Full wwPDB EM Validation Report ⓘ

Nov 27, 2023 – 02:24 PM JST

PDB ID	:	8IUN
EMDB ID	:	EMD-35727
Title	:	Cryo-EM structure of the CRT-LESS RC-LH core complex from roseiflexus castenholzii
Authors	:	Wang, G.-L.; Qi, C.-H.; Yu, L.-J.
Deposited on	:	2023-03-24
Resolution	:	2.85 Å(reported)

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

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

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

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

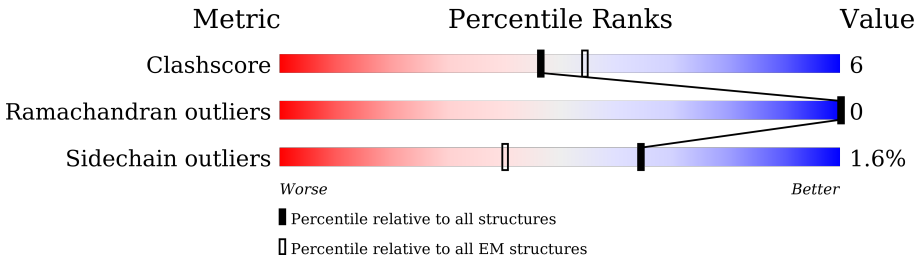
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	55	5% 80% 9% 9%
1	2	55	16% 80% 11% 9%
1	4	55	5% 87% 9%
1	6	55	82% 9% 9%
1	8	55	69% 22% 9%
1	B	55	91% 9%
1	E	55	80% 11% 9%
1	G	55	7% 85% 5% 9%

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Mol	Chain	Length	Quality of chain
1	I	55	75% 15% 9%
1	K	55	82% 9% 9%
1	O	55	87% 9%
1	Q	55	71% 20% 9%
1	S	55	80% 9% 9%
1	U	55	76% 15% 9%
1	W	55	73% 18% 9%
2	L	641	42% 55%
2	M	641	41% 6% 52%
3	1	42	12% 81% 10% 10%
3	3	42	5% 79% 14% 7%
3	5	42	81% 12% 7%
3	7	42	10% 83% 10% 7%
3	9	42	81% 10% 10%
3	A	42	83% 7% 10%
3	D	42	76% 14% 7%
3	F	42	76% 14% 10%
3	H	42	5% 79% 12% 7%
3	J	42	83% 10% 7%
3	N	42	83% 10% 7%
3	P	42	76% 17% 7%
3	R	42	86% 7% 7%
3	T	42	83% 7% 10%
3	V	42	7% 69% 21% 10%
4	Y	39	77% 5% 18%

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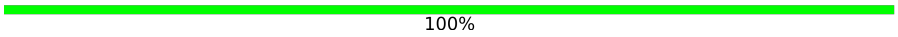
Mol	Chain	Length	Quality of chain
5	h	63	
6	C	320	
7	Z	10	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	UNL	9	103	-	-	X	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 24285 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 Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	W	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	U	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	S	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	Q	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	O	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	K	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	I	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	G	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	E	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	B	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	0	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	8	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	6	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	4	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	2	50	Total	C	N	O	S	0	0
			416	280	69	66	1		

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	306	Total	C	N	O	S	0	0
			2488	1673	399	409	7		
2	L	286	Total	C	N	O	S	0	0
			2278	1527	367	376	8		

- Molecule 3 is a protein called Alpha subunit of light-harvesting 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	J	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	N	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	P	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	R	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	T	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
3	V	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
3	1	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
3	3	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	5	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	7	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	9	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
3	A	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
3	D	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	F	38	Total	C	N	O	S	0	0
			300	201	51	47	1		

- Molecule 4 is a protein called reaction center small polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Y	32	Total	C	N	O	S	0	0
			259	181	36	39	3		

- Molecule 5 is a protein called reaction center small polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	47	Total	C	N	O	S	0	0
			362	242	59	60	1		

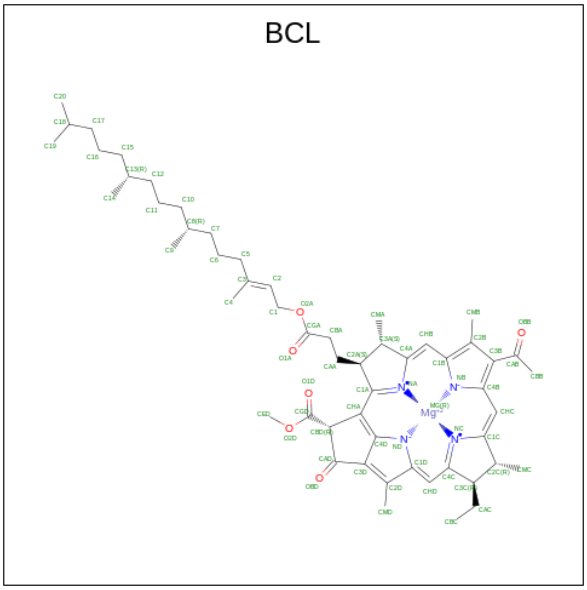
- Molecule 6 is a protein called Cytochrome subunit of photosynthetic reaction center.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	308	Total	C	N	O	S	0	0
			2347	1492	400	433	22		

- Molecule 7 is a protein called reaction center unknown polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Z	10	Total	C	N	O	0	0
			51	31	10	10		

- Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
8	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
8	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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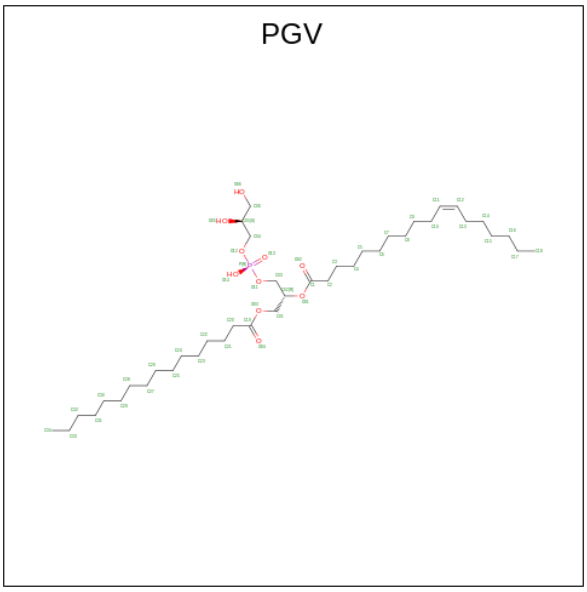
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 9 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
9	U	1	Total	C	O	P	0
			44	33	10	1	
9	U	1	Total	C	O	P	0
			44	33	10	1	
9	S	1	Total	C	O	P	0
			44	33	10	1	
9	O	1	Total	C	O	P	0
			44	33	10	1	
9	K	1	Total	C	O	P	0
			44	33	10	1	
9	K	1	Total	C	O	P	0
			44	33	10	1	
9	I	1	Total	C	O	P	0
			44	33	10	1	

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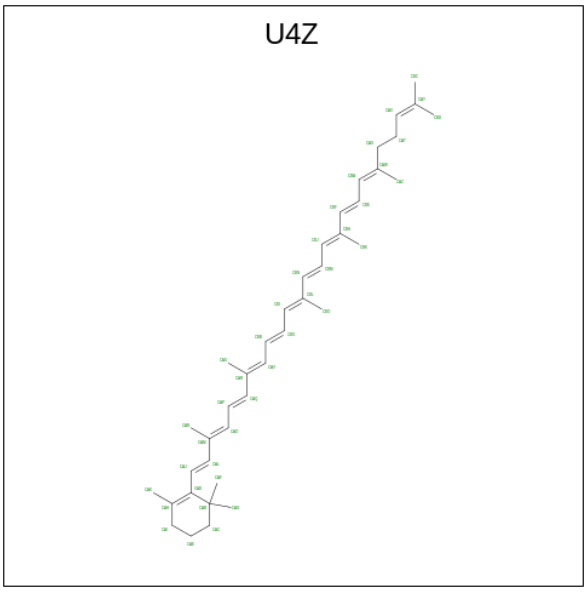
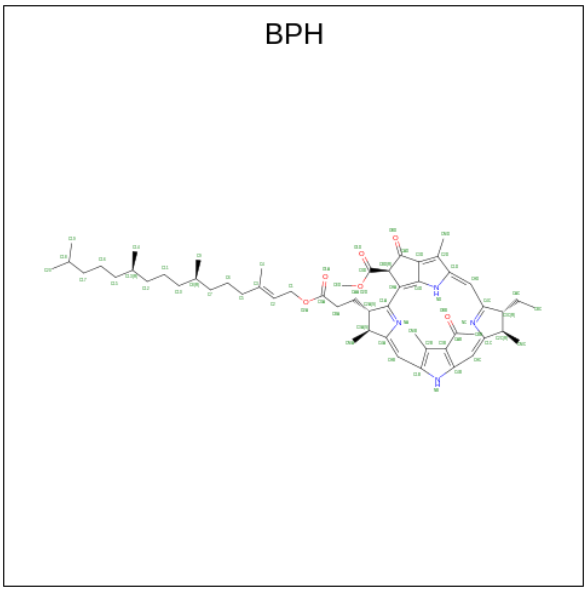
Mol	Chain	Residues	Atoms				AltConf
9	E	1	Total	C	O	P	0
			44	33	10	1	
9	E	1	Total	C	O	P	0
			44	33	10	1	
9	0	1	Total	C	O	P	0
			44	33	10	1	
9	0	1	Total	C	O	P	0
			44	33	10	1	
9	8	1	Total	C	O	P	0
			44	33	10	1	
9	6	1	Total	C	O	P	0
			44	33	10	1	
9	4	1	Total	C	O	P	0
			44	33	10	1	
9	M	1	Total	C	O	P	0
			35	24	10	1	
9	L	1	Total	C	O	P	0
			51	40	10	1	
9	L	1	Total	C	O	P	0
			33	23	9	1	
9	L	1	Total	C	O	P	0
			35	24	10	1	
9	N	1	Total	C	O	P	0
			24	13	10	1	
9	1	1	Total	C	O	P	0
			36	27	8	1	
9	h	1	Total	C	O	P	0
			46	37	8	1	
9	C	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 10 is gamma-Carotene (three-letter code: U4Z) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
10	0	1	Total C 40 40	0
10	J	1	Total C 40 40	0
10	R	1	Total C 40 40	0
10	3	1	Total C 40 40	0
10	D	1	Total C 40 40	0

- Molecule 11 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).

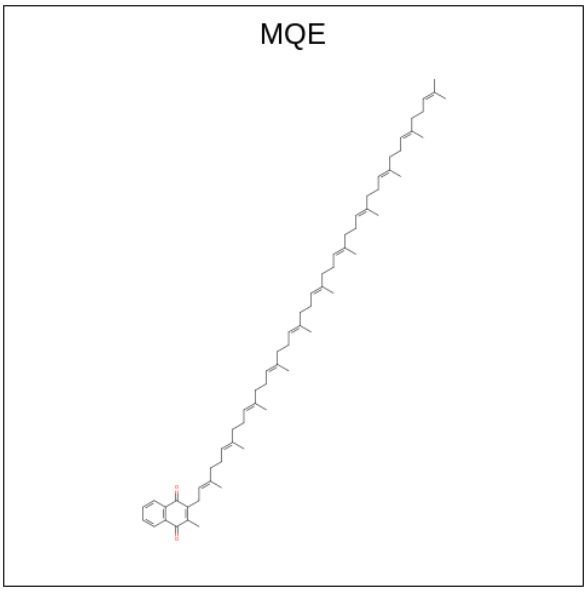


Mol	Chain	Residues	Atoms				AltConf
11	M	1	Total	C	N	O	0
			65	55	4	6	
11	L	1	Total	C	N	O	0
			65	55	4	6	
11	L	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

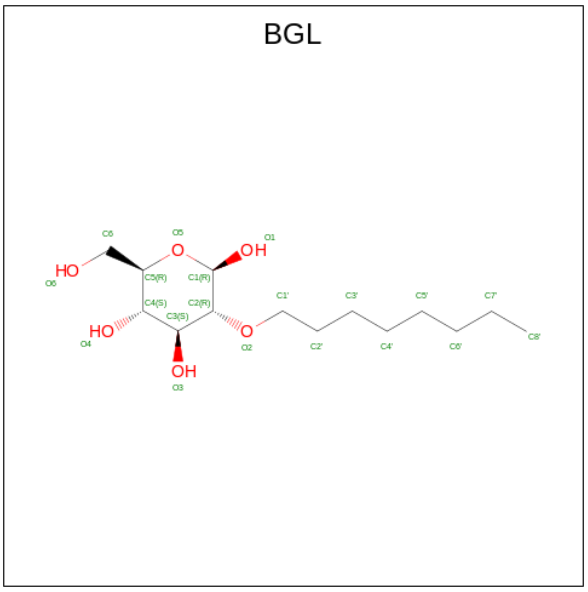
Mol	Chain	Residues	Atoms		AltConf
12	M	1	Total	Mn	0
			1	1	

- Molecule 13 is 2-methyl-3-[(2E,6E,10E,14E,18E,22E,26E,30E,34E,38E)-3,7,11,15,19,23,27,31,35,39,43-undecamethyltetratetraconta-2,6,10,1 4,18,22,26,30,34,38,42-undecaen-1-yl]naphthalene-1,4-dione (three-letter code: MQE) (formula: $C_{66}H_{96}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
13	M	1	Total C O 68 66 2	0
13	L	1	Total C O 53 51 2	0

- Molecule 14 is 2-O-octyl-beta-D-glucopyranose (three-letter code: BGL) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	AltConf
14	M	1	Total C O 20 14 6	0

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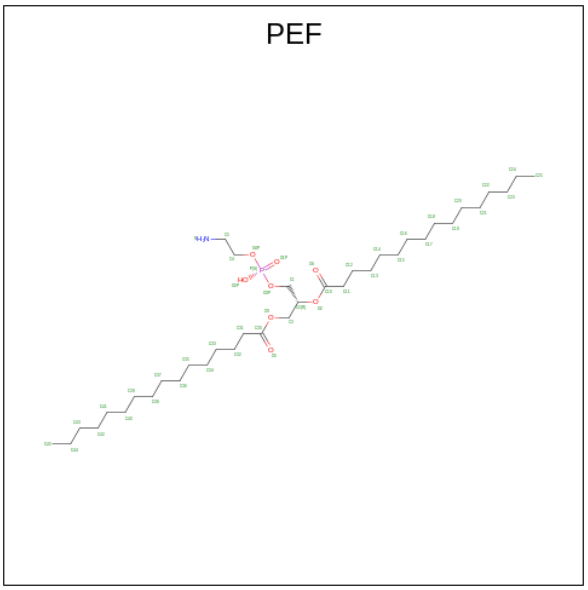
Mol	Chain	Residues	Atoms	AltConf
14	M	1	Total C O 20 14 6	0
14	M	1	Total C O 20 14 6	0
14	L	1	Total C O 20 14 6	0
14	L	1	Total C O 20 14 6	0
14	L	1	Total C O 20 14 6	0
14	L	1	Total C O 20 14 6	0
14	H	1	Total C O 20 14 6	0
14	Y	1	Total C O 20 14 6	0
14	Y	1	Total C O 20 14 6	0
14	C	1	Total C O 20 14 6	0

- Molecule 15 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
15	M	1	Total C N O P 21 11 1 8 1	0

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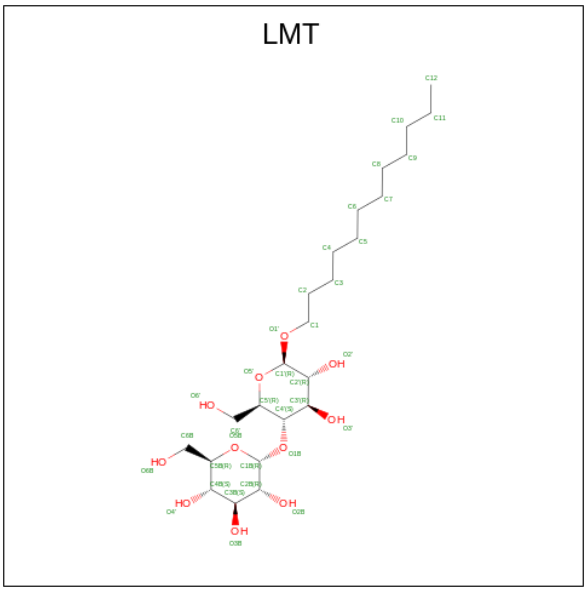
Mol	Chain	Residues	Atoms					AltConf
15	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
15	L	1	Total	C	N	O	P	0
			41	31	1	8	1	
15	h	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 16 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			35	24	11	
16	H	1	Total	C	O	0
			35	24	11	
16	T	1	Total	C	O	0
			35	24	11	
16	1	1	Total	C	O	0
			35	24	11	
16	D	1	Total	C	O	0
			35	24	11	

- Molecule 17 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		AltConf
17	M	3	Total	C	0
			44	44	

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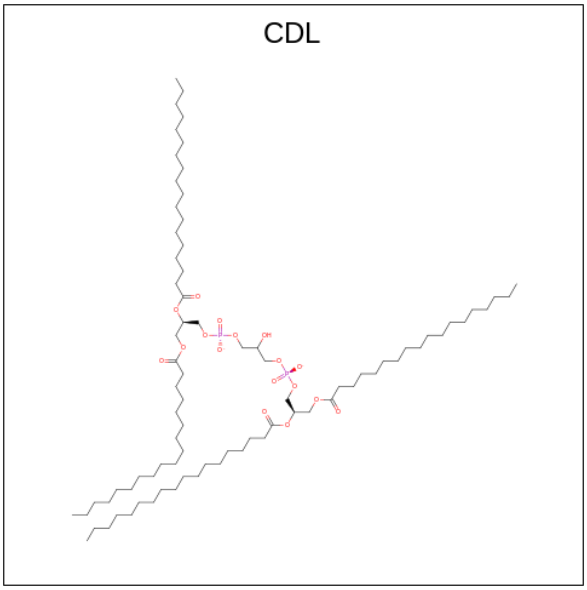
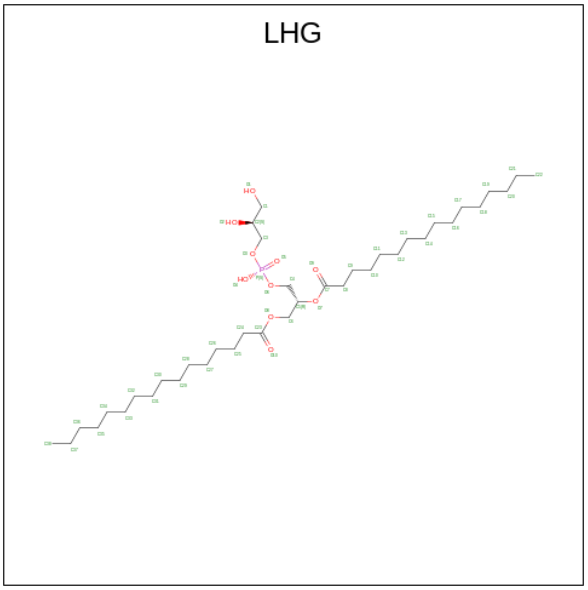
Mol	Chain	Residues	Atoms	AltConf
17	L	3	Total C 30 30	0
17	H	1	Total C 13 13	0
17	V	2	Total C 26 26	0
17	1	1	Total C 18 18	0
17	9	2	Total C 36 36	0
17	A	1	Total C 18 18	0
17	D	1	Total C 12 12	0
17	F	1	Total C 15 15	0
17	Y	1	Total C 14 14	0
17	h	2	Total C 24 24	0
17	C	2	Total C 34 34	0

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



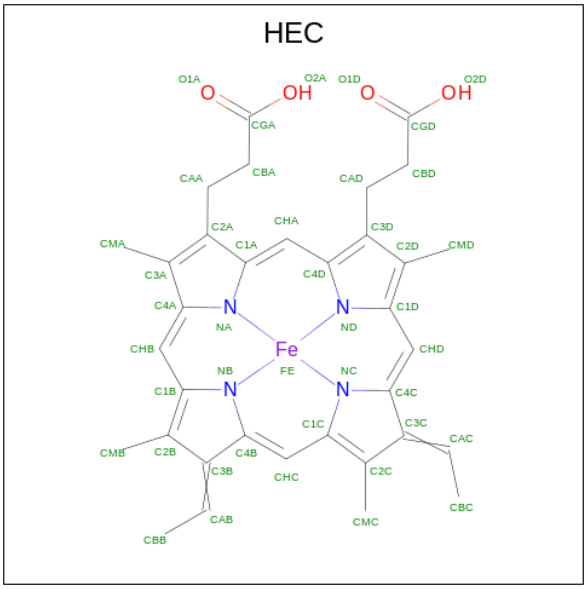
Mol	Chain	Residues	Atoms				AltConf
18	P	1	Total	C	O	P	0
			50	31	17	2	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
19	h	1	Total	C	O	0
			24	20	4	

- Molecule 20 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 21 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
21	C	1	Total	Ca	0
			1	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Antenna complex alpha/beta subunit

Chain W:

• Molecule 1: Antenna complex alpha/beta subunit

Chain U:

• Molecule 1: Antenna complex alpha/beta subunit

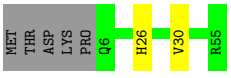
Chain S:

• Molecule 1: Antenna complex alpha/beta subunit

Chain Q:

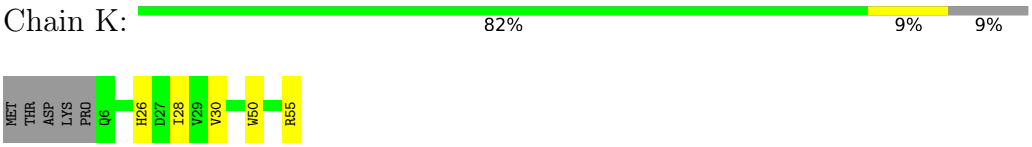
• Molecule 1: Antenna complex alpha/beta subunit

Chain O:



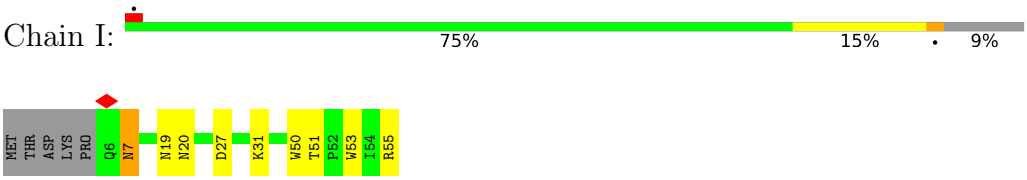
• Molecule 1: Antenna complex alpha/beta subunit

Chain K:



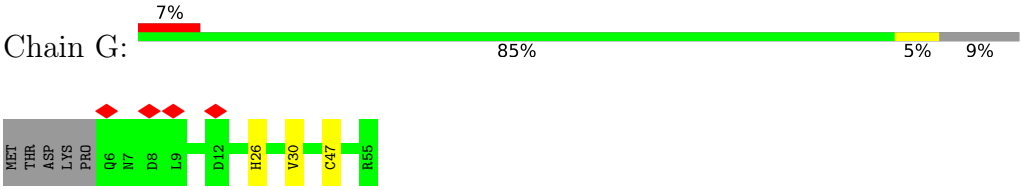
• Molecule 1: Antenna complex alpha/beta subunit

Chain I:



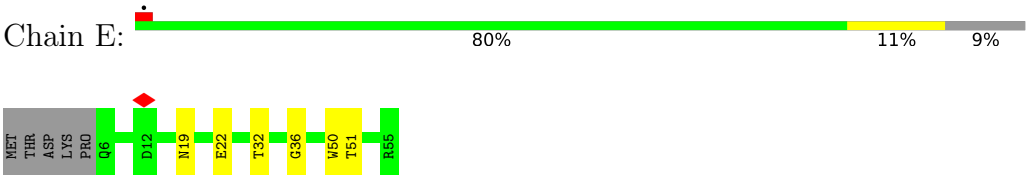
• Molecule 1: Antenna complex alpha/beta subunit

Chain G:



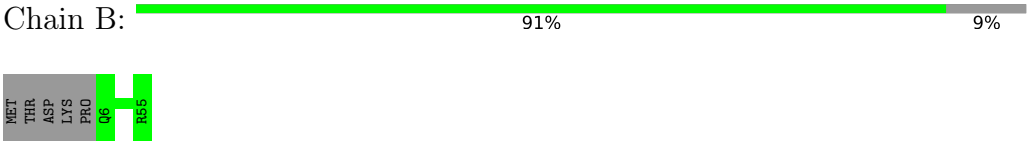
• Molecule 1: Antenna complex alpha/beta subunit

Chain E:



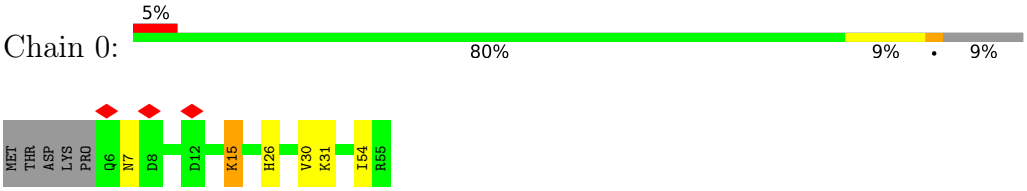
• Molecule 1: Antenna complex alpha/beta subunit

Chain B:



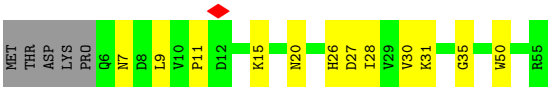
• Molecule 1: Antenna complex alpha/beta subunit

Chain 0:



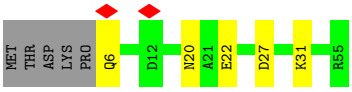
• Molecule 1: Antenna complex alpha/beta subunit

Chain 8:



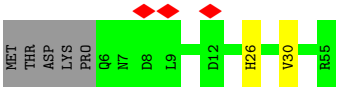
• Molecule 1: Antenna complex alpha/beta subunit

Chain 6:



• Molecule 1: Antenna complex alpha/beta subunit

Chain 4:

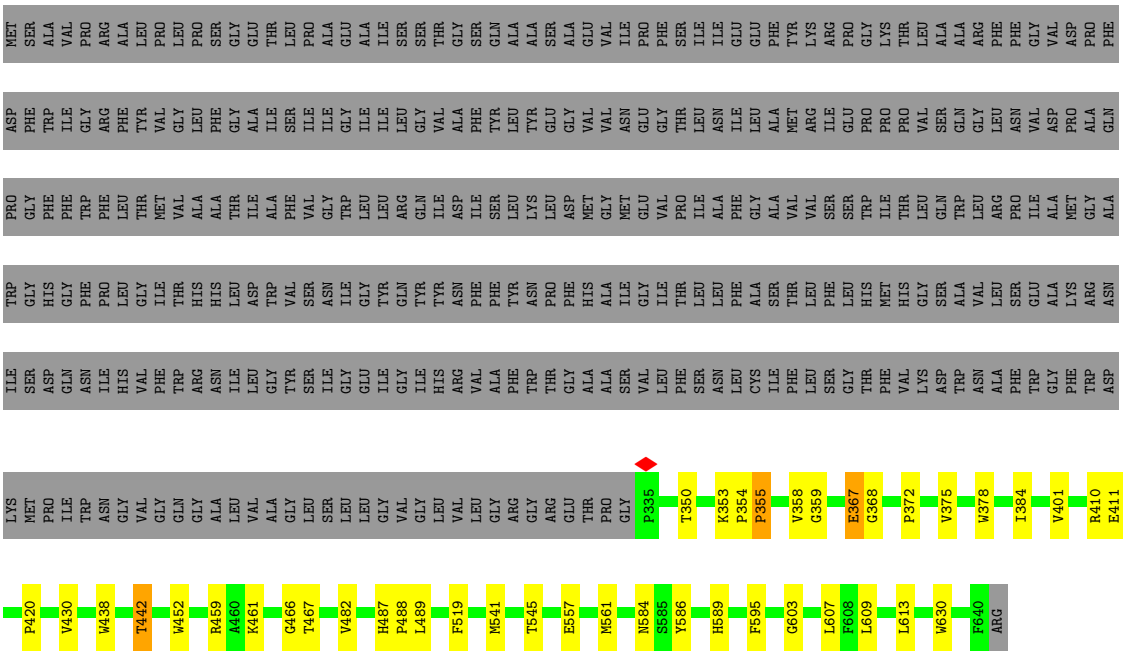


• Molecule 1: Antenna complex alpha/beta subunit

Chain 2:

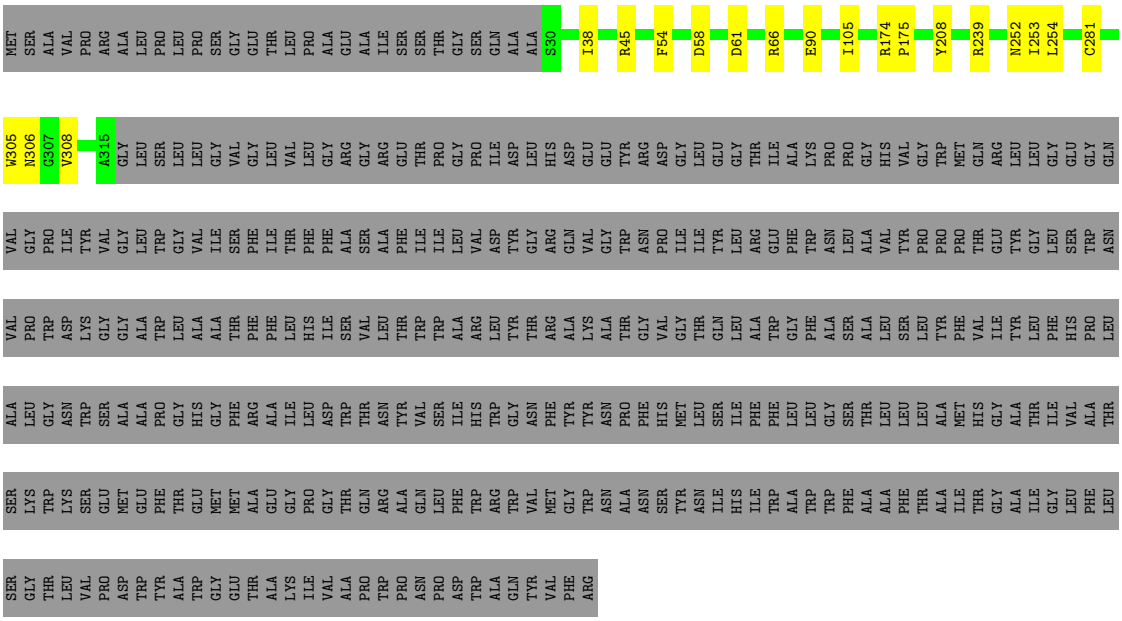
• Molecule 2: Reaction center protein L chain

