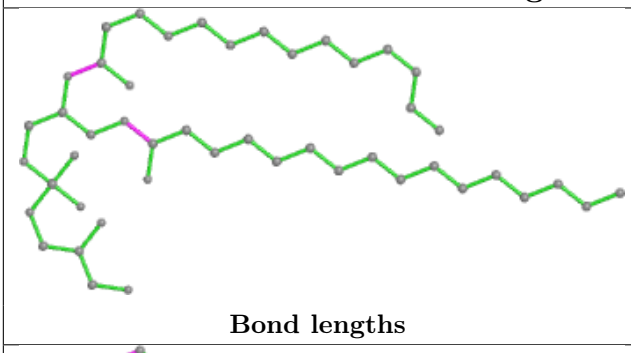
Ligand BCL 9 103



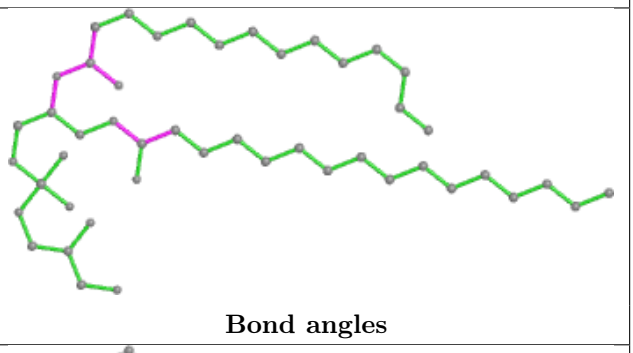
Ligand H4X K 103



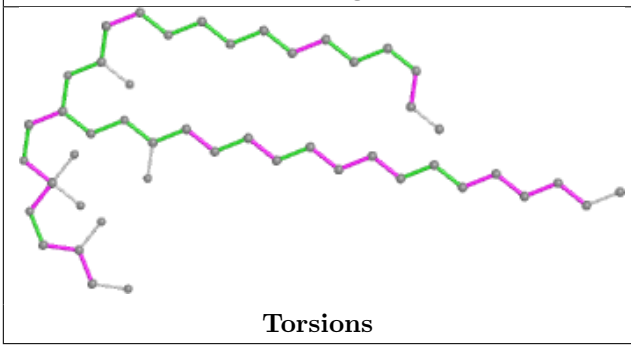
Ligand PGV 9 101



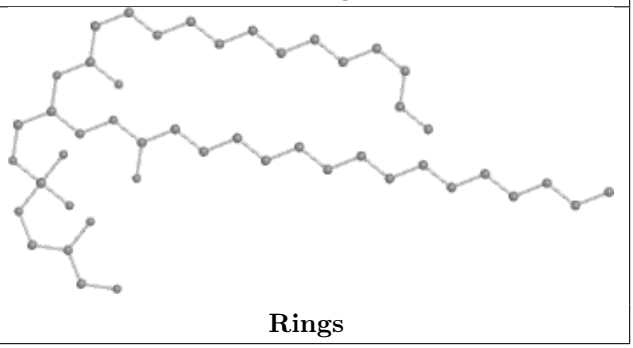
Bond lengths



Bond angles

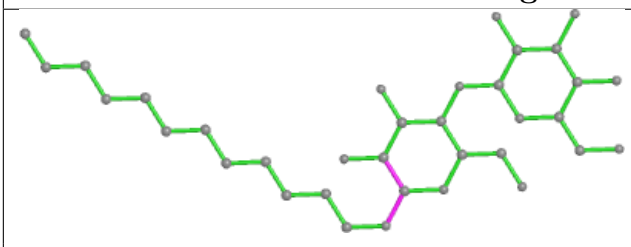


Torsions

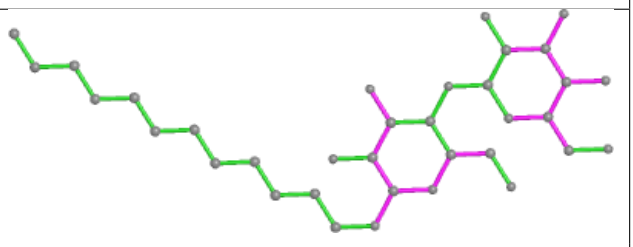


Rings

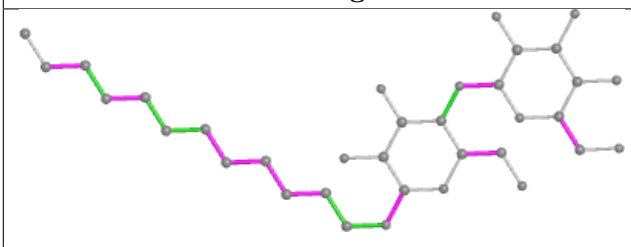
Ligand LMT G 102



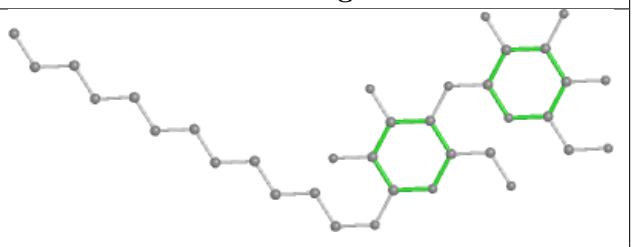
Bond lengths



Bond angles

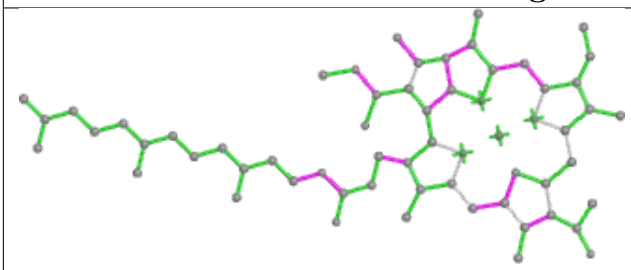


Torsions

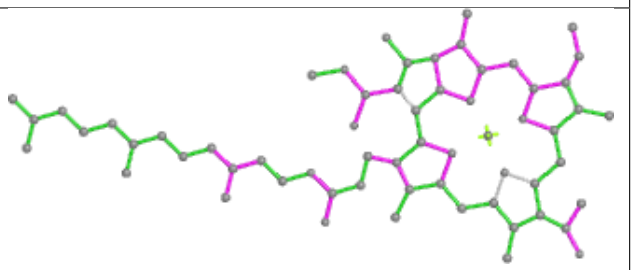


Rings

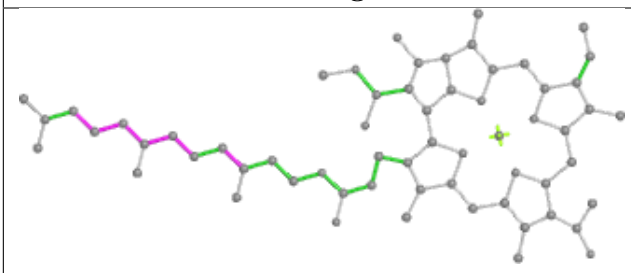
Ligand BCL 7 102



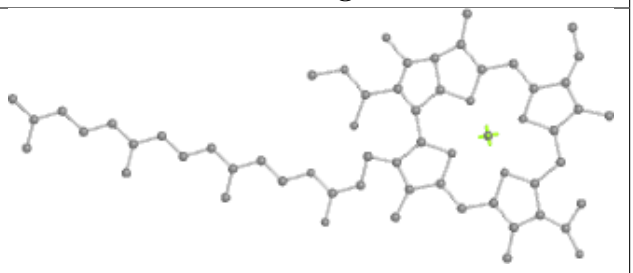
Bond lengths



Bond angles

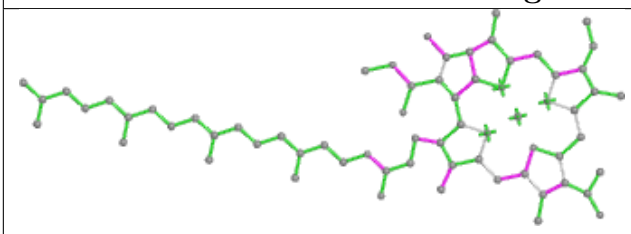


Torsions

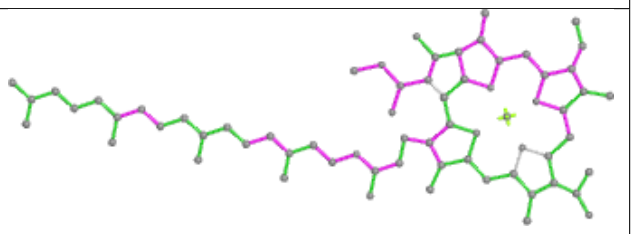


Rings

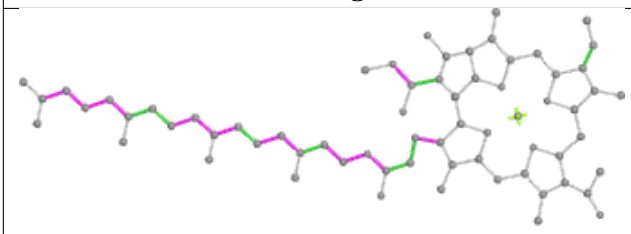
Ligand BCL K 105



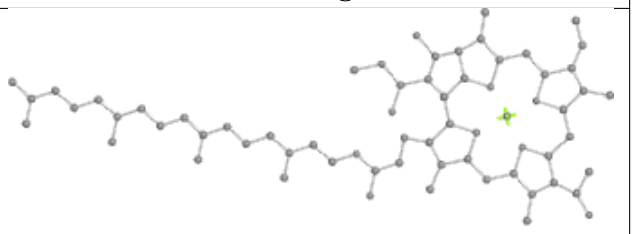
Bond lengths



Bond angles

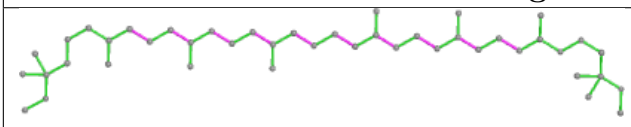


Torsions

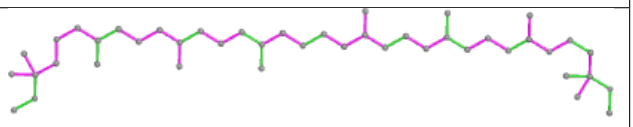


Rings

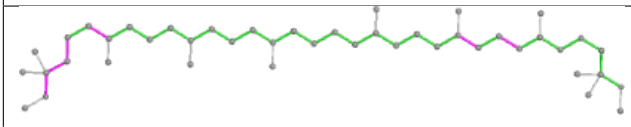
Ligand H4X 2 101



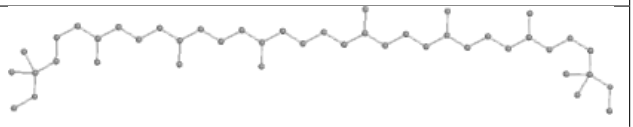
Bond lengths



Bond angles

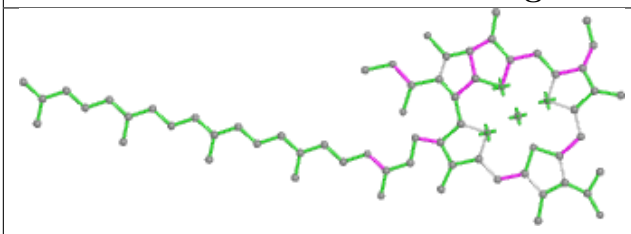


Torsions