Chain M:



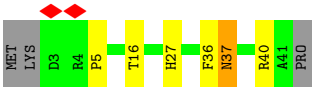
• Molecule 2: Reaction center protein L chain

Chain L:



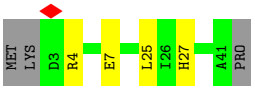
• Molecule 3: Alpha subunit of light-harvesting 1

Chain H:



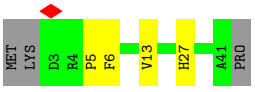
• Molecule 3: Alpha subunit of light-harvesting 1

Chain J:



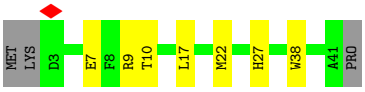
• Molecule 3: Alpha subunit of light-harvesting 1

Chain N:



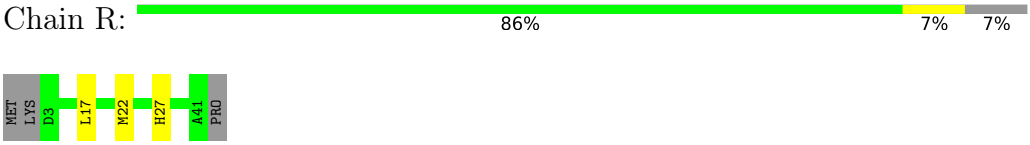
• Molecule 3: Alpha subunit of light-harvesting 1

Chain P:



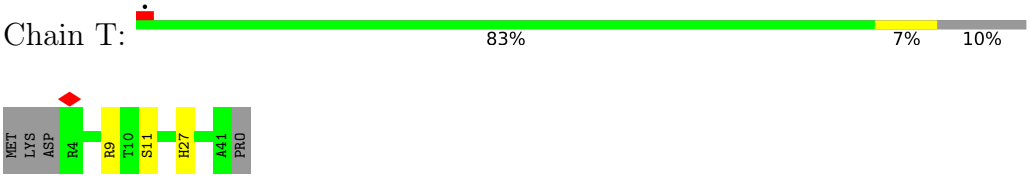
• Molecule 3: Alpha subunit of light-harvesting 1

Chain R:



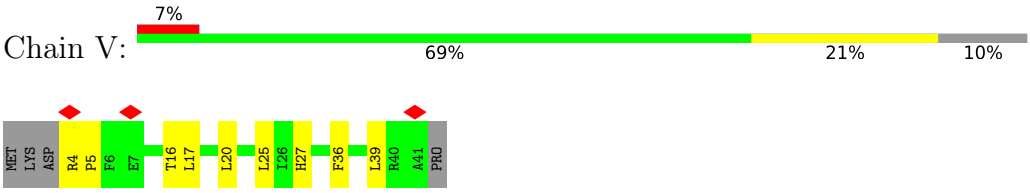
• Molecule 3: Alpha subunit of light-harvesting 1

Chain T:



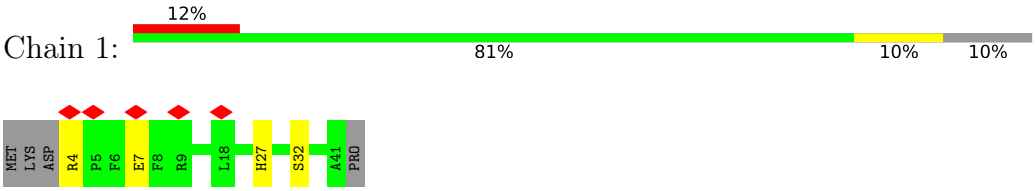
• Molecule 3: Alpha subunit of light-harvesting 1

Chain V:



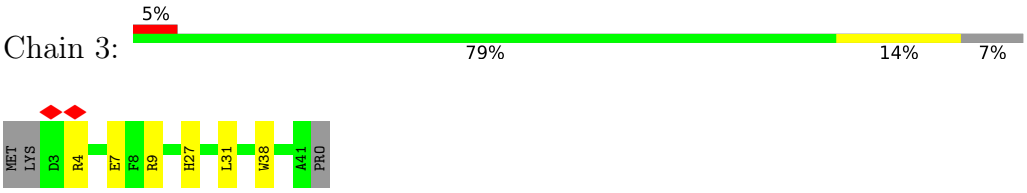
• Molecule 3: Alpha subunit of light-harvesting 1

Chain 1:



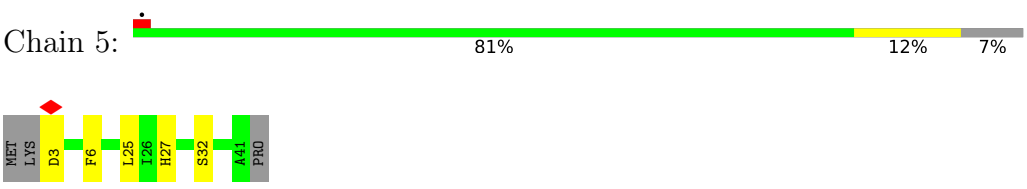
• Molecule 3: Alpha subunit of light-harvesting 1

Chain 3:



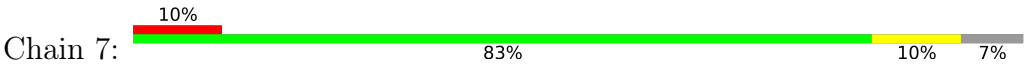
• Molecule 3: Alpha subunit of light-harvesting 1

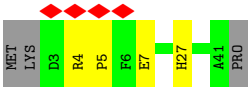
Chain 5:



• Molecule 3: Alpha subunit of light-harvesting 1

Chain 7:



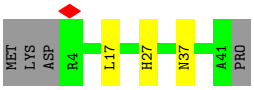


• Molecule 3: Alpha subunit of light-harvesting 1

Chain 9:

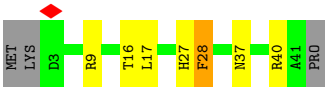
• Molecule 3: Alpha subunit of light-harvesting 1

Chain A:



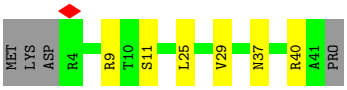
• Molecule 3: Alpha subunit of light-harvesting 1

Chain D:



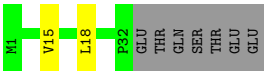
• Molecule 3: Alpha subunit of light-harvesting 1

Chain F:



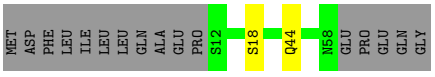
• Molecule 4: reaction center small polypeptide

Chain Y:



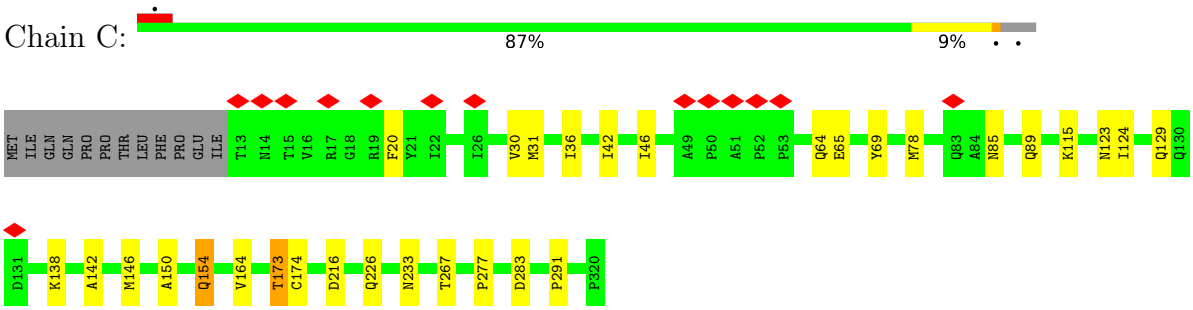
• Molecule 5: reaction center small polypeptide

Chain h:



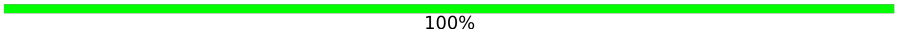
• Molecule 6: Cytochrome subunit of photosynthetic reaction center

Chain C:



• Molecule 7: reaction center unknown polypeptide

Chain Z:



There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	373675	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.500	Depositor
Minimum map value	-1.414	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.307	Depositor
Map size (Å)	320.4, 320.4, 320.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89, 0.89, 0.89	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PGV, UNL, U4Z, PEF, LMT, LHG, CDL, MQE, MN, BGL, BPH, HEC, BCL, CA

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	0	0.30	0/432	0.44	0/597
1	2	0.26	0/432	0.41	0/597
1	4	0.28	0/432	0.41	0/597
1	6	0.28	0/432	0.41	0/597
1	8	0.29	0/432	0.42	0/597
1	B	0.29	0/432	0.43	0/597
1	E	0.29	0/432	0.43	0/597
1	G	0.27	0/432	0.41	0/597
1	I	0.28	0/432	0.42	0/597
1	K	0.29	0/432	0.42	0/597
1	O	0.29	0/432	0.42	0/597
1	Q	0.30	0/432	0.43	0/597
1	S	0.29	0/432	0.42	0/597
1	U	0.29	0/432	0.42	0/597
1	W	0.27	0/432	0.40	0/597
2	L	0.37	0/2360	0.53	0/3220
2	M	0.68	1/2597 (0.0%)	0.54	1/3566 (0.0%)
3	1	0.28	0/307	0.51	0/417
3	3	0.29	0/315	0.52	0/428
3	5	0.30	0/315	0.49	0/428
3	7	0.31	0/315	0.52	0/428
3	9	0.29	0/307	0.53	0/417
3	A	0.30	0/307	0.53	0/417
3	D	0.29	0/315	0.50	0/428
3	F	0.30	0/307	0.52	0/417
3	H	0.33	0/315	0.52	0/428
3	J	0.30	0/315	0.50	0/428
3	N	0.37	0/315	0.63	0/428
3	P	0.29	0/315	0.53	0/428
3	R	0.30	0/315	0.50	0/428
3	T	0.33	0/307	0.52	0/417
3	V	0.28	0/307	0.49	0/417

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	Y	0.29	0/268	0.43	0/370
5	h	0.30	0/374	0.48	0/513
6	C	0.38	0/2409	0.54	0/3288
7	Z	0.80	0/51	0.97	0/70
All	All	0.39	1/19216 (0.0%)	0.50	1/26336 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	355	PRO	N-CD	-29.82	1.06	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	355	PRO	N-CD-CG	7.76	114.85	103.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	416	0	413	6	0
1	2	416	0	413	4	0
1	4	416	0	413	1	0
1	6	416	0	413	3	0
1	8	416	0	413	12	0
1	B	416	0	413	0	0
1	E	416	0	413	5	0
1	G	416	0	413	2	0
1	I	416	0	413	9	0
1	K	416	0	413	6	0
1	O	416	0	413	1	0
1	Q	416	0	413	7	0
1	S	416	0	413	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	416	0	413	5	0
1	W	416	0	413	6	0
2	L	2278	0	2235	16	0
2	M	2488	0	2373	25	0
3	1	300	0	316	3	0
3	3	308	0	320	5	0
3	5	308	0	320	4	0
3	7	308	0	320	3	0
3	9	300	0	316	12	0
3	A	300	0	316	2	0
3	D	308	0	320	8	0
3	F	300	0	316	6	0
3	H	308	0	320	7	0
3	J	308	0	320	3	0
3	N	308	0	320	4	0
3	P	308	0	320	5	0
3	R	308	0	320	2	0
3	T	300	0	316	3	0
3	V	300	0	316	13	0
4	Y	259	0	272	1	0
5	h	362	0	365	0	0
6	C	2347	0	2301	28	0
7	Z	51	0	49	0	0
8	0	132	0	148	9	0
8	1	66	0	74	3	0
8	2	132	0	148	11	0
8	3	132	0	148	1	0
8	4	66	0	74	7	0
8	5	66	0	74	2	0
8	6	132	0	148	5	0
8	7	66	0	74	1	0
8	8	132	0	148	6	0
8	9	66	0	74	0	0
8	A	132	0	148	4	0
8	B	66	0	74	2	0
8	D	66	0	74	3	0
8	E	132	0	148	11	0
8	F	66	0	74	3	0
8	G	132	0	148	3	0
8	H	66	0	74	1	0
8	I	132	0	148	6	0
8	J	66	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	K	132	0	148	2	0
8	L	132	0	148	3	0
8	M	66	0	74	2	0
8	N	66	0	74	3	0
8	O	132	0	148	4	0
8	P	66	0	74	2	0
8	Q	132	0	148	5	0
8	R	66	0	74	3	0
8	S	132	0	148	6	0
8	T	66	0	74	0	0
8	U	132	0	148	8	0
8	V	66	0	74	8	0
8	W	132	0	148	7	0
9	0	88	0	122	2	0
9	1	36	0	43	1	0
9	4	44	0	61	1	0
9	6	44	0	61	1	0
9	8	44	0	61	1	0
9	C	51	0	76	1	0
9	E	88	0	122	2	0
9	I	44	0	61	3	0
9	K	88	0	122	3	0
9	L	119	0	154	2	0
9	M	35	0	38	5	0
9	N	24	0	18	0	0
9	O	44	0	61	1	0
9	S	44	0	61	1	0
9	U	88	0	122	2	0
9	h	46	0	69	0	0
10	0	40	0	0	0	0
10	3	40	0	0	2	0
10	D	40	0	0	0	0
10	J	40	0	0	0	0
10	R	40	0	0	1	0
11	L	130	0	152	2	0
11	M	65	0	76	2	0
12	M	1	0	0	0	0
13	L	53	0	0	0	0
13	M	68	0	0	1	0
14	C	20	0	28	0	0
14	H	20	0	28	0	0
14	L	80	0	112	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	M	60	0	84	2	0
14	Y	40	0	56	0	0
15	L	88	0	131	3	0
15	M	21	0	15	0	0
15	h	41	0	55	0	0
16	1	35	0	46	1	0
16	D	35	0	46	3	0
16	H	35	0	46	2	0
16	M	35	0	46	2	0
16	T	35	0	46	1	0
17	1	18	0	0	0	0
17	9	36	0	0	10	0
17	A	18	0	0	0	0
17	C	34	0	0	0	0
17	D	12	0	0	0	0
17	F	15	0	0	0	0
17	H	13	0	0	0	0
17	L	30	0	0	0	0
17	M	44	0	0	0	0
17	V	26	0	0	0	0
17	Y	14	0	0	0	0
17	h	24	0	0	0	0
18	P	50	0	44	2	0
19	h	24	0	34	0	0
20	C	172	0	120	7	0
21	C	1	0	0	0	0
All	All	24285	0	24535	304	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 6.

All (304) 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)
3:9:31:LEU:HD23	17:9:103:UNL:C11	1.59	1.32
3:9:31:LEU:HD21	17:9:103:UNL:C14	1.62	1.27
3:9:31:LEU:CD2	17:9:103:UNL:C11	2.23	1.16
8:2:102:BCL:HBB2	6:C:20:PHE:CE1	1.85	1.10
3:V:20:LEU:HD12	8:V:101:BCL:C4	1.86	1.05
3:H:37:ASN:HD21	3:H:40:ARG:HD2	1.18	1.04
6:C:164:VAL:HG12	20:C:504:HEC:O1D	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:37:ASN:ND2	3:H:40:ARG:HD2	1.75	1.02
3:9:31:LEU:CD2	17:9:103:UNL:C14	2.38	1.02
8:2:102:BCL:HBB2	6:C:20:PHE:CZ	1.99	0.98
6:C:164:VAL:CG1	20:C:504:HEC:O1D	2.13	0.95
8:2:102:BCL:CBB	6:C:20:PHE:CZ	2.50	0.94
6:C:64:GLN:HG2	6:C:65:GLU:HG2	1.56	0.88
3:V:20:LEU:HD12	8:V:101:BCL:H43	1.58	0.84
1:0:7:ASN:HB3	1:0:15:LYS:HD2	1.61	0.82
3:V:20:LEU:CD1	8:V:101:BCL:C4	2.59	0.81
8:O:102:BCL:HMB1	8:O:102:BCL:HBB3	1.63	0.79
1:I:7:ASN:OD1	1:I:7:ASN:O	2.03	0.77
2:M:466:GLY:HA2	9:M:705:PGV:H061	1.67	0.75
8:U:102:BCL:HBB3	8:U:102:BCL:HMB1	1.69	0.74
1:K:55:ARG:HH11	1:K:55:ARG:HG2	1.51	0.74
3:9:31:LEU:HD22	17:9:103:UNL:C11	2.15	0.74
8:8:102:BCL:HBB3	8:8:102:BCL:HMB1	1.70	0.73
1:8:9:LEU:HD13	1:8:20:ASN:CG	2.10	0.72
1:K:50:TRP:HB2	9:K:104:PGV:H22	1.72	0.71
8:2:102:BCL:HBB1	6:C:20:PHE:CZ	2.24	0.70
2:M:359:GLY:H	14:M:710:BGL:H4	1.57	0.69
2:L:306:ASN:O	3:5:32:SER:OG	2.09	0.69
13:M:704:MQE:CCP	3:R:22:MET:HG3	2.22	0.68
6:C:150:ALA:O	6:C:154:GLN:HB2	1.93	0.68
3:V:20:LEU:CD1	8:V:101:BCL:H41	2.22	0.68
15:L:713:PEF:H232	15:L:713:PEF:H453	1.75	0.68
1:K:55:ARG:HG2	1:K:55:ARG:NH1	2.10	0.67
1:I:7:ASN:O	1:I:7:ASN:CG	2.34	0.66
8:O:102:BCL:HMB1	8:O:102:BCL:CBB	2.24	0.66
1:S:8:ASP:OD1	1:S:9:LEU:CD1	2.44	0.66
8:0:102:BCL:HMB1	8:0:102:BCL:HBB3	1.77	0.65
8:S:102:BCL:HBB3	8:S:102:BCL:HMB1	1.78	0.65
2:L:66:ARG:HE	9:L:711:PGV:H061	1.60	0.65
2:L:58:ASP:HB3	2:L:61:ASP:HB2	1.79	0.65
8:B:101:BCL:H43	1:0:31:LYS:HE3	1.80	0.64
8:Q:101:BCL:H51	8:P:101:BCL:H72	1.80	0.64
1:8:9:LEU:HD13	1:8:20:ASN:OD1	1.98	0.63
2:M:489:LEU:HD21	3:D:28:PHE:CE2	2.34	0.62
3:9:31:LEU:HD23	17:9:103:UNL:C12	2.26	0.62
9:M:705:PGV:H041	2:L:239:ARG:HH22	1.64	0.62
6:C:164:VAL:HG11	20:C:504:HEC:O1D	1.98	0.62
3:D:28:PHE:HD1	3:D:28:PHE:O	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:38:ILE:HD12	2:L:38:ILE:N	2.16	0.61
8:S:102:BCL:H2	8:S:102:BCL:HAA2	1.82	0.60
8:2:102:BCL:CBB	6:C:20:PHE:CE1	2.70	0.60
8:0:102:BCL:HMB1	8:0:102:BCL:CBB	2.32	0.59
6:C:85:ASN:OD1	6:C:89:GLN:OE1	2.20	0.59
2:L:208:TYR:HA	9:C:506:PGV:H241	1.84	0.59
6:C:123:ASN:ND2	6:C:129:GLN:OE1	2.34	0.59
1:6:6:GLN:O	1:6:20:ASN:ND2	2.36	0.58
1:U:36:GLY:HA3	8:U:101:BCL:H52	1.85	0.58
1:Q:54:ILE:HG22	9:O:103:PGV:H031	1.86	0.58
8:I:102:BCL:HBB3	8:I:102:BCL:HMB1	1.86	0.57
2:M:384:ILE:HD12	3:A:17:LEU:HD23	1.86	0.57
3:F:37:ASN:OD1	3:F:40:ARG:NH1	2.37	0.57
16:H:102:LMT:H101	3:J:25:LEU:HD11	1.86	0.57
3:3:4:ARG:NH2	3:3:7:GLU:OE1	2.38	0.57
8:U:102:BCL:HMB1	8:U:102:BCL:CBB	2.34	0.57
2:M:438:TRP:O	2:M:442:THR:OG1	2.18	0.57
1:S:8:ASP:OD1	1:S:9:LEU:HD12	2.04	0.56
3:V:36:PHE:O	3:V:39:LEU:N	2.33	0.56
1:W:7:ASN:O	1:W:15:LYS:NZ	2.30	0.56
1:I:55:ARG:HB2	3:F:37:ASN:HD22	1.71	0.56
6:C:142:ALA:O	6:C:146:MET:HG3	2.06	0.55
1:U:9:LEU:HG	1:U:20:ASN:ND2	2.23	0.54
8:L:703:BCL:H151	11:L:704:BPH:H5C2	1.88	0.54
1:8:9:LEU:HD12	1:8:9:LEU:N	2.23	0.53
3:N:5:PRO:HD2	3:N:6:PHE:H	1.73	0.53
1:W:36:GLY:HA3	8:W:101:BCL:H52	1.89	0.53
1:I:51:THR:HG23	3:H:36:PHE:CE1	2.44	0.53
8:6:102:BCL:CAB	10:3:102:U4Z:CAE	2.86	0.53
3:N:13:VAL:HG22	8:N:101:BCL:H201	1.90	0.53
1:I:53:TRP:HZ2	9:I:103:PGV:H281	1.73	0.53
1:8:7:ASN:O	1:8:15:LYS:NZ	2.29	0.53
3:P:38:TRP:CZ2	8:P:101:BCL:HHC	2.44	0.53
3:V:16:THR:HG23	8:V:101:BCL:H62	1.91	0.53
2:M:410:ARG:HG2	2:M:411:GLU:HG2	1.91	0.53
2:M:461:LYS:NZ	9:M:705:PGV:O05	2.32	0.53
3:H:5:PRO:O	3:F:9:ARG:NE	2.38	0.53
3:D:17:LEU:HD11	16:D:104:LMT:H51	1.91	0.53
1:0:7:ASN:HD22	1:0:15:LYS:HG3	1.73	0.52
1:K:26:HIS:O	1:K:30:VAL:HG13	2.10	0.52
1:I:19:ASN:OD1	1:I:20:ASN:N	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:609:LEU:HD22	2:M:613:LEU:HD12	1.91	0.52
3:9:31:LEU:HB2	3:9:38:TRP:CZ3	2.45	0.52
2:M:420:PRO:HB3	2:M:430:VAL:HG11	1.92	0.51
9:K:103:PGV:H21	1:I:50:TRP:HB2	1.91	0.51
3:H:37:ASN:ND2	3:H:40:ARG:CD	2.61	0.51
6:C:173:THR:O	6:C:174:CYS:HB2	2.11	0.51
2:M:489:LEU:HD21	3:D:28:PHE:CZ	2.46	0.51
6:C:277:PRO:HG2	6:C:283:ASP:HB2	1.93	0.51
8:8:102:BCL:HMB1	8:8:102:BCL:CBB	2.41	0.51
3:5:3:ASP:N	3:5:3:ASP:OD1	2.44	0.50
3:T:9:ARG:HH22	3:V:5:PRO:HG2	1.74	0.50
2:M:358:VAL:HG13	14:M:710:BGL:H2	1.93	0.50
2:L:54:PHE:HE1	3:V:17:LEU:HD12	1.76	0.50
8:O:101:BCL:HMD1	3:N:27:HIS:CE1	2.47	0.50
2:M:557:GLU:O	2:M:561:MET:HG3	2.11	0.50
1:S:55:ARG:HG3	1:S:55:ARG:HH11	1.77	0.49
1:Q:7:ASN:ND2	1:Q:18:PHE:O	2.45	0.49
3:V:20:LEU:HD13	8:V:101:BCL:H41	1.94	0.49
1:S:26:HIS:O	1:S:30:VAL:HG13	2.12	0.49
2:L:90:GLU:HG2	2:L:105:ILE:HG23	1.93	0.49
8:4:101:BCL:CBB	8:4:101:BCL:HMB1	2.42	0.49
3:A:27:HIS:CE1	8:A:101:BCL:HMD1	2.47	0.49
1:G:26:HIS:O	1:G:30:VAL:HG13	2.13	0.49
8:K:102:BCL:HBD	8:K:102:BCL:HBA1	1.94	0.49
2:M:367:GLU:OE1	2:M:368:GLY:N	2.46	0.48
8:E:101:BCL:H111	8:E:101:BCL:H142	1.67	0.48
1:Q:6:GLN:N	1:Q:8:ASP:OD1	2.46	0.48
8:0:101:BCL:HMD1	3:9:27:HIS:CE1	2.48	0.48
8:A:102:BCL:H141	8:A:102:BCL:H161	1.74	0.48
1:E:19:ASN:HB3	1:E:22:GLU:HG3	1.95	0.48
8:S:102:BCL:H112	1:Q:32:THR:HA	1.96	0.48
8:K:101:BCL:HMD1	3:J:27:HIS:CE1	2.49	0.48
9:S:103:PGV:H21	1:Q:50:TRP:HB2	1.95	0.47
8:6:101:BCL:HMD1	3:5:27:HIS:CE1	2.49	0.47
3:9:31:LEU:CD2	17:9:103:UNL:C13	2.91	0.47
9:I:103:PGV:H61	1:G:47:CYS:SG	2.54	0.47
8:E:101:BCL:H111	8:E:101:BCL:H91	1.69	0.47
1:8:27:ASP:OD2	1:8:31:LYS:NZ	2.35	0.47
2:L:38:ILE:HD12	2:L:38:ILE:H	1.76	0.47
3:D:9:ARG:HD3	16:D:104:LMT:H2B	1.96	0.47
8:2:102:BCL:H143	8:2:102:BCL:H162	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:0:104:PGV:H21	1:8:50:TRP:HB2	1.96	0.47
8:2:102:BCL:H62	8:2:102:BCL:H2	1.50	0.47
16:M:709:LMT:H22	3:F:29:VAL:HG22	1.95	0.47
1:W:26:HIS:O	1:W:30:VAL:HG13	2.15	0.47
8:0:102:BCL:H62	8:0:102:BCL:H93	1.66	0.47
2:M:557:GLU:OE2	2:M:589:HIS:HE1	1.97	0.47
2:M:603:GLY:HA2	8:M:701:BCL:HED3	1.97	0.47
8:7:101:BCL:H192	8:7:101:BCL:H162	1.75	0.47
8:S:102:BCL:HMB1	8:S:102:BCL:CBB	2.45	0.47
8:F:101:BCL:H161	8:F:101:BCL:H202	1.60	0.47
8:Q:101:BCL:HMD1	3:P:27:HIS:CE1	2.49	0.46
8:I:101:BCL:HMD1	3:H:27:HIS:CE1	2.50	0.46
8:G:101:BCL:H91	8:G:101:BCL:H111	1.79	0.46
8:I:102:BCL:H122	8:I:102:BCL:H162	1.66	0.46
8:E:101:BCL:H41	8:E:101:BCL:H62	1.60	0.46
16:H:102:LMT:H1B	16:H:102:LMT:H3'	1.52	0.46
3:N:5:PRO:CD	3:N:6:PHE:H	2.28	0.46
1:6:27:ASP:OD1	1:6:31:LYS:HE3	2.15	0.46
9:1:102:PGV:H132	6:C:36:ILE:HG12	1.96	0.46
9:L:711:PGV:H222	9:L:711:PGV:H251	1.74	0.46
9:E:103:PGV:O12	9:E:103:PGV:O06	2.28	0.46
3:H:16:THR:HG22	8:H:101:BCL:H172	1.97	0.46
3:3:27:HIS:CE1	8:3:101:BCL:HMD1	2.51	0.46
8:D:102:BCL:H141	3:F:11:SER:HB2	1.97	0.46
1:8:9:LEU:HD13	1:8:20:ASN:ND2	2.29	0.46
8:2:101:BCL:HMD1	3:1:27:HIS:CE1	2.51	0.46
2:M:467:THR:HG23	9:M:705:PGV:H062	1.97	0.46
9:U:103:PGV:H21	1:S:50:TRP:HB2	1.96	0.46
3:1:4:ARG:NH1	3:3:4:ARG:O	2.49	0.46
8:S:102:BCL:H111	8:S:102:BCL:H151	1.36	0.46
8:G:102:BCL:H72	1:E:32:THR:HA	1.98	0.46
8:E:102:BCL:H162	8:E:102:BCL:H121	1.45	0.46
3:9:31:LEU:HD23	17:9:103:UNL:C14	2.40	0.45
1:2:12:ASP:HA	1:2:15:LYS:HG3	1.98	0.45
8:B:101:BCL:H91	8:B:101:BCL:H111	1.80	0.45
8:1:101:BCL:H62	8:1:101:BCL:H93	1.66	0.45
2:L:38:ILE:H	2:L:38:ILE:CD1	2.29	0.45
2:M:584:ASN:HB3	2:M:586:TYR:H	1.82	0.45
8:U:101:BCL:H41	8:U:101:BCL:H61	1.77	0.45
2:L:54:PHE:CE1	3:V:17:LEU:HD12	2.51	0.45
2:L:38:ILE:N	2:L:38:ILE:CD1	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:19:ASN:HB3	1:Q:22:GLU:HG3	1.99	0.45
8:O:102:BCL:H2	1:K:28:ILE:HG23	1.99	0.45
16:1:104:LMT:H1B	16:1:104:LMT:H3'	1.72	0.45
8:5:101:BCL:H142	8:5:101:BCL:H111	1.72	0.45
8:S:101:BCL:HMD1	3:R:27:HIS:CE1	2.52	0.45
8:W:101:BCL:HMD1	3:V:27:HIS:CE1	2.52	0.45
2:M:541:MET:O	2:M:545:THR:HG22	2.17	0.45
6:C:233:ASN:C	6:C:233:ASN:OD1	2.55	0.45
8:W:102:BCL:CAB	10:R:101:U4Z:CAC	2.94	0.44
8:8:102:BCL:HHD	8:8:102:BCL:HAC2	1.81	0.44
1:4:26:HIS:O	1:4:30:VAL:HG13	2.17	0.44
1:2:11:PRO:HG2	1:2:14:TRP:HE3	1.82	0.44
8:2:102:BCL:HMB1	8:2:102:BCL:HBB3	1.99	0.44
8:W:101:BCL:HBA2	8:W:101:BCL:HBD	1.98	0.44
8:W:102:BCL:H151	1:U:39:ILE:HD12	1.99	0.44
8:U:101:BCL:HMD1	3:T:27:HIS:CE1	2.53	0.44
8:I:101:BCL:HAA1	9:I:103:PGV:H331	2.00	0.44
8:6:102:BCL:H62	8:6:102:BCL:H41	1.59	0.44
2:M:378:TRP:HE1	16:D:104:LMT:H6D	1.81	0.44
3:1:7:GLU:OE1	3:1:7:GLU:N	2.46	0.44
3:9:31:LEU:HD22	17:9:103:UNL:C10	2.48	0.44
8:4:101:BCL:OBB	8:4:101:BCL:HHC	2.17	0.44
6:C:78:MET:HG3	20:C:501:HEC:HMB3	1.99	0.44
1:K:55:ARG:HH11	1:K:55:ARG:CG	2.26	0.44
8:0:102:BCL:H91	1:8:35:GLY:HA3	1.98	0.44
2:M:452:TRP:HZ3	11:M:702:BPH:H102	1.81	0.44
2:M:487:HIS:HB3	2:M:488:PRO:HD3	2.00	0.44
8:N:101:BCL:H111	8:N:101:BCL:H142	1.77	0.44
6:C:267:THR:HG22	6:C:291:PRO:HG2	2.00	0.44
8:0:102:BCL:H2	1:8:28:ILE:HG23	2.00	0.44
1:8:26:HIS:O	1:8:30:VAL:HG13	2.18	0.44
8:4:101:BCL:H171	8:4:101:BCL:H13	1.76	0.44
3:7:4:ARG:HH21	3:7:7:GLU:HG3	1.81	0.44
1:0:54:ILE:HG21	9:0:104:PGV:O02	2.17	0.44
8:F:101:BCL:H93	8:F:101:BCL:H112	1.74	0.44
3:3:31:LEU:HB2	3:3:38:TRP:CZ3	2.53	0.43
8:U:101:BCL:H141	8:U:101:BCL:H161	1.86	0.43
1:I:27:ASP:OD2	1:I:31:LYS:NZ	2.50	0.43
8:6:102:BCL:C3B	10:3:102:U4Z:CAC	2.96	0.43
6:C:69:TYR:CE2	6:C:115:LYS:HD2	2.53	0.43
8:8:101:BCL:HMD1	3:7:27:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:709:LMT:H1B	16:M:709:LMT:H3'	1.72	0.43
1:E:50:TRP:CG	1:E:51:THR:HG23	2.53	0.43
8:Q:102:BCL:H91	8:Q:102:BCL:H111	1.75	0.43
8:G:102:BCL:H41	8:G:102:BCL:H61	1.63	0.43
1:0:26:HIS:O	1:0:30:VAL:HG13	2.19	0.43
8:1:101:BCL:H152	8:1:101:BCL:H112	1.49	0.43
6:C:226:GLN:HE22	20:C:503:HEC:HMB2	1.84	0.43
8:8:101:BCL:HAA1	9:8:103:PGV:H342	2.01	0.43
6:C:233:ASN:HB3	20:C:503:HEC:HMC2	2.00	0.43
1:E:50:TRP:CD1	1:E:51:THR:HG23	2.54	0.43
8:0:102:BCL:H91	8:0:102:BCL:H111	1.86	0.43
9:M:705:PGV:H041	2:L:239:ARG:NH2	2.32	0.43
8:A:102:BCL:H142	8:A:102:BCL:H111	1.93	0.43
2:M:354:PRO:HA	2:M:355:PRO:HD3	1.72	0.42
6:C:138:LYS:HA	6:C:138:LYS:HD3	1.71	0.42
8:Q:101:BCL:H142	8:Q:101:BCL:H111	1.77	0.42
8:E:101:BCL:HMD1	3:D:27:HIS:CE1	2.55	0.42
8:4:101:BCL:H13	8:4:101:BCL:H102	1.72	0.42
3:P:9:ARG:H	3:P:9:ARG:HG3	1.62	0.42
8:R:102:BCL:H111	8:R:102:BCL:H143	1.75	0.42
3:P:7:GLU:HB2	3:P:10:THR:HG23	2.00	0.42
3:V:20:LEU:CD1	8:V:101:BCL:H43	2.35	0.42
8:U:102:BCL:H101	8:U:102:BCL:H162	2.01	0.42
2:M:482:VAL:HG12	2:M:607:LEU:HD23	2.02	0.42
8:1:101:BCL:H121	8:1:101:BCL:H8	1.85	0.42
6:C:78:MET:HG3	20:C:501:HEC:CMB	2.49	0.42
8:I:102:BCL:HMB1	8:I:102:BCL:CBB	2.49	0.42
8:4:101:BCL:H61	8:4:101:BCL:H41	1.44	0.42
1:O:26:HIS:O	1:O:30:VAL:HG13	2.19	0.42
8:0:102:BCL:H12	1:8:31:LYS:HE2	2.02	0.42
8:4:101:BCL:H2	1:2:28:ILE:HG12	2.02	0.42
6:C:30:VAL:HG23	6:C:31:MET:CE	2.50	0.42
8:M:701:BCL:H112	8:M:701:BCL:H72	1.99	0.42
3:P:17:LEU:CD1	18:P:102:CDL:H531	2.49	0.42
3:9:31:LEU:CD2	17:9:103:UNL:C12	2.93	0.42
8:W:102:BCL:H203	8:W:102:BCL:H161	1.89	0.42
8:E:101:BCL:H203	8:E:101:BCL:H161	1.87	0.42
1:E:36:GLY:HA3	8:E:101:BCL:H52	2.01	0.42
3:J:4:ARG:NH2	3:J:7:GLU:OE1	2.53	0.42
8:Q:102:BCL:H193	8:Q:102:BCL:H162	1.76	0.42
8:4:101:BCL:H61	8:4:101:BCL:H92	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2:102:BCL:CBB	8:2:102:BCL:HMB1	2.50	0.42
2:L:174:ARG:HB3	2:L:175:PRO:HD3	2.01	0.42
1:W:27:ASP:O	1:W:31:LYS:HG2	2.20	0.41
8:E:102:BCL:H41	8:E:102:BCL:H62	1.59	0.41
1:8:11:PRO:O	1:8:15:LYS:HG2	2.19	0.41
1:S:55:ARG:HG3	1:S:55:ARG:NH1	2.33	0.41
2:M:459:ARG:HB2	2:L:253:ILE:HD11	2.01	0.41
3:V:4:ARG:HB3	3:V:5:PRO:HD3	2.02	0.41
8:E:102:BCL:H142	8:E:102:BCL:H112	1.82	0.41
8:L:702:BCL:H92	8:L:702:BCL:H62	1.79	0.41
15:L:717:PEF:H331	4:Y:18:LEU:HD23	2.02	0.41
8:U:102:BCL:H41	8:U:102:BCL:H62	1.76	0.41
2:L:253:ILE:HG22	2:L:254:LEU:HG	2.02	0.41
8:N:101:BCL:H2	8:N:101:BCL:H61	1.90	0.41
8:E:101:BCL:H93	8:E:101:BCL:H61	1.77	0.41
1:0:7:ASN:ND2	1:0:15:LYS:HG3	2.35	0.41
11:M:702:BPH:H6C1	11:M:702:BPH:H4C1	1.71	0.41
3:D:16:THR:HG23	8:D:102:BCL:H61	2.03	0.41
8:D:102:BCL:H41	8:D:102:BCL:H62	1.80	0.41
6:C:42:ILE:O	6:C:46:ILE:HG12	2.21	0.41
1:W:8:ASP:N	1:W:8:ASP:OD1	2.52	0.41
1:U:26:HIS:O	1:U:30:VAL:HG13	2.21	0.41
8:E:101:BCL:CBB	9:E:103:PGV:H91	2.50	0.41
1:2:18:PHE:CE2	8:2:102:BCL:HMB3	2.55	0.41
2:M:350:THR:HB	2:M:372:PRO:HB2	2.03	0.41
6:C:124:ILE:HD13	6:C:124:ILE:HA	1.93	0.41
8:W:101:BCL:H161	8:W:101:BCL:H192	1.88	0.41
9:4:102:PGV:H272	9:4:102:PGV:H241	1.86	0.41
15:L:713:PEF:H252	15:L:717:PEF:H371	2.03	0.41
18:P:102:CDL:H141	18:P:102:CDL:H111	1.89	0.41
9:K:103:PGV:O12	9:K:103:PGV:O06	2.27	0.41
8:0:102:BCL:H61	8:0:102:BCL:H41	1.49	0.41
1:6:22:GLU:HG3	3:7:5:PRO:HG3	2.02	0.41
8:V:101:BCL:H41	8:V:101:BCL:H61	1.40	0.41
3:3:9:ARG:HG3	3:5:6:PHE:CE1	2.56	0.41
8:A:102:BCL:H122	8:A:102:BCL:H8	1.78	0.41
1:U:54:ILE:HG21	9:U:103:PGV:O02	2.21	0.40
1:I:55:ARG:HB2	3:F:37:ASN:ND2	2.34	0.40
8:6:101:BCL:HAA1	9:6:103:PGV:H342	2.03	0.40
8:5:101:BCL:H203	8:5:101:BCL:H161	1.82	0.40
8:F:101:BCL:H142	8:F:101:BCL:H111	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:53:TRP:CD1	1:W:54:ILE:HG13	2.57	0.40
8:I:102:BCL:HHD	8:I:102:BCL:HAC2	1.87	0.40
6:C:216:ASP:OD1	6:C:216:ASP:N	2.48	0.40
1:Q:15:LYS:N	1:Q:16:PRO:HD2	2.37	0.40
14:L:715:BGL:O1	16:T:102:LMT:O2'	2.34	0.40
8:R:102:BCL:H171	3:T:11:SER:HA	2.03	0.40
8:8:102:BCL:H8	8:8:102:BCL:H122	1.69	0.40
8:L:703:BCL:H52	11:L:704:BPH:HBB2	2.04	0.40
8:R:102:BCL:H13	8:R:102:BCL:H172	1.95	0.40
3:D:37:ASN:OD1	3:D:40:ARG:HG3	2.22	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	0	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	2	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
1	4	48/55 (87%)	48 (100%)	0	0	100	100
1	6	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
1	8	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
1	B	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
1	E	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	G	48/55 (87%)	43 (90%)	5 (10%)	0	100	100
1	I	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	K	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	O	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	Q	48/55 (87%)	47 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	U	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	W	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
2	L	284/641 (44%)	272 (96%)	12 (4%)	0	100	100
2	M	304/641 (47%)	294 (97%)	10 (3%)	0	100	100
3	1	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
3	3	37/42 (88%)	34 (92%)	3 (8%)	0	100	100
3	5	37/42 (88%)	36 (97%)	1 (3%)	0	100	100
3	7	37/42 (88%)	34 (92%)	3 (8%)	0	100	100
3	9	36/42 (86%)	36 (100%)	0	0	100	100
3	A	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
3	D	37/42 (88%)	37 (100%)	0	0	100	100
3	F	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
3	H	37/42 (88%)	36 (97%)	1 (3%)	0	100	100
3	J	37/42 (88%)	35 (95%)	2 (5%)	0	100	100
3	N	37/42 (88%)	37 (100%)	0	0	100	100
3	P	37/42 (88%)	37 (100%)	0	0	100	100
3	R	37/42 (88%)	37 (100%)	0	0	100	100
3	T	36/42 (86%)	36 (100%)	0	0	100	100
3	V	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
4	Y	30/39 (77%)	29 (97%)	1 (3%)	0	100	100
5	h	45/63 (71%)	45 (100%)	0	0	100	100
6	C	306/320 (96%)	290 (95%)	16 (5%)	0	100	100
7	Z	8/10 (80%)	8 (100%)	0	0	100	100
All	All	2246/3169 (71%)	2166 (96%)	80 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	44/49 (90%)	43 (98%)	1 (2%)	50	78
1	2	44/49 (90%)	44 (100%)	0	100	100
1	4	44/49 (90%)	44 (100%)	0	100	100
1	6	44/49 (90%)	44 (100%)	0	100	100
1	8	44/49 (90%)	44 (100%)	0	100	100
1	B	44/49 (90%)	44 (100%)	0	100	100
1	E	44/49 (90%)	44 (100%)	0	100	100
1	G	44/49 (90%)	44 (100%)	0	100	100
1	I	44/49 (90%)	43 (98%)	1 (2%)	50	78
1	K	44/49 (90%)	44 (100%)	0	100	100
1	O	44/49 (90%)	44 (100%)	0	100	100
1	Q	44/49 (90%)	44 (100%)	0	100	100
1	S	44/49 (90%)	43 (98%)	1 (2%)	50	78
1	U	44/49 (90%)	43 (98%)	1 (2%)	50	78
1	W	44/49 (90%)	44 (100%)	0	100	100
2	L	232/511 (45%)	227 (98%)	5 (2%)	52	79
2	M	244/511 (48%)	236 (97%)	8 (3%)	38	68
3	1	33/37 (89%)	32 (97%)	1 (3%)	41	72
3	3	34/37 (92%)	34 (100%)	0	100	100
3	5	34/37 (92%)	33 (97%)	1 (3%)	42	72
3	7	34/37 (92%)	34 (100%)	0	100	100
3	9	33/37 (89%)	32 (97%)	1 (3%)	41	72
3	A	33/37 (89%)	32 (97%)	1 (3%)	41	72
3	D	34/37 (92%)	33 (97%)	1 (3%)	42	72
3	F	33/37 (89%)	32 (97%)	1 (3%)	41	72
3	H	34/37 (92%)	33 (97%)	1 (3%)	42	72
3	J	34/37 (92%)	34 (100%)	0	100	100
3	N	34/37 (92%)	34 (100%)	0	100	100
3	P	34/37 (92%)	33 (97%)	1 (3%)	42	72
3	R	34/37 (92%)	33 (97%)	1 (3%)	42	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	T	33/37 (89%)	33 (100%)	0	100 100
3	V	33/37 (89%)	32 (97%)	1 (3%)	41 72
4	Y	29/36 (81%)	28 (97%)	1 (3%)	37 67
5	h	36/50 (72%)	34 (94%)	2 (6%)	21 47
6	C	250/262 (95%)	248 (99%)	2 (1%)	81 93
7	Z	1/1 (100%)	1 (100%)	0	100 100
All	All	1956/2661 (74%)	1924 (98%)	32 (2%)	64 84

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	12	ASP
1	S	9	LEU
1	I	7	ASN
1	0	15	LYS
2	M	353	LYS
2	M	367	GLU
2	M	375	VAL
2	M	401	VAL
2	M	442	THR
2	M	519	PHE
2	M	595	PHE
2	M	630	TRP
2	L	45	ARG
2	L	252	ASN
2	L	281	CYS
2	L	305	TRP
2	L	308	VAL
3	H	37	ASN
3	P	22	MET
3	R	17	LEU
3	V	25	LEU
3	1	32	SER
3	5	25	LEU
3	9	18	LEU
3	A	37	ASN
3	D	28	PHE
3	F	25	LEU
4	Y	15	VAL
5	h	18	SER

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Mol	Chain	Res	Type
5	h	44	GLN
6	C	154	GLN
6	C	173	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	525	HIS
3	H	37	ASN
6	C	89	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 128 ligands modelled in this entry, 2 are monoatomic and 20 are unknown - leaving 106 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	$\#\|Z\| > 2$
8	BCL	N	101	-	64,74,74	1.67	12 (18%)	78,115,115	2.26	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	HEC	C	501	6	32,50,50	2.15	3 (9%)	24,82,82	1.47	2 (8%)
8	BCL	2	102	-	64,74,74	1.67	12 (18%)	78,115,115	2.39	23 (29%)
10	U4Z	3	102	-	40,40,40	1.76	9 (22%)	50,51,51	1.66	14 (28%)
9	PGV	I	103	-	43,43,50	0.97	2 (4%)	46,49,56	1.27	4 (8%)
13	MQE	M	704	-	69,69,69	0.37	0	84,87,87	0.41	0
16	LMT	1	104	-	36,36,36	0.39	0	47,47,47	0.79	1 (2%)
8	BCL	0	101	-	64,74,74	1.71	12 (18%)	78,115,115	2.18	21 (26%)
16	LMT	H	102	-	36,36,36	0.40	0	47,47,47	0.73	1 (2%)
13	MQE	L	705	-	54,54,69	0.34	0	66,69,87	0.60	1 (1%)
8	BCL	4	101	-	64,74,74	1.66	14 (21%)	78,115,115	2.29	22 (28%)
9	PGV	L	712	-	34,34,50	1.09	2 (5%)	37,40,56	1.20	4 (10%)
11	BPH	L	704	-	51,70,70	0.67	1 (1%)	52,101,101	0.74	1 (1%)
8	BCL	3	101	-	64,74,74	1.72	12 (18%)	78,115,115	2.27	24 (30%)
9	PGV	L	706	-	50,50,50	0.90	2 (4%)	53,56,56	0.99	2 (3%)
14	BGL	L	715	-	20,20,20	0.34	0	24,25,25	0.94	1 (4%)
8	BCL	S	102	-	64,74,74	1.70	16 (25%)	78,115,115	2.37	25 (32%)
9	PGV	U	104	-	43,43,50	0.98	2 (4%)	46,49,56	1.10	4 (8%)
18	CDL	P	102	-	49,49,99	1.28	4 (8%)	55,61,111	1.29	5 (9%)
8	BCL	O	102	-	64,74,74	1.64	12 (18%)	78,115,115	2.31	23 (29%)
8	BCL	W	102	-	64,74,74	1.64	12 (18%)	78,115,115	2.35	24 (30%)
11	BPH	M	702	-	51,70,70	0.62	1 (1%)	52,101,101	0.76	0
8	BCL	L	703	-	64,74,74	1.70	13 (20%)	78,115,115	2.36	22 (28%)
8	BCL	U	101	-	64,74,74	1.71	13 (20%)	78,115,115	2.16	23 (29%)
8	BCL	F	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.25	18 (23%)
20	HEC	C	504	6	32,50,50	2.13	3 (9%)	24,82,82	1.57	3 (12%)
8	BCL	G	101	-	64,74,74	1.69	11 (17%)	78,115,115	2.17	25 (32%)
15	PEF	L	717	-	40,40,46	1.01	2 (5%)	43,45,51	1.07	2 (4%)
8	BCL	T	101	-	64,74,74	1.67	13 (20%)	78,115,115	2.31	18 (23%)
14	BGL	Y	103	-	20,20,20	0.40	0	24,25,25	0.65	0
8	BCL	1	101	-	64,74,74	1.67	12 (18%)	78,115,115	2.30	19 (24%)
8	BCL	8	101	-	64,74,74	1.73	11 (17%)	78,115,115	2.06	21 (26%)
9	PGV	0	104	-	43,43,50	0.98	2 (4%)	46,49,56	1.16	4 (8%)
8	BCL	I	101	-	64,74,74	1.71	12 (18%)	78,115,115	2.13	21 (26%)
16	LMT	M	709	-	36,36,36	0.37	0	47,47,47	0.97	3 (6%)
14	BGL	L	708	-	20,20,20	0.40	0	24,25,25	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BCL	3	103	-	64,74,74	1.69	13 (20%)	78,115,115	2.30	18 (23%)
8	BCL	K	102	-	64,74,74	1.70	13 (20%)	78,115,115	2.24	23 (29%)
8	BCL	E	101	-	64,74,74	1.69	10 (15%)	78,115,115	2.07	20 (25%)
8	BCL	M	701	-	64,74,74	1.71	14 (21%)	78,115,115	2.46	20 (25%)
20	HEC	C	503	6	32,50,50	2.14	3 (9%)	24,82,82	1.59	4 (16%)
14	BGL	M	706	-	20,20,20	0.44	0	24,25,25	0.63	0
8	BCL	J	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.25	18 (23%)
8	BCL	H	101	-	64,74,74	1.69	12 (18%)	78,115,115	2.40	19 (24%)
8	BCL	A	102	-	64,74,74	1.69	12 (18%)	78,115,115	2.21	19 (24%)
9	PGV	N	102	-	23,23,50	1.32	2 (8%)	26,29,56	1.38	3 (11%)
8	BCL	U	102	-	64,74,74	1.68	14 (21%)	78,115,115	2.64	25 (32%)
9	PGV	8	103	-	43,43,50	0.98	2 (4%)	46,49,56	1.16	4 (8%)
8	BCL	K	101	-	64,74,74	1.70	11 (17%)	78,115,115	2.07	22 (28%)
8	BCL	B	101	-	64,74,74	1.78	16 (25%)	78,115,115	2.33	22 (28%)
8	BCL	V	101	-	64,74,74	1.65	13 (20%)	78,115,115	2.16	19 (24%)
8	BCL	P	101	-	64,74,74	1.69	12 (18%)	78,115,115	2.26	19 (24%)
11	BPH	L	701	-	51,70,70	0.56	0	52,101,101	0.81	1 (1%)
9	PGV	0	105	-	43,43,50	0.97	2 (4%)	46,49,56	1.16	4 (8%)
14	BGL	M	707	-	20,20,20	0.35	0	24,25,25	0.84	1 (4%)
10	U4Z	0	103	-	40,40,40	1.73	9 (22%)	50,51,51	1.62	13 (26%)
14	BGL	H	103	-	20,20,20	0.36	0	24,25,25	0.61	0
8	BCL	O	101	-	64,74,74	1.73	13 (20%)	78,115,115	2.17	20 (25%)
9	PGV	K	104	-	43,43,50	0.98	2 (4%)	46,49,56	1.03	2 (4%)
9	PGV	L	711	-	32,32,50	0.85	1 (3%)	34,37,56	1.09	3 (8%)
8	BCL	5	101	-	64,74,74	1.67	11 (17%)	78,115,115	2.24	19 (24%)
8	BCL	G	102	-	64,74,74	1.69	13 (20%)	78,115,115	2.39	21 (26%)
14	BGL	L	709	-	20,20,20	0.39	0	24,25,25	0.49	0
9	PGV	O	103	-	43,43,50	0.98	2 (4%)	46,49,56	1.14	3 (6%)
9	PGV	S	103	-	43,43,50	0.98	2 (4%)	46,49,56	1.12	5 (10%)
16	LMT	D	104	-	36,36,36	0.39	0	47,47,47	0.76	0
8	BCL	S	101	-	64,74,74	1.72	12 (18%)	78,115,115	2.10	20 (25%)
8	BCL	Q	102	-	64,74,74	1.69	12 (18%)	78,115,115	2.27	20 (25%)
8	BCL	A	101	-	64,74,74	1.71	11 (17%)	78,115,115	2.21	21 (26%)
14	BGL	L	714	-	20,20,20	0.37	0	24,25,25	0.56	0
8	BCL	W	101	-	64,74,74	1.74	13 (20%)	78,115,115	2.12	18 (23%)
8	BCL	0	102	-	64,74,74	1.65	13 (20%)	78,115,115	2.29	22 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	PGV	6	103	-	43,43,50	0.99	2 (4%)	46,49,56	1.14	2 (4%)
8	BCL	Q	101	-	64,74,74	1.70	12 (18%)	78,115,115	2.17	20 (25%)
9	PGV	C	506	21	50,50,50	0.86	2 (4%)	53,56,56	1.10	4 (7%)
9	PGV	M	705	-	34,34,50	1.12	2 (5%)	37,40,56	1.10	2 (5%)
8	BCL	L	702	-	64,74,74	1.70	12 (18%)	78,115,115	2.33	20 (25%)
8	BCL	2	101	-	64,74,74	1.71	11 (17%)	78,115,115	2.06	21 (26%)
14	BGL	M	710	-	20,20,20	0.39	0	24,25,25	0.60	0
14	BGL	Y	101	-	20,20,20	0.38	0	24,25,25	0.77	0
15	PEF	M	708	-	20,20,46	1.52	2 (10%)	23,25,51	1.58	3 (13%)
9	PGV	K	103	-	43,43,50	0.98	2 (4%)	46,49,56	1.03	3 (6%)
19	LHG	h	101	5	23,23,48	0.30	0	24,24,54	0.71	1 (4%)
16	LMT	T	102	-	36,36,36	0.51	1 (2%)	47,47,47	1.04	3 (6%)
8	BCL	9	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.29	21 (26%)
15	PEF	L	713	-	46,46,46	0.95	2 (4%)	49,51,51	1.09	4 (8%)
9	PGV	E	103	-	43,43,50	0.97	2 (4%)	46,49,56	1.12	3 (6%)
9	PGV	E	104	-	43,43,50	0.97	2 (4%)	46,49,56	1.09	4 (8%)
8	BCL	6	102	-	64,74,74	1.65	12 (18%)	78,115,115	2.30	20 (25%)
10	U4Z	J	101	-	40,40,40	1.73	10 (25%)	50,51,51	1.63	14 (28%)
8	BCL	8	102	-	64,74,74	1.61	12 (18%)	78,115,115	2.33	24 (30%)
10	U4Z	R	101	-	40,40,40	1.71	9 (22%)	50,51,51	1.57	12 (24%)
10	U4Z	D	101	-	40,40,40	1.71	10 (25%)	50,51,51	1.59	11 (22%)
8	BCL	I	102	-	64,74,74	1.67	14 (21%)	78,115,115	2.26	20 (25%)
8	BCL	6	101	-	64,74,74	1.70	12 (18%)	78,115,115	2.09	21 (26%)
9	PGV	1	102	-	35,35,50	1.11	2 (5%)	38,40,56	1.18	4 (10%)
8	BCL	R	102	-	64,74,74	1.70	13 (20%)	78,115,115	2.29	18 (23%)
9	PGV	4	102	-	43,43,50	0.97	2 (4%)	46,49,56	1.06	4 (8%)
8	BCL	7	101	-	64,74,74	1.68	14 (21%)	78,115,115	2.31	21 (26%)
8	BCL	D	102	-	64,74,74	1.70	13 (20%)	78,115,115	2.34	22 (28%)
9	PGV	U	103	-	43,43,50	0.97	2 (4%)	46,49,56	1.09	4 (8%)
8	BCL	E	102	-	64,74,74	1.70	12 (18%)	78,115,115	2.36	20 (25%)
14	BGL	C	507	-	20,20,20	0.37	0	24,25,25	0.63	0
9	PGV	h	102	-	45,45,50	0.97	2 (4%)	49,50,56	1.19	5 (10%)
15	PEF	h	103	-	40,40,46	1.02	2 (5%)	43,45,51	1.13	3 (6%)
20	HEC	C	502	6	32,50,50	2.09	3 (9%)	24,82,82	1.69	6 (25%)