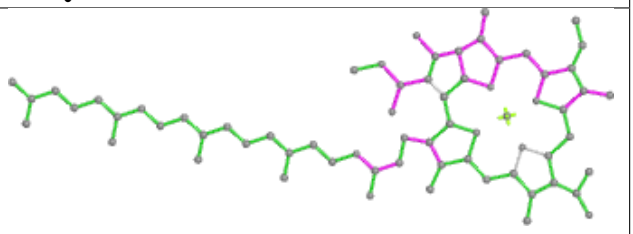


Rings

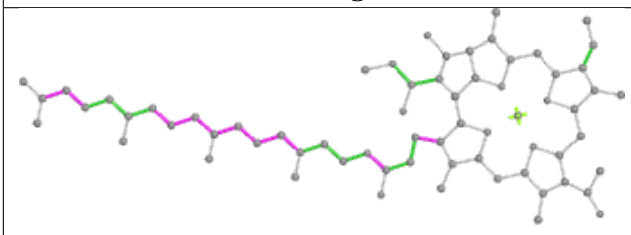
Ligand BCL Q 103



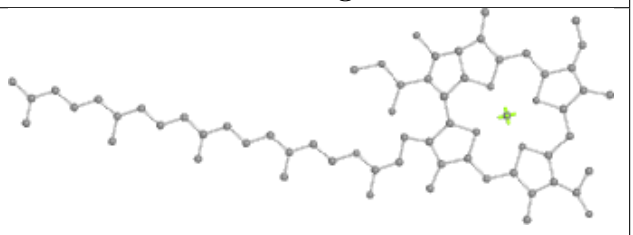
Bond lengths



Bond angles

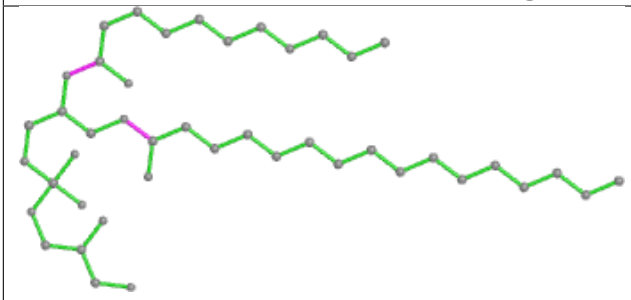


Torsions

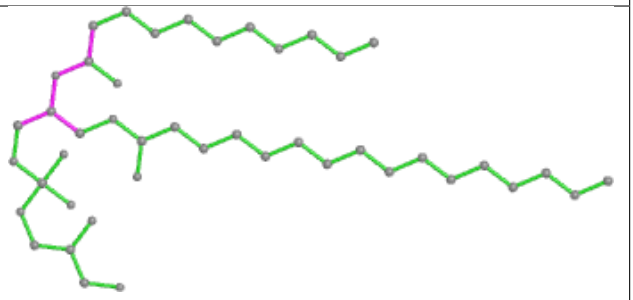


Rings

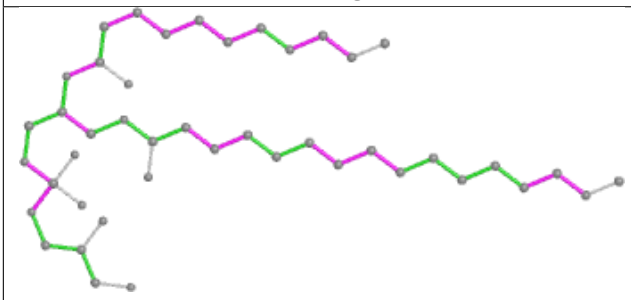
Ligand PGV O 102



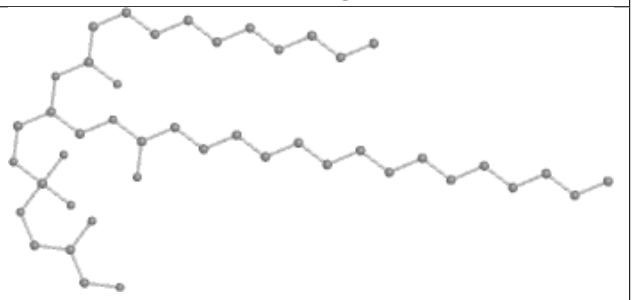
Bond lengths



Bond angles

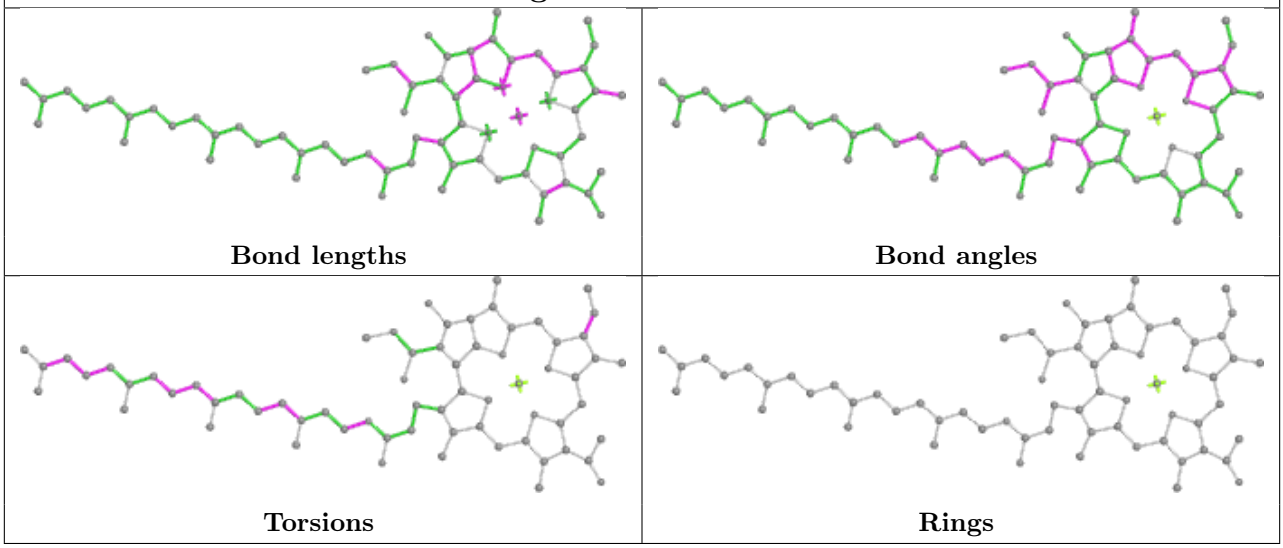


Torsions

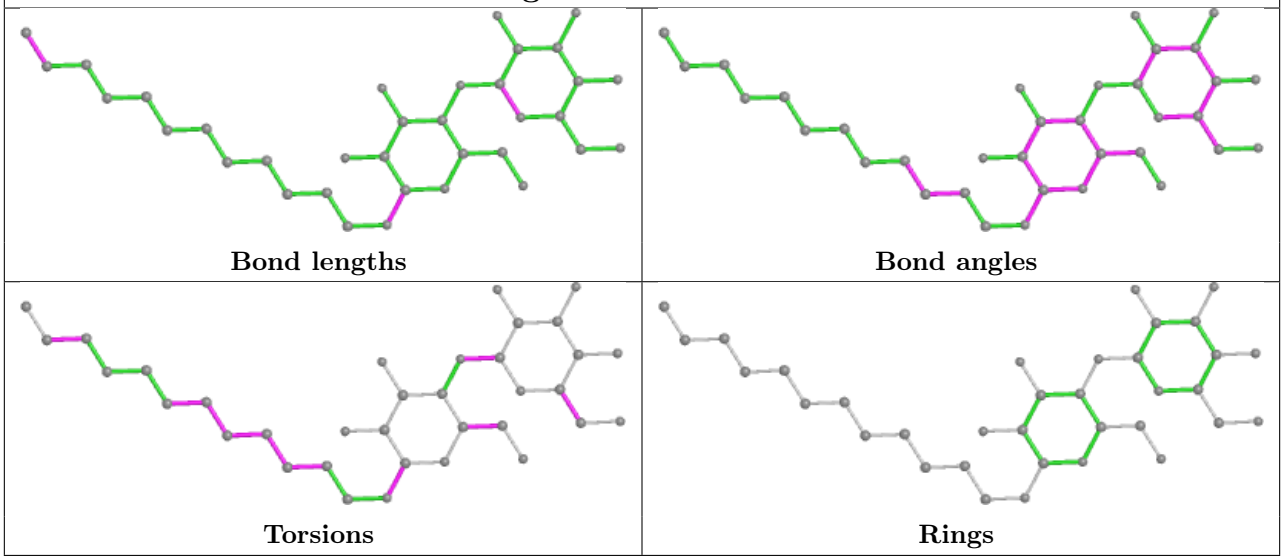


Rings

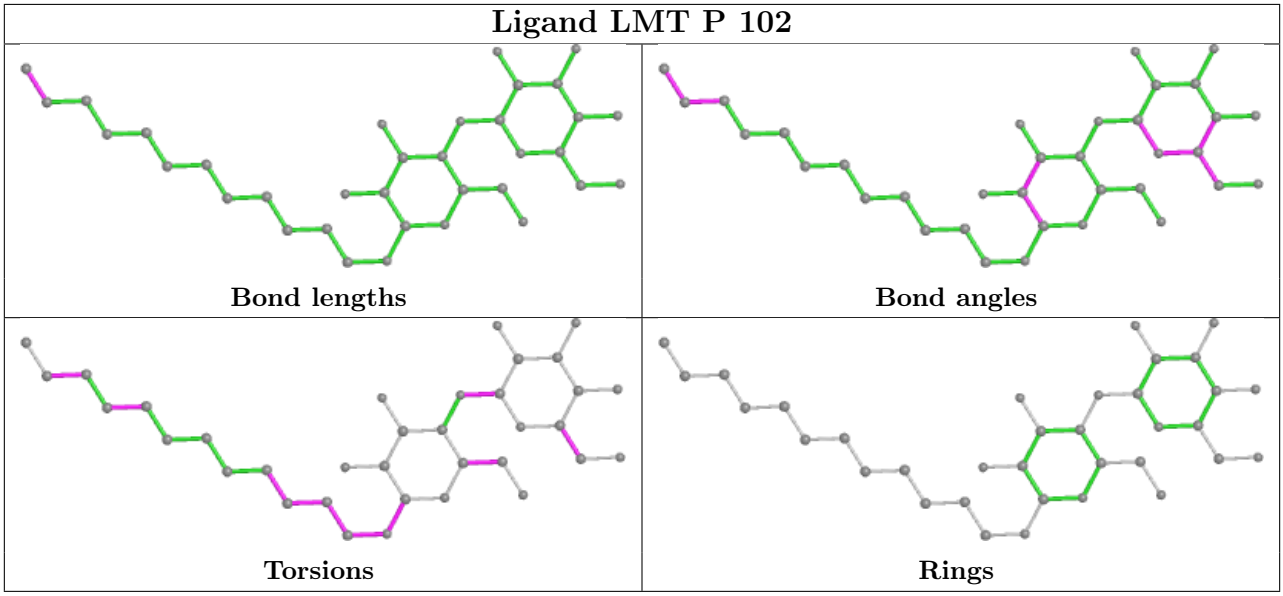
Ligand BCL 5 103



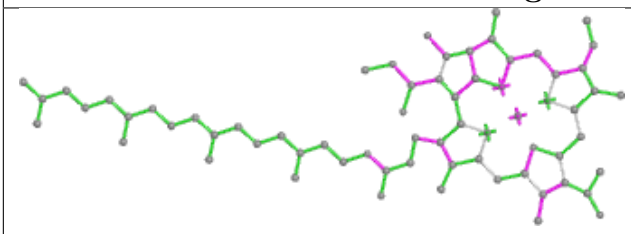
Ligand LMT B 104



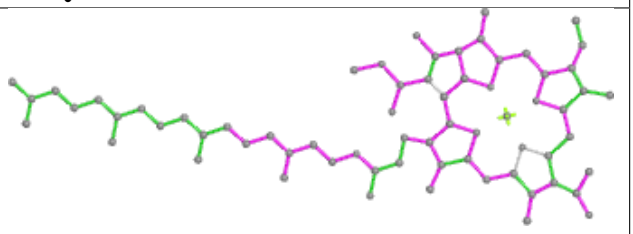
Ligand LMT P 102



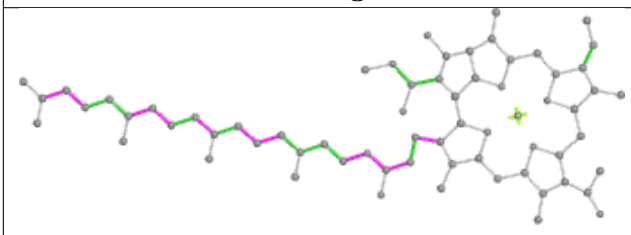
Ligand BCL Q 104



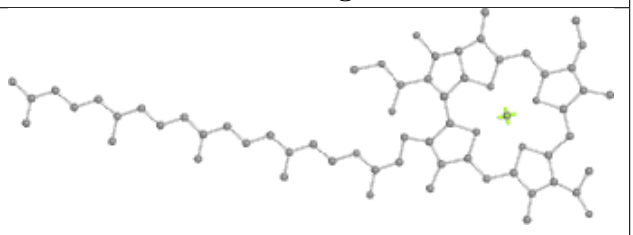
Bond lengths



Bond angles

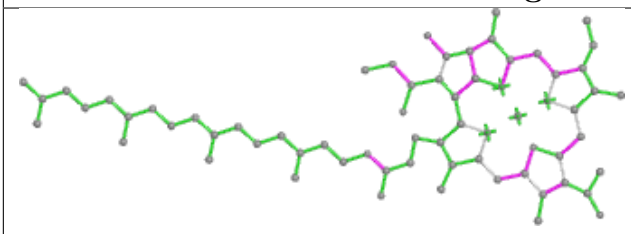


Torsions

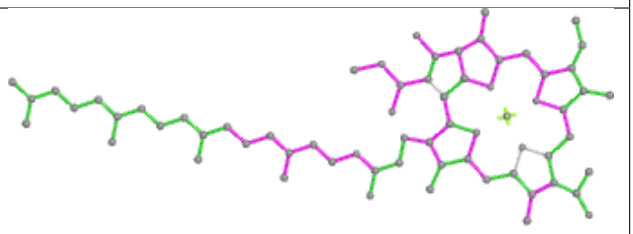


Rings

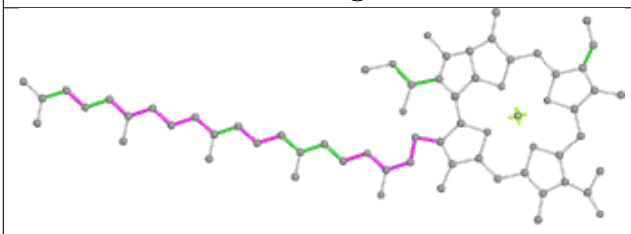
Ligand BCL O 105



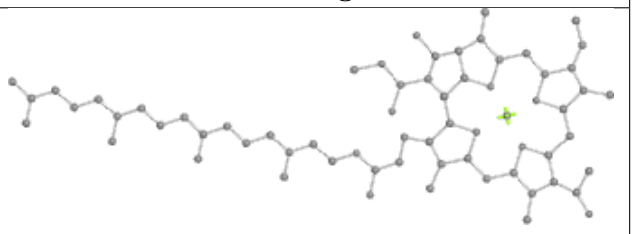
Bond lengths



Bond angles

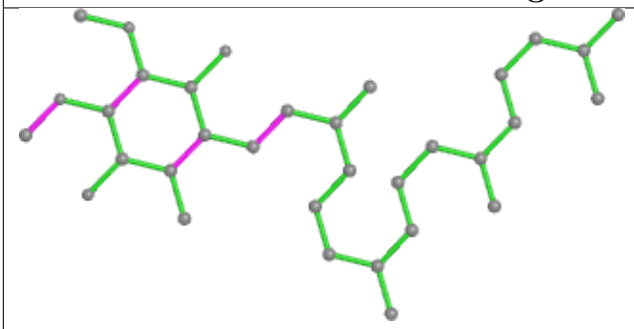


Torsions

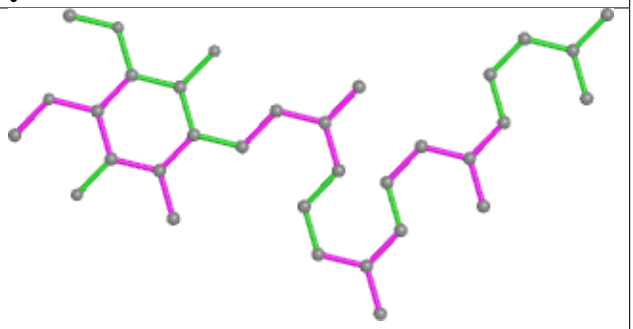


Rings

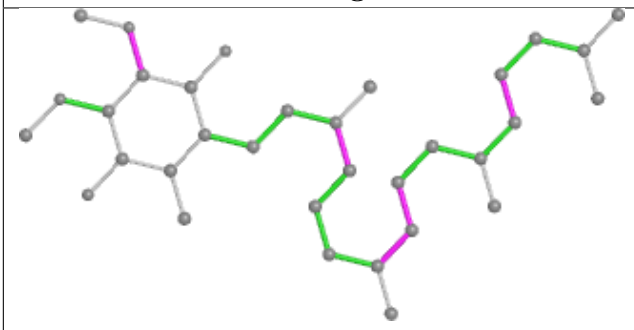
Ligand UQ8 L 303



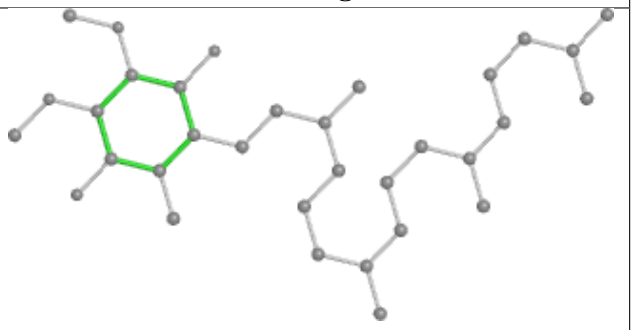
Bond lengths



Bond angles

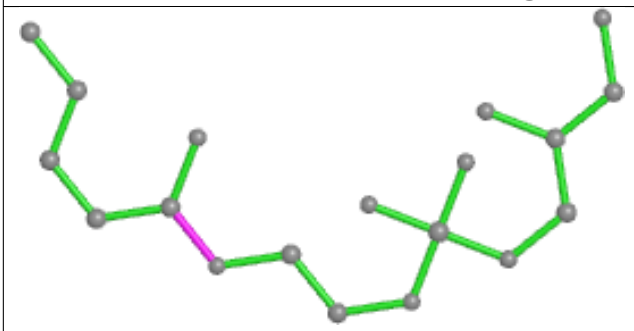


Torsions

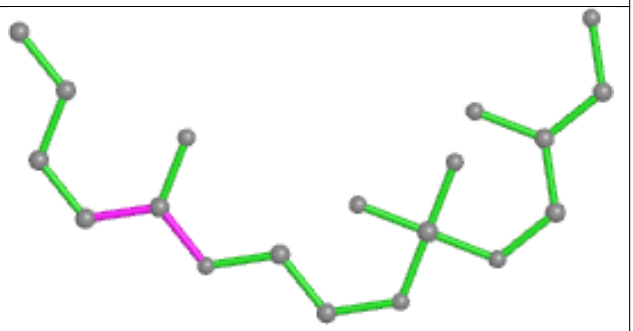


Rings

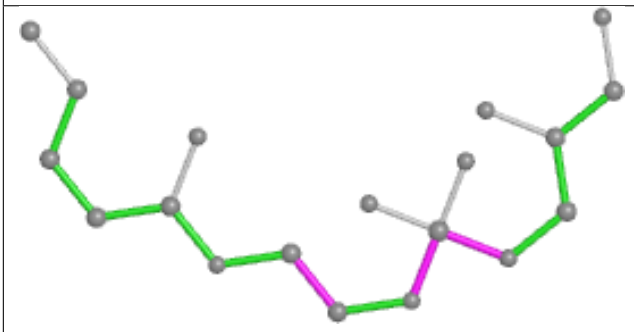
Ligand PGV K 102



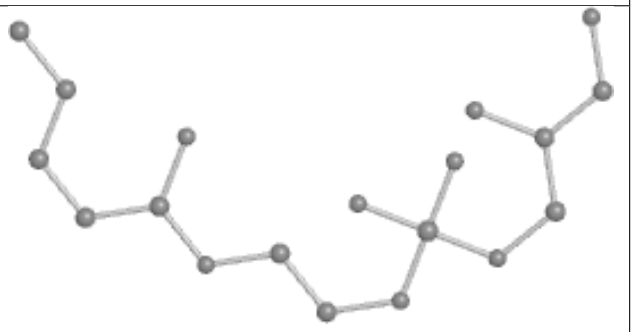
Bond lengths



Bond angles

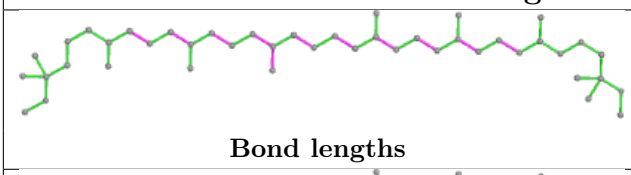


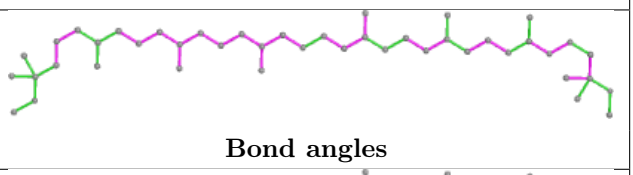
Torsions

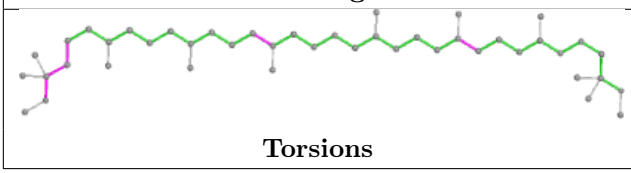


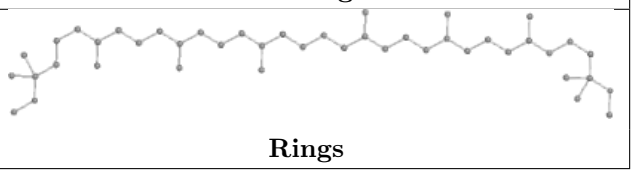
Rings

Ligand H4X K 107

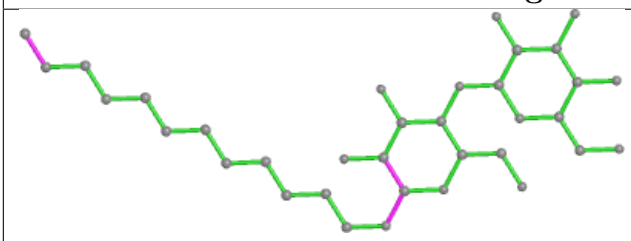

Bond lengths

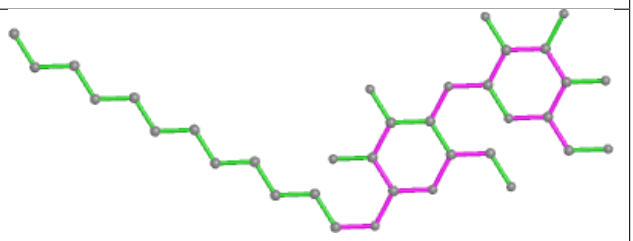

Bond angles

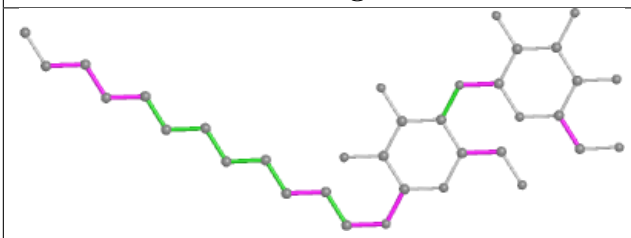

Torsions

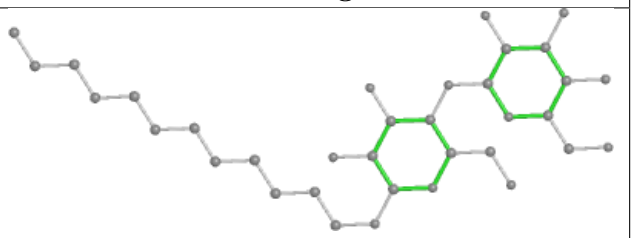

Rings

Ligand LMT 4 102

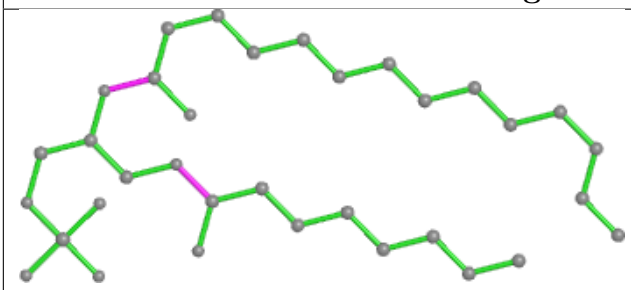

Bond lengths

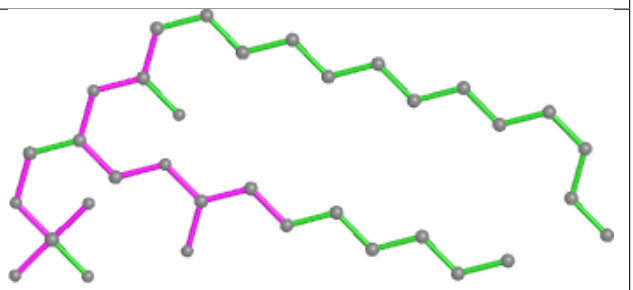

Bond angles

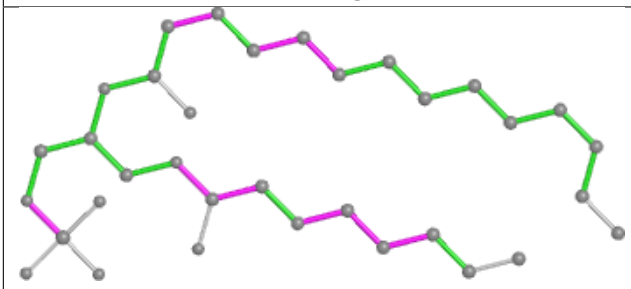

Torsions

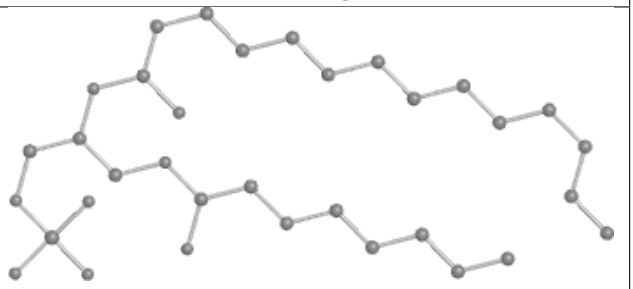

Rings

Ligand PGV F 101

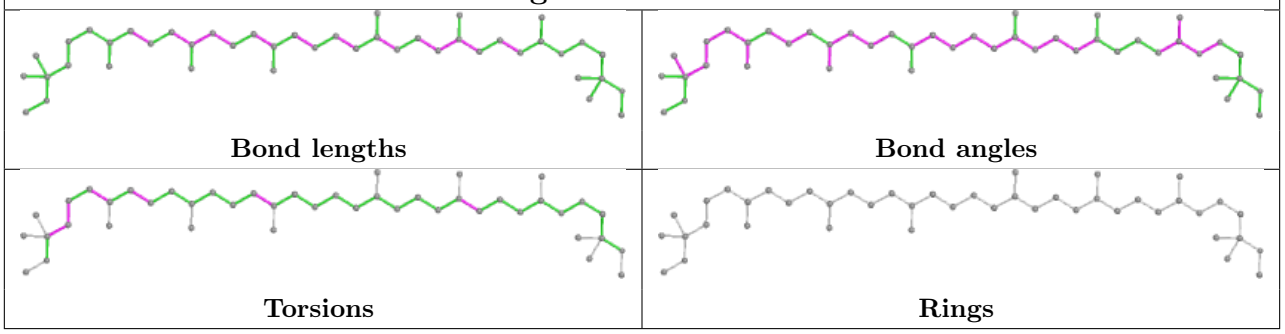

Bond lengths


Bond angles

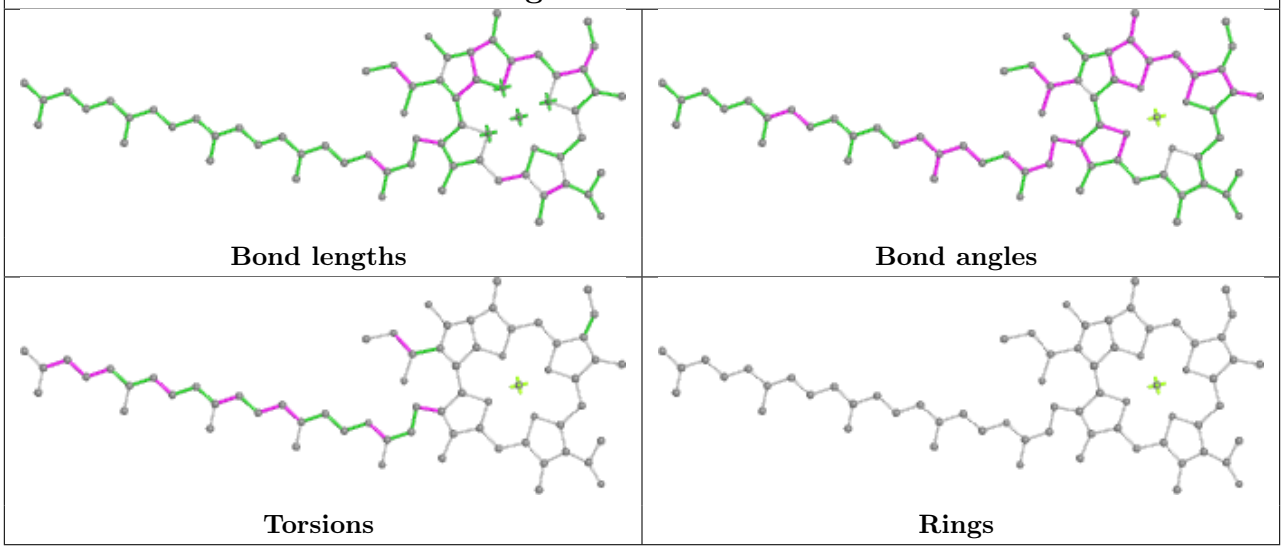

Torsions


Rings

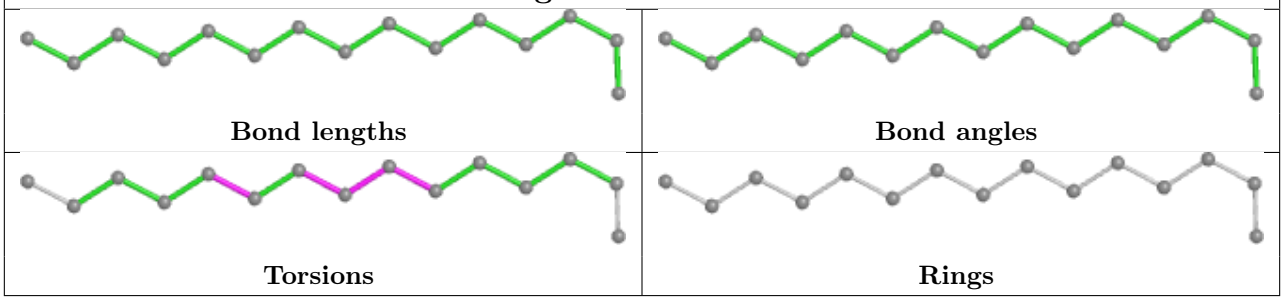
Ligand H4X 4 101



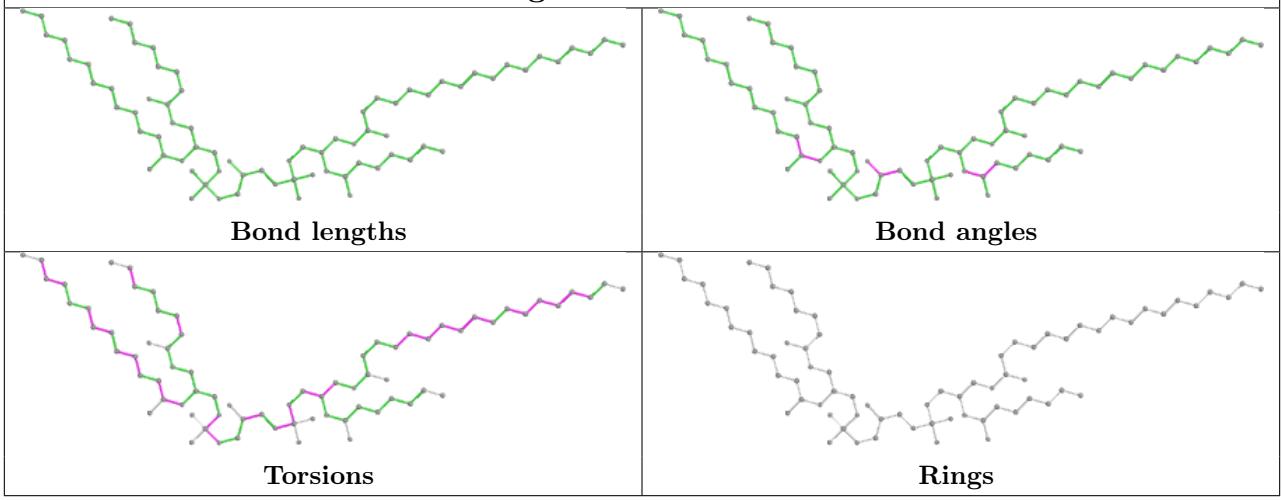
Ligand BCL U 102



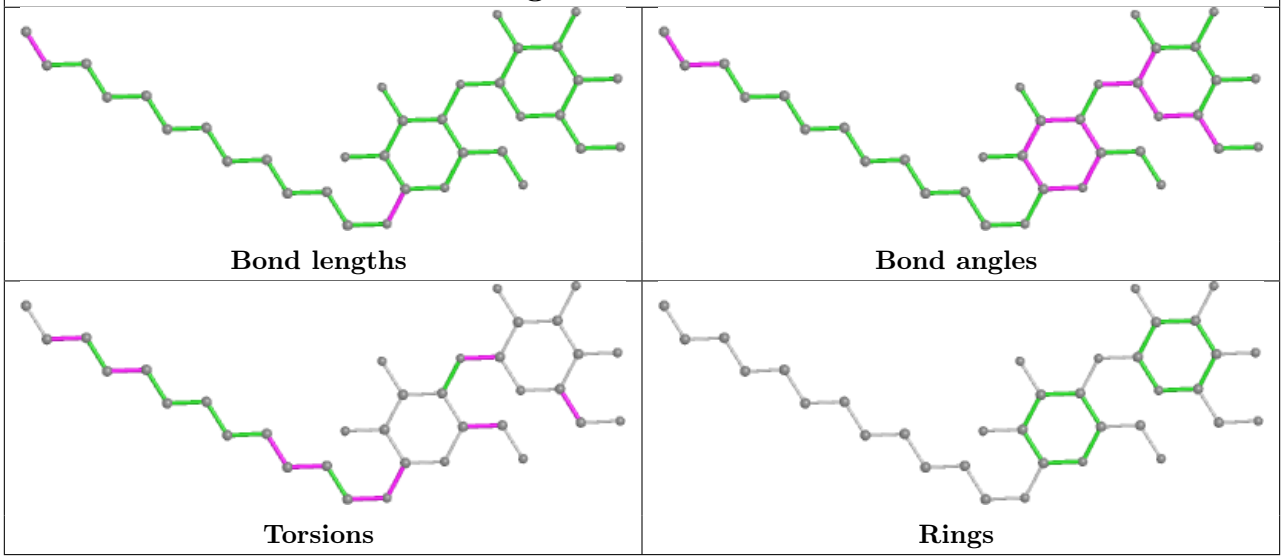