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
8	BCL	N	101	-	-	18/37/137/137	-
20	HEC	C	501	6	-	2/10/54/54	-
8	BCL	2	102	-	-	21/37/137/137	-
10	U4Z	3	102	-	-	4/36/53/53	0/1/1/1
9	PGV	I	103	-	-	11/48/48/55	-
13	MQE	M	704	-	-	12/65/85/85	0/2/2/2
16	LMT	1	104	-	-	3/21/61/61	0/2/2/2
8	BCL	0	101	-	-	11/37/137/137	-
16	LMT	H	102	-	-	6/21/61/61	0/2/2/2
13	MQE	L	705	-	-	6/47/67/85	0/2/2/2
8	BCL	4	101	-	-	17/37/137/137	-
9	PGV	L	712	-	-	15/39/39/55	-
11	BPH	L	704	-	-	11/37/105/105	0/5/6/6
8	BCL	3	101	-	-	11/37/137/137	-
9	PGV	L	706	-	-	16/55/55/55	-
14	BGL	L	715	-	-	1/11/31/31	0/1/1/1
8	BCL	S	102	-	-	19/37/137/137	-
9	PGV	U	104	-	-	14/48/48/55	-
18	CDL	P	102	-	-	23/60/60/110	-
8	BCL	O	102	-	-	18/37/137/137	-
8	BCL	W	102	-	-	17/37/137/137	-
11	BPH	M	702	-	-	23/37/105/105	0/5/6/6
8	BCL	L	703	-	-	17/37/137/137	-
8	BCL	U	101	-	-	11/37/137/137	-
8	BCL	F	101	-	-	21/37/137/137	-
20	HEC	C	504	6	-	3/10/54/54	-
8	BCL	G	101	-	-	16/37/137/137	-
15	PEF	L	717	-	-	12/44/44/50	-
8	BCL	T	101	-	-	17/37/137/137	-
14	BGL	Y	103	-	-	3/11/31/31	0/1/1/1
8	BCL	1	101	-	-	13/37/137/137	-
8	BCL	8	101	-	-	14/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PGV	0	104	-	-	15/48/48/55	-
8	BCL	I	101	-	-	10/37/137/137	-
16	LMT	M	709	-	-	12/21/61/61	0/2/2/2
14	BGL	L	708	-	-	3/11/31/31	0/1/1/1
8	BCL	3	103	-	-	14/37/137/137	-
8	BCL	K	102	-	-	18/37/137/137	-
8	BCL	E	101	-	-	15/37/137/137	-
8	BCL	M	701	-	-	20/37/137/137	-
20	HEC	C	503	6	-	0/10/54/54	-
14	BGL	M	706	-	-	3/11/31/31	0/1/1/1
8	BCL	J	102	-	-	14/37/137/137	-
8	BCL	H	101	-	-	16/37/137/137	-
8	BCL	A	102	-	-	13/37/137/137	-
9	PGV	N	102	-	-	2/28/28/55	-
8	BCL	U	102	-	-	23/37/137/137	-
9	PGV	8	103	-	-	15/48/48/55	-
8	BCL	K	101	-	-	15/37/137/137	-
8	BCL	B	101	-	-	17/37/137/137	-
8	BCL	V	101	-	-	19/37/137/137	-
8	BCL	P	101	-	-	10/37/137/137	-
11	BPH	L	701	-	-	14/37/105/105	0/5/6/6
9	PGV	0	105	-	-	11/48/48/55	-
14	BGL	M	707	-	-	1/11/31/31	0/1/1/1
10	U4Z	0	103	-	-	2/36/53/53	0/1/1/1
14	BGL	H	103	-	-	2/11/31/31	0/1/1/1
8	BCL	O	101	-	-	12/37/137/137	-
9	PGV	K	104	-	-	15/48/48/55	-
9	PGV	L	711	-	-	11/36/36/55	-
8	BCL	5	101	-	-	16/37/137/137	-
8	BCL	G	102	-	-	23/37/137/137	-
14	BGL	L	709	-	-	0/11/31/31	0/1/1/1
9	PGV	O	103	-	-	17/48/48/55	-
9	PGV	S	103	-	-	11/48/48/55	-
16	LMT	D	104	-	-	7/21/61/61	0/2/2/2
8	BCL	S	101	-	-	17/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	Q	102	-	-	20/37/137/137	-
8	BCL	A	101	-	-	15/37/137/137	-
14	BGL	L	714	-	-	2/11/31/31	0/1/1/1
8	BCL	W	101	-	-	18/37/137/137	-
8	BCL	0	102	-	-	20/37/137/137	-
9	PGV	6	103	-	-	16/48/48/55	-
8	BCL	Q	101	-	-	15/37/137/137	-
9	PGV	C	506	21	-	21/55/55/55	-
9	PGV	M	705	-	-	11/39/39/55	-
8	BCL	L	702	-	-	14/37/137/137	-
8	BCL	2	101	-	-	14/37/137/137	-
14	BGL	M	710	-	-	1/11/31/31	0/1/1/1
14	BGL	Y	101	-	-	2/11/31/31	0/1/1/1
15	PEF	M	708	-	-	8/23/23/50	-
9	PGV	K	103	-	-	13/48/48/55	-
19	LHG	h	101	5	-	19/23/23/53	-
16	LMT	T	102	-	-	8/21/61/61	0/2/2/2
8	BCL	9	101	-	-	13/37/137/137	-
15	PEF	L	713	-	-	14/50/50/50	-
9	PGV	E	103	-	-	15/48/48/55	-
9	PGV	E	104	-	-	11/48/48/55	-
8	BCL	6	102	-	-	20/37/137/137	-
10	U4Z	J	101	-	-	4/36/53/53	0/1/1/1
8	BCL	8	102	-	-	12/37/137/137	-
10	U4Z	R	101	-	-	4/36/53/53	0/1/1/1
10	U4Z	D	101	-	-	4/36/53/53	0/1/1/1
8	BCL	I	102	-	-	23/37/137/137	-
8	BCL	6	101	-	-	10/37/137/137	-
9	PGV	1	102	-	-	11/37/37/55	-
8	BCL	R	102	-	-	13/37/137/137	-
9	PGV	4	102	-	-	15/48/48/55	-
8	BCL	7	101	-	-	16/37/137/137	-
8	BCL	D	102	-	-	15/37/137/137	-
9	PGV	U	103	-	-	12/48/48/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	E	102	-	-	23/37/137/137	-
14	BGL	C	507	-	-	1/11/31/31	0/1/1/1
9	PGV	h	102	-	-	11/47/47/55	-
15	PEF	h	103	-	-	18/44/44/50	-
20	HEC	C	502	6	-	0/10/54/54	-

All (718) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	501	HEC	C2B-C3B	-6.58	1.33	1.40
20	C	503	HEC	C2B-C3B	-6.42	1.34	1.40
20	C	504	HEC	C2B-C3B	-6.00	1.34	1.40
20	C	502	HEC	C2B-C3B	-5.93	1.34	1.40
20	C	501	HEC	C3C-C2C	-5.87	1.34	1.40
20	C	502	HEC	C3C-C2C	-5.86	1.34	1.40
20	C	503	HEC	C3C-C2C	-5.84	1.34	1.40
20	C	504	HEC	C3C-C2C	-5.78	1.34	1.40
20	C	504	HEC	C3D-C2D	5.57	1.54	1.37
20	C	502	HEC	C3D-C2D	5.32	1.53	1.37
20	C	501	HEC	C3D-C2D	5.31	1.53	1.37
20	C	503	HEC	C3D-C2D	5.29	1.53	1.37
8	A	101	BCL	C3B-C2B	5.26	1.48	1.39
8	E	101	BCL	C3B-C2B	5.23	1.48	1.39
8	G	102	BCL	O2D-CGD	5.17	1.45	1.33
8	0	101	BCL	C3B-C2B	5.13	1.48	1.39
8	W	101	BCL	C3B-C2B	5.12	1.48	1.39
8	L	703	BCL	O2D-CGD	5.12	1.45	1.33
8	8	101	BCL	C3B-C2B	5.12	1.48	1.39
8	B	101	BCL	C3D-C4D	-5.09	1.32	1.44
8	G	101	BCL	C3B-C2B	5.08	1.48	1.39
8	B	101	BCL	C3B-C2B	5.07	1.48	1.39
8	6	101	BCL	C3B-C2B	5.07	1.48	1.39
8	S	101	BCL	C3B-C2B	5.06	1.48	1.39
8	M	701	BCL	O2D-CGD	5.06	1.45	1.33
8	0	102	BCL	O2D-CGD	5.05	1.45	1.33
8	3	101	BCL	C3B-C2B	5.05	1.48	1.39
8	O	101	BCL	C3B-C2B	5.04	1.48	1.39
8	K	101	BCL	C3B-C2B	5.02	1.48	1.39
8	2	101	BCL	C3B-C2B	5.02	1.48	1.39
8	L	702	BCL	C3D-C4D	-5.01	1.32	1.44
8	G	102	BCL	C3D-C4D	-5.00	1.32	1.44
8	W	102	BCL	O2D-CGD	5.00	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	102	BCL	C3D-C4D	-4.98	1.32	1.44
8	R	102	BCL	O2D-CGD	4.98	1.45	1.33
8	9	101	BCL	O2D-CGD	4.98	1.45	1.33
8	K	102	BCL	C3D-C4D	-4.97	1.32	1.44
8	U	101	BCL	O2D-CGD	4.97	1.45	1.33
8	Q	102	BCL	C3D-C4D	-4.96	1.33	1.44
8	8	102	BCL	O2D-CGD	4.96	1.45	1.33
8	I	101	BCL	C3B-C2B	4.96	1.48	1.39
8	0	102	BCL	C3D-C4D	-4.96	1.33	1.44
8	U	101	BCL	C3B-C2B	4.96	1.48	1.39
8	Q	101	BCL	C3B-C2B	4.96	1.48	1.39
8	S	101	BCL	O2D-CGD	4.95	1.45	1.33
8	E	102	BCL	C3D-C4D	-4.95	1.33	1.44
8	I	101	BCL	O2D-CGD	4.95	1.45	1.33
8	L	702	BCL	C3B-C2B	4.94	1.48	1.39
8	W	101	BCL	O2D-CGD	4.93	1.45	1.33
8	T	101	BCL	O2D-CGD	4.93	1.45	1.33
8	U	102	BCL	O2D-CGD	4.93	1.45	1.33
8	0	101	BCL	O2D-CGD	4.93	1.45	1.33
8	2	101	BCL	O2D-CGD	4.93	1.45	1.33
8	2	102	BCL	O2D-CGD	4.91	1.45	1.33
8	V	101	BCL	O2D-CGD	4.91	1.45	1.33
8	L	703	BCL	C3B-C2B	4.91	1.48	1.39
8	S	102	BCL	C3D-C4D	-4.91	1.33	1.44
8	O	101	BCL	O2D-CGD	4.90	1.45	1.33
8	A	102	BCL	C3D-C4D	-4.90	1.33	1.44
8	S	102	BCL	O2D-CGD	4.89	1.45	1.33
8	7	101	BCL	O2D-CGD	4.88	1.45	1.33
8	G	102	BCL	C3B-C2B	4.88	1.48	1.39
8	4	101	BCL	O2D-CGD	4.88	1.45	1.33
8	P	101	BCL	O2D-CGD	4.87	1.45	1.33
8	6	102	BCL	O2D-CGD	4.87	1.45	1.33
8	Q	102	BCL	C3B-C2B	4.87	1.48	1.39
8	F	101	BCL	O2D-CGD	4.86	1.45	1.33
8	D	102	BCL	O2D-CGD	4.86	1.45	1.33
8	N	101	BCL	O2D-CGD	4.86	1.45	1.33
8	6	102	BCL	C3D-C4D	-4.86	1.33	1.44
8	A	102	BCL	O2D-CGD	4.84	1.45	1.33
8	A	101	BCL	O2D-CGD	4.84	1.45	1.33
8	3	103	BCL	O2D-CGD	4.84	1.45	1.33
8	4	101	BCL	C3D-C4D	-4.83	1.33	1.44
8	8	101	BCL	O2D-CGD	4.82	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	3	101	BCL	O2D-CGD	4.82	1.45	1.33
8	5	101	BCL	O2D-CGD	4.82	1.45	1.33
8	Q	101	BCL	O2D-CGD	4.82	1.45	1.33
8	V	101	BCL	C3D-C4D	-4.82	1.33	1.44
8	8	102	BCL	C3D-C4D	-4.82	1.33	1.44
8	O	102	BCL	C3D-C4D	-4.81	1.33	1.44
8	5	101	BCL	C3D-C4D	-4.81	1.33	1.44
8	K	101	BCL	O2D-CGD	4.81	1.44	1.33
8	G	101	BCL	O2D-CGD	4.80	1.44	1.33
8	E	101	BCL	O2D-CGD	4.78	1.44	1.33
8	W	102	BCL	C3D-C4D	-4.78	1.33	1.44
8	H	101	BCL	O2D-CGD	4.78	1.44	1.33
8	J	102	BCL	C3D-C4D	-4.77	1.33	1.44
8	J	102	BCL	O2D-CGD	4.77	1.44	1.33
8	M	701	BCL	C3B-C2B	4.77	1.48	1.39
8	Q	101	BCL	C3D-C4D	-4.77	1.33	1.44
8	8	101	BCL	C3D-C4D	-4.77	1.33	1.44
8	6	101	BCL	O2D-CGD	4.76	1.44	1.33
8	D	102	BCL	C3B-C2B	4.76	1.48	1.39
8	9	101	BCL	C3D-C4D	-4.76	1.33	1.44
8	R	102	BCL	C3D-C4D	-4.75	1.33	1.44
8	3	103	BCL	C3D-C4D	-4.75	1.33	1.44
8	O	102	BCL	O2D-CGD	4.75	1.44	1.33
8	7	101	BCL	C3B-C2B	4.74	1.47	1.39
8	M	701	BCL	C3D-C4D	-4.74	1.33	1.44
8	A	101	BCL	C3D-C4D	-4.74	1.33	1.44
8	U	101	BCL	C3D-C4D	-4.74	1.33	1.44
8	E	101	BCL	C3D-C4D	-4.73	1.33	1.44
8	0	101	BCL	C3D-C4D	-4.73	1.33	1.44
8	K	102	BCL	O2D-CGD	4.73	1.44	1.33
8	T	101	BCL	C3D-C4D	-4.72	1.33	1.44
8	H	101	BCL	C3D-C4D	-4.72	1.33	1.44
8	P	101	BCL	C3D-C4D	-4.71	1.33	1.44
8	F	101	BCL	C3D-C4D	-4.71	1.33	1.44
8	D	102	BCL	C3D-C4D	-4.71	1.33	1.44
8	3	103	BCL	C3B-C2B	4.70	1.47	1.39
8	7	101	BCL	C3D-C4D	-4.69	1.33	1.44
8	S	101	BCL	C3D-C4D	-4.69	1.33	1.44
8	3	101	BCL	C3D-C4D	-4.69	1.33	1.44
8	E	102	BCL	C3B-C2B	4.68	1.47	1.39
8	E	102	BCL	O2D-CGD	4.68	1.44	1.33
8	W	101	BCL	C3D-C4D	-4.68	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	O	101	BCL	C3D-C4D	-4.67	1.33	1.44
8	2	102	BCL	C3D-C4D	-4.67	1.33	1.44
15	M	708	PEF	O2-C10	4.66	1.45	1.35
8	N	101	BCL	C3D-C4D	-4.66	1.33	1.44
8	N	101	BCL	C3B-C2B	4.66	1.47	1.39
8	F	101	BCL	C3B-C2B	4.65	1.47	1.39
8	U	102	BCL	C3D-C4D	-4.65	1.33	1.44
8	G	101	BCL	C3D-C4D	-4.65	1.33	1.44
8	2	101	BCL	C3D-C4D	-4.64	1.33	1.44
8	I	102	BCL	O2D-CGD	4.64	1.44	1.33
8	K	101	BCL	C3D-C4D	-4.64	1.33	1.44
8	I	101	BCL	C3D-C4D	-4.63	1.33	1.44
8	6	102	BCL	C3B-C2B	4.62	1.47	1.39
8	L	703	BCL	C3D-C4D	-4.62	1.33	1.44
8	6	101	BCL	C3D-C4D	-4.61	1.33	1.44
8	Q	102	BCL	O2D-CGD	4.61	1.44	1.33
8	A	102	BCL	C3B-C2B	4.61	1.47	1.39
8	H	101	BCL	C3B-C2B	4.61	1.47	1.39
8	1	101	BCL	C3D-C4D	-4.61	1.33	1.44
8	R	102	BCL	C3B-C2B	4.58	1.47	1.39
8	P	101	BCL	C3B-C2B	4.57	1.47	1.39
8	B	101	BCL	O2D-CGD	4.57	1.44	1.33
8	J	102	BCL	C3B-C2B	4.56	1.47	1.39
8	T	101	BCL	C3B-C2B	4.54	1.47	1.39
8	M	701	BCL	O2A-CGA	4.50	1.46	1.33
8	1	101	BCL	C3B-C2B	4.50	1.47	1.39
8	1	101	BCL	O2D-CGD	4.49	1.44	1.33
8	8	101	BCL	C1D-ND	-4.49	1.32	1.37
8	E	101	BCL	O2A-CGA	4.48	1.46	1.33
8	K	102	BCL	O2A-CGA	4.48	1.46	1.33
8	L	703	BCL	O2A-CGA	4.45	1.46	1.33
8	2	102	BCL	O2A-CGA	4.44	1.46	1.33
8	9	101	BCL	C3B-C2B	4.43	1.47	1.39
8	E	102	BCL	O2A-CGA	4.40	1.46	1.33
8	B	101	BCL	O2A-CGA	4.39	1.46	1.33
8	L	702	BCL	O2D-CGD	4.39	1.43	1.33
8	W	102	BCL	O2A-CGA	4.38	1.46	1.33
8	2	102	BCL	C3B-C2B	4.36	1.47	1.39
8	O	102	BCL	O2A-CGA	4.35	1.46	1.33
8	5	101	BCL	C3B-C2B	4.35	1.47	1.39
9	M	705	PGV	O03-C19	4.35	1.46	1.33
8	I	102	BCL	C3B-C2B	4.32	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	8	101	BCL	O2A-CGA	4.32	1.46	1.33
8	U	101	BCL	O2A-CGA	4.31	1.45	1.33
8	I	102	BCL	O2A-CGA	4.30	1.45	1.33
8	V	101	BCL	O2A-CGA	4.30	1.45	1.33
9	0	104	PGV	O03-C19	4.30	1.45	1.33
9	U	104	PGV	O03-C19	4.29	1.45	1.33
9	1	102	PGV	O03-C19	4.28	1.45	1.33
9	O	103	PGV	O03-C19	4.27	1.45	1.33
18	P	102	CDL	OB8-CB7	4.27	1.45	1.33
9	8	103	PGV	O03-C19	4.27	1.45	1.33
8	V	101	BCL	C3B-C2B	4.26	1.47	1.39
15	L	713	PEF	O3-C30	4.26	1.45	1.33
15	h	103	PEF	O3-C30	4.26	1.45	1.33
9	6	103	PGV	O03-C19	4.25	1.45	1.33
9	K	103	PGV	O03-C19	4.24	1.45	1.33
9	U	103	PGV	O03-C19	4.24	1.45	1.33
9	E	104	PGV	O03-C19	4.24	1.45	1.33
8	S	102	BCL	O2A-CGA	4.24	1.45	1.33
9	I	103	PGV	O03-C19	4.23	1.45	1.33
9	4	102	PGV	O03-C19	4.23	1.45	1.33
9	0	105	PGV	O03-C19	4.23	1.45	1.33
8	A	102	BCL	O2A-CGA	4.23	1.45	1.33
8	1	101	BCL	O2A-CGA	4.23	1.45	1.33
9	E	103	PGV	O03-C19	4.22	1.45	1.33
8	6	102	BCL	O2A-CGA	4.21	1.45	1.33
9	S	103	PGV	O03-C19	4.21	1.45	1.33
9	N	102	PGV	O03-C19	4.21	1.45	1.33
15	M	708	PEF	O3-C30	4.20	1.45	1.33
9	K	104	PGV	O03-C19	4.20	1.45	1.33
9	L	711	PGV	O03-C19	4.20	1.45	1.33
15	L	717	PEF	O3-C30	4.19	1.45	1.33
9	6	103	PGV	O01-C1	4.19	1.46	1.34
18	P	102	CDL	OA8-CA7	4.18	1.45	1.33
8	K	101	BCL	O2A-CGA	4.18	1.45	1.33
8	K	102	BCL	C3B-C2B	4.17	1.46	1.39
8	6	101	BCL	O2A-CGA	4.17	1.45	1.33
9	K	104	PGV	O01-C1	4.17	1.46	1.34
18	P	102	CDL	OB6-CB5	4.16	1.46	1.34
8	4	101	BCL	O2A-CGA	4.16	1.45	1.33
8	2	101	BCL	O2A-CGA	4.15	1.45	1.33
8	4	101	BCL	C3B-C2B	4.14	1.46	1.39
9	S	103	PGV	O01-C1	4.14	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	101	BCL	O2A-CGA	4.13	1.45	1.33
8	6	101	BCL	C1D-ND	-4.13	1.32	1.37
9	U	104	PGV	O01-C1	4.13	1.45	1.34
8	J	102	BCL	O2A-CGA	4.12	1.45	1.33
8	I	101	BCL	O2A-CGA	4.12	1.45	1.33
8	Q	102	BCL	O2A-CGA	4.12	1.45	1.33
9	0	105	PGV	O01-C1	4.12	1.45	1.34
8	2	101	BCL	C1D-ND	-4.12	1.32	1.37
8	F	101	BCL	O2A-CGA	4.12	1.45	1.33
9	O	103	PGV	O01-C1	4.11	1.45	1.34
9	h	102	PGV	O01-C1	4.11	1.45	1.34
8	K	101	BCL	C1D-ND	-4.10	1.32	1.37
9	M	705	PGV	O01-C1	4.10	1.45	1.34
9	h	102	PGV	O03-C19	4.10	1.45	1.33
9	L	712	PGV	O03-C19	4.09	1.45	1.33
8	Q	101	BCL	O2A-CGA	4.09	1.45	1.33
9	K	103	PGV	O01-C1	4.09	1.45	1.34
9	L	706	PGV	O03-C19	4.09	1.45	1.33
8	H	101	BCL	O2A-CGA	4.09	1.45	1.33
8	W	102	BCL	C3B-C2B	4.09	1.46	1.39
8	G	102	BCL	O2A-CGA	4.09	1.45	1.33
9	U	103	PGV	O01-C1	4.09	1.45	1.34
9	8	103	PGV	O01-C1	4.08	1.45	1.34
8	0	101	BCL	O2A-CGA	4.08	1.45	1.33
9	E	103	PGV	O01-C1	4.08	1.45	1.34
8	9	101	BCL	O2A-CGA	4.07	1.45	1.33
9	L	706	PGV	O01-C1	4.07	1.45	1.34
9	I	103	PGV	O01-C1	4.06	1.45	1.34
9	L	712	PGV	O01-C1	4.06	1.45	1.34
8	Q	101	BCL	C1D-ND	-4.06	1.32	1.37
9	0	104	PGV	O01-C1	4.06	1.45	1.34
8	U	101	BCL	C1D-ND	-4.06	1.32	1.37
15	h	103	PEF	O2-C10	4.06	1.45	1.34
8	N	101	BCL	O2A-CGA	4.05	1.45	1.33
9	N	102	PGV	O01-C1	4.05	1.45	1.34
8	5	101	BCL	O2A-CGA	4.05	1.45	1.33
8	A	101	BCL	C1D-ND	-4.05	1.32	1.37
9	C	506	PGV	O03-C19	4.04	1.45	1.33
9	4	102	PGV	O01-C1	4.04	1.45	1.34
8	I	101	BCL	C1D-ND	-4.04	1.32	1.37
8	G	101	BCL	C1D-ND	-4.03	1.32	1.37
8	3	103	BCL	O2A-CGA	4.03	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	717	PEF	O2-C10	4.03	1.45	1.34
8	R	102	BCL	O2A-CGA	4.03	1.45	1.33
8	L	702	BCL	O2A-CGA	4.03	1.45	1.33
8	U	102	BCL	O2A-CGA	4.02	1.45	1.33
8	W	101	BCL	O2A-CGA	4.02	1.45	1.33
8	0	102	BCL	O2A-CGA	4.02	1.45	1.33
8	S	101	BCL	O2A-CGA	4.02	1.45	1.33
9	E	104	PGV	O01-C1	4.02	1.45	1.34
8	S	101	BCL	C1D-ND	-4.01	1.32	1.37
8	S	102	BCL	C3B-C2B	4.00	1.46	1.39
8	8	102	BCL	O2A-CGA	4.00	1.45	1.33
8	7	101	BCL	O2A-CGA	4.00	1.45	1.33
8	P	101	BCL	O2A-CGA	3.99	1.45	1.33
8	D	102	BCL	O2A-CGA	3.99	1.45	1.33
8	O	101	BCL	O2A-CGA	3.98	1.45	1.33
18	P	102	CDL	OA6-CA5	3.98	1.45	1.34
8	G	101	BCL	O2A-CGA	3.97	1.45	1.33
8	0	102	BCL	C3B-C2B	3.95	1.46	1.39
9	1	102	PGV	O01-C1	3.92	1.45	1.34
8	0	101	BCL	C1D-ND	-3.92	1.33	1.37
15	L	713	PEF	O2-C10	3.92	1.45	1.34
8	O	101	BCL	C1D-ND	-3.92	1.33	1.37
8	W	101	BCL	C1D-ND	-3.91	1.33	1.37
8	E	101	BCL	C1D-ND	-3.90	1.33	1.37
8	3	101	BCL	O2A-CGA	3.87	1.44	1.33
8	8	102	BCL	C3B-C2B	3.86	1.46	1.39
8	T	101	BCL	O2A-CGA	3.85	1.44	1.33
8	3	101	BCL	C1D-ND	-3.83	1.33	1.37
8	O	102	BCL	C3B-C2B	3.78	1.46	1.39
10	3	102	U4Z	CBJ-CBH	3.76	1.40	1.35
10	3	102	U4Z	CAV-CAR	3.72	1.40	1.35
10	3	102	U4Z	CBI-CBL	3.62	1.40	1.35
8	U	102	BCL	C1B-NB	-3.59	1.32	1.35
10	R	101	U4Z	CBJ-CBH	3.56	1.40	1.35
9	C	506	PGV	O01-C1	3.56	1.44	1.34
10	J	101	U4Z	CBI-CBL	3.51	1.40	1.35
10	J	101	U4Z	CBJ-CBH	3.49	1.40	1.35
10	3	102	U4Z	CAO-CAM	3.48	1.40	1.35
10	R	101	U4Z	CBI-CBL	3.48	1.40	1.35
8	H	101	BCL	C1D-ND	-3.46	1.33	1.37
10	0	103	U4Z	CBJ-CBH	3.46	1.40	1.35
8	K	102	BCL	CHD-C1D	3.46	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	101	U4Z	CBJ-CBH	3.44	1.40	1.35
8	A	102	BCL	CHD-C1D	3.44	1.45	1.38
10	0	103	U4Z	CAL-CAM	-3.43	1.38	1.45
10	J	101	U4Z	CAV-CAR	3.43	1.40	1.35
8	L	702	BCL	C1D-ND	-3.43	1.33	1.37
10	0	103	U4Z	CAV-CAR	3.42	1.40	1.35
10	0	103	U4Z	CBI-CBL	3.42	1.40	1.35
10	R	101	U4Z	CAV-CAR	3.42	1.40	1.35
8	L	703	BCL	CHD-C1D	3.41	1.45	1.38
8	U	102	BCL	C3B-C2B	3.41	1.45	1.39
10	J	101	U4Z	CAO-CAM	3.40	1.40	1.35
8	0	102	BCL	CHD-C1D	3.39	1.45	1.38
10	D	101	U4Z	CBI-CBL	3.36	1.40	1.35
8	3	103	BCL	C1D-ND	-3.35	1.33	1.37
10	D	101	U4Z	CAV-CAR	3.35	1.40	1.35
8	M	701	BCL	C1D-ND	-3.34	1.33	1.37
8	U	102	BCL	CHD-C1D	3.34	1.44	1.38
8	V	101	BCL	CHD-C1D	3.33	1.44	1.38
10	J	101	U4Z	CAL-CAM	-3.33	1.38	1.45
8	P	101	BCL	C1D-ND	-3.32	1.33	1.37
8	J	102	BCL	C1D-ND	-3.32	1.33	1.37
8	1	101	BCL	CHD-C1D	3.32	1.44	1.38
8	F	101	BCL	C1D-ND	-3.31	1.33	1.37
10	D	101	U4Z	CAL-CAM	-3.31	1.38	1.45
10	R	101	U4Z	CAO-CAM	3.29	1.40	1.35
8	7	101	BCL	CHD-C1D	3.29	1.44	1.38
8	D	102	BCL	OBD-CAD	3.28	1.28	1.22
8	R	102	BCL	CHD-C1D	3.28	1.44	1.38
10	0	103	U4Z	CAO-CAM	3.27	1.40	1.35
10	D	101	U4Z	CAO-CAM	3.26	1.40	1.35
8	B	101	BCL	C1D-ND	-3.25	1.33	1.37
8	5	101	BCL	C1D-ND	-3.25	1.33	1.37
10	R	101	U4Z	CAL-CAM	-3.25	1.39	1.45
8	M	701	BCL	CHD-C1D	3.25	1.44	1.38
8	Q	102	BCL	CHD-C1D	3.23	1.44	1.38
8	S	102	BCL	CHD-C1D	3.23	1.44	1.38
8	O	102	BCL	CHD-C1D	3.22	1.44	1.38
8	1	101	BCL	C1D-ND	-3.19	1.33	1.37
8	B	101	BCL	CHD-C1D	3.19	1.44	1.38
8	N	101	BCL	CHD-C1D	3.19	1.44	1.38
8	L	702	BCL	C3D-C2D	3.19	1.47	1.39
8	J	102	BCL	CHD-C1D	3.19	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	102	U4Z	CAL-CAM	-3.18	1.39	1.45
8	O	101	BCL	OBD-CAD	3.18	1.28	1.22
8	F	101	BCL	CHD-C1D	3.17	1.44	1.38
8	T	101	BCL	CHD-C1D	3.17	1.44	1.38
8	L	702	BCL	CHD-C1D	3.17	1.44	1.38
8	9	101	BCL	CHD-C1D	3.16	1.44	1.38
8	J	102	BCL	OBD-CAD	3.16	1.27	1.22
8	D	102	BCL	CHD-C1D	3.16	1.44	1.38
8	S	102	BCL	OBD-CAD	3.15	1.27	1.22
8	4	101	BCL	CHD-C1D	3.15	1.44	1.38
8	P	101	BCL	CHD-C1D	3.15	1.44	1.38
8	9	101	BCL	C1D-ND	-3.14	1.33	1.37
8	I	102	BCL	CHD-C1D	3.14	1.44	1.38
8	Q	102	BCL	C1D-ND	-3.13	1.33	1.37
8	D	102	BCL	C1D-ND	-3.13	1.33	1.37
8	2	102	BCL	CHD-C1D	3.13	1.44	1.38
8	5	101	BCL	CHD-C1D	3.12	1.44	1.38
8	G	102	BCL	CHD-C1D	3.12	1.44	1.38
8	3	101	BCL	OBD-CAD	3.12	1.27	1.22
8	1	101	BCL	OBD-CAD	3.10	1.27	1.22
8	3	103	BCL	OBD-CAD	3.09	1.27	1.22
8	6	101	BCL	OBD-CAD	3.08	1.27	1.22
8	R	102	BCL	C1D-ND	-3.08	1.34	1.37
8	W	102	BCL	CHD-C1D	3.08	1.44	1.38
8	9	101	BCL	OBD-CAD	3.08	1.27	1.22
8	E	102	BCL	CHD-C1D	3.07	1.44	1.38
8	F	101	BCL	OBD-CAD	3.07	1.27	1.22
8	3	103	BCL	CHD-C1D	3.06	1.44	1.38
8	N	101	BCL	C1D-ND	-3.06	1.34	1.37
8	8	102	BCL	CHD-C1D	3.05	1.44	1.38
8	2	102	BCL	OBD-CAD	3.05	1.27	1.22
8	Q	101	BCL	OBD-CAD	3.05	1.27	1.22
8	R	102	BCL	OBD-CAD	3.05	1.27	1.22
8	A	102	BCL	C1D-ND	-3.05	1.34	1.37
8	R	102	BCL	C3D-C2D	3.04	1.47	1.39
8	N	101	BCL	OBD-CAD	3.03	1.27	1.22
8	V	101	BCL	C1D-ND	-3.02	1.34	1.37
8	A	102	BCL	C3D-C2D	3.02	1.47	1.39
8	O	101	BCL	C3D-C2D	3.01	1.47	1.39
8	U	101	BCL	C3D-C2D	3.01	1.47	1.39
8	T	101	BCL	C1D-ND	-3.00	1.34	1.37
8	2	101	BCL	C3D-C2D	3.00	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	7	101	BCL	OBD-CAD	3.00	1.27	1.22
8	1	101	BCL	C3D-C2D	3.00	1.47	1.39
8	O	102	BCL	C1D-ND	-2.99	1.34	1.37
8	M	701	BCL	OBD-CAD	2.98	1.27	1.22
8	E	102	BCL	OBD-CAD	2.98	1.27	1.22
8	K	101	BCL	OBD-CAD	2.98	1.27	1.22
8	S	101	BCL	C3D-C2D	2.98	1.47	1.39
8	H	101	BCL	OBD-CAD	2.97	1.27	1.22
8	I	101	BCL	OBD-CAD	2.97	1.27	1.22
8	2	101	BCL	OBD-CAD	2.97	1.27	1.22
8	G	101	BCL	OBD-CAD	2.97	1.27	1.22
8	U	101	BCL	OBD-CAD	2.96	1.27	1.22
8	A	101	BCL	OBD-CAD	2.95	1.27	1.22
8	0	101	BCL	C3D-C2D	2.95	1.47	1.39
8	8	101	BCL	C3D-C2D	2.95	1.47	1.39
8	Q	102	BCL	C3D-C2D	2.95	1.47	1.39
8	W	101	BCL	C3D-C2D	2.94	1.47	1.39
8	6	102	BCL	CHD-C1D	2.94	1.44	1.38
8	3	103	BCL	C3D-C2D	2.94	1.47	1.39
8	E	101	BCL	C3D-C2D	2.93	1.47	1.39
8	9	101	BCL	C3D-C2D	2.93	1.47	1.39
8	Q	101	BCL	C3D-C2D	2.93	1.47	1.39
8	E	101	BCL	OBD-CAD	2.93	1.27	1.22
8	L	702	BCL	OBD-CAD	2.92	1.27	1.22
8	I	102	BCL	C1D-ND	-2.92	1.34	1.37
8	N	101	BCL	C3D-C2D	2.91	1.47	1.39
8	F	101	BCL	C3D-C2D	2.91	1.47	1.39
8	P	101	BCL	OBD-CAD	2.91	1.27	1.22
8	H	101	BCL	CHD-C1D	2.91	1.44	1.38
8	A	101	BCL	C3D-C2D	2.90	1.47	1.39
8	K	101	BCL	C3D-C2D	2.90	1.47	1.39
8	6	101	BCL	C3D-C2D	2.90	1.47	1.39
8	V	101	BCL	OBD-CAD	2.90	1.27	1.22
8	5	101	BCL	OBD-CAD	2.90	1.27	1.22
8	U	102	BCL	OBD-CAD	2.89	1.27	1.22
8	D	102	BCL	C3D-C2D	2.89	1.47	1.39
8	B	101	BCL	MG-NA	-2.88	1.99	2.06
8	2	101	BCL	CHD-C1D	2.88	1.44	1.38
8	S	102	BCL	C1D-ND	-2.88	1.34	1.37
8	B	101	BCL	C3D-C2D	2.88	1.47	1.39
8	V	101	BCL	C3D-C2D	2.88	1.47	1.39
8	8	101	BCL	OBD-CAD	2.88	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	703	BCL	OBD-CAD	2.88	1.27	1.22
8	3	101	BCL	C3D-C2D	2.88	1.47	1.39
8	O	102	BCL	OBD-CAD	2.88	1.27	1.22
8	L	703	BCL	C1D-ND	-2.88	1.34	1.37
8	T	101	BCL	OBD-CAD	2.87	1.27	1.22
8	E	102	BCL	C1D-ND	-2.87	1.34	1.37
8	I	101	BCL	C3D-C2D	2.87	1.47	1.39
8	H	101	BCL	MG-NA	-2.87	1.99	2.06
8	P	101	BCL	C3D-C2D	2.86	1.46	1.39
8	L	703	BCL	C3D-C2D	2.86	1.46	1.39
8	7	101	BCL	C3D-C2D	2.86	1.46	1.39
8	8	102	BCL	C1D-ND	-2.85	1.34	1.37
8	5	101	BCL	C3D-C2D	2.84	1.46	1.39
8	S	101	BCL	CHD-C1D	2.84	1.43	1.38
8	J	102	BCL	C3D-C2D	2.84	1.46	1.39
8	O	102	BCL	C3D-C2D	2.83	1.46	1.39
8	K	102	BCL	C3D-C2D	2.83	1.46	1.39
10	3	102	U4Z	CAH-CAD	2.83	1.39	1.34
8	4	101	BCL	C1D-ND	-2.83	1.34	1.37
8	H	101	BCL	C3D-C2D	2.82	1.46	1.39
8	M	701	BCL	C3D-C2D	2.82	1.46	1.39
8	U	102	BCL	C3D-C2D	2.82	1.46	1.39
8	0	102	BCL	C3D-C2D	2.82	1.46	1.39
10	D	101	U4Z	CAQ-CAR	-2.81	1.39	1.45
11	L	704	BPH	C3A-C2A	-2.81	1.52	1.54
8	K	101	BCL	CHD-C1D	2.81	1.43	1.38
8	T	101	BCL	C3D-C2D	2.81	1.46	1.39
8	K	102	BCL	C1D-ND	-2.81	1.34	1.37
10	0	103	U4Z	CAQ-CAR	-2.81	1.39	1.45
10	J	101	U4Z	CAH-CAD	2.81	1.39	1.34
8	W	102	BCL	OBD-CAD	2.80	1.27	1.22
8	6	102	BCL	C1D-ND	-2.79	1.34	1.37
8	0	102	BCL	C1D-ND	-2.79	1.34	1.37
11	M	702	BPH	C3A-C2A	-2.79	1.52	1.54
8	U	102	BCL	C4B-NB	-2.79	1.32	1.35
8	4	101	BCL	C3D-C2D	2.78	1.46	1.39
8	0	101	BCL	OBD-CAD	2.78	1.27	1.22
8	U	102	BCL	C1D-ND	-2.78	1.34	1.37
8	S	101	BCL	OBD-CAD	2.77	1.27	1.22
8	4	101	BCL	OBD-CAD	2.76	1.27	1.22
8	2	102	BCL	C1D-ND	-2.75	1.34	1.37
8	7	101	BCL	C1D-ND	-2.75	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	102	BCL	C3D-C2D	2.75	1.46	1.39
8	W	101	BCL	OBD-CAD	2.75	1.27	1.22
8	G	101	BCL	C3D-C2D	2.75	1.46	1.39
8	S	102	BCL	C3D-C2D	2.73	1.46	1.39
8	2	102	BCL	C3D-C2D	2.73	1.46	1.39
10	R	101	U4Z	CAQ-CAR	-2.73	1.40	1.45
8	A	101	BCL	CHD-C1D	2.73	1.43	1.38
8	I	102	BCL	C3D-C2D	2.73	1.46	1.39
8	6	102	BCL	C3D-C2D	2.72	1.46	1.39
8	U	101	BCL	CHD-C1D	2.72	1.43	1.38
8	B	101	BCL	CHD-C4C	2.69	1.46	1.39
8	8	102	BCL	OBD-CAD	2.69	1.27	1.22
8	A	102	BCL	OBD-CAD	2.68	1.27	1.22
8	O	101	BCL	CHD-C1D	2.67	1.43	1.38
8	0	101	BCL	CHD-C1D	2.67	1.43	1.38
8	6	101	BCL	CHD-C1D	2.67	1.43	1.38
8	8	101	BCL	CHD-C1D	2.67	1.43	1.38
8	E	102	BCL	C3D-C2D	2.66	1.46	1.39
8	E	101	BCL	CHD-C1D	2.65	1.43	1.38
10	J	101	U4Z	CAQ-CAR	-2.65	1.40	1.45
8	W	102	BCL	C3D-C2D	2.65	1.46	1.39
8	3	101	BCL	CHD-C1D	2.65	1.43	1.38
8	L	702	BCL	MG-NA	-2.65	2.00	2.06
8	W	102	BCL	C1D-ND	-2.64	1.34	1.37
10	3	102	U4Z	CAQ-CAR	-2.64	1.40	1.45
10	0	103	U4Z	CAH-CAD	2.63	1.39	1.34
8	3	103	BCL	MG-NA	-2.62	2.00	2.06
8	K	102	BCL	CHD-C4C	2.62	1.46	1.39
8	W	101	BCL	CHD-C1D	2.61	1.43	1.38
8	8	102	BCL	C3D-C2D	2.61	1.46	1.39
10	D	101	U4Z	CBN-CBL	-2.61	1.40	1.45
8	Q	101	BCL	CHD-C1D	2.60	1.43	1.38
8	I	101	BCL	CHD-C1D	2.60	1.43	1.38
8	E	102	BCL	CHD-C4C	2.59	1.46	1.39
8	V	101	BCL	CHD-C4C	2.59	1.46	1.39
8	7	101	BCL	CHD-C4C	2.58	1.46	1.39
8	1	101	BCL	CHD-C4C	2.57	1.46	1.39
8	O	102	BCL	CHD-C4C	2.56	1.46	1.39
8	B	101	BCL	C4B-NB	-2.56	1.32	1.35
8	3	101	BCL	MG-NA	-2.56	2.00	2.06
8	U	102	BCL	CHD-C4C	2.56	1.46	1.39
8	G	102	BCL	C1D-ND	-2.55	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	102	BCL	CHD-C4C	2.55	1.46	1.39
8	I	102	BCL	OBD-CAD	2.54	1.26	1.22
8	Q	102	BCL	CHD-C4C	2.54	1.46	1.39
10	R	101	U4Z	CBN-CBL	-2.54	1.40	1.45
8	G	101	BCL	CHD-C1D	2.53	1.43	1.38
10	D	101	U4Z	CBF-CBH	-2.53	1.40	1.45
8	W	101	BCL	MG-NA	-2.53	2.00	2.06
8	Q	102	BCL	MG-NA	-2.53	2.00	2.06
8	S	102	BCL	CHD-C4C	2.53	1.46	1.39
8	W	101	BCL	C3C-C4C	-2.53	1.48	1.51
10	J	101	U4Z	CBN-CBL	-2.53	1.40	1.45
8	R	102	BCL	CHD-C4C	2.52	1.46	1.39
8	B	101	BCL	MG-NC	-2.52	2.00	2.06
10	R	101	U4Z	CAH-CAD	2.52	1.38	1.34
8	P	101	BCL	MG-NA	-2.51	2.00	2.06
8	L	702	BCL	CHD-C4C	2.51	1.46	1.39
8	E	102	BCL	MG-NA	-2.51	2.00	2.06
10	J	101	U4Z	CBF-CBH	-2.51	1.40	1.45
8	O	101	BCL	MG-NC	-2.50	2.00	2.06
8	0	102	BCL	CHD-C4C	2.50	1.46	1.39
8	W	102	BCL	CHD-C4C	2.50	1.46	1.39
8	W	101	BCL	MG-NC	-2.49	2.00	2.06
10	0	103	U4Z	CBF-CBH	-2.49	1.40	1.45
8	B	101	BCL	OBD-CAD	2.49	1.26	1.22
10	3	102	U4Z	CBF-CBH	-2.48	1.40	1.45
8	4	101	BCL	CHD-C4C	2.48	1.46	1.39
10	3	102	U4Z	CBN-CBL	-2.47	1.40	1.45
10	0	103	U4Z	CBN-CBL	-2.47	1.40	1.45
8	M	701	BCL	MG-NA	-2.47	2.00	2.06
10	R	101	U4Z	CBF-CBH	-2.46	1.40	1.45
8	8	102	BCL	CHD-C4C	2.45	1.46	1.39
8	I	102	BCL	CHD-C4C	2.45	1.46	1.39
8	T	101	BCL	CHD-C4C	2.44	1.46	1.39
8	6	102	BCL	C1B-CHB	2.44	1.47	1.41
8	U	102	BCL	MG-NA	-2.43	2.00	2.06
8	2	101	BCL	MG-NA	-2.43	2.00	2.06
8	9	101	BCL	C3C-C4C	-2.43	1.48	1.51
8	S	101	BCL	MG-NA	-2.43	2.00	2.06
8	K	102	BCL	MG-NA	-2.42	2.00	2.06
8	D	102	BCL	MG-NA	-2.42	2.00	2.06
8	G	102	BCL	CHD-C4C	2.42	1.46	1.39
8	O	101	BCL	MG-NA	-2.42	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	3	101	BCL	MG-NC	-2.41	2.00	2.06
8	D	102	BCL	CHD-C4C	2.41	1.46	1.39
8	2	102	BCL	CHD-C4C	2.41	1.46	1.39
8	U	101	BCL	MG-NA	-2.40	2.00	2.06
8	K	102	BCL	OBD-CAD	2.40	1.26	1.22
8	N	101	BCL	CHD-C4C	2.40	1.46	1.39
8	R	102	BCL	MG-NA	-2.40	2.00	2.06
8	U	101	BCL	MG-NC	-2.40	2.00	2.06
8	Q	102	BCL	OBD-CAD	2.39	1.26	1.22
10	D	101	U4Z	CAH-CAD	2.39	1.38	1.34
8	0	101	BCL	MG-NA	-2.39	2.00	2.06
8	0	102	BCL	OBD-CAD	2.38	1.26	1.22
8	J	102	BCL	CHD-C4C	2.38	1.45	1.39
8	6	102	BCL	CHD-C4C	2.37	1.45	1.39
8	P	101	BCL	CHD-C4C	2.36	1.45	1.39
8	F	101	BCL	CHD-C4C	2.36	1.45	1.39
8	E	102	BCL	C1D-C2D	2.36	1.50	1.45
8	L	703	BCL	CHD-C4C	2.36	1.45	1.39
8	V	101	BCL	MG-NC	-2.36	2.00	2.06
8	9	101	BCL	CHD-C4C	2.36	1.45	1.39
8	H	101	BCL	C3C-C4C	-2.36	1.48	1.51
8	0	102	BCL	C1D-C2D	2.35	1.50	1.45
8	5	101	BCL	CHD-C4C	2.35	1.45	1.39
8	3	103	BCL	CHD-C4C	2.34	1.45	1.39
8	S	101	BCL	MG-NC	-2.34	2.00	2.06
8	L	703	BCL	C1D-C2D	2.34	1.49	1.45
8	4	101	BCL	C3C-C4C	-2.34	1.48	1.51
8	F	101	BCL	C3C-C4C	-2.33	1.48	1.51
8	9	101	BCL	MG-NA	-2.32	2.00	2.06
8	I	101	BCL	MG-NC	-2.32	2.00	2.06
8	A	101	BCL	MG-NC	-2.32	2.00	2.06
8	K	102	BCL	C1D-C2D	2.32	1.49	1.45
8	5	101	BCL	MG-NA	-2.32	2.00	2.06
8	7	101	BCL	MG-NC	-2.32	2.00	2.06
8	4	101	BCL	MG-NC	-2.31	2.00	2.06
8	2	101	BCL	CHD-C4C	2.31	1.45	1.39
8	T	101	BCL	MG-NC	-2.31	2.00	2.06
8	U	102	BCL	MG-NC	-2.31	2.00	2.06
8	S	102	BCL	MG-NA	-2.31	2.00	2.06
8	S	101	BCL	CHD-C4C	2.30	1.45	1.39
8	T	101	BCL	MG-NA	-2.30	2.00	2.06
8	E	102	BCL	MG-NC	-2.29	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	701	BCL	C1D-C2D	2.29	1.49	1.45
8	6	102	BCL	OBD-CAD	2.29	1.26	1.22
8	L	703	BCL	MG-NC	-2.29	2.00	2.06
8	Q	101	BCL	MG-NA	-2.28	2.00	2.06
8	8	101	BCL	C3C-C4C	-2.28	1.48	1.51
8	A	102	BCL	MG-NA	-2.28	2.00	2.06
8	U	102	BCL	C1D-C2D	2.27	1.49	1.45
8	H	101	BCL	CHD-C4C	2.27	1.45	1.39
8	S	102	BCL	C1D-C2D	2.27	1.49	1.45
8	O	102	BCL	C1D-C2D	2.27	1.49	1.45
8	I	101	BCL	MG-NA	-2.26	2.00	2.06
8	A	101	BCL	MG-NA	-2.26	2.00	2.06
8	4	101	BCL	MG-NA	-2.26	2.00	2.06
8	K	102	BCL	MG-NC	-2.26	2.00	2.06
8	6	101	BCL	MG-NC	-2.26	2.00	2.06
8	G	101	BCL	MG-NA	-2.26	2.00	2.06
8	1	101	BCL	MG-NA	-2.25	2.00	2.06
8	B	101	BCL	C1D-C2D	2.25	1.49	1.45
8	7	101	BCL	C3C-C4C	-2.25	1.48	1.51
8	J	102	BCL	MG-NA	-2.24	2.00	2.06
8	Q	102	BCL	MG-NC	-2.24	2.00	2.06
8	G	102	BCL	OBD-CAD	2.24	1.26	1.22
8	S	102	BCL	CAA-C2A	-2.23	1.50	1.54
8	2	102	BCL	C1D-C2D	2.23	1.49	1.45
8	B	101	BCL	CAA-C2A	-2.22	1.50	1.54
8	1	101	BCL	MG-NC	-2.22	2.01	2.06
8	W	102	BCL	MG-NC	-2.21	2.01	2.06
8	G	102	BCL	C1D-C2D	2.21	1.49	1.45
8	G	102	BCL	MG-NC	-2.21	2.01	2.06
8	D	102	BCL	C3C-C4C	-2.21	1.48	1.51
8	M	701	BCL	CHD-C4C	2.21	1.45	1.39
8	0	101	BCL	MG-NC	-2.21	2.01	2.06
8	8	102	BCL	MG-NC	-2.20	2.01	2.06
8	L	702	BCL	C4B-CHC	2.20	1.47	1.41
8	N	101	BCL	MG-NA	-2.20	2.01	2.06
8	L	702	BCL	MG-NC	-2.20	2.01	2.06
8	3	101	BCL	CAA-C2A	-2.19	1.50	1.54
8	7	101	BCL	C1D-C2D	2.19	1.49	1.45
8	O	102	BCL	MG-NC	-2.19	2.01	2.06
8	G	102	BCL	MG-NA	-2.19	2.01	2.06
8	Q	102	BCL	C1D-C2D	2.19	1.49	1.45
8	8	101	BCL	MG-NA	-2.18	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	8	101	BCL	MG-NC	-2.18	2.01	2.06
8	4	101	BCL	C1D-C2D	2.18	1.49	1.45
8	I	102	BCL	MG-NA	-2.18	2.01	2.06
8	F	101	BCL	MG-NA	-2.18	2.01	2.06
8	O	101	BCL	C4B-CHC	2.18	1.47	1.41
8	K	101	BCL	CHD-C4C	2.17	1.45	1.39
8	O	101	BCL	C3C-C4C	-2.17	1.48	1.51
8	W	102	BCL	C1D-C2D	2.17	1.49	1.45
8	I	101	BCL	C4B-CHC	2.16	1.47	1.41
8	O	102	BCL	MG-NA	-2.16	2.01	2.06
8	A	101	BCL	CHD-C4C	2.16	1.45	1.39
8	3	103	BCL	C1B-CHB	2.16	1.47	1.41
8	0	101	BCL	CHD-C4C	2.16	1.45	1.39
8	6	102	BCL	C1D-C2D	2.16	1.49	1.45
8	P	101	BCL	C3C-C4C	-2.16	1.48	1.51
8	I	102	BCL	C1B-CHB	2.15	1.47	1.41
8	2	102	BCL	C4B-NB	-2.15	1.33	1.35
8	8	102	BCL	C1D-C2D	2.15	1.49	1.45
8	5	101	BCL	C3C-C4C	-2.15	1.48	1.51
8	6	101	BCL	MG-NA	-2.15	2.01	2.06
8	H	101	BCL	C1B-CHB	2.14	1.46	1.41
8	U	101	BCL	CHD-C4C	2.14	1.45	1.39
8	W	101	BCL	CHD-C4C	2.14	1.45	1.39
8	1	101	BCL	C1D-C2D	2.14	1.49	1.45
8	0	102	BCL	C3C-C4C	-2.13	1.48	1.51
8	B	101	BCL	C3A-C2A	-2.13	1.48	1.54
8	G	102	BCL	C3C-C4C	-2.13	1.48	1.51
8	V	101	BCL	C1D-C2D	2.13	1.49	1.45
8	I	102	BCL	MG-NC	-2.13	2.01	2.06
8	3	103	BCL	C1D-C2D	2.13	1.49	1.45
8	E	101	BCL	MG-NC	-2.12	2.01	2.06
8	4	101	BCL	C4B-NB	-2.12	1.33	1.35
8	O	101	BCL	CHD-C4C	2.12	1.45	1.39
8	K	101	BCL	MG-NC	-2.12	2.01	2.06
8	7	101	BCL	MG-NA	-2.11	2.01	2.06
8	N	101	BCL	C1D-C2D	2.11	1.49	1.45
8	F	101	BCL	MG-NC	-2.11	2.01	2.06
8	J	102	BCL	C3C-C4C	-2.11	1.48	1.51
8	Q	101	BCL	CHD-C4C	2.11	1.45	1.39
8	7	101	BCL	C4B-CHC	2.10	1.46	1.41
8	S	102	BCL	C3C-C4C	-2.10	1.48	1.51
8	G	101	BCL	MG-NC	-2.10	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	102	BCL	C1D-C2D	2.10	1.49	1.45
8	3	101	BCL	CHD-C4C	2.10	1.45	1.39
16	T	102	LMT	O1'-C1'	2.10	1.43	1.40
8	0	101	BCL	C4B-CHC	2.09	1.46	1.41
8	6	102	BCL	MG-NA	-2.09	2.01	2.06
8	0	102	BCL	MG-NC	-2.09	2.01	2.06
8	S	102	BCL	MG-NC	-2.09	2.01	2.06
8	G	101	BCL	CHD-C4C	2.09	1.45	1.39
8	S	102	BCL	C3A-C2A	-2.09	1.48	1.54
8	I	101	BCL	CHD-C4C	2.09	1.45	1.39
8	M	701	BCL	MG-NC	-2.09	2.01	2.06
8	A	102	BCL	MG-NC	-2.08	2.01	2.06
8	T	101	BCL	C3C-C4C	-2.08	1.49	1.51
8	W	102	BCL	MG-NA	-2.08	2.01	2.06
8	T	101	BCL	C1D-C2D	2.08	1.49	1.45
8	A	102	BCL	C1D-C2D	2.08	1.49	1.45
8	I	102	BCL	C1D-C2D	2.08	1.49	1.45
8	U	101	BCL	C1B-CHB	2.08	1.46	1.41
8	V	101	BCL	MG-NA	-2.08	2.01	2.06
8	K	102	BCL	C3A-C2A	-2.07	1.48	1.54
8	L	703	BCL	MG-NA	-2.07	2.01	2.06
8	R	102	BCL	MG-NC	-2.07	2.01	2.06
8	W	101	BCL	C4B-CHC	2.07	1.46	1.41
8	L	703	BCL	C4B-CHC	2.06	1.46	1.41
8	D	102	BCL	MG-NC	-2.06	2.01	2.06
10	D	101	U4Z	CAI-CAH	-2.05	1.46	1.51
8	S	102	BCL	C1B-CHB	2.05	1.46	1.41
8	Q	101	BCL	C4B-CHC	2.05	1.46	1.41
8	D	102	BCL	C1B-CHB	2.05	1.46	1.41
8	U	101	BCL	C4B-CHC	2.05	1.46	1.41
8	J	102	BCL	C1D-C2D	2.05	1.49	1.45
8	9	101	BCL	C1B-CHB	2.04	1.46	1.41
8	6	101	BCL	CHD-C4C	2.04	1.45	1.39
8	K	101	BCL	MG-NA	-2.04	2.01	2.06
8	2	101	BCL	MG-NC	-2.04	2.01	2.06
8	M	701	BCL	C4B-CHC	2.04	1.46	1.41
8	3	103	BCL	C3C-C4C	-2.04	1.49	1.51
8	E	101	BCL	CHD-C4C	2.04	1.44	1.39
8	I	102	BCL	C3A-C2A	-2.03	1.48	1.54
8	B	101	BCL	C4B-CHC	2.03	1.46	1.41
8	S	101	BCL	C4B-CHC	2.03	1.46	1.41
8	F	101	BCL	C1B-CHB	2.03	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	101	BCL	C4B-NB	-2.03	1.33	1.35
8	Q	101	BCL	C1B-CHB	2.03	1.46	1.41
8	M	701	BCL	C1B-CHB	2.03	1.46	1.41
8	R	102	BCL	C3C-C4C	-2.03	1.49	1.51
8	8	102	BCL	MG-NA	-2.02	2.01	2.06
8	6	101	BCL	C1B-CHB	2.02	1.46	1.41
8	9	101	BCL	MG-NC	-2.02	2.01	2.06
10	J	101	U4Z	CAI-CAH	-2.01	1.47	1.51
8	N	101	BCL	MG-NC	-2.01	2.01	2.06
8	V	101	BCL	C4B-CHC	2.01	1.46	1.41
8	0	102	BCL	MG-NA	-2.01	2.01	2.06
8	2	102	BCL	MG-NC	-2.01	2.01	2.06
8	J	102	BCL	C4B-CHC	2.00	1.46	1.41