Ligand 8K6 5 106



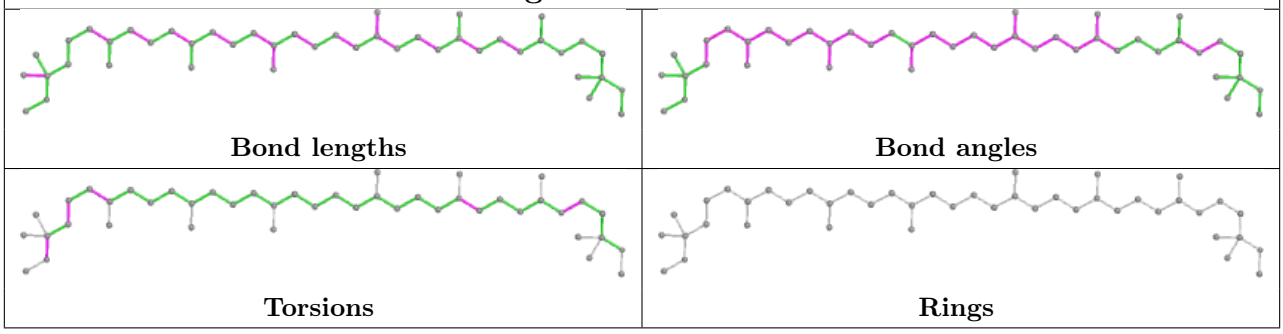
Ligand CDL S 101



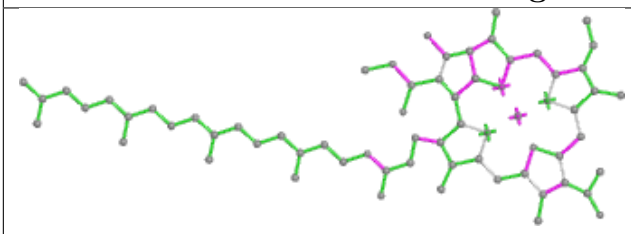
Ligand LMT 0 101



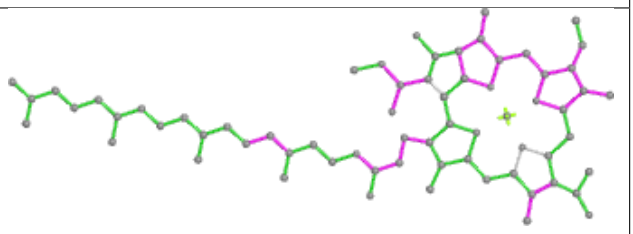
Ligand H4X G 101



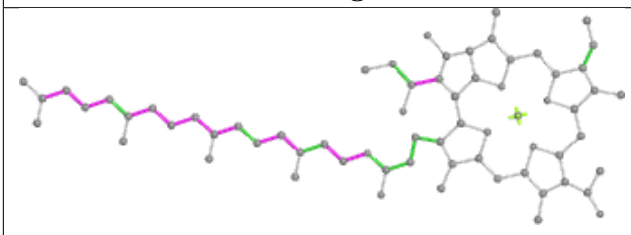
Ligand BCL 3 103



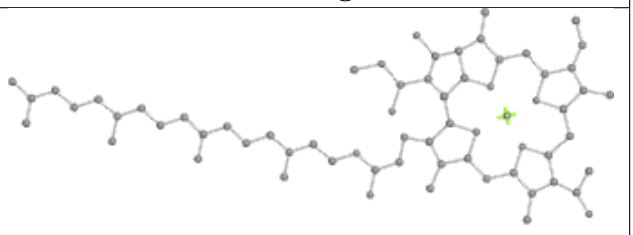
Bond lengths



Bond angles

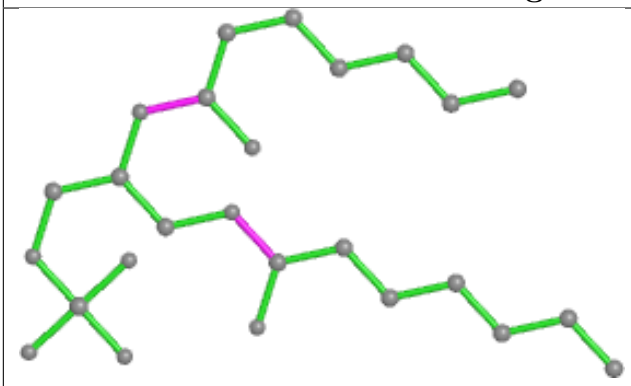


Torsions

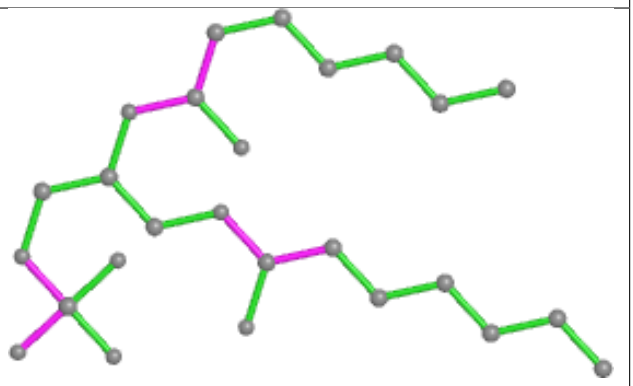


Rings

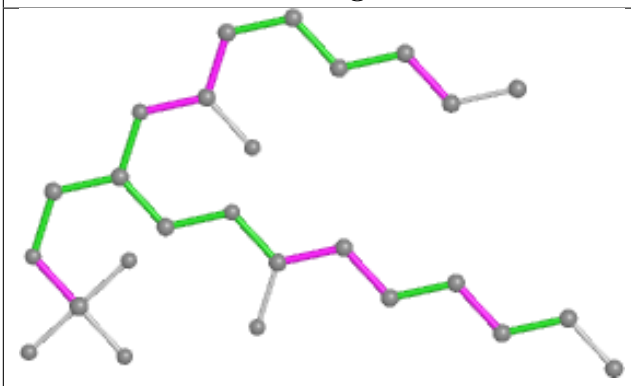
Ligand PGV 1 103



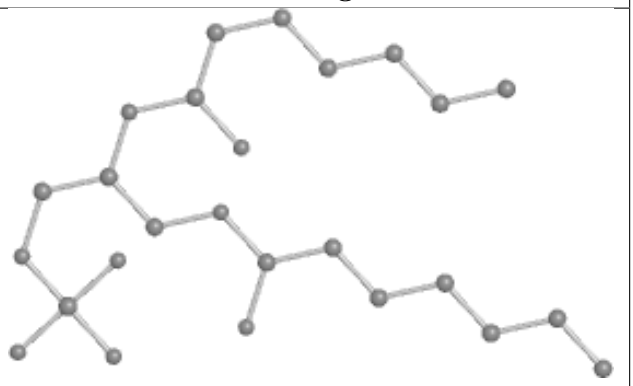
Bond lengths



Bond angles

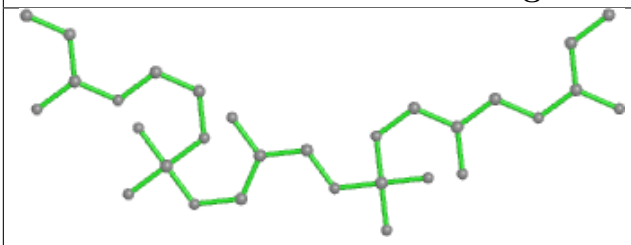


Torsions

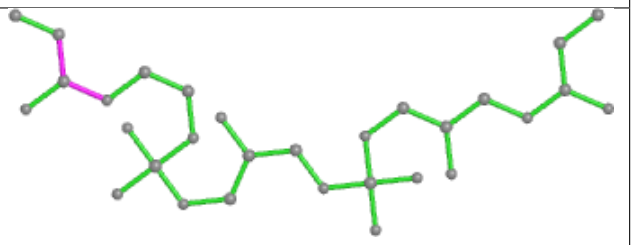


Rings

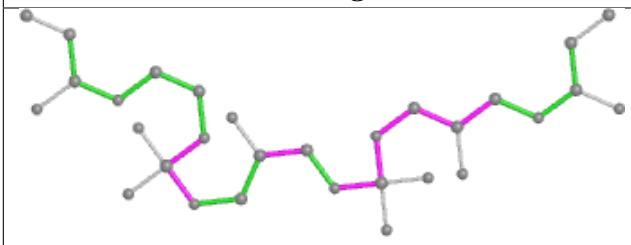
Ligand CDL Y 103



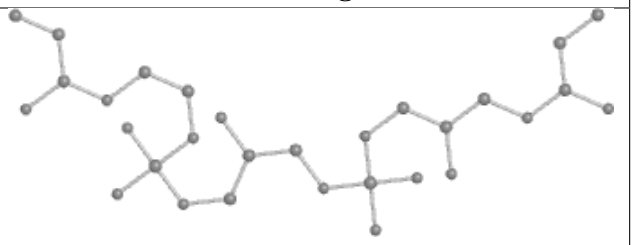
Bond lengths



Bond angles

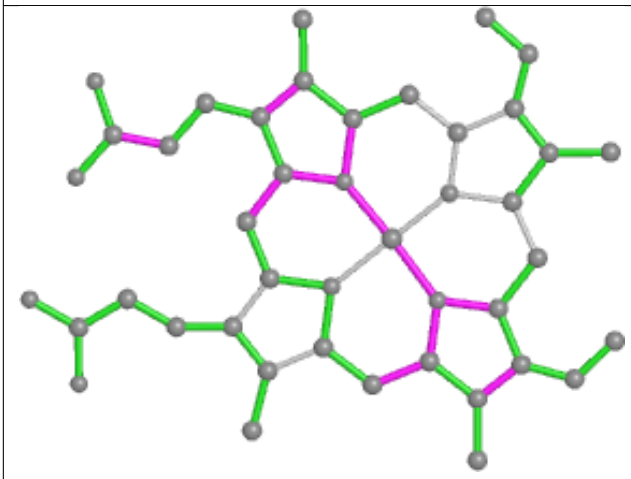


Torsions

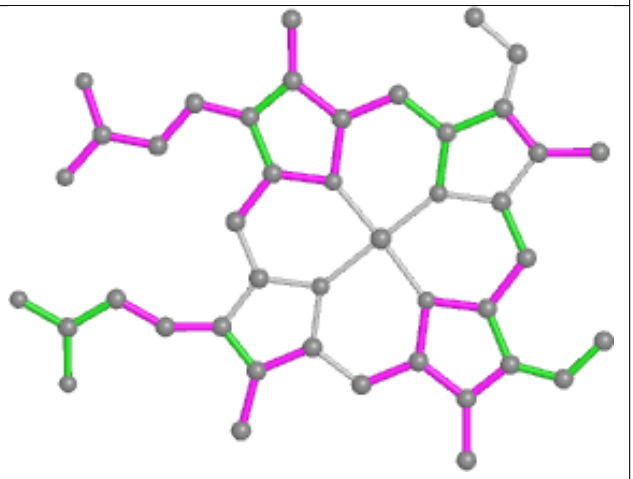


Rings

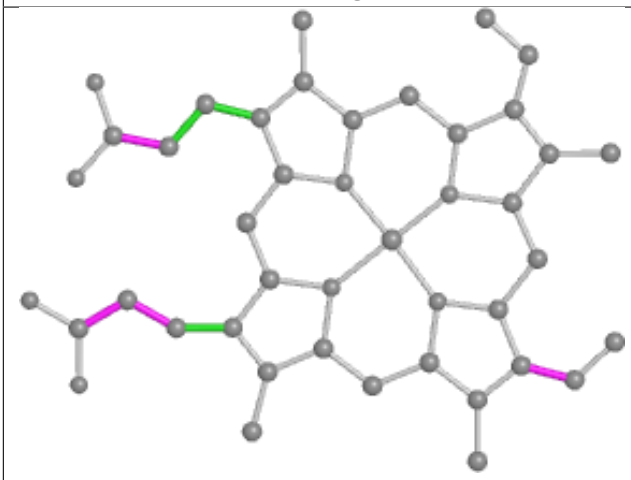
Ligand HEM C 401



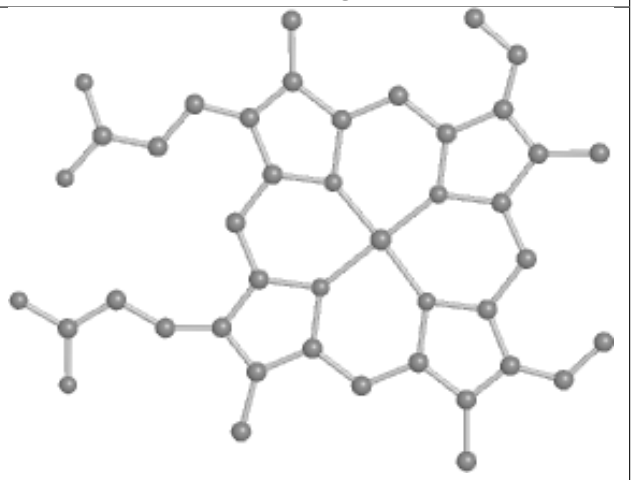
Bond lengths



Bond angles

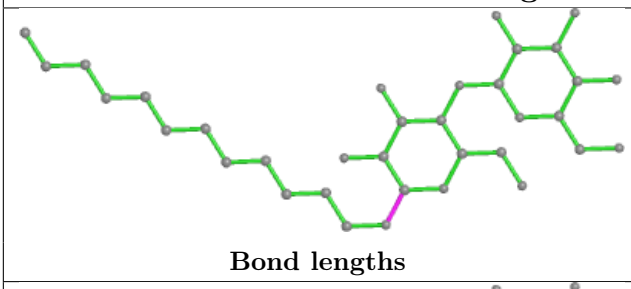


Torsions

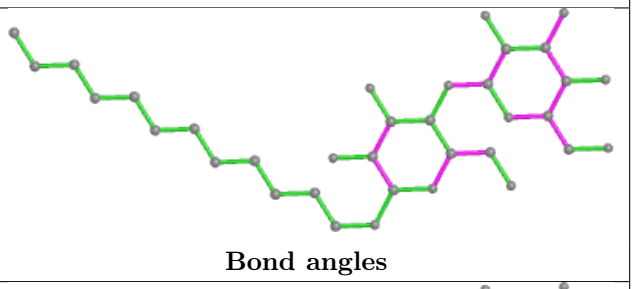


Rings

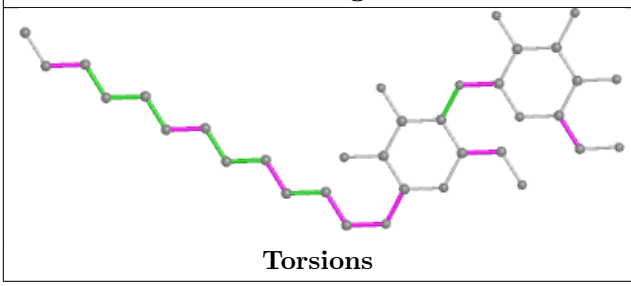
Ligand LMT N 101



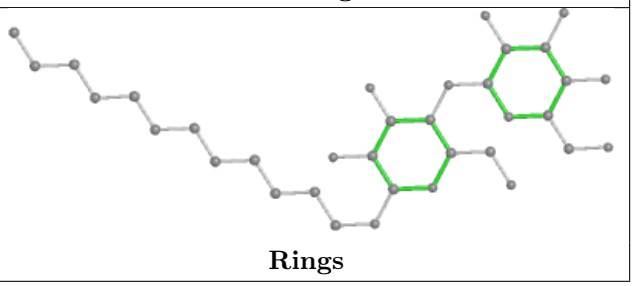