All (1187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	U	102	BCL	C4A-NA-C1A	8.90	110.71	106.71
8	M	701	BCL	CHD-C1D-ND	-8.74	116.42	124.45
8	B	101	BCL	CHD-C1D-ND	-8.60	116.55	124.45
8	Q	102	BCL	CHD-C1D-ND	-8.48	116.66	124.45
8	E	102	BCL	CHD-C1D-ND	-8.46	116.68	124.45
8	S	102	BCL	CHD-C1D-ND	-8.40	116.74	124.45
8	K	102	BCL	CHD-C1D-ND	-8.30	116.83	124.45
8	7	101	BCL	CHD-C1D-ND	-8.29	116.84	124.45
8	E	102	BCL	CMD-C2D-C1D	8.21	139.19	124.71
8	H	101	BCL	CHD-C1D-ND	-8.19	116.93	124.45
8	3	103	BCL	CHD-C1D-ND	-8.17	116.95	124.45
8	0	102	BCL	CHD-C1D-ND	-8.16	116.96	124.45
8	8	102	BCL	CMD-C2D-C1D	8.15	139.07	124.71
8	U	102	BCL	CHD-C1D-ND	-8.13	116.98	124.45
8	D	102	BCL	CHD-C1D-ND	-8.12	116.99	124.45
8	L	703	BCL	CHD-C1D-ND	-8.06	117.04	124.45
8	R	102	BCL	CHD-C1D-ND	-8.05	117.06	124.45
8	1	101	BCL	CHD-C1D-ND	-8.03	117.08	124.45
8	6	102	BCL	CMD-C2D-C1D	8.03	138.86	124.71
8	8	102	BCL	CHD-C1D-ND	-8.02	117.08	124.45
8	4	101	BCL	CMD-C2D-C1D	8.01	138.84	124.71
8	W	102	BCL	CMD-C2D-C1D	8.01	138.83	124.71
8	G	102	BCL	CMD-C2D-C1D	7.97	138.76	124.71
8	O	102	BCL	CHD-C1D-ND	-7.96	117.14	124.45
8	T	101	BCL	CHD-C1D-ND	-7.95	117.15	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2	102	BCL	CMD-C2D-C1D	7.93	138.69	124.71
8	S	102	BCL	CMD-C2D-C1D	7.89	138.62	124.71
8	B	101	BCL	CMD-C2D-C1D	7.87	138.59	124.71
8	O	102	BCL	CMD-C2D-C1D	7.87	138.59	124.71
8	I	102	BCL	CHD-C1D-ND	-7.87	117.22	124.45
8	0	102	BCL	CMD-C2D-C1D	7.87	138.58	124.71
8	4	101	BCL	CHD-C1D-ND	-7.83	117.26	124.45
8	K	102	BCL	CMD-C2D-C1D	7.78	138.43	124.71
8	W	102	BCL	CHD-C1D-ND	-7.78	117.30	124.45
8	6	102	BCL	CHD-C1D-ND	-7.75	117.33	124.45
8	G	102	BCL	CHD-C1D-ND	-7.73	117.35	124.45
8	P	101	BCL	CHD-C1D-ND	-7.72	117.36	124.45
8	L	703	BCL	CMD-C2D-C1D	7.70	138.28	124.71
8	I	102	BCL	CMD-C2D-C1D	7.70	138.28	124.71
8	U	102	BCL	CMD-C2D-C1D	7.67	138.23	124.71
8	2	102	BCL	CHD-C1D-ND	-7.67	117.41	124.45
8	V	101	BCL	CHD-C1D-ND	-7.65	117.43	124.45
8	A	102	BCL	CHD-C1D-ND	-7.63	117.44	124.45
8	F	101	BCL	CHD-C1D-ND	-7.61	117.46	124.45
8	N	101	BCL	CHD-C1D-ND	-7.60	117.47	124.45
8	9	101	BCL	CHD-C1D-ND	-7.55	117.51	124.45
8	5	101	BCL	CHD-C1D-ND	-7.54	117.52	124.45
8	7	101	BCL	CMD-C2D-C1D	7.54	138.00	124.71
8	L	702	BCL	CHD-C1D-ND	-7.53	117.53	124.45
8	M	701	BCL	CMD-C2D-C1D	7.48	137.89	124.71
8	J	102	BCL	CHD-C1D-ND	-7.47	117.59	124.45
8	Q	102	BCL	CMD-C2D-C1D	7.43	137.81	124.71
8	T	101	BCL	CMD-C2D-C1D	7.42	137.78	124.71
8	N	101	BCL	CMD-C2D-C1D	7.27	137.52	124.71
8	1	101	BCL	O2D-CGD-CBD	7.14	123.95	111.27
8	V	101	BCL	CMD-C2D-C1D	7.05	137.14	124.71
8	D	102	BCL	CMD-C2D-C1D	6.99	137.04	124.71
8	1	101	BCL	CMD-C2D-C1D	6.99	137.03	124.71
8	F	101	BCL	CMD-C2D-C1D	6.99	137.03	124.71
8	H	101	BCL	CMD-C2D-C1D	6.97	136.99	124.71
8	R	102	BCL	CMD-C2D-C1D	6.96	136.98	124.71
8	3	103	BCL	CMD-C2D-C1D	6.89	136.85	124.71
8	A	102	BCL	CMD-C2D-C1D	6.88	136.84	124.71
8	J	102	BCL	CMD-C2D-C1D	6.87	136.83	124.71
8	9	101	BCL	CMD-C2D-C1D	6.85	136.78	124.71
8	5	101	BCL	CMD-C2D-C1D	6.78	136.67	124.71
8	P	101	BCL	CMD-C2D-C1D	6.72	136.56	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	101	BCL	C2D-C1D-ND	6.70	115.04	110.10
8	Q	101	BCL	C2D-C1D-ND	6.66	115.01	110.10
8	O	101	BCL	C2D-C1D-ND	6.47	114.87	110.10
8	6	101	BCL	C2D-C1D-ND	6.42	114.84	110.10
8	2	101	BCL	CHD-C1D-ND	-6.40	118.57	124.45
8	A	101	BCL	CHD-C1D-ND	-6.40	118.57	124.45
8	W	101	BCL	CHD-C1D-ND	-6.37	118.60	124.45
8	3	101	BCL	C2D-C1D-ND	6.37	114.80	110.10
8	S	101	BCL	CHD-C1D-ND	-6.35	118.62	124.45
8	G	101	BCL	C2D-C1D-ND	6.30	114.75	110.10
8	I	101	BCL	C2D-C1D-ND	6.27	114.73	110.10
8	U	101	BCL	CHD-C1D-ND	-6.23	118.73	124.45
8	L	702	BCL	CMD-C2D-C1D	6.20	135.64	124.71
8	S	101	BCL	C2D-C1D-ND	6.16	114.64	110.10
8	K	101	BCL	C2D-C1D-ND	6.12	114.61	110.10
8	S	102	BCL	O2D-CGD-CBD	6.11	122.13	111.27
8	0	101	BCL	C2D-C1D-ND	6.06	114.57	110.10
8	8	101	BCL	C2D-C1D-ND	6.06	114.57	110.10
8	M	701	BCL	O2D-CGD-CBD	6.04	122.00	111.27
8	L	702	BCL	O2D-CGD-CBD	6.03	121.98	111.27
8	E	101	BCL	C2D-C1D-ND	6.02	114.54	110.10
8	3	101	BCL	CHD-C1D-ND	-6.00	118.94	124.45
8	W	101	BCL	C2D-C1D-ND	6.00	114.53	110.10
8	O	101	BCL	CHD-C1D-ND	-5.96	118.98	124.45
8	U	101	BCL	C2D-C1D-ND	5.95	114.49	110.10
8	5	101	BCL	O2D-CGD-CBD	5.93	121.80	111.27
8	D	102	BCL	C2D-C1D-ND	5.91	114.46	110.10
8	F	101	BCL	C2D-C1D-ND	5.91	114.46	110.10
8	J	102	BCL	O2D-CGD-CBD	5.90	121.76	111.27
8	H	101	BCL	C2D-C1D-ND	5.88	114.44	110.10
8	I	101	BCL	CHD-C1D-ND	-5.86	119.07	124.45
8	L	703	BCL	C2D-C1D-ND	5.79	114.37	110.10
8	Q	101	BCL	CHD-C1D-ND	-5.79	119.13	124.45
8	3	103	BCL	C2D-C1D-ND	5.79	114.37	110.10
8	0	101	BCL	CHD-C1D-ND	-5.79	119.14	124.45
8	L	702	BCL	CMB-C2B-C3B	5.78	135.49	124.68
8	M	701	BCL	C2D-C1D-ND	5.77	114.36	110.10
8	A	102	BCL	O2D-CGD-CBD	5.75	121.49	111.27
8	0	101	BCL	CMB-C2B-C3B	5.74	135.42	124.68
8	U	102	BCL	O2D-CGD-CBD	5.71	121.41	111.27
8	9	101	BCL	O2D-CGD-CBD	5.70	121.40	111.27
8	W	102	BCL	C2D-C1D-ND	5.70	114.30	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	T	101	BCL	C2D-C1D-ND	5.70	114.30	110.10
8	E	102	BCL	C2D-C1D-ND	5.67	114.28	110.10
8	9	101	BCL	C2D-C1D-ND	5.67	114.28	110.10
8	6	102	BCL	C2D-C1D-ND	5.65	114.27	110.10
8	8	102	BCL	C2D-C1D-ND	5.63	114.26	110.10
8	G	102	BCL	C3D-C2D-C1D	-5.63	98.15	105.83
8	U	102	BCL	C2D-C1D-ND	5.62	114.24	110.10
8	8	102	BCL	O2D-CGD-CBD	5.59	121.20	111.27
8	6	102	BCL	C3D-C2D-C1D	-5.58	98.21	105.83
8	G	102	BCL	O2D-CGD-CBD	5.57	121.16	111.27
8	7	101	BCL	C2D-C1D-ND	5.56	114.20	110.10
8	8	102	BCL	C3D-C2D-C1D	-5.55	98.25	105.83
8	N	101	BCL	C2D-C1D-ND	5.55	114.19	110.10
8	I	101	BCL	CMB-C2B-C3B	5.54	135.04	124.68
8	0	102	BCL	O2D-CGD-CBD	5.53	121.09	111.27
8	G	102	BCL	C2D-C1D-ND	5.52	114.17	110.10
8	J	102	BCL	C2D-C1D-ND	5.52	114.17	110.10
8	8	101	BCL	CMB-C2B-C3B	5.52	135.00	124.68
8	E	102	BCL	C3D-C2D-C1D	-5.52	98.30	105.83
8	N	101	BCL	O2D-CGD-CBD	5.51	121.05	111.27
8	2	101	BCL	C2D-C1D-ND	5.50	114.15	110.10
8	G	101	BCL	CHD-C1D-ND	-5.49	119.41	124.45
8	P	101	BCL	C2D-C1D-ND	5.49	114.15	110.10
8	R	102	BCL	C2D-C1D-ND	5.48	114.15	110.10
8	G	101	BCL	CMB-C2B-C3B	5.48	134.93	124.68
8	R	102	BCL	O2D-CGD-CBD	5.47	120.99	111.27
8	Q	102	BCL	C3D-C2D-C1D	-5.45	98.39	105.83
8	O	102	BCL	O2D-CGD-CBD	5.45	120.95	111.27
8	W	102	BCL	C3D-C2D-C1D	-5.45	98.40	105.83
8	K	101	BCL	CMB-C2B-C3B	5.43	134.84	124.68
8	6	101	BCL	CHD-C1D-ND	-5.42	119.47	124.45
8	K	101	BCL	CHD-C1D-ND	-5.40	119.50	124.45
8	I	102	BCL	C2D-C1D-ND	5.39	114.08	110.10
8	4	101	BCL	C3D-C2D-C1D	-5.39	98.48	105.83
8	2	101	BCL	CMB-C2B-C3B	5.38	134.75	124.68
8	Q	102	BCL	C2D-C1D-ND	5.38	114.07	110.10
8	S	101	BCL	CMB-C2B-C3B	5.38	134.74	124.68
8	I	102	BCL	C3D-C2D-C1D	-5.36	98.51	105.83
8	D	102	BCL	O2D-CGD-CBD	5.35	120.77	111.27
8	W	101	BCL	CMB-C2B-C3B	5.34	134.67	124.68
8	F	101	BCL	O2D-CGD-CBD	5.34	120.75	111.27
8	1	101	BCL	C2D-C1D-ND	5.33	114.03	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	0	102	BCL	C3D-C2D-C1D	-5.33	98.56	105.83
8	W	102	BCL	O2D-CGD-CBD	5.33	120.74	111.27
8	3	101	BCL	CMB-C2B-C3B	5.33	134.65	124.68
8	T	101	BCL	O2D-CGD-CBD	5.31	120.71	111.27
8	O	101	BCL	CMB-C2B-C3B	5.31	134.61	124.68
8	Q	102	BCL	CMB-C2B-C3B	5.30	134.60	124.68
8	L	703	BCL	C3D-C2D-C1D	-5.29	98.61	105.83
8	S	102	BCL	C3D-C2D-C1D	-5.29	98.61	105.83
9	I	103	PGV	O01-C1-C2	5.29	122.91	111.50
8	3	103	BCL	O2D-CGD-CBD	5.27	120.64	111.27
8	A	101	BCL	CMB-C2B-C3B	5.27	134.53	124.68
8	U	101	BCL	CMB-C2B-C3B	5.26	134.52	124.68
8	O	102	BCL	C3D-C2D-C1D	-5.26	98.66	105.83
8	I	102	BCL	O2D-CGD-CBD	5.23	120.57	111.27
8	L	703	BCL	CMB-C2B-C3B	5.23	134.46	124.68
8	7	101	BCL	O2D-CGD-CBD	5.23	120.56	111.27
8	U	102	BCL	CMB-C2B-C3B	5.23	134.46	124.68
8	W	101	BCL	O2D-CGD-CBD	5.22	120.55	111.27
8	H	101	BCL	CHD-C4C-NC	5.22	130.88	125.08
8	B	101	BCL	C3D-C2D-C1D	-5.22	98.71	105.83
8	S	102	BCL	C2D-C1D-ND	5.22	113.95	110.10
8	O	102	BCL	C2D-C1D-ND	5.21	113.94	110.10
8	Q	101	BCL	CMB-C2B-C3B	5.21	134.42	124.68
8	T	101	BCL	C3D-C2D-C1D	-5.20	98.73	105.83
8	H	101	BCL	O2D-CGD-CBD	5.20	120.50	111.27
8	B	101	BCL	CMB-C2B-C3B	5.19	134.40	124.68
8	2	102	BCL	C3D-C2D-C1D	-5.17	98.77	105.83
8	U	102	BCL	C3D-C2D-C1D	-5.15	98.80	105.83
8	L	702	BCL	C2D-C1D-ND	5.15	113.90	110.10
8	2	102	BCL	C2D-C1D-ND	5.15	113.90	110.10
8	4	101	BCL	C2D-C1D-ND	5.15	113.90	110.10
8	5	101	BCL	C2D-C1D-ND	5.15	113.90	110.10
8	E	102	BCL	CMB-C2B-C3B	5.13	134.28	124.68
8	K	102	BCL	C3D-C2D-C1D	-5.13	98.83	105.83
8	V	101	BCL	C2D-C1D-ND	5.13	113.89	110.10
8	H	101	BCL	C3C-C4C-CHD	-5.13	112.43	123.39
8	F	101	BCL	C3D-C2D-C1D	-5.12	98.84	105.83
8	M	701	BCL	C3D-C2D-C1D	-5.12	98.84	105.83
8	E	101	BCL	CHD-C1D-ND	-5.09	119.78	124.45
8	D	102	BCL	C3D-C2D-C1D	-5.09	98.89	105.83
8	9	101	BCL	C3D-C2D-C1D	-5.08	98.90	105.83
8	H	101	BCL	C3D-C2D-C1D	-5.05	98.93	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	101	BCL	O2D-CGD-CBD	5.04	120.23	111.27
8	V	101	BCL	O2D-CGD-CBD	5.04	120.23	111.27
8	6	101	BCL	CMB-C2B-C3B	5.04	134.11	124.68
8	3	103	BCL	C3D-C2D-C1D	-5.03	98.97	105.83
8	2	102	BCL	O2D-CGD-CBD	5.02	120.19	111.27
8	N	101	BCL	C3D-C2D-C1D	-5.02	98.99	105.83
8	8	101	BCL	CHD-C1D-ND	-5.01	119.85	124.45
8	7	101	BCL	C3D-C2D-C1D	-5.01	98.99	105.83
8	I	101	BCL	CMD-C2D-C1D	4.99	133.51	124.71
8	P	101	BCL	C3D-C2D-C1D	-4.99	99.02	105.83
8	A	102	BCL	C2D-C1D-ND	4.97	113.77	110.10
8	J	102	BCL	C3D-C2D-C1D	-4.97	99.05	105.83
8	E	101	BCL	CMB-C2B-C3B	4.97	133.98	124.68
8	G	101	BCL	C3C-C4C-CHD	-4.95	112.83	123.39
8	A	101	BCL	CMD-C2D-C1D	4.94	133.43	124.71
8	G	101	BCL	CMD-C2D-C1D	4.94	133.42	124.71
8	Q	101	BCL	C3C-C4C-CHD	-4.93	112.86	123.39
8	W	101	BCL	CMD-C2D-C1D	4.93	133.40	124.71
8	A	102	BCL	C3D-C2D-C1D	-4.93	99.11	105.83
8	V	101	BCL	C3D-C2D-C1D	-4.93	99.11	105.83
8	0	102	BCL	C2D-C1D-ND	4.91	113.72	110.10
8	3	101	BCL	CMD-C2D-C1D	4.91	133.37	124.71
8	A	101	BCL	C3D-C2D-C1D	-4.90	99.14	105.83
8	A	101	BCL	O2D-CGD-CBD	4.90	119.98	111.27
8	4	101	BCL	O2D-CGD-CBD	4.90	119.97	111.27
8	O	101	BCL	C3C-C4C-CHD	-4.88	112.96	123.39
8	A	101	BCL	C1D-ND-C4D	-4.88	102.87	106.33
8	8	101	BCL	C3C-C4C-CHD	-4.88	112.96	123.39
8	D	102	BCL	CHD-C4C-NC	4.88	130.50	125.08
8	K	102	BCL	O2D-CGD-CBD	4.88	119.93	111.27
8	B	101	BCL	O2D-CGD-CBD	4.88	119.93	111.27
8	3	103	BCL	CHD-C4C-NC	4.85	130.46	125.08
8	0	101	BCL	CMD-C2D-C1D	4.85	133.26	124.71
8	U	101	BCL	CMD-C2D-C1D	4.84	133.25	124.71
8	2	101	BCL	CMD-C2D-C1D	4.84	133.24	124.71
8	Q	101	BCL	C3D-C2D-C1D	-4.84	99.23	105.83
8	1	101	BCL	C3D-C2D-C1D	-4.83	99.24	105.83
8	6	102	BCL	O2D-CGD-CBD	4.83	119.84	111.27
8	1	101	BCL	CMB-C2B-C3B	4.82	133.69	124.68
8	O	101	BCL	C3D-C2D-C1D	-4.82	99.26	105.83
8	R	102	BCL	C3D-C2D-C1D	-4.81	99.27	105.83
8	G	102	BCL	CMB-C2B-C3B	4.81	133.68	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	102	BCL	CHD-C4C-NC	4.80	130.41	125.08
9	0	105	PGV	O01-C1-C2	4.79	121.83	111.50
8	0	101	BCL	C3C-C4C-CHD	-4.79	113.17	123.39
15	M	708	PEF	O2-C10-C11	4.78	119.89	111.09
8	5	101	BCL	C3D-C2D-C1D	-4.78	99.31	105.83
8	S	101	BCL	CMD-C2D-C1D	4.78	133.13	124.71
8	6	101	BCL	C3C-C4C-CHD	-4.78	113.19	123.39
8	7	101	BCL	CMB-C2B-C3B	4.78	133.61	124.68
8	Q	101	BCL	CMD-C2D-C1D	4.77	133.12	124.71
8	3	103	BCL	C3C-C4C-CHD	-4.77	113.20	123.39
8	L	702	BCL	C3D-C2D-C1D	-4.76	99.33	105.83
8	L	702	BCL	O2D-CGD-O1D	-4.76	114.53	123.84
8	3	101	BCL	C3C-C4C-CHD	-4.76	113.22	123.39
8	R	102	BCL	CMB-C2B-C3B	4.75	133.56	124.68
8	6	101	BCL	C1D-ND-C4D	-4.74	102.97	106.33
8	4	101	BCL	CHD-C4C-NC	4.73	130.34	125.08
8	3	101	BCL	C1D-ND-C4D	-4.73	102.97	106.33
8	A	101	BCL	C3C-C4C-CHD	-4.73	113.29	123.39
8	9	101	BCL	CHD-C4C-NC	4.72	130.32	125.08
8	I	101	BCL	C3C-C4C-CHD	-4.72	113.30	123.39
8	0	101	BCL	C3D-C2D-C1D	-4.72	99.39	105.83
8	J	102	BCL	C3C-C4C-CHD	-4.72	113.32	123.39
8	2	102	BCL	CMB-C2B-C3B	4.70	133.47	124.68
8	J	102	BCL	CHD-C4C-NC	4.69	130.29	125.08
8	M	701	BCL	CMB-C2B-C3B	4.69	133.45	124.68
8	3	101	BCL	O2D-CGD-CBD	4.68	119.58	111.27
8	Q	101	BCL	C1D-ND-C4D	-4.68	103.01	106.33
8	I	101	BCL	C3D-C2D-C1D	-4.67	99.45	105.83
8	M	701	BCL	C4A-NA-C1A	4.67	108.81	106.71
9	6	103	PGV	O01-C1-C2	4.67	121.57	111.50
8	3	101	BCL	C3D-C2D-C1D	-4.67	99.46	105.83
9	8	103	PGV	O01-C1-C2	4.66	121.55	111.50
8	E	101	BCL	CMD-C2D-C1D	4.66	132.93	124.71
8	9	101	BCL	C3C-C4C-CHD	-4.66	113.44	123.39
8	K	101	BCL	C3D-C2D-C1D	-4.66	99.47	105.83
8	M	701	BCL	CHD-C4C-NC	4.65	130.24	125.08
8	2	102	BCL	C4A-NA-C1A	4.65	108.80	106.71
8	A	102	BCL	CMB-C2B-C3B	4.65	133.37	124.68
8	S	101	BCL	C3D-C2D-C1D	-4.64	99.49	105.83
8	G	101	BCL	C3D-C2D-C1D	-4.64	99.50	105.83
8	E	101	BCL	C3C-C4C-CHD	-4.64	113.48	123.39
8	U	101	BCL	C3C-C4C-CHD	-4.64	113.48	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	102	BCL	CHD-C4C-NC	4.63	130.22	125.08
8	E	101	BCL	C3D-C2D-C1D	-4.63	99.51	105.83
8	E	102	BCL	O2D-CGD-CBD	4.62	119.48	111.27
8	U	101	BCL	O2D-CGD-CBD	4.62	119.48	111.27
8	S	101	BCL	C3C-C4C-CHD	-4.61	113.54	123.39
8	K	101	BCL	C3C-C4C-CHD	-4.61	113.54	123.39
8	D	102	BCL	C3C-C4C-CHD	-4.61	113.54	123.39
8	F	101	BCL	CHD-C4C-NC	4.60	130.19	125.08
8	W	101	BCL	C3D-C2D-C1D	-4.60	99.55	105.83
8	F	101	BCL	C3C-C4C-CHD	-4.60	113.57	123.39
18	P	102	CDL	OB6-CB5-C51	4.59	121.40	111.50
8	J	102	BCL	CMB-C2B-C3B	4.59	133.27	124.68
9	0	104	PGV	O01-C1-C2	4.59	121.40	111.50
8	E	101	BCL	O2D-CGD-CBD	4.58	119.40	111.27
8	L	703	BCL	CHD-C4C-NC	4.57	130.15	125.08
9	O	103	PGV	O01-C1-C2	4.56	121.33	111.50
8	T	101	BCL	CHD-C4C-NC	4.54	130.12	125.08
8	B	101	BCL	C2D-C1D-ND	4.54	113.45	110.10
8	7	101	BCL	C1D-ND-C4D	-4.53	103.12	106.33
8	O	101	BCL	CMD-C2D-C1D	4.52	132.68	124.71
8	I	102	BCL	CHD-C4C-NC	4.52	130.09	125.08
8	7	101	BCL	CHD-C4C-NC	4.51	130.09	125.08
8	0	101	BCL	O2D-CGD-CBD	4.51	119.29	111.27
8	D	102	BCL	CMB-C2B-C3B	4.50	133.10	124.68
8	M	701	BCL	C3C-C4C-CHD	-4.50	113.78	123.39
8	F	101	BCL	CMB-C2B-C3B	4.50	133.09	124.68
9	C	506	PGV	O01-C1-C2	4.50	121.19	111.50
8	Q	101	BCL	O2D-CGD-CBD	4.49	119.25	111.27
8	8	101	BCL	O2D-CGD-CBD	4.49	119.25	111.27
8	2	102	BCL	CHD-C4C-NC	4.48	130.05	125.08
8	P	101	BCL	CMB-C2B-C3B	4.48	133.05	124.68
8	6	101	BCL	C3D-C2D-C1D	-4.48	99.72	105.83
8	U	101	BCL	C3D-C2D-C1D	-4.47	99.73	105.83
8	D	102	BCL	C1D-ND-C4D	-4.47	103.16	106.33
8	1	101	BCL	CHD-C4C-NC	4.47	130.04	125.08
8	5	101	BCL	CHD-C4C-NC	4.47	130.04	125.08
9	E	103	PGV	O01-C1-C2	4.47	121.13	111.50
8	K	101	BCL	CMD-C2D-C1D	4.46	132.58	124.71
8	5	101	BCL	C3C-C4C-CHD	-4.46	113.86	123.39
8	S	102	BCL	CHD-C4C-NC	4.46	130.03	125.08
8	N	101	BCL	C3C-C4C-CHD	-4.45	113.88	123.39
8	H	101	BCL	CMB-C2B-C3B	4.45	133.00	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	K	102	BCL	C2D-C1D-ND	4.44	113.38	110.10
8	7	101	BCL	C3C-C4C-CHD	-4.44	113.92	123.39
8	M	701	BCL	C1D-ND-C4D	-4.44	103.18	106.33
8	G	102	BCL	C3C-C4C-CHD	-4.42	113.95	123.39
8	Q	102	BCL	O2D-CGD-CBD	4.41	119.10	111.27
8	O	101	BCL	C1D-ND-C4D	-4.41	103.20	106.33
8	5	101	BCL	CMB-C2B-C3B	4.41	132.92	124.68
8	6	101	BCL	O2D-CGD-CBD	4.40	119.09	111.27
8	G	101	BCL	C1D-ND-C4D	-4.38	103.22	106.33
8	R	102	BCL	C1D-ND-C4D	-4.38	103.22	106.33
8	S	101	BCL	C1D-ND-C4D	-4.38	103.22	106.33
8	U	102	BCL	CHD-C4C-NC	4.38	129.94	125.08
8	6	102	BCL	C3C-C4C-CHD	-4.38	114.03	123.39
8	3	103	BCL	C1D-ND-C4D	-4.38	103.23	106.33
8	G	101	BCL	CHD-C4C-NC	4.37	129.93	125.08
8	3	103	BCL	CMB-C2B-C3B	4.37	132.85	124.68
8	H	101	BCL	C4A-NA-C1A	4.37	108.67	106.71
8	T	101	BCL	C3C-C4C-CHD	-4.37	114.06	123.39
8	2	101	BCL	C3D-C2D-C1D	-4.36	99.87	105.83
8	6	102	BCL	CHD-C4C-NC	4.36	129.92	125.08
8	I	101	BCL	O2D-CGD-CBD	4.36	119.01	111.27
8	H	101	BCL	C1C-NC-C4C	-4.35	104.75	106.71
8	I	101	BCL	C1D-ND-C4D	-4.35	103.25	106.33
8	E	102	BCL	C1D-ND-C4D	-4.35	103.25	106.33
8	R	102	BCL	CHD-C4C-NC	4.35	129.91	125.08
8	P	101	BCL	CHD-C4C-NC	4.35	129.91	125.08
8	P	101	BCL	C3C-C4C-CHD	-4.35	114.11	123.39
8	4	101	BCL	C3C-C4C-CHD	-4.34	114.12	123.39
8	T	101	BCL	CMB-C2B-C3B	4.33	132.78	124.68
8	A	102	BCL	CHD-C4C-NC	4.33	129.88	125.08
8	8	102	BCL	CHD-C4C-NC	4.33	129.88	125.08
9	U	103	PGV	O01-C1-C2	4.32	120.81	111.50
8	8	101	BCL	C3D-C2D-C1D	-4.32	99.94	105.83
8	G	101	BCL	O2D-CGD-CBD	4.30	118.91	111.27
8	I	102	BCL	C3C-C4C-CHD	-4.30	114.20	123.39
8	W	101	BCL	C3C-C4C-CHD	-4.30	114.21	123.39
8	0	101	BCL	CHD-C4C-NC	4.30	129.85	125.08
8	W	102	BCL	CMB-C2B-C3B	4.29	132.71	124.68
9	U	104	PGV	O01-C1-C2	4.29	120.75	111.50
8	U	101	BCL	C1D-ND-C4D	-4.29	103.29	106.33
8	1	101	BCL	C3C-C4C-CHD	-4.28	114.24	123.39
8	2	102	BCL	C3C-C4C-CHD	-4.27	114.28	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	W	102	BCL	C1D-ND-C4D	-4.25	103.31	106.33
8	Q	102	BCL	CHD-C4C-NC	4.25	129.80	125.08
8	O	101	BCL	CHD-C4C-NC	4.25	129.80	125.08
8	Q	101	BCL	CHD-C4C-NC	4.24	129.79	125.08
8	N	101	BCL	CHD-C4C-NC	4.24	129.79	125.08
8	V	101	BCL	CHD-C4C-NC	4.24	129.79	125.08
8	0	102	BCL	CHD-C4C-NC	4.23	129.78	125.08
8	E	102	BCL	C3C-C4C-CHD	-4.23	114.35	123.39
9	4	102	PGV	O01-C1-C2	4.23	120.61	111.50
9	S	103	PGV	O01-C1-C2	4.23	120.61	111.50
8	L	703	BCL	C3C-C4C-CHD	-4.23	114.36	123.39
8	2	101	BCL	C3C-C4C-CHD	-4.22	114.37	123.39
8	6	101	BCL	CMD-C2D-C1D	4.22	132.15	124.71
8	S	102	BCL	C3C-C4C-CHD	-4.22	114.38	123.39
8	9	101	BCL	CMB-C2B-C3B	4.21	132.56	124.68
8	8	101	BCL	CHD-C4C-NC	4.21	129.75	125.08
8	R	102	BCL	C3C-C4C-CHD	-4.21	114.41	123.39
8	K	102	BCL	CHD-C4C-NC	4.20	129.75	125.08
8	6	102	BCL	C1C-NC-C4C	-4.20	104.82	106.71
8	A	101	BCL	CHD-C4C-NC	4.20	129.74	125.08
8	U	102	BCL	C1D-ND-C4D	-4.20	103.35	106.33
8	L	702	BCL	CHD-C4C-NC	4.19	129.73	125.08
9	K	104	PGV	O01-C1-C2	4.18	120.52	111.50
8	O	101	BCL	O2D-CGD-CBD	4.18	118.70	111.27
8	L	703	BCL	C1D-ND-C4D	-4.18	103.37	106.33
8	B	101	BCL	CHD-C4C-NC	4.18	129.72	125.08
9	E	104	PGV	O01-C1-C2	4.18	120.50	111.50
9	h	102	PGV	O01-C1-C2	4.17	120.50	111.50
15	L	713	PEF	O2-C10-C11	4.17	120.49	111.50
8	N	101	BCL	CMB-C2B-C3B	4.16	132.46	124.68
8	6	101	BCL	CHD-C4C-NC	4.15	129.69	125.08
8	0	101	BCL	C1D-ND-C4D	-4.15	103.39	106.33
8	O	102	BCL	CHD-C4C-NC	4.14	129.68	125.08
9	L	712	PGV	O01-C1-C2	4.14	120.43	111.50