Bond lengths



Bond angles

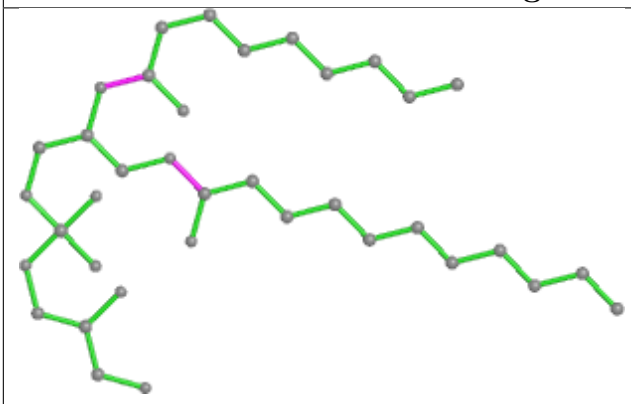


Torsions

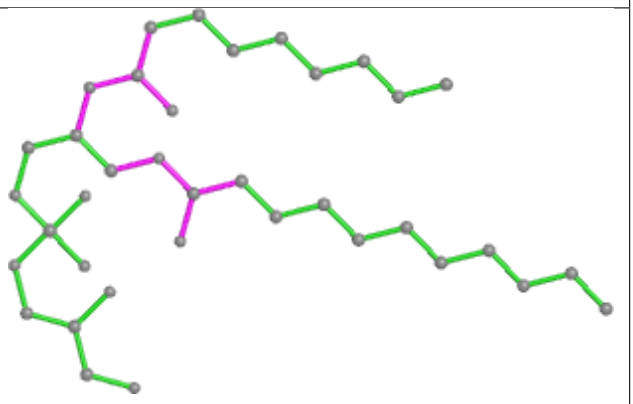


Rings

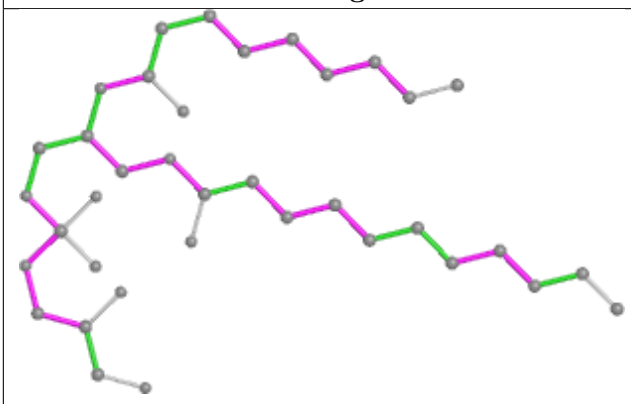
Ligand PGV F 104



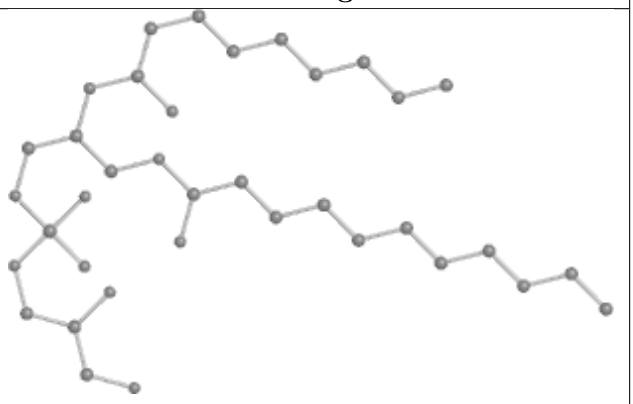
Bond lengths



Bond angles

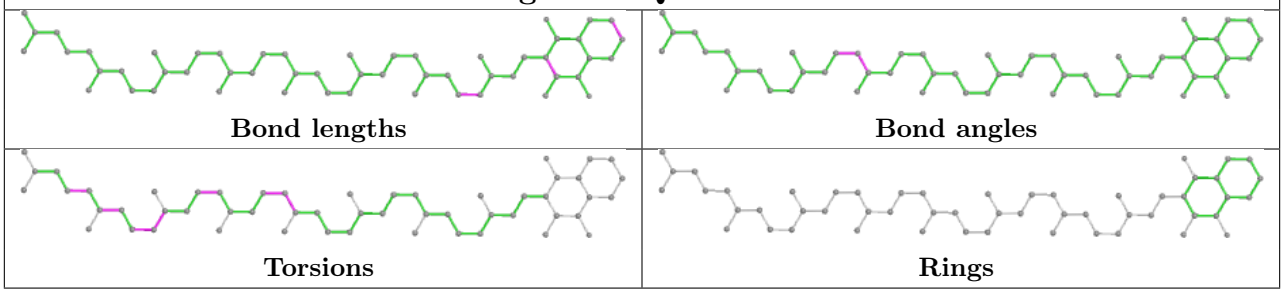


Torsions

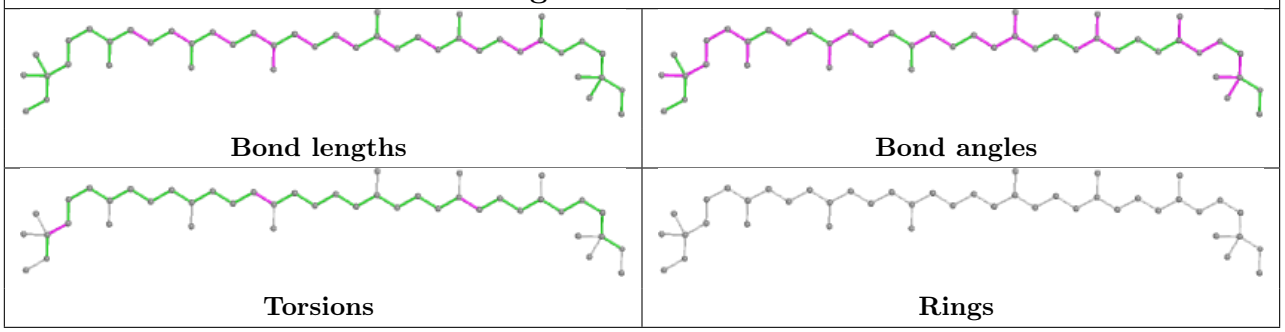


Rings

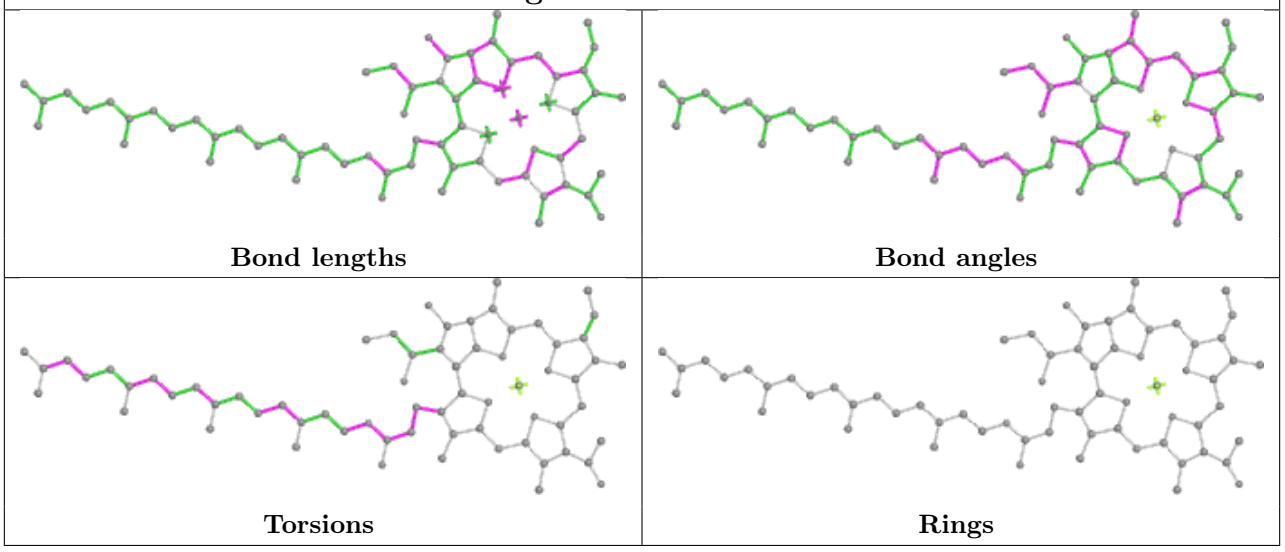
Ligand MQ8 M 405



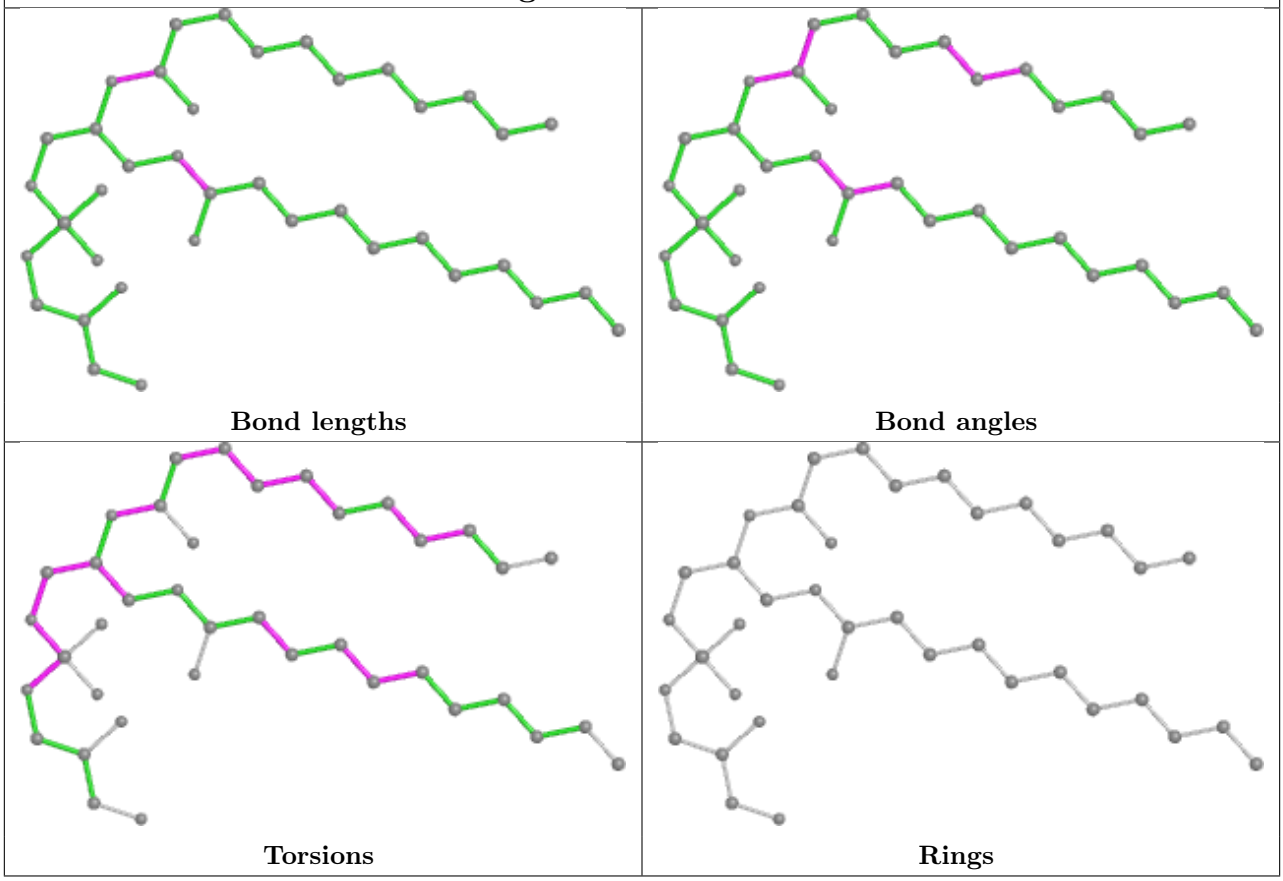
Ligand H4X 6 101



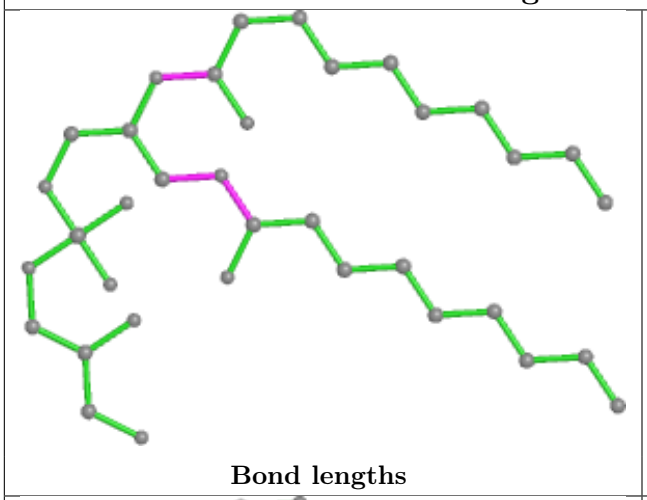
Ligand BCL D 104



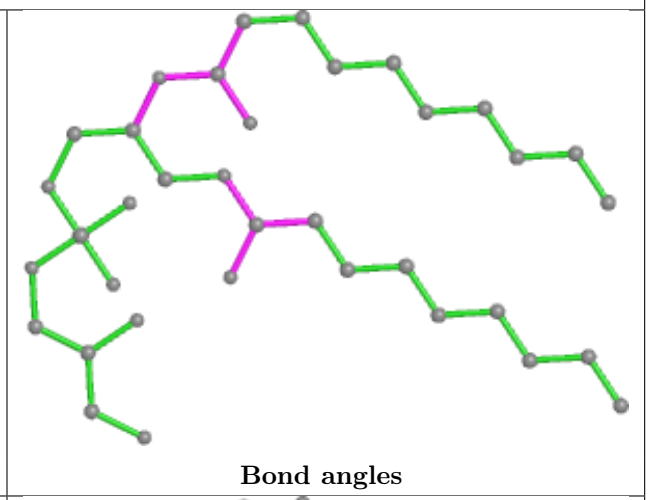
Ligand PGV M 406



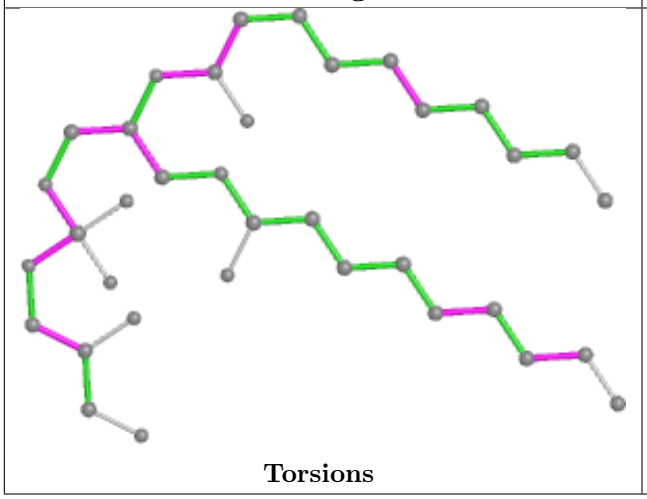
Ligand PGV H 301



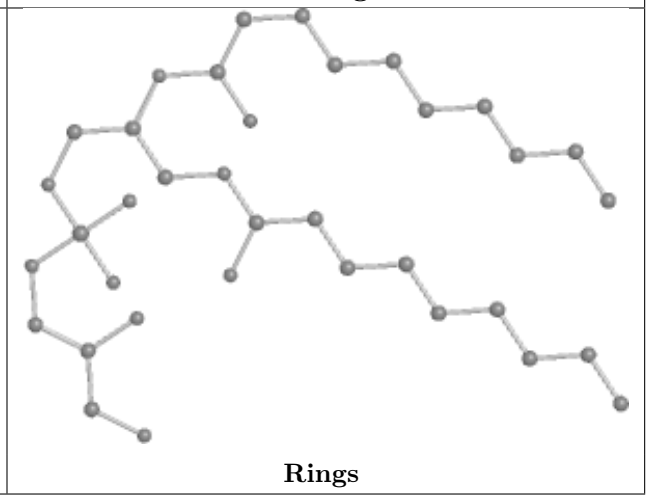
Bond lengths



Bond angles

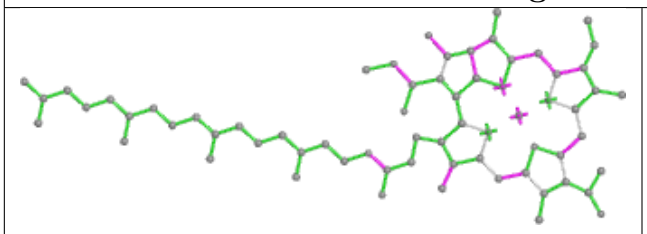


Torsions

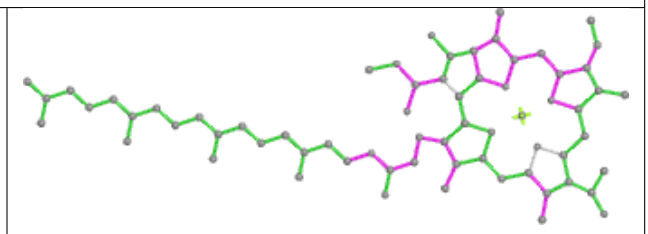


Rings

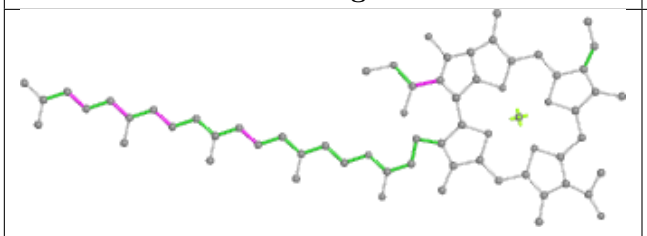
Ligand BCL S 103



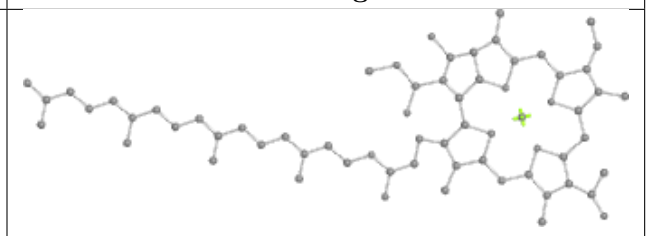
Bond lengths



Bond angles

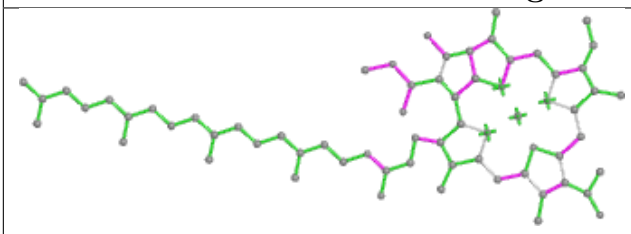


Torsions

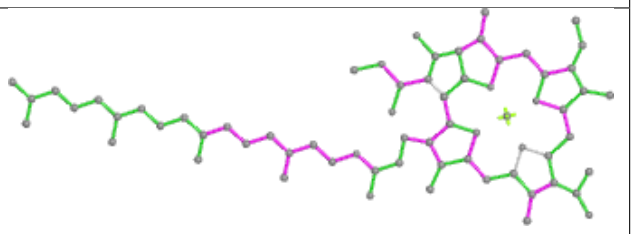


Rings

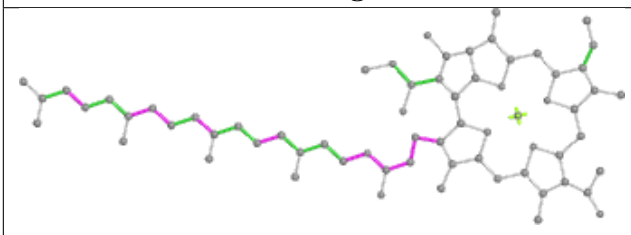
Ligand BCL F 105



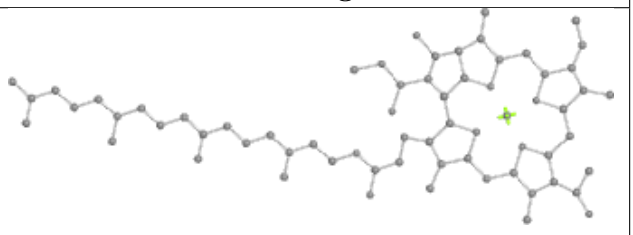
Bond lengths



Bond angles

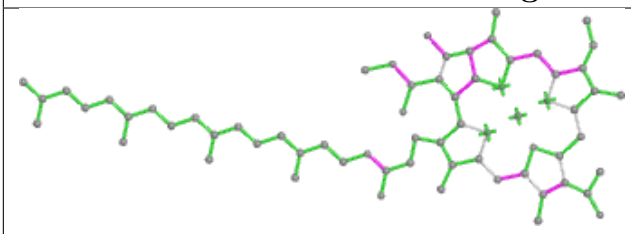