8	W	102	BCL	CHD-C4C-NC	4.14	129.68	125.08
8	L	702	BCL	C3C-C4C-CHD	-4.14	114.55	123.39
8	F	101	BCL	C1D-ND-C4D	-4.14	103.40	106.33
8	T	101	BCL	C1D-ND-C4D	-4.13	103.40	106.33
8	9	101	BCL	C1D-ND-C4D	-4.13	103.40	106.33
8	3	101	BCL	CHD-C4C-NC	4.12	129.66	125.08
8	J	102	BCL	C1D-ND-C4D	-4.12	103.41	106.33
8	L	703	BCL	O2D-CGD-CBD	4.12	118.59	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	504	HEC	CMC-C2C-C1C	-4.12	122.14	128.46
9	N	102	PGV	O01-C1-C2	4.11	120.35	111.50
8	A	102	BCL	C3C-C4C-CHD	-4.10	114.64	123.39
8	S	101	BCL	CHD-C4C-NC	4.10	129.63	125.08
8	N	101	BCL	C1D-ND-C4D	-4.09	103.43	106.33
8	H	101	BCL	C1D-ND-C4D	-4.09	103.43	106.33
8	K	101	BCL	C1D-ND-C4D	-4.08	103.43	106.33
8	V	101	BCL	C3C-C4C-CHD	-4.08	114.67	123.39
8	8	101	BCL	C1D-ND-C4D	-4.06	103.45	106.33
8	B	101	BCL	C1B-CHB-C4A	-4.04	122.12	130.12
8	L	702	BCL	C1D-ND-C4D	-4.03	103.47	106.33
15	h	103	PEF	O2-C10-C11	4.02	120.17	111.50
8	8	102	BCL	C3C-C4C-CHD	-4.01	114.82	123.39
8	W	101	BCL	C1D-ND-C4D	-4.01	103.48	106.33
8	I	101	BCL	CHD-C4C-NC	4.00	129.52	125.08
8	Q	102	BCL	C3C-C4C-CHD	-3.99	114.86	123.39
8	W	101	BCL	CHD-C4C-NC	3.99	129.51	125.08
8	E	101	BCL	CHD-C4C-NC	3.99	129.51	125.08
8	2	101	BCL	C1-C2-C3	-3.99	119.14	126.04
8	2	102	BCL	C1C-NC-C4C	-3.99	104.91	106.71
8	U	101	BCL	CHD-C4C-NC	3.98	129.50	125.08
8	U	102	BCL	CHC-C1C-NC	3.98	130.01	124.51
8	S	101	BCL	O2D-CGD-CBD	3.98	118.34	111.27
9	K	103	PGV	O01-C1-C2	3.98	120.07	111.50
9	M	705	PGV	O01-C1-C2	3.96	120.04	111.50
8	G	102	BCL	C1D-ND-C4D	-3.96	103.52	106.33
8	0	102	BCL	C3C-C4C-CHD	-3.93	115.00	123.39
8	O	102	BCL	C3C-C4C-CHD	-3.92	115.02	123.39
9	L	706	PGV	O01-C1-C2	3.92	119.94	111.50
8	K	101	BCL	CHD-C4C-NC	3.90	129.41	125.08
8	U	102	BCL	C4-C3-C2	-3.90	113.68	123.68
8	G	102	BCL	C1-C2-C3	-3.90	119.30	126.04
8	U	102	BCL	C3C-C4C-CHD	-3.89	115.07	123.39
8	I	102	BCL	C1D-ND-C4D	-3.89	103.57	106.33
8	E	101	BCL	C1C-NC-C4C	-3.87	104.97	106.71
8	1	101	BCL	C1D-ND-C4D	-3.87	103.59	106.33
8	8	101	BCL	CMD-C2D-C1D	3.85	131.51	124.71
8	P	101	BCL	C1D-ND-C4D	-3.85	103.60	106.33
8	E	101	BCL	C1D-ND-C4D	-3.85	103.60	106.33
8	V	101	BCL	C1D-ND-C4D	-3.85	103.60	106.33
18	P	102	CDL	OA6-CA5-C11	3.83	119.75	111.50
8	2	101	BCL	CHD-C4C-NC	3.83	129.33	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	5	101	BCL	C1D-ND-C4D	-3.82	103.62	106.33
8	K	102	BCL	C3C-C4C-CHD	-3.81	115.24	123.39
8	S	102	BCL	C1D-ND-C4D	-3.81	103.63	106.33
8	8	102	BCL	C1D-ND-C4D	-3.79	103.64	106.33
8	1	101	BCL	O2D-CGD-O1D	-3.78	116.44	123.84
8	6	102	BCL	C1D-ND-C4D	-3.78	103.65	106.33
8	W	102	BCL	C3C-C4C-CHD	-3.78	115.31	123.39
10	D	101	U4Z	CAN-CAM-CAO	-3.77	117.64	122.92
8	2	101	BCL	C1D-ND-C4D	-3.77	103.66	106.33
8	O	101	BCL	C4-C3-C5	3.77	121.61	115.27
10	3	102	U4Z	CAN-CAM-CAO	-3.75	117.67	122.92
10	3	102	U4Z	CBB-CBG-CBI	3.75	131.15	123.47
10	R	101	U4Z	CAN-CAM-CAO	-3.73	117.69	122.92
15	L	717	PEF	O2-C10-C11	3.72	119.52	111.50
8	L	703	BCL	CED-O2D-CGD	3.71	124.33	115.94
10	D	101	U4Z	CBB-CBG-CBI	3.69	131.03	123.47
8	U	101	BCL	C1-C2-C3	-3.68	119.68	126.04
8	M	701	BCL	C1-C2-C3	-3.66	119.72	126.04
8	O	102	BCL	O2D-CGD-O1D	-3.65	116.70	123.84
8	L	702	BCL	C3D-C4D-ND	3.65	116.14	110.24
8	B	101	BCL	C2A-C3A-C4A	-3.63	96.00	101.87
8	S	102	BCL	C4-C3-C5	3.63	121.38	115.27
8	9	101	BCL	C1-C2-C3	-3.61	119.79	126.04
8	A	102	BCL	C1D-ND-C4D	-3.60	103.78	106.33
8	K	101	BCL	O2D-CGD-CBD	3.58	117.63	111.27
8	O	102	BCL	C1D-ND-C4D	-3.56	103.81	106.33
10	J	101	U4Z	CAN-CAM-CAO	-3.56	117.94	122.92
8	P	101	BCL	C1C-NC-C4C	-3.56	105.11	106.71
10	0	103	U4Z	CAN-CAM-CAO	-3.55	117.94	122.92
20	C	501	HEC	CMC-C2C-C1C	-3.55	123.00	128.46
8	I	102	BCL	CMB-C2B-C3B	3.54	131.29	124.68
8	I	102	BCL	O2D-CGD-O1D	-3.54	116.93	123.84
8	W	102	BCL	C4-C3-C5	3.52	121.20	115.27
8	K	102	BCL	O2D-CGD-O1D	-3.52	116.96	123.84
8	E	102	BCL	O2D-CGD-O1D	-3.50	117.00	123.84
8	A	102	BCL	O2D-CGD-O1D	-3.50	117.00	123.84
8	K	102	BCL	CMB-C2B-C3B	3.49	131.20	124.68
8	2	102	BCL	C1D-ND-C4D	-3.48	103.86	106.33
8	A	101	BCL	C1-C2-C3	-3.48	120.03	126.04
8	3	103	BCL	C1-C2-C3	-3.47	120.04	126.04
9	1	102	PGV	O01-C1-C2	3.47	118.97	111.50
8	3	101	BCL	C4-C3-C5	3.47	121.10	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	5	101	BCL	O2D-CGD-O1D	-3.46	117.07	123.84
8	Q	102	BCL	C1D-ND-C4D	-3.45	103.89	106.33
8	K	102	BCL	CAA-C2A-C3A	-3.45	103.34	112.78
8	J	102	BCL	O2D-CGD-O1D	-3.44	117.12	123.84
15	M	708	PEF	C2-O2-C10	-3.43	111.50	117.90
8	3	101	BCL	O2D-CGD-O1D	-3.43	117.13	123.84
8	R	102	BCL	C3D-C4D-ND	3.43	115.78	110.24
8	B	101	BCL	C3C-C4C-CHD	-3.42	116.08	123.39
9	N	102	PGV	O03-C19-C20	3.42	120.35	111.38
8	S	102	BCL	CMB-C2B-C3B	3.41	131.06	124.68
9	I	103	PGV	C02-O01-C1	-3.41	109.40	117.79
8	0	102	BCL	C1D-ND-C4D	-3.40	103.92	106.33
8	6	101	BCL	C3D-C4D-ND	3.40	115.74	110.24
8	8	102	BCL	CMB-C2B-C3B	3.40	131.03	124.68
8	7	101	BCL	C3D-C4D-ND	3.39	115.72	110.24
8	M	701	BCL	C3D-C4D-ND	3.39	115.72	110.24
8	6	102	BCL	CMB-C2B-C3B	3.38	131.01	124.68
10	J	101	U4Z	CBB-CBG-CBI	3.38	130.40	123.47
8	E	101	BCL	O2D-CGD-O1D	-3.37	117.24	123.84
8	9	101	BCL	O2A-CGA-CBA	3.37	122.48	111.91
8	A	101	BCL	C3D-C4D-ND	3.36	115.68	110.24
8	8	102	BCL	C4-C3-C5	3.36	120.92	115.27
8	B	101	BCL	CAA-CBA-CGA	-3.36	103.44	113.25
8	4	101	BCL	O2D-CGD-O1D	-3.35	117.28	123.84
8	V	101	BCL	CMB-C2B-C3B	3.34	130.93	124.68
8	S	101	BCL	C3D-C4D-ND	3.34	115.64	110.24
10	D	101	U4Z	CBO-CBL-CBI	-3.33	118.26	122.92
16	M	709	LMT	C1-O1'-C1'	-3.32	108.33	113.84
8	3	101	BCL	C1-C2-C3	-3.32	120.30	126.04
8	3	103	BCL	C3D-C4D-ND	3.32	115.60	110.24
8	0	102	BCL	C1-C2-C3	-3.31	120.31	126.04
8	M	701	BCL	C1C-NC-C4C	-3.31	105.22	106.71
8	M	701	BCL	O2D-CGD-O1D	-3.31	117.36	123.84
8	S	102	BCL	C1C-NC-C4C	-3.31	105.22	106.71
8	G	102	BCL	C4-C3-C5	3.31	120.84	115.27
10	0	103	U4Z	CBB-CBG-CBI	3.31	130.25	123.47
8	Q	101	BCL	C1-C2-C3	-3.30	120.33	126.04
8	U	101	BCL	C3D-C4D-ND	3.30	115.58	110.24
8	4	101	BCL	C1D-ND-C4D	-3.29	104.00	106.33
8	3	101	BCL	C3D-C4D-ND	3.29	115.56	110.24
8	6	102	BCL	O2D-CGD-O1D	-3.29	117.41	123.84
8	2	101	BCL	O2D-CGD-CBD	3.29	117.11	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	702	BCL	O2A-CGA-CBA	3.28	122.20	111.91
10	0	103	U4Z	CBO-CBL-CBI	-3.28	118.33	122.92
16	T	102	LMT	C1'-C2'-C3'	3.27	116.81	110.00
8	Q	102	BCL	O2D-CGD-O1D	-3.27	117.44	123.84
8	D	102	BCL	C3D-C4D-ND	3.27	115.52	110.24
8	A	102	BCL	C4-C3-C5	3.25	120.74	115.27
8	Q	101	BCL	C3D-C4D-ND	3.25	115.50	110.24
10	R	101	U4Z	CBB-CBG-CBI	3.25	130.13	123.47
8	L	702	BCL	C1-C2-C3	-3.25	120.43	126.04
8	B	101	BCL	O2D-CGD-O1D	-3.25	117.49	123.84
10	3	102	U4Z	CBO-CBL-CBI	-3.24	118.38	122.92
8	S	102	BCL	O2A-CGA-CBA	3.24	122.08	111.91
8	O	102	BCL	CMB-C2B-C3B	3.24	130.74	124.68
8	U	102	BCL	O2D-CGD-O1D	-3.24	117.51	123.84
8	0	101	BCL	C1-C2-C3	-3.24	120.45	126.04
8	P	101	BCL	C4A-NA-C1A	3.23	108.16	106.71
8	O	102	BCL	C4-C3-C5	3.23	120.70	115.27
8	2	102	BCL	O2D-CGD-O1D	-3.23	117.53	123.84
8	I	101	BCL	C1-C2-C3	-3.23	120.46	126.04
8	W	102	BCL	C4-C3-C2	-3.23	115.40	123.68
20	C	503	HEC	CMC-C2C-C1C	-3.23	123.50	128.46
8	8	102	BCL	C1-C2-C3	-3.22	120.47	126.04
8	2	101	BCL	C3D-C4D-ND	3.22	115.44	110.24
8	T	101	BCL	C4-C3-C5	3.20	120.66	115.27
10	R	101	U4Z	CBO-CBL-CBI	-3.19	118.45	122.92
8	9	101	BCL	C3D-C4D-ND	3.19	115.40	110.24
20	C	502	HEC	CMC-C2C-C1C	-3.19	123.56	128.46
10	J	101	U4Z	CBO-CBL-CBI	-3.19	118.46	122.92
8	3	101	BCL	C4D-CHA-C1A	-3.18	117.37	121.25
10	0	103	U4Z	CBK-CBH-CBJ	-3.18	118.46	122.92
8	8	101	BCL	C3D-C4D-ND	3.18	115.39	110.24
8	1	101	BCL	C3D-C4D-ND	3.18	115.39	110.24
10	D	101	U4Z	CAI-CAH-CAD	-3.18	118.11	122.73
8	J	102	BCL	C3D-C4D-ND	3.18	115.38	110.24
8	I	101	BCL	C3D-C4D-ND	3.18	115.38	110.24
8	O	101	BCL	C3D-C4D-ND	3.18	115.38	110.24
8	3	103	BCL	O2D-CGD-O1D	-3.18	117.63	123.84
10	J	101	U4Z	CAI-CAH-CAD	-3.18	118.12	122.73
8	N	101	BCL	C3D-C4D-ND	3.18	115.37	110.24
8	V	101	BCL	C3D-C4D-ND	3.17	115.37	110.24
8	A	101	BCL	O2D-CGD-O1D	-3.17	117.64	123.84
19	h	101	LHG	O7-C7-O9	-3.17	121.53	125.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	0	101	BCL	O2D-CGD-O1D	-3.17	117.64	123.84
8	W	102	BCL	CHB-C4A-NA	3.17	128.90	124.51
9	L	711	PGV	O01-C1-C2	3.17	120.67	109.56
8	A	102	BCL	C3D-C4D-ND	3.17	115.36	110.24
10	R	101	U4Z	CAI-CAH-CAD	-3.16	118.14	122.73
8	0	101	BCL	C4-C3-C5	3.16	120.59	115.27
8	2	102	BCL	CHC-C1C-NC	3.16	128.88	124.51
8	0	102	BCL	C4-C3-C5	3.16	120.58	115.27
8	K	101	BCL	C3D-C4D-ND	3.15	115.33	110.24
8	T	101	BCL	O2A-CGA-CBA	3.15	121.79	111.91
8	2	102	BCL	CHB-C4A-NA	3.15	128.86	124.51
10	3	102	U4Z	CAU-CAR-CAV	-3.14	118.52	122.92
10	3	102	U4Z	CAI-CAH-CAD	-3.14	118.17	122.73
8	L	702	BCL	CMB-C2B-C1B	-3.13	123.65	128.46
8	E	102	BCL	C3D-C4D-ND	3.13	115.30	110.24
8	K	102	BCL	CAA-CBA-CGA	-3.13	104.11	113.25
8	5	101	BCL	C3D-C4D-ND	3.12	115.29	110.24
20	C	502	HEC	CMB-C2B-C1B	-3.12	123.67	128.46
9	L	712	PGV	O03-C19-C20	3.11	121.67	111.91
10	0	103	U4Z	CAU-CAR-CAV	-3.11	118.57	122.92
8	K	101	BCL	C1C-NC-C4C	-3.11	105.31	106.71
10	R	101	U4Z	CBK-CBH-CBJ	-3.10	118.58	122.92
8	K	101	BCL	CBA-CAA-C2A	-3.10	104.71	113.86
8	V	101	BCL	C1-C2-C3	-3.09	120.69	126.04
8	F	101	BCL	C3D-C4D-ND	3.09	115.24	110.24
8	G	101	BCL	C3D-C4D-ND	3.09	115.24	110.24
8	0	101	BCL	C3D-C4D-ND	3.08	115.22	110.24
8	U	102	BCL	C4-C3-C5	3.08	120.45	115.27
8	4	101	BCL	CMB-C2B-C3B	3.08	130.44	124.68
8	T	101	BCL	C3D-C4D-ND	3.07	115.21	110.24
9	C	506	PGV	C02-O01-C1	-3.07	110.23	117.79
8	E	101	BCL	C1-C2-C3	-3.07	120.74	126.04
8	U	101	BCL	O2D-CGD-O1D	-3.07	117.84	123.84
8	P	101	BCL	O2D-CGD-O1D	-3.07	117.84	123.84
8	K	101	BCL	O2A-CGA-CBA	3.06	121.50	111.91
8	D	102	BCL	C1-C2-C3	-3.05	120.76	126.04
8	P	101	BCL	C3D-C4D-ND	3.05	115.18	110.24
8	H	101	BCL	C1-C2-C3	-3.05	120.76	126.04
10	3	102	U4Z	CBK-CBH-CBJ	-3.05	118.65	122.92
10	J	101	U4Z	CAU-CAR-CAV	-3.04	118.66	122.92
8	3	103	BCL	C4-C3-C5	3.04	120.39	115.27
8	N	101	BCL	O2D-CGD-O1D	-3.04	117.90	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	7	101	BCL	C1-C2-C3	-3.04	120.79	126.04
8	K	102	BCL	C1B-CHB-C4A	-3.04	124.10	130.12
8	O	102	BCL	O2A-CGA-CBA	3.04	121.44	111.91
10	D	101	U4Z	CAB-CAD-CAH	-3.04	118.34	122.61
10	0	103	U4Z	CAI-CAH-CAD	-3.03	118.33	122.73
8	H	101	BCL	C3D-C4D-ND	3.03	115.14	110.24
8	L	703	BCL	C3D-C4D-ND	3.03	115.14	110.24
8	9	101	BCL	O2D-CGD-O1D	-3.03	117.91	123.84
8	U	102	BCL	C3D-C4D-ND	3.03	115.14	110.24
8	P	101	BCL	C4-C3-C5	3.03	120.36	115.27
8	4	101	BCL	C4-C3-C5	3.02	120.35	115.27
20	C	503	HEC	CMB-C2B-C1B	-3.02	123.82	128.46
8	W	101	BCL	C3D-C4D-ND	3.02	115.12	110.24
8	D	102	BCL	O2D-CGD-O1D	-3.02	117.94	123.84
10	D	101	U4Z	CBK-CBH-CBJ	-3.02	118.70	122.92
10	J	101	U4Z	CAB-CAD-CAH	-3.02	118.36	122.61
13	L	705	MQE	CAY-CAX-CBQ	3.02	121.73	118.50
8	6	102	BCL	C4-C3-C5	3.01	120.34	115.27
8	W	102	BCL	C3D-C4D-ND	3.01	115.11	110.24
8	N	101	BCL	O2A-CGA-CBA	3.01	121.35	111.91
8	L	703	BCL	C4-C3-C2	-3.01	115.96	123.68
8	S	102	BCL	O2D-CGD-O1D	-3.01	117.96	123.84
8	I	102	BCL	C1-C2-C3	-3.00	120.85	126.04
8	O	102	BCL	C4-C3-C2	-3.00	115.99	123.68
8	K	102	BCL	C1D-ND-C4D	-3.00	104.20	106.33
8	R	102	BCL	C1-C2-C3	-3.00	120.86	126.04
8	8	101	BCL	C1C-NC-C4C	-3.00	105.36	106.71
10	0	103	U4Z	CAB-CAD-CAH	-2.99	118.40	122.61
8	S	102	BCL	C3D-C4D-ND	2.99	115.08	110.24
8	0	102	BCL	CMB-C2B-C3B	2.99	130.28	124.68
10	3	102	U4Z	CAB-CAD-CAH	-2.99	118.40	122.61
8	W	101	BCL	O2D-CGD-O1D	-2.99	117.99	123.84
8	U	102	BCL	CHB-C4A-NA	2.99	128.64	124.51
8	0	101	BCL	CMB-C2B-C1B	-2.99	123.87	128.46
10	R	101	U4Z	CAU-CAR-CAV	-2.98	118.74	122.92
8	I	102	BCL	C3D-C4D-ND	2.98	115.06	110.24
8	O	101	BCL	C1-C2-C3	-2.98	120.89	126.04
8	S	101	BCL	O2A-CGA-CBA	2.98	121.26	111.91
8	Q	102	BCL	C1B-CHB-C4A	-2.98	124.22	130.12
8	G	101	BCL	O2D-CGD-O1D	-2.98	118.02	123.84
8	R	102	BCL	C4-C3-C5	2.97	120.27	115.27
8	K	102	BCL	C2A-C3A-C4A	-2.97	97.07	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	101	U4Z	CBK-CBH-CBJ	-2.97	118.77	122.92
8	N	101	BCL	C1C-NC-C4C	-2.96	105.37	106.71
8	Q	101	BCL	O2A-CGA-CBA	2.96	121.20	111.91
8	8	101	BCL	O2D-CGD-O1D	-2.96	118.06	123.84
8	R	102	BCL	O2D-CGD-O1D	-2.95	118.06	123.84
8	Q	101	BCL	O2D-CGD-O1D	-2.95	118.07	123.84
20	C	504	HEC	CMB-C2B-C1B	-2.95	123.93	128.46
8	3	101	BCL	CAA-CBA-CGA	-2.95	104.63	113.25
8	3	101	BCL	CHB-C4A-NA	2.95	128.59	124.51
8	2	102	BCL	CAA-CBA-CGA	-2.95	104.64	113.25
8	K	101	BCL	CHB-C4A-NA	2.94	128.58	124.51
8	M	701	BCL	O2A-CGA-CBA	2.94	121.14	111.91
10	0	103	U4Z	CBG-CBB-CAV	2.94	129.50	123.47
8	A	102	BCL	O2A-CGA-CBA	2.94	121.14	111.91
8	0	101	BCL	C4D-CHA-C1A	-2.94	117.67	121.25
8	U	101	BCL	O2A-CGA-CBA	2.93	121.11	111.91
8	E	102	BCL	CHC-C1C-NC	2.93	128.57	124.51
8	8	101	BCL	C1-C2-C3	-2.93	120.97	126.04
8	Q	101	BCL	C1C-NC-C4C	-2.93	105.39	106.71
8	2	101	BCL	CED-O2D-CGD	2.93	122.56	115.94
8	0	102	BCL	C3D-C4D-ND	2.92	114.97	110.24
9	h	102	PGV	O03-C19-C20	2.92	121.08	111.91
10	D	101	U4Z	CAU-CAR-CAV	-2.92	118.83	122.92
8	L	703	BCL	CHC-C1C-NC	2.91	128.54	124.51
8	M	701	BCL	CED-O2D-CGD	2.91	122.52	115.94
8	8	102	BCL	CHB-C4A-NA	2.90	128.53	124.51
8	U	101	BCL	C4-C3-C5	2.90	120.14	115.27
8	O	102	BCL	C3D-C4D-ND	2.90	114.92	110.24
8	7	101	BCL	C4-C3-C5	2.89	120.14	115.27
8	H	101	BCL	CHC-C1C-NC	2.89	128.51	124.51
8	A	101	BCL	CHB-C4A-NA	2.89	128.51	124.51
8	G	101	BCL	CHB-C4A-NA	2.89	128.51	124.51
20	C	502	HEC	CBD-CAD-C3D	-2.89	107.68	112.62
8	2	101	BCL	O2A-CGA-CBA	2.89	120.98	111.91
8	D	102	BCL	O2A-CGA-CBA	2.89	120.97	111.91
8	U	102	BCL	O2A-CGA-CBA	2.88	120.96	111.91
8	I	101	BCL	CMB-C2B-C1B	-2.88	124.04	128.46
8	2	101	BCL	C1C-NC-C4C	-2.88	105.41	106.71
8	L	703	BCL	CHB-C4A-NA	2.88	128.49	124.51
8	G	102	BCL	C3D-C4D-ND	2.88	114.89	110.24
8	K	102	BCL	C3D-C4D-ND	2.87	114.89	110.24
8	V	101	BCL	C4-C3-C5	2.87	120.10	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	T	101	BCL	O2D-CGD-O1D	-2.86	118.25	123.84
8	Q	102	BCL	C3D-C4D-ND	2.86	114.86	110.24
9	E	103	PGV	O03-C19-C20	2.86	120.87	111.91
8	6	101	BCL	C1-C2-C3	-2.85	121.11	126.04
8	H	101	BCL	O2D-CGD-O1D	-2.84	118.28	123.84
8	E	101	BCL	C3D-C4D-ND	2.84	114.83	110.24
15	M	708	PEF	O3-C30-C31	2.84	120.82	111.91
8	3	101	BCL	C4A-NA-C1A	2.84	107.98	106.71
8	N	101	BCL	C1-C2-C3	-2.84	121.14	126.04
8	J	102	BCL	C4-C3-C5	2.83	120.04	115.27
9	0	104	PGV	O03-C19-C20	2.83	120.80	111.91
8	I	101	BCL	O2D-CGD-O1D	-2.83	118.30	123.84
8	O	102	BCL	C4A-NA-C1A	2.82	107.97	106.71
8	G	101	BCL	C1C-NC-C4C	-2.82	105.44	106.71
9	1	102	PGV	O03-C19-C20	2.82	120.75	111.91
8	S	101	BCL	CMB-C2B-C1B	-2.82	124.14	128.46
15	L	717	PEF	O3-C30-C31	2.81	120.71	111.91
8	H	101	BCL	C4-C3-C5	2.81	119.99	115.27
8	8	101	BCL	CMB-C2B-C1B	-2.80	124.16	128.46
8	L	703	BCL	O2A-CGA-CBA	2.80	120.69	111.91
18	P	102	CDL	OB8-CB7-C71	2.79	120.68	111.91
8	S	101	BCL	C4D-CHA-C1A	-2.79	117.85	121.25
15	L	713	PEF	C2-O2-C10	-2.79	110.92	117.79
8	F	101	BCL	O2D-CGD-O1D	-2.79	118.38	123.84
15	h	103	PEF	O3-C30-C31	2.79	120.67	111.91
10	J	101	U4Z	CBG-CBB-CAV	2.79	129.18	123.47
10	3	102	U4Z	CBG-CBB-CAV	2.78	129.17	123.47
8	G	101	BCL	CBA-CAA-C2A	-2.77	105.68	113.86
8	0	101	BCL	CHB-C4A-NA	2.77	128.35	124.51
8	O	101	BCL	O2D-CGD-O1D	-2.77	118.42	123.84
8	V	101	BCL	CHC-C1C-NC	2.77	128.35	124.51
10	3	102	U4Z	CBN-CBL-CBI	2.77	123.19	118.94
10	D	101	U4Z	CBN-CBL-CBI	2.77	123.19	118.94
8	7	101	BCL	O2D-CGD-O1D	-2.77	118.42	123.84
8	Q	101	BCL	CHB-C4A-NA	2.77	128.34	124.51
8	V	101	BCL	CHB-C4A-NA	2.76	128.33	124.51
8	M	701	BCL	C1-O2A-CGA	2.76	123.68	116.44
9	U	104	PGV	O03-C19-C20	2.76	120.56	111.91
8	6	101	BCL	O2D-CGD-O1D	-2.76	118.45	123.84
8	A	101	BCL	O2A-CGA-CBA	2.76	120.56	111.91
8	I	102	BCL	O2A-CGA-CBA	2.76	120.55	111.91
8	V	101	BCL	O2D-CGD-O1D	-2.75	118.45	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	8	101	BCL	CHB-C4A-NA	2.75	128.31	124.51
8	G	101	BCL	C4D-CHA-C1A	-2.74	117.91	121.25
8	F	101	BCL	C1-C2-C3	-2.74	121.30	126.04
8	O	101	BCL	CHB-C4A-NA	2.74	128.30	124.51
8	6	101	BCL	CHB-C4A-NA	2.74	128.30	124.51
8	0	102	BCL	O2D-CGD-O1D	-2.73	118.49	123.84
9	8	103	PGV	O03-C19-C20	2.73	120.48	111.91
10	R	101	U4Z	CBG-CBB-CAV	2.73	129.07	123.47
8	L	703	BCL	C1-O2A-CGA	2.73	123.61	116.44
8	B	101	BCL	C1D-ND-C4D	-2.73	104.39	106.33
8	G	101	BCL	CMB-C2B-C1B	-2.72	124.28	128.46
8	L	702	BCL	C4-C3-C5	2.72	119.85	115.27
8	G	102	BCL	C1D-CHD-C4C	-2.72	120.05	126.62
8	W	101	BCL	CMB-C2B-C1B	-2.72	124.28	128.46
8	W	102	BCL	O2A-CGA-CBA	2.72	120.45	111.91
8	B	101	BCL	C3D-C4D-ND	2.72	114.64	110.24
9	U	103	PGV	O03-C19-C20	2.72	120.45	111.91
8	5	101	BCL	C1-C2-C3	-2.72	121.34	126.04
9	8	103	PGV	C02-O01-C1	-2.72	111.10	117.79
8	U	101	BCL	CHB-C4A-NA	2.72	128.27	124.51
10	3	102	U4Z	CAQ-CAR-CAV	2.71	123.11	118.94
8	S	101	BCL	CHB-C4A-NA	2.71	128.26	124.51
8	G	102	BCL	O2A-CGA-CBA	2.71	120.41	111.91
15	L	713	PEF	O3-C30-C31	2.70	120.39	111.91
8	6	101	BCL	C1C-NC-C4C	-2.70	105.49	106.71
8	8	102	BCL	C4A-NA-C1A	2.70	107.92	106.71
10	0	103	U4Z	CAQ-CAR-CAV	2.70	123.08	118.94
8	8	102	BCL	C3D-C4D-ND	2.70	114.60	110.24
8	5	101	BCL	C4-C3-C5	2.70	119.81	115.27
9	S	103	PGV	O03-C19-C20	2.70	120.37	111.91
8	I	101	BCL	O2A-CGA-CBA	2.69	120.36	111.91
8	F	101	BCL	O2A-CGA-CBA	2.69	120.35	111.91
8	B	101	BCL	C4B-CHC-C1C	-2.69	124.80	130.12
8	Q	102	BCL	CHC-C1C-NC	2.68	128.22	124.51
8	8	101	BCL	O2A-CGA-CBA	2.68	120.32	111.91
8	4	101	BCL	C1-C2-C3	-2.68	121.41	126.04
8	H	101	BCL	C1D-CHD-C4C	-2.68	120.16	126.62
9	6	103	PGV	O03-C19-C20	2.68	120.31	111.91
8	5	101	BCL	C1C-NC-C4C	-2.67	105.50	106.71
8	8	101	BCL	C4-C3-C5	2.67	119.77	115.27
8	6	102	BCL	C3D-C4D-ND	2.67	114.56	110.24
8	1	101	BCL	C1-C2-C3	-2.67	121.42	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	Q	102	BCL	C4-C3-C5	2.67	119.77	115.27
8	4	101	BCL	C3D-C4D-ND	2.67	114.56	110.24
9	E	104	PGV	O03-C19-C20	2.67	120.29	111.91
15	h	103	PEF	C2-O2-C10	-2.67	111.22	117.79
8	I	101	BCL	CHB-C4A-NA	2.67	128.20	124.51
8	6	102	BCL	C1-C2-C3	-2.67	121.43	126.04
8	0	102	BCL	C1C-NC-C4C	-2.67	105.51	106.71
8	4	101	BCL	O2A-CGA-CBA	2.67	120.28	111.91
8	2	102	BCL	C3D-C4D-ND	2.67	114.55	110.24