Torsions

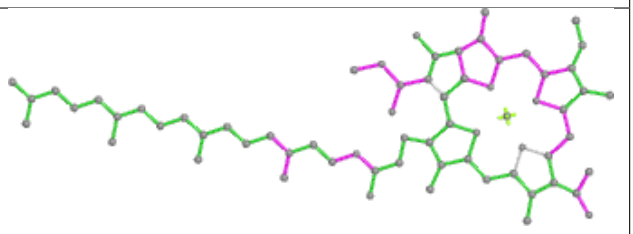


Rings

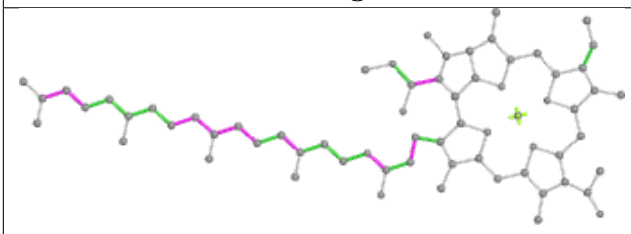
Ligand BCL M 402



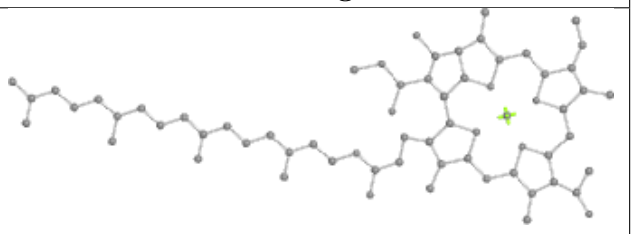
Bond lengths



Bond angles

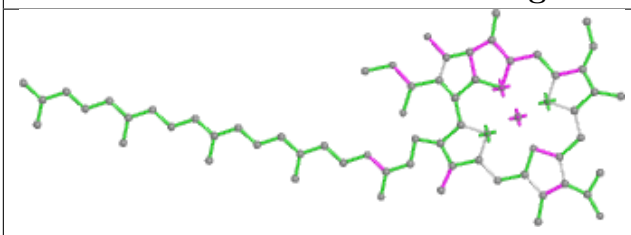


Torsions

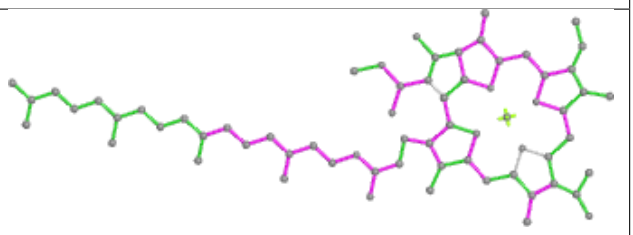


Rings

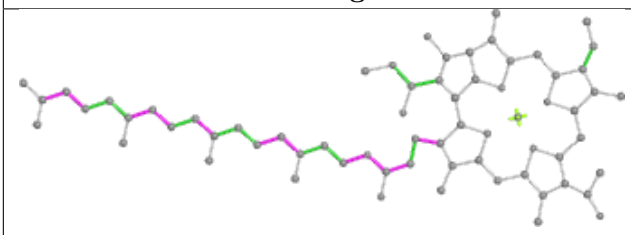
Ligand BCL J 101



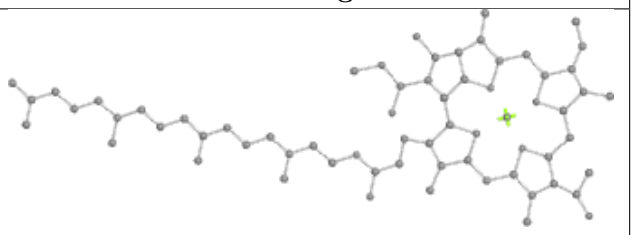
Bond lengths



Bond angles

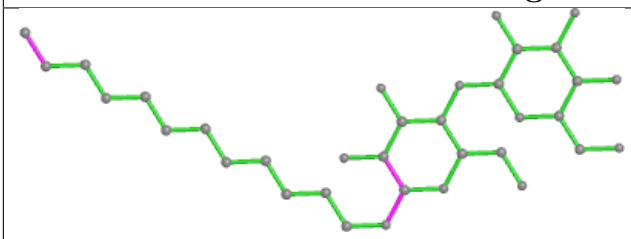


Torsions

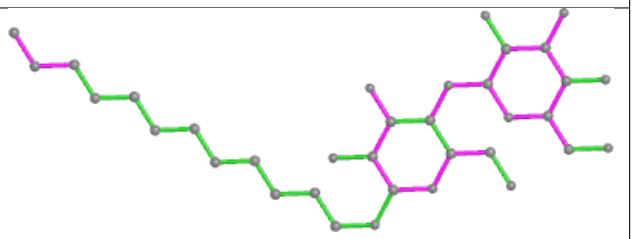


Rings

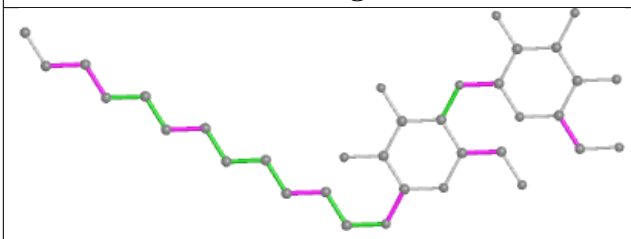
Ligand LMT 2 103



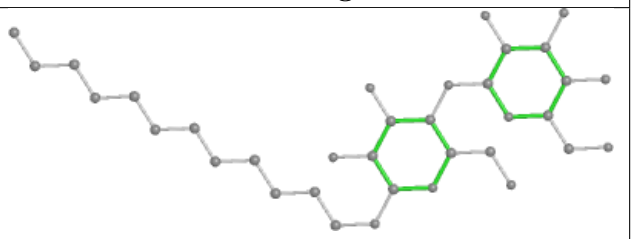
Bond lengths



Bond angles

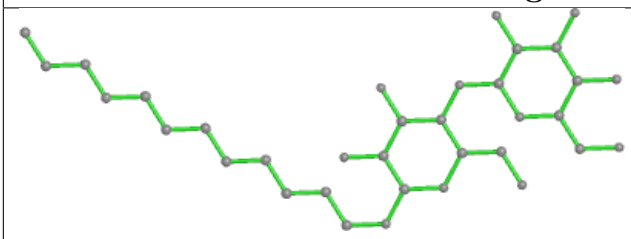


Torsions

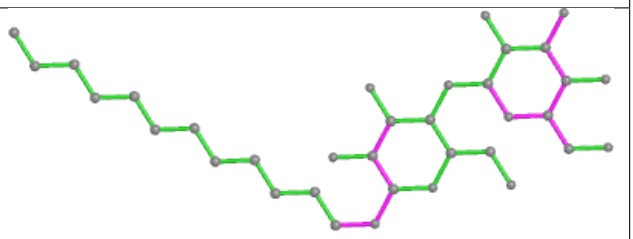


Rings

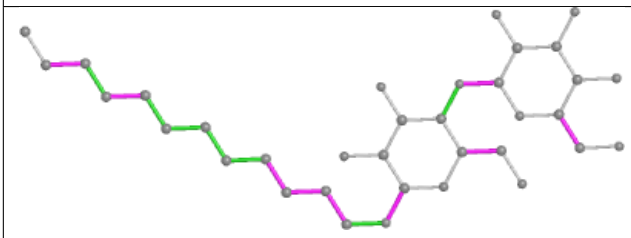
Ligand LMT 8 102



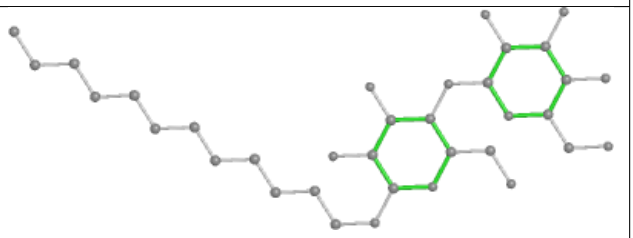
Bond lengths



Bond angles

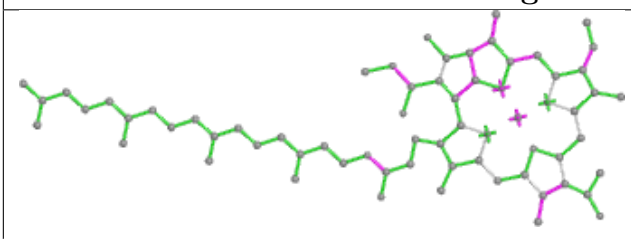


Torsions

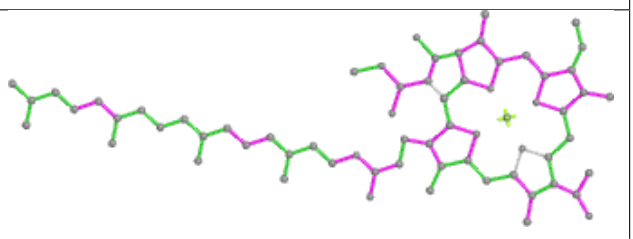


Rings

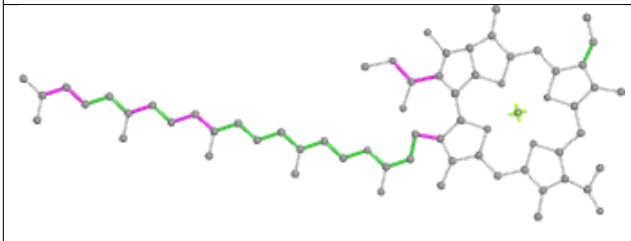
Ligand BCL M 403



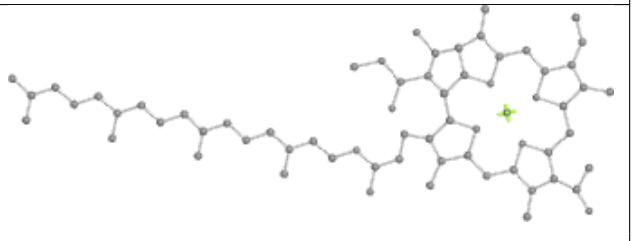
Bond lengths



Bond angles

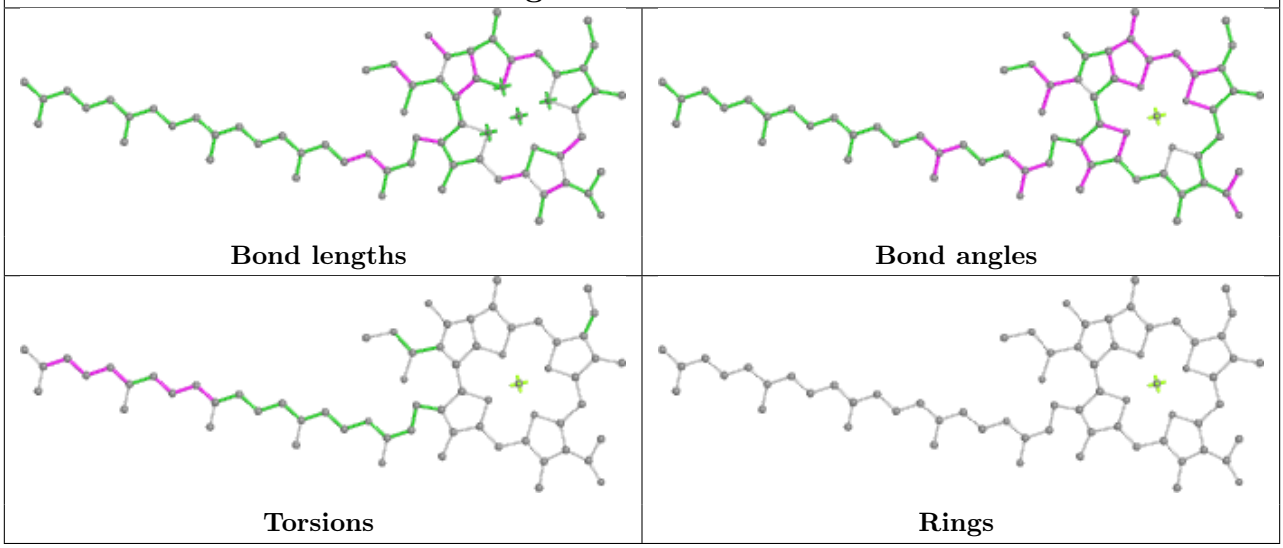


Torsions

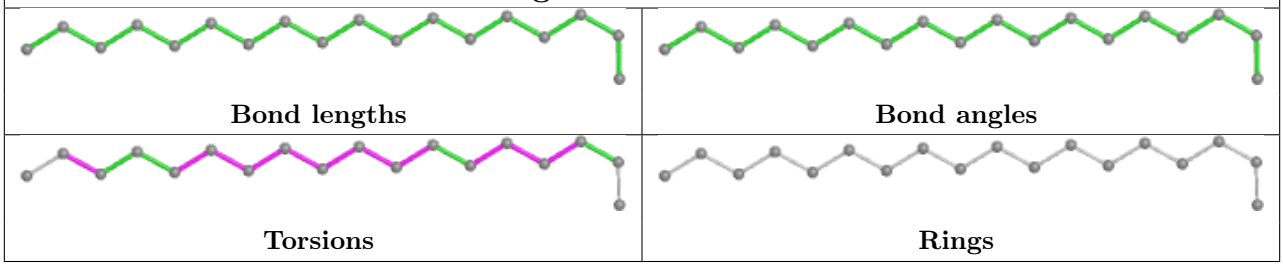


Rings

Ligand BCL Y 102

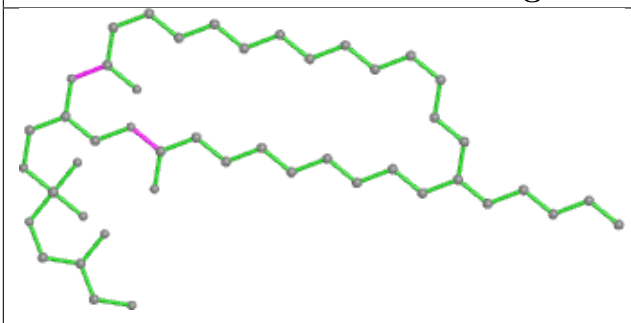


Ligand 8K6 L 307

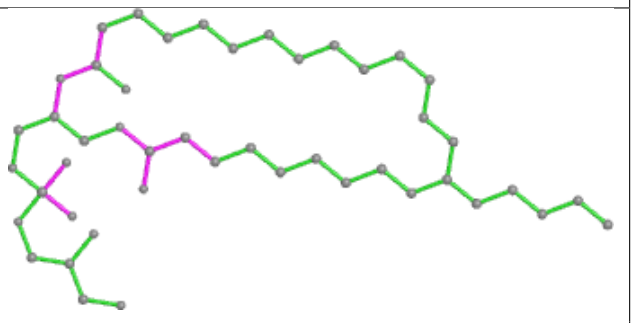


Ligand H4X P 101

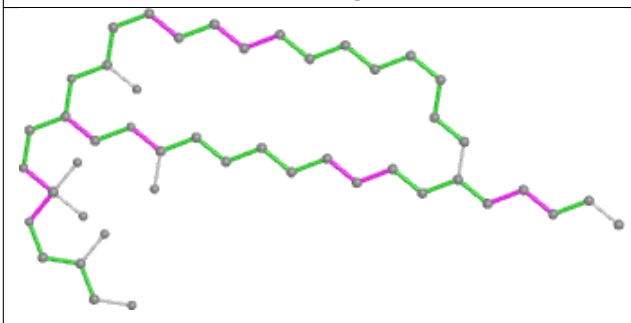
Ligand PGV L 305



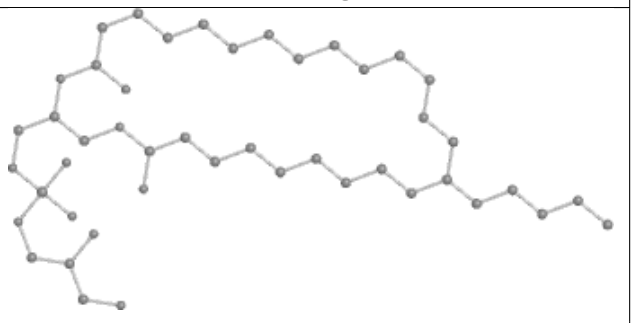
Bond lengths



Bond angles

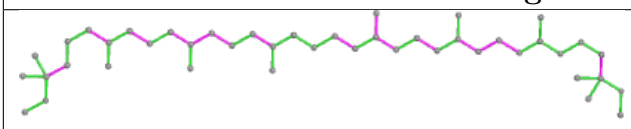


Torsions

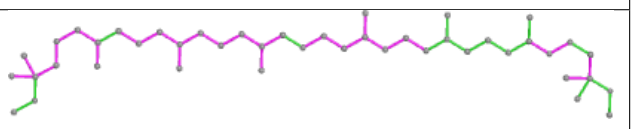


Rings

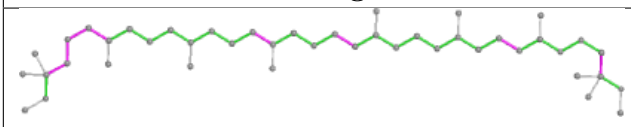
Ligand H4X O 101



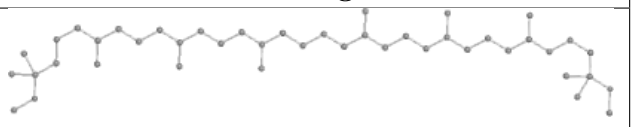
Bond lengths



Bond angles

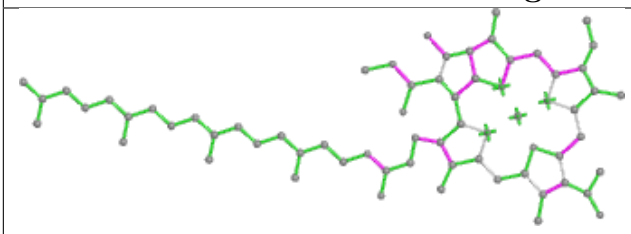


Torsions

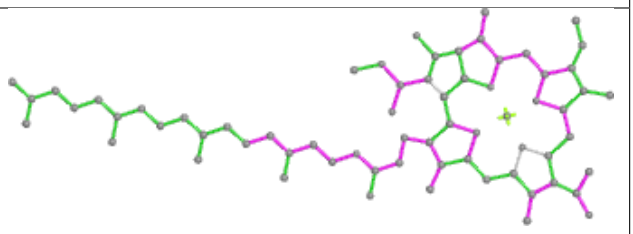


Rings

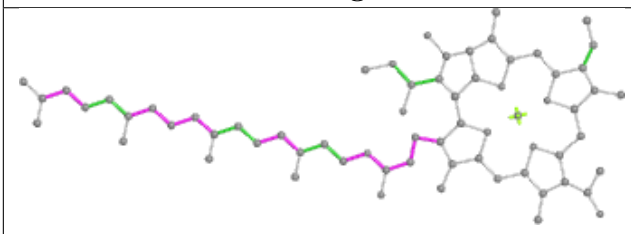
Ligand BCL X 101



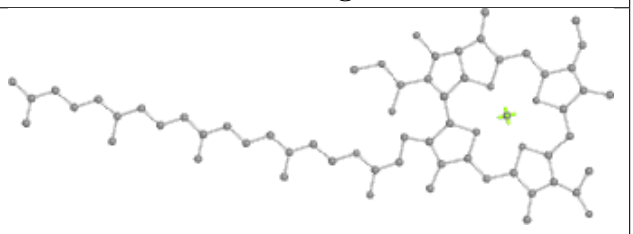
Bond lengths



Bond angles

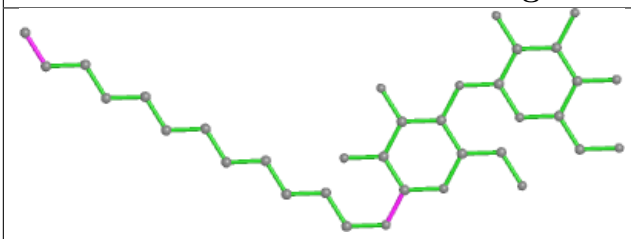


Torsions

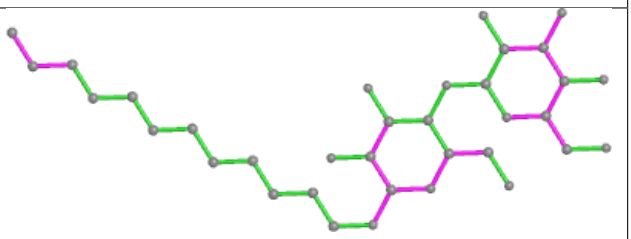


Rings

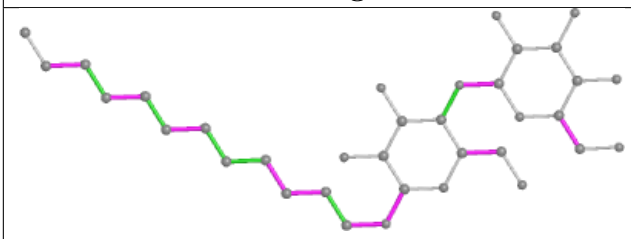
Ligand LMT E 102



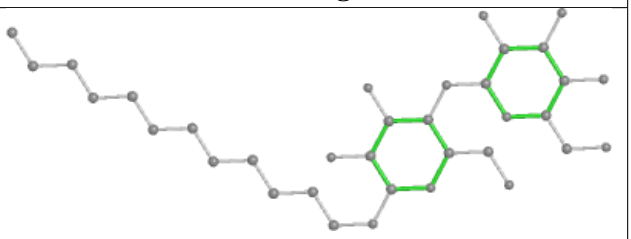
Bond lengths



Bond angles

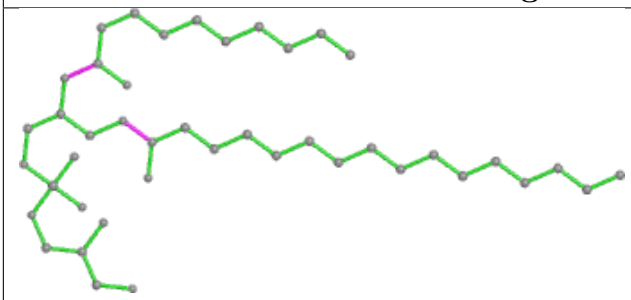


Torsions

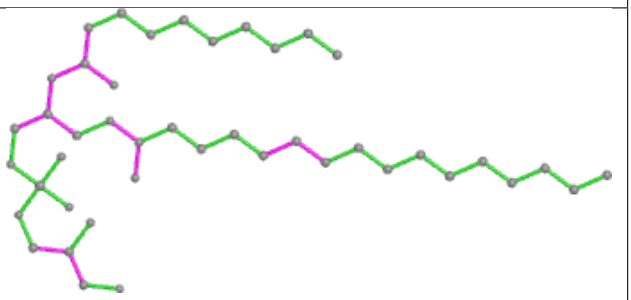


Rings

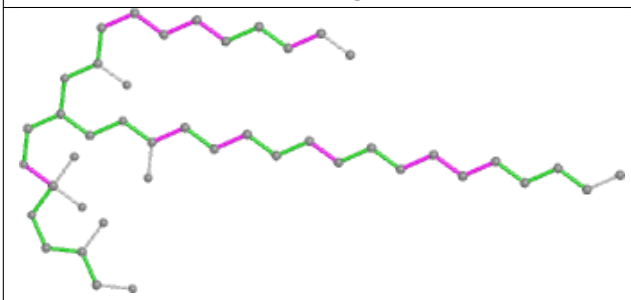
Ligand PGV D 101



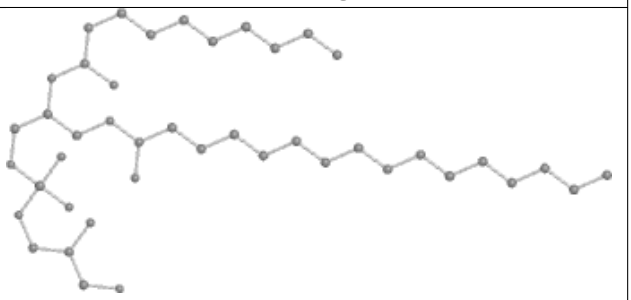
Bond lengths



Bond angles

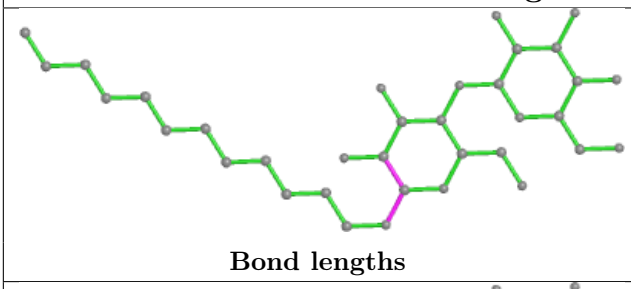


Torsions

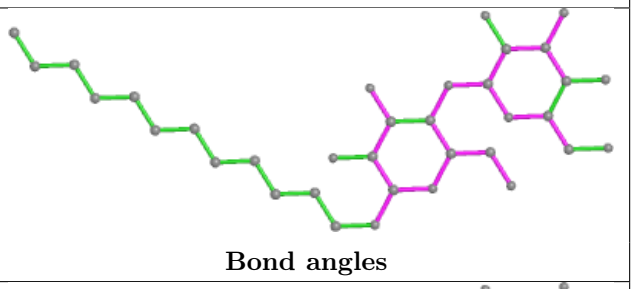


Rings

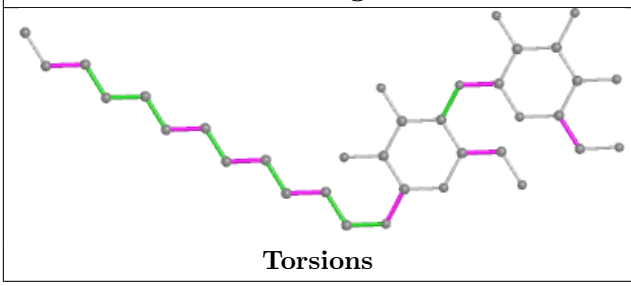
Ligand LMT J 102



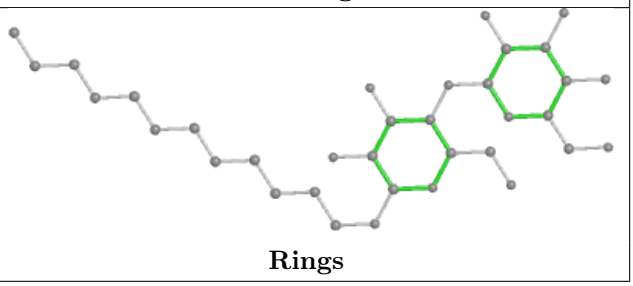
Bond lengths



Bond angles

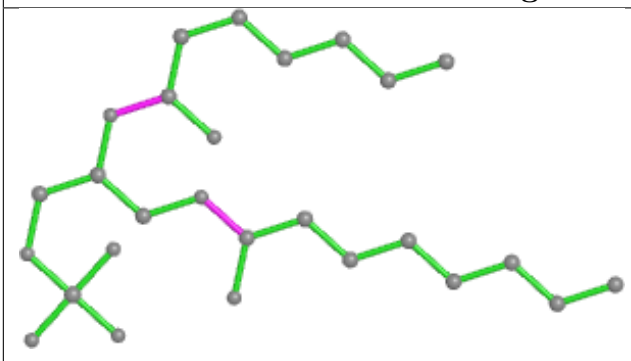


Torsions

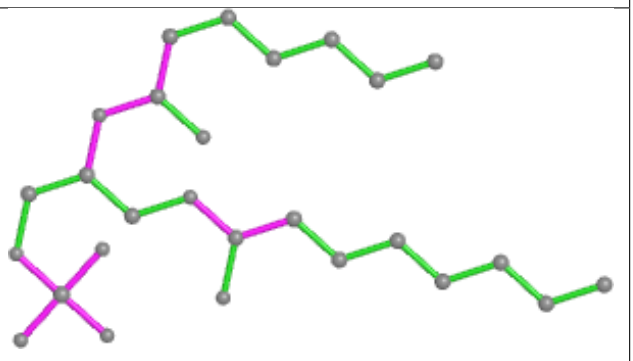


Rings

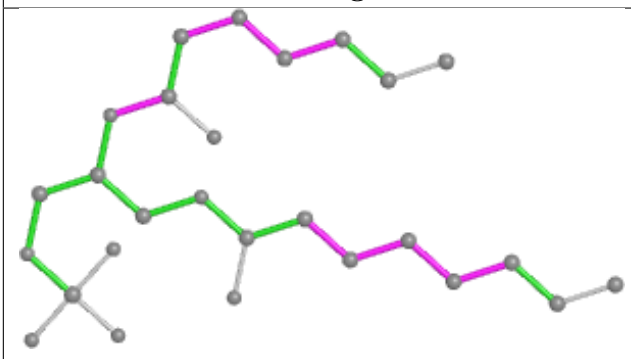
Ligand PGV Y 105



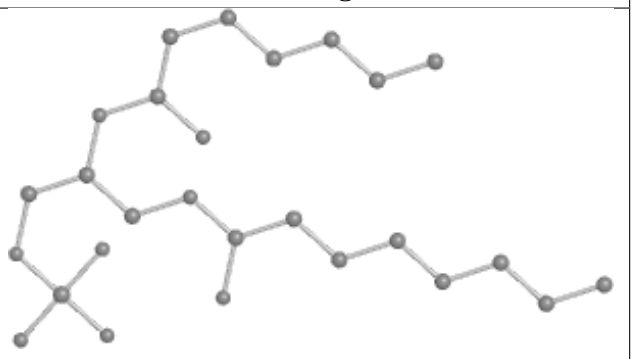
Bond lengths



Bond angles

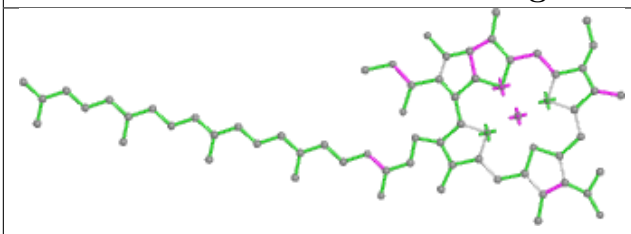


Torsions

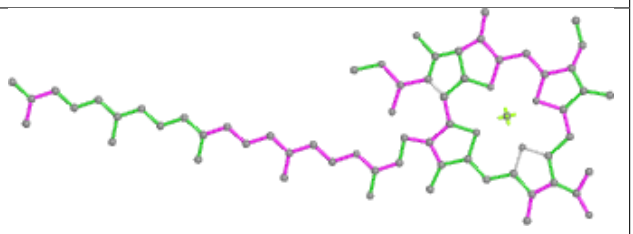


Rings

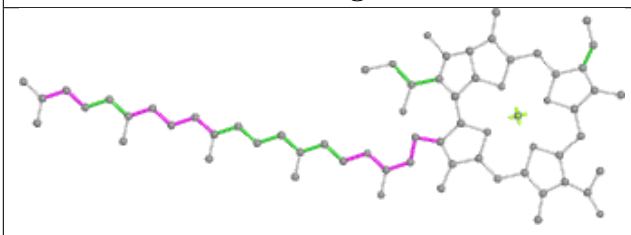
Ligand BCL 2 102



Bond lengths



Bond angles



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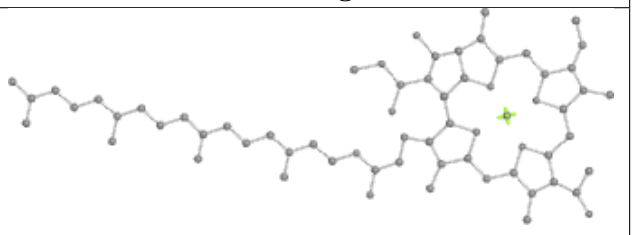
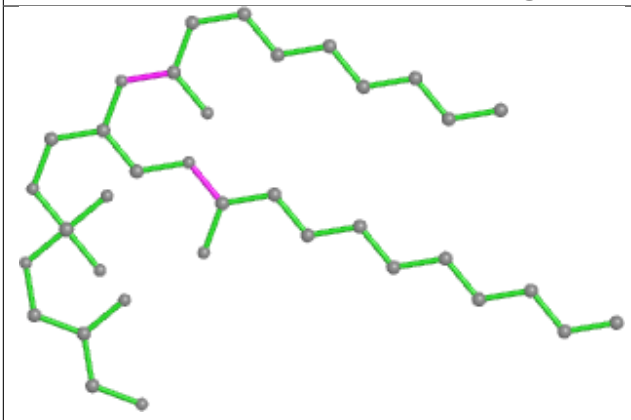
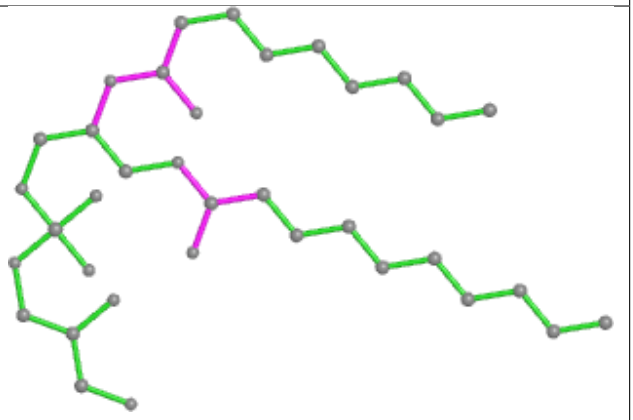


Rings

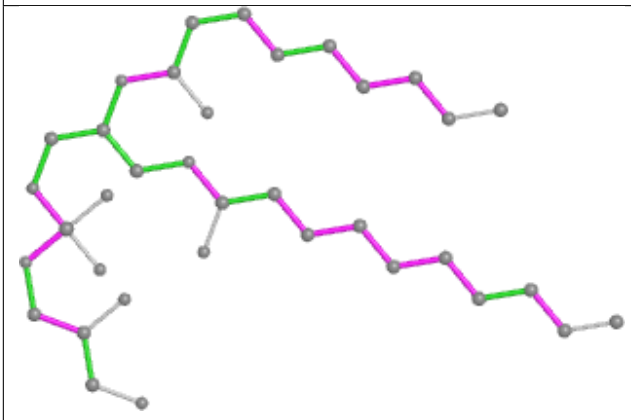
Ligand PGV K 101



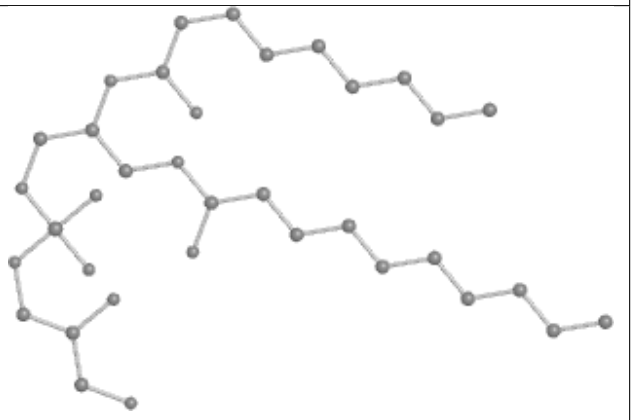
Bond lengths



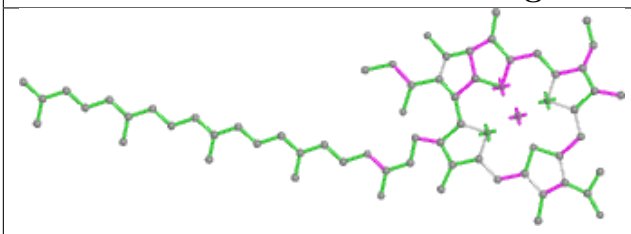
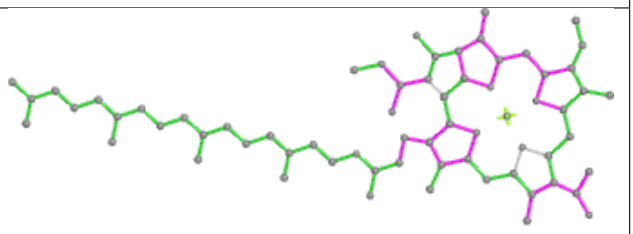
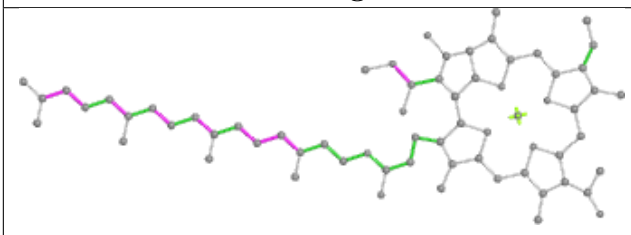
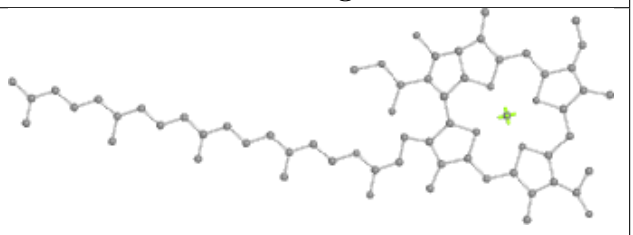
Bond angles



Torsions



Rings

Ligand BCL O 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30314. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.