8	U	102	BCL	C4B-CHC-C1C	-2.67	124.84	130.12
8	8	101	BCL	C1D-CHD-C4C	-2.67	120.19	126.62
8	4	101	BCL	CAA-CBA-CGA	-2.66	105.48	113.25
8	0	102	BCL	CED-O2D-CGD	2.66	121.95	115.94
8	3	103	BCL	O2A-CGA-CBA	2.66	120.25	111.91
8	K	101	BCL	CMB-C2B-C1B	-2.66	124.38	128.46
8	E	101	BCL	C4-C3-C5	2.65	119.73	115.27
8	W	101	BCL	C1C-NC-C4C	-2.65	105.52	106.71
9	O	103	PGV	O03-C19-C20	2.65	120.21	111.91
9	L	711	PGV	O03-C19-C20	2.64	120.21	111.91
9	1	102	PGV	C02-O01-C1	-2.64	111.28	117.79
8	E	101	BCL	C1D-CHD-C4C	-2.64	120.24	126.62
8	L	702	BCL	C1-O2A-CGA	2.64	123.38	116.44
8	P	101	BCL	O2A-CGA-CBA	2.64	120.19	111.91
8	W	101	BCL	C1D-CHD-C4C	-2.64	120.26	126.62
9	K	104	PGV	O03-C19-C20	2.64	120.18	111.91
8	P	101	BCL	CHB-C4A-NA	2.64	128.16	124.51
8	0	102	BCL	CHC-C1C-NC	2.63	128.15	124.51
8	O	102	BCL	CHB-C4A-NA	2.63	128.15	124.51
10	0	103	U4Z	CBN-CBL-CBI	2.63	122.98	118.94
8	O	101	BCL	C1D-CHD-C4C	-2.63	120.27	126.62
8	9	101	BCL	CHB-C4A-NA	2.63	128.15	124.51
8	2	102	BCL	O2A-CGA-CBA	2.63	120.15	111.91
9	L	706	PGV	O03-C19-C20	2.63	120.15	111.91
18	P	102	CDL	OA8-CA7-C31	2.62	120.14	111.91
8	I	102	BCL	CHC-C1C-NC	2.62	128.14	124.51
8	N	101	BCL	C4-C3-C5	2.62	119.68	115.27
8	G	102	BCL	CMB-C2B-C1B	-2.62	124.44	128.46
8	U	101	BCL	C4D-CHA-C1A	-2.62	118.06	121.25
8	6	102	BCL	C1D-CHD-C4C	-2.61	120.32	126.62
8	3	101	BCL	CBA-CAA-C2A	-2.61	106.16	113.86
8	I	102	BCL	CAA-CBA-CGA	-2.61	105.63	113.25
8	2	101	BCL	CMB-C2B-C1B	-2.61	124.45	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	U	101	BCL	CMB-C2B-C1B	-2.60	124.46	128.46
8	A	101	BCL	C4D-CHA-C1A	-2.60	118.08	121.25
8	W	102	BCL	O2D-CGD-O1D	-2.60	118.75	123.84
8	2	101	BCL	O2A-CGA-O1A	-2.60	117.03	123.59
8	4	101	BCL	C4A-NA-C1A	2.60	107.87	106.71
8	W	101	BCL	C4D-CHA-C1A	-2.59	118.09	121.25
8	6	101	BCL	C1D-CHD-C4C	-2.59	120.37	126.62
8	G	102	BCL	O1D-CGD-CBD	-2.59	119.18	124.48
8	W	102	BCL	CAA-CBA-CGA	-2.59	105.68	113.25
8	W	101	BCL	CHB-C4A-NA	2.59	128.09	124.51
8	J	102	BCL	O2A-CGA-CBA	2.59	120.03	111.91
8	3	101	BCL	CMB-C2B-C1B	-2.59	124.49	128.46
8	E	102	BCL	C4-C3-C5	2.59	119.62	115.27
8	K	102	BCL	O2A-CGA-CBA	2.58	120.02	111.91
8	Q	102	BCL	C1D-CHD-C4C	-2.58	120.39	126.62
8	H	101	BCL	O2A-CGA-CBA	2.58	120.01	111.91
8	1	101	BCL	C4-C3-C5	2.58	119.61	115.27
8	E	101	BCL	C4D-CHA-C1A	-2.57	118.12	121.25
8	O	101	BCL	C4D-CHA-C1A	-2.57	118.12	121.25
16	1	104	LMT	C1B-O1B-C4'	-2.57	111.60	117.96
8	G	101	BCL	C1D-CHD-C4C	-2.57	120.42	126.62
8	K	101	BCL	C1D-CHD-C4C	-2.57	120.43	126.62
8	6	101	BCL	C4-C3-C5	2.57	119.59	115.27
8	Q	102	BCL	CMB-C2B-C1B	-2.56	124.52	128.46
10	R	101	U4Z	CBN-CBL-CBI	2.56	122.87	118.94
9	E	104	PGV	C02-O01-C1	-2.56	111.48	117.79
8	E	102	BCL	O2A-CGA-CBA	2.56	119.95	111.91
9	I	103	PGV	O03-C19-C20	2.56	119.94	111.91
8	5	101	BCL	O2A-CGA-CBA	2.55	119.92	111.91
8	3	101	BCL	C1C-NC-C4C	-2.55	105.56	106.71
8	V	101	BCL	O2A-CGA-CBA	2.55	119.90	111.91
8	I	101	BCL	C1D-CHD-C4C	-2.54	120.49	126.62
20	C	502	HEC	CBA-CAA-C2A	-2.54	108.32	112.60
8	B	101	BCL	CAA-C2A-C3A	-2.54	105.82	112.78
10	J	101	U4Z	CBN-CBL-CBI	2.54	122.84	118.94
8	0	102	BCL	O2A-CGA-CBA	2.54	119.87	111.91
10	R	101	U4Z	CAQ-CAR-CAV	2.54	122.83	118.94
8	L	702	BCL	CHC-C1C-NC	2.54	128.02	124.51
8	I	101	BCL	C4D-CHA-C1A	-2.54	118.16	121.25
8	U	101	BCL	C6-C7-C8	-2.53	107.73	115.92
8	K	102	BCL	C6-C7-C8	-2.53	107.73	115.92
8	S	102	BCL	C1D-CHD-C4C	-2.53	120.51	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	101	BCL	CHB-C4A-NA	2.53	128.01	124.51
8	L	702	BCL	C1D-CHD-C4C	-2.53	120.52	126.62
8	2	101	BCL	C4-C3-C5	2.53	119.53	115.27
16	T	102	LMT	O5'-C5'-C6'	2.53	112.73	106.44
8	S	101	BCL	CED-O2D-CGD	2.53	121.66	115.94
8	6	101	BCL	O2A-CGA-CBA	2.53	119.84	111.91
8	D	102	BCL	CHC-C1C-NC	2.53	128.00	124.51
8	L	703	BCL	C4D-CHA-C1A	-2.53	118.18	121.25
8	D	102	BCL	C6-C5-C3	-2.52	106.84	113.45
8	T	101	BCL	C1-C2-C3	-2.52	121.68	126.04
8	B	101	BCL	O2A-C1-C2	2.52	115.25	108.64
11	L	701	BPH	C1-C2-C3	-2.52	121.69	126.04
8	4	101	BCL	CHC-C1C-NC	2.52	127.99	124.51
10	R	101	U4Z	CBF-CBH-CBJ	2.51	122.79	118.94
8	I	102	BCL	C1D-CHD-C4C	-2.51	120.57	126.62
8	P	101	BCL	C1-C2-C3	-2.51	121.71	126.04
9	0	104	PGV	C02-O01-C1	-2.51	111.62	117.79
9	C	506	PGV	O01-C1-O02	-2.50	117.65	123.70
10	3	102	U4Z	CBF-CBH-CBJ	2.50	122.78	118.94
8	S	102	BCL	CHC-C1C-NC	2.50	127.97	124.51
9	N	102	PGV	C02-O01-C1	-2.50	111.64	117.79
8	1	101	BCL	CHC-C1C-NC	2.50	127.97	124.51
8	7	101	BCL	O2A-CGA-CBA	2.50	119.74	111.91
8	8	102	BCL	O2D-CGD-O1D	-2.49	118.96	123.84
9	4	102	PGV	C02-O01-C1	-2.49	111.66	117.79
8	R	102	BCL	O2A-CGA-CBA	2.49	119.72	111.91
8	U	102	BCL	O2A-CGA-O1A	-2.49	117.31	123.59
8	4	101	BCL	C1D-CHD-C4C	-2.49	120.62	126.62
8	2	101	BCL	CHB-C4A-NA	2.49	127.95	124.51
8	O	101	BCL	CMB-C2B-C1B	-2.49	124.64	128.46
8	O	102	BCL	CHC-C1C-NC	2.48	127.94	124.51
10	J	101	U4Z	CAQ-CAR-CAV	2.48	122.75	118.94
8	L	702	BCL	C6-C5-C3	-2.48	106.95	113.45
8	U	101	BCL	C1D-CHD-C4C	-2.48	120.64	126.62
8	8	102	BCL	CHC-C1C-NC	2.48	127.94	124.51
10	0	103	U4Z	CBF-CBH-CBJ	2.48	122.74	118.94
8	2	102	BCL	C1D-CHD-C4C	-2.47	120.65	126.62
8	S	101	BCL	O2A-C1-C2	2.47	115.14	108.64
8	Q	101	BCL	C4D-CHA-C1A	-2.47	118.24	121.25
8	8	101	BCL	C4D-CHA-C1A	-2.47	118.24	121.25
8	0	101	BCL	C1D-CHD-C4C	-2.47	120.67	126.62
8	L	702	BCL	C2A-C3A-C4A	-2.46	97.89	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	506	PGV	O03-C19-C20	2.46	119.64	111.91
9	K	103	PGV	O03-C19-C20	2.46	119.64	111.91
8	I	101	BCL	C4-C3-C5	2.46	119.41	115.27
8	3	103	BCL	CHC-C1C-NC	2.46	127.91	124.51
8	0	102	BCL	C1D-CHD-C4C	-2.46	120.69	126.62
20	C	501	HEC	CMB-C2B-C1B	-2.46	124.69	128.46
8	8	102	BCL	CAA-CBA-CGA	-2.46	106.08	113.25
8	B	101	BCL	O2A-CGA-CBA	2.46	119.61	111.91
8	Q	101	BCL	C1D-CHD-C4C	-2.45	120.71	126.62
10	D	101	U4Z	CBG-CBB-CAV	2.45	128.50	123.47
8	I	102	BCL	CHB-C4A-NA	2.45	127.90	124.51
8	3	101	BCL	C1D-CHD-C4C	-2.44	120.72	126.62
20	C	504	HEC	CBA-CAA-C2A	-2.44	108.49	112.60
8	D	102	BCL	C4A-NA-C1A	2.44	107.80	106.71
9	L	712	PGV	C02-O01-C1	-2.43	111.81	117.79
9	0	105	PGV	O03-C19-C20	2.43	119.53	111.91
8	M	701	BCL	CHB-C4A-NA	2.43	127.87	124.51
8	6	102	BCL	CHB-C4A-NA	2.42	127.86	124.51
8	6	101	BCL	C4D-CHA-C1A	-2.42	118.30	121.25
8	6	101	BCL	CMB-C2B-C1B	-2.42	124.75	128.46
8	J	102	BCL	C1-O2A-CGA	2.42	122.79	116.44
8	S	101	BCL	O2D-CGD-O1D	-2.42	119.11	123.84
8	1	101	BCL	O2A-CGA-CBA	2.42	119.49	111.91
8	A	102	BCL	CHC-C1C-NC	2.41	127.85	124.51
8	3	101	BCL	O2A-CGA-CBA	2.41	119.47	111.91
8	U	101	BCL	O2A-C1-C2	2.41	114.97	108.64
8	M	701	BCL	CHC-C1C-NC	2.41	127.84	124.51
9	1	102	PGV	O14-P-O13	2.40	120.08	110.68
8	1	101	BCL	CHB-C4A-NA	2.40	127.83	124.51
8	8	102	BCL	C1C-NC-C4C	-2.40	105.63	106.71
8	4	101	BCL	C1C-NC-C4C	-2.39	105.63	106.71
8	K	102	BCL	C1-O2A-CGA	2.39	122.72	116.44
8	E	101	BCL	CHB-C4A-NA	2.39	127.82	124.51
8	L	703	BCL	CMB-C2B-C1B	-2.39	124.80	128.46
8	E	102	BCL	CMB-C2B-C1B	-2.39	124.80	128.46
8	1	101	BCL	O1D-CGD-CBD	-2.38	119.61	124.48
8	5	101	BCL	CHB-C4A-NA	2.38	127.81	124.51
8	L	703	BCL	CBA-CAA-C2A	-2.38	106.83	113.86
8	I	101	BCL	C1C-NC-C4C	-2.38	105.64	106.71
8	W	102	BCL	C1D-CHD-C4C	-2.38	120.88	126.62
8	G	102	BCL	CED-O2D-CGD	2.38	121.32	115.94
8	K	101	BCL	C1-C2-C3	-2.38	121.93	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	0	102	BCL	C4B-CHC-C1C	-2.38	125.41	130.12
8	S	102	BCL	CED-O2D-CGD	2.38	121.31	115.94
8	O	102	BCL	C1C-NC-C4C	-2.37	105.64	106.71
8	6	102	BCL	CHC-C1C-NC	2.37	127.79	124.51
8	R	102	BCL	C6-C5-C3	-2.37	107.25	113.45
8	8	102	BCL	O2A-CGA-CBA	2.37	119.34	111.91
8	D	102	BCL	C1D-CHD-C4C	-2.37	120.91	126.62
8	K	102	BCL	C1D-CHD-C4C	-2.36	120.93	126.62
8	O	102	BCL	O2A-CGA-O1A	-2.36	117.64	123.59
9	h	102	PGV	O14-P-O13	2.36	119.92	110.68
8	2	101	BCL	CHC-C1C-NC	2.36	127.77	124.51
8	I	102	BCL	C1C-NC-C4C	-2.36	105.65	106.71
8	N	101	BCL	C4A-NA-C1A	2.36	107.77	106.71
9	U	104	PGV	C02-O01-C1	-2.36	111.99	117.79
8	9	101	BCL	C4-C3-C5	2.36	119.23	115.27
8	A	102	BCL	CHB-C4A-NA	2.35	127.77	124.51
8	T	101	BCL	CHB-C4A-NA	2.35	127.76	124.51
8	U	102	BCL	C5-C3-C2	2.35	125.87	121.12
8	A	101	BCL	C1D-CHD-C4C	-2.35	120.96	126.62
8	R	102	BCL	CHB-C4A-NA	2.35	127.76	124.51
8	L	703	BCL	C4-C3-C5	2.35	119.22	115.27
8	W	101	BCL	C6-C5-C3	-2.34	107.31	113.45
8	6	102	BCL	C1-O2A-CGA	2.34	122.58	116.44
10	J	101	U4Z	CBF-CBH-CBJ	2.34	122.53	118.94
8	A	101	BCL	CMB-C2B-C1B	-2.34	124.87	128.46
8	G	101	BCL	CED-O2D-CGD	2.34	121.22	115.94
9	4	102	PGV	O03-C19-C20	2.33	119.21	111.91
8	0	101	BCL	CAA-CBA-CGA	-2.33	106.45	113.25
10	3	102	U4Z	CAE-CAI-CAH	2.33	118.23	114.08
8	O	101	BCL	C1C-NC-C4C	-2.32	105.66	106.71
8	3	101	BCL	C2A-C1A-CHA	-2.32	119.80	123.86
8	O	102	BCL	C4B-CHC-C1C	-2.32	125.52	130.12
8	G	101	BCL	O2A-CGA-CBA	2.32	119.19	111.91
8	9	101	BCL	C1D-CHD-C4C	-2.32	121.03	126.62
8	Q	102	BCL	O2A-CGA-CBA	2.32	119.17	111.91
8	5	101	BCL	C1D-CHD-C4C	-2.31	121.04	126.62
8	0	102	BCL	CAA-CBA-CGA	-2.31	106.49	113.25
8	S	101	BCL	O2A-CGA-O1A	-2.31	117.76	123.59
8	N	101	BCL	C1D-CHD-C4C	-2.31	121.06	126.62
8	E	101	BCL	CMB-C2B-C1B	-2.31	124.92	128.46
9	I	103	PGV	O01-C1-O02	-2.30	118.14	123.70
8	E	102	BCL	C1D-CHD-C4C	-2.30	121.07	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	503	HEC	CBD-CAD-C3D	-2.30	108.70	112.62
8	F	101	BCL	C4-C3-C5	2.30	119.14	115.27
8	3	103	BCL	C1C-NC-C4C	-2.30	105.67	106.71
10	D	101	U4Z	CAQ-CAR-CAV	2.30	122.47	118.94
8	4	101	BCL	CHB-C4A-NA	2.30	127.69	124.51
8	Q	101	BCL	C4-C3-C5	2.29	119.12	115.27
8	D	102	BCL	C4-C3-C5	2.29	119.12	115.27
9	L	711	PGV	C1-O01-C02	-2.29	110.14	115.40
8	B	101	BCL	C1D-CHD-C4C	-2.29	121.11	126.62
9	O	103	PGV	C02-O01-C1	-2.28	112.17	117.79
8	S	102	BCL	O2A-CGA-O1A	-2.28	117.83	123.59
8	2	101	BCL	C1D-CHD-C4C	-2.28	121.12	126.62
10	0	103	U4Z	CAN-CAM-CAL	2.28	121.67	118.08
10	J	101	U4Z	CAN-CAM-CAL	2.28	121.66	118.08
8	S	101	BCL	C1D-CHD-C4C	-2.27	121.14	126.62
8	R	102	BCL	CHC-C1C-NC	2.27	127.65	124.51
8	3	101	BCL	CHC-C1C-NC	2.27	127.65	124.51
8	3	103	BCL	C1D-CHD-C4C	-2.27	121.14	126.62
8	S	101	BCL	CHC-C1C-NC	2.27	127.65	124.51
8	8	102	BCL	O1D-CGD-CBD	-2.27	119.84	124.48
8	W	102	BCL	CED-O2D-CGD	2.27	121.07	115.94
8	8	102	BCL	C1D-CHD-C4C	-2.27	121.15	126.62
8	9	101	BCL	C1C-NC-C4C	-2.27	105.69	106.71
10	0	103	U4Z	CAE-CAI-CAH	2.26	118.12	114.08
8	F	101	BCL	CHC-C1C-NC	2.26	127.64	124.51
8	G	101	BCL	C2A-C1A-CHA	-2.26	119.91	123.86
9	M	705	PGV	O03-C19-C20	2.26	119.00	111.91
8	J	102	BCL	C1D-CHD-C4C	-2.26	121.17	126.62
8	P	101	BCL	C1D-CHD-C4C	-2.26	121.18	126.62
8	0	102	BCL	CHB-C4A-NA	2.26	127.63	124.51
8	Q	102	BCL	C1-O2A-CGA	2.25	122.36	116.44
9	h	102	PGV	C02-O01-C1	-2.25	112.25	117.79
8	H	101	BCL	C6-C5-C3	-2.25	107.55	113.45
8	7	101	BCL	CHB-C4A-NA	2.25	127.62	124.51
8	A	102	BCL	C1-C2-C3	-2.25	122.16	126.04
8	F	101	BCL	C1D-CHD-C4C	-2.25	121.20	126.62
8	E	102	BCL	CHB-C4A-NA	2.25	127.62	124.51
8	V	101	BCL	C1D-CHD-C4C	-2.24	121.21	126.62
8	K	102	BCL	C4B-CHC-C1C	-2.24	125.67	130.12
8	4	101	BCL	C1B-CHB-C4A	-2.24	125.68	130.12
8	I	101	BCL	CED-O2D-CGD	2.24	121.00	115.94
10	J	101	U4Z	CAE-CAI-CAH	2.24	118.07	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	101	BCL	C1C-NC-C4C	-2.24	105.70	106.71
8	A	102	BCL	C1D-CHD-C4C	-2.24	121.23	126.62
8	I	101	BCL	O2A-CGA-O1A	-2.24	117.95	123.59
8	S	102	BCL	O1D-CGD-CBD	-2.23	119.91	124.48
8	2	102	BCL	C4-C3-C5	2.23	119.02	115.27
8	Q	101	BCL	CMB-C2B-C1B	-2.23	125.04	128.46
8	L	703	BCL	O2D-CGD-O1D	-2.23	119.48	123.84
10	D	101	U4Z	CBF-CBH-CBJ	2.23	122.36	118.94
8	T	101	BCL	O2A-CGA-O1A	-2.22	117.98	123.59
8	U	102	BCL	C4D-CHA-C1A	-2.22	118.54	121.25
8	E	102	BCL	CMD-C2D-C3D	-2.22	122.50	127.61
8	D	102	BCL	CHB-C4A-NA	2.22	127.58	124.51
8	U	101	BCL	CHC-C1C-NC	2.22	127.58	124.51
8	T	101	BCL	C1C-NC-C4C	-2.22	105.71	106.71
8	E	102	BCL	C1-C2-C3	-2.22	122.20	126.04
8	M	701	BCL	C1D-CHD-C4C	-2.22	121.27	126.62
8	G	102	BCL	CHC-C1C-NC	2.22	127.58	124.51
8	T	101	BCL	C1D-CHD-C4C	-2.22	121.27	126.62
8	W	102	BCL	CHC-C1C-NC	2.22	127.58	124.51
20	C	502	HEC	C1D-C2D-C3D	-2.21	105.45	107.00
8	K	101	BCL	CED-O2D-CGD	2.21	120.94	115.94
8	G	101	BCL	C6-C7-C8	-2.21	108.77	115.92
8	2	102	BCL	CMD-C2D-C3D	-2.21	122.53	127.61
10	R	101	U4Z	CAE-CAI-CAH	2.21	118.02	114.08
8	J	102	BCL	CHC-C1C-NC	2.20	127.56	124.51
8	A	102	BCL	C1C-NC-C4C	-2.20	105.72	106.71
8	J	102	BCL	CHB-C4A-NA	2.20	127.56	124.51
8	G	102	BCL	C1B-CHB-C4A	-2.20	125.76	130.12
9	L	712	PGV	O03-C19-O04	-2.19	118.05	123.59
8	E	101	BCL	O2A-CGA-CBA	2.19	118.79	111.91
10	R	101	U4Z	CAN-CAM-CAL	2.19	121.53	118.08
8	E	102	BCL	C1-O2A-CGA	2.19	122.19	116.44
8	A	101	BCL	C4-C3-C5	2.19	118.95	115.27
8	A	101	BCL	CHC-C1C-NC	2.19	127.53	124.51
15	L	713	PEF	O2-C10-O4	-2.18	118.42	123.70
8	2	102	BCL	CAA-C2A-C1A	2.18	119.13	111.97
8	9	101	BCL	CED-O2D-CGD	2.18	120.87	115.94
8	Q	102	BCL	C1-C2-C3	-2.18	122.28	126.04
9	8	103	PGV	O01-C1-O02	-2.18	118.44	123.70
18	P	102	CDL	OA6-CA5-OA7	-2.17	118.45	123.70
8	S	102	BCL	C4B-CHC-C1C	-2.17	125.81	130.12
8	V	101	BCL	C4B-CHC-C1C	-2.17	125.82	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	101	BCL	CMB-C2B-C1B	-2.17	125.13	128.46
8	J	102	BCL	C1C-NC-C4C	-2.17	105.73	106.71
8	O	102	BCL	C1D-CHD-C4C	-2.17	121.40	126.62
10	3	102	U4Z	CAK-CAH-CAD	2.16	126.96	124.53
8	G	101	BCL	C4-C3-C5	2.16	118.91	115.27
8	G	101	BCL	C1-C2-C3	-2.16	122.31	126.04
8	E	101	BCL	CHC-C1C-NC	2.16	127.50	124.51
8	8	102	BCL	C4B-CHC-C1C	-2.16	125.84	130.12
8	8	101	BCL	CHC-C1C-NC	2.15	127.49	124.51
8	7	101	BCL	CHC-C1C-NC	2.15	127.49	124.51
10	3	102	U4Z	CAN-CAM-CAL	2.15	121.47	118.08
8	W	101	BCL	CHC-C1C-NC	2.15	127.48	124.51
8	1	101	BCL	CMB-C2B-C1B	-2.15	125.16	128.46
8	8	102	BCL	CMD-C2D-C3D	-2.15	122.68	127.61
8	U	102	BCL	C1C-NC-C4C	-2.15	105.74	106.71
8	4	101	BCL	CMD-C2D-C3D	-2.14	122.68	127.61
8	2	102	BCL	C1-O2A-CGA	2.14	122.07	116.44
8	B	101	BCL	CHD-C1D-C2D	2.14	129.97	125.48
8	G	102	BCL	O2D-CGD-O1D	-2.14	119.66	123.84
8	B	101	BCL	CMD-C2D-C3D	-2.14	122.69	127.61
8	F	101	BCL	CED-O2D-CGD	2.13	120.77	115.94
8	G	102	BCL	C4-C3-C2	-2.13	118.21	123.68
8	I	102	BCL	C4-C3-C5	2.13	118.86	115.27
8	I	102	BCL	CAA-C2A-C3A	-2.13	106.94	112.78
10	J	101	U4Z	CAK-CAH-CAD	2.13	126.92	124.53
8	2	101	BCL	O2D-CGD-O1D	-2.13	119.67	123.84
8	Q	102	BCL	C1C-NC-C4C	-2.13	105.75	106.71
9	S	103	PGV	O01-C1-O02	-2.13	118.56	123.70
8	U	102	BCL	C1D-CHD-C4C	-2.13	121.49	126.62
8	9	101	BCL	O2A-CGA-O1A	-2.12	118.24	123.59
8	K	102	BCL	CMD-C2D-C3D	-2.12	122.74	127.61
14	M	707	BGL	C1'-O2-C2	-2.12	109.27	114.32
8	9	101	BCL	CHC-C1C-NC	2.12	127.44	124.51
8	6	102	BCL	O2A-CGA-CBA	2.12	118.56	111.91
11	L	704	BPH	CMB-C2B-C3B	2.12	128.64	124.68
8	O	102	BCL	CMD-C2D-C3D	-2.11	122.75	127.61
9	h	102	PGV	O03-C19-O04	-2.11	118.27	123.59
8	W	102	BCL	CMD-C2D-C3D	-2.11	122.77	127.61
9	U	103	PGV	C02-O01-C1	-2.11	112.61	117.79
20	C	502	HEC	CMB-C2B-C3B	2.10	128.29	125.82
8	5	101	BCL	C16-C15-C13	-2.10	109.12	115.92
8	S	102	BCL	CMD-C2D-C3D	-2.10	122.78	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	0	105	PGV	C02-O01-C1	-2.10	112.61	117.79
9	E	103	PGV	C02-O01-C1	-2.10	112.62	117.79
8	O	102	BCL	CAA-C2A-C1A	2.10	118.86	111.97
14	L	715	BGL	O5-C5-C4	2.10	113.51	109.69
8	K	101	BCL	O2D-CGD-O1D	-2.10	119.73	123.84
8	0	101	BCL	C11-C10-C8	-2.10	109.13	115.92
8	A	102	BCL	C2A-C1A-CHA	-2.10	120.19	123.86
9	4	102	PGV	O01-C1-O02	-2.10	118.63	123.70
8	1	101	BCL	C1D-CHD-C4C	-2.10	121.56	126.62
8	7	101	BCL	C1D-CHD-C4C	-2.10	121.56	126.62
8	G	101	BCL	CHC-C1C-NC	2.09	127.41	124.51
8	R	102	BCL	C1D-CHD-C4C	-2.09	121.57	126.62
8	W	102	BCL	C1C-NC-C4C	-2.09	105.77	106.71
8	5	101	BCL	CHC-C1C-NC	2.09	127.41	124.51
8	L	703	BCL	C1D-CHD-C4C	-2.09	121.58	126.62
8	O	101	BCL	CED-O2D-CGD	2.09	120.66	115.94
8	V	101	BCL	C2A-C1A-CHA	-2.09	120.20	123.86
8	2	102	BCL	C4B-CHC-C1C	-2.09	125.98	130.12
8	7	101	BCL	CAC-C3C-C4C	-2.08	107.96	112.58
9	S	103	PGV	C02-O01-C1	-2.08	112.67	117.79
8	U	102	BCL	CED-O2D-CGD	2.08	120.64	115.94
9	0	105	PGV	O01-C1-O02	-2.08	118.69	123.70
8	7	101	BCL	CBA-CAA-C2A	-2.07	107.74	113.86
9	0	104	PGV	O01-C1-O02	-2.07	118.70	123.70
8	U	101	BCL	C2A-C1A-CHA	-2.07	120.24	123.86
16	M	709	LMT	O1'-C1'-C2'	2.07	111.53	108.30
8	0	102	BCL	CMD-C2D-C3D	-2.06	122.86	127.61
8	3	103	BCL	C6-C5-C3	-2.06	108.05	113.45
8	W	102	BCL	C1-O2A-CGA	2.06	121.85	116.44
8	K	101	BCL	C11-C12-C13	-2.06	109.26	115.92
8	U	101	BCL	CED-O2D-CGD	2.06	120.59	115.94
8	P	101	BCL	CED-O2D-CGD	2.06	120.59	115.94
8	K	102	BCL	CHC-C1C-NC	2.06	127.36	124.51
8	0	101	BCL	CED-O2D-CGD	2.06	120.59	115.94
8	A	101	BCL	C2A-C1A-CHA	-2.06	120.26	123.86
9	U	103	PGV	O01-C1-O02	-2.05	118.74	123.70
8	6	101	BCL	CHC-C1C-NC	2.05	127.35	124.51
9	U	104	PGV	O01-C1-O02	-2.05	118.75	123.70
8	0	101	BCL	CHC-C1C-NC	2.05	127.35	124.51
8	K	102	BCL	CHD-C1D-C2D	2.05	129.78	125.48
20	C	503	HEC	CMB-C2B-C3B	2.05	128.23	125.82
8	D	102	BCL	CED-O2D-CGD	2.04	120.56	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	M	709	LMT	C3B-C4B-C5B	2.04	113.88	110.24
16	H	102	LMT	C1B-O1B-C4'	-2.04	112.92	117.96
8	9	101	BCL	C4A-NA-C1A	2.04	107.62	106.71
8	Q	101	BCL	CED-O2D-CGD	2.04	120.54	115.94
8	W	102	BCL	C11-C10-C8	-2.04	109.34	115.92
8	6	102	BCL	CMD-C2D-C3D	-2.04	122.93	127.61
8	D	102	BCL	C1C-NC-C4C	-2.04	105.79	106.71
16	T	102	LMT	O1B-C4'-C3'	2.03	112.69	107.28
8	S	102	BCL	C6-C5-C3	-2.03	108.12	113.45
8	K	101	BCL	C4-C3-C5	2.03	118.69	115.27
8	7	101	BCL	C2A-C1A-CHA	-2.03	120.31	123.86
8	W	102	BCL	C11-C12-C13	-2.03	109.37	115.92
8	U	102	BCL	CMD-C2D-C3D	-2.02	122.96	127.61
8	8	101	BCL	CED-O2D-CGD	2.02	120.51	115.94
8	O	101	BCL	C11-C10-C8	-2.02	109.39	115.92
8	K	101	BCL	C4D-CHA-C1A	-2.02	118.79	121.25
9	E	104	PGV	O01-C1-O02	-2.02	118.82	123.70
8	G	101	BCL	C4A-NA-C1A	2.02	107.61	106.71
8	F	101	BCL	C1C-NC-C4C	-2.02	105.80	106.71
8	D	102	BCL	O2A-CGA-O1A	-2.02	118.50	123.59
8	S	102	BCL	CAA-C2A-C3A	-2.02	107.26	112.78
8	S	102	BCL	C4-C3-C2	-2.01	118.51	123.68
8	6	101	BCL	CED-O2D-CGD	2.01	120.49	115.94
8	8	102	BCL	CED-O2D-CGD	2.01	120.49	115.94
9	K	103	PGV	O01-C1-O02	-2.01	118.84	123.70
9	S	103	PGV	C03-C02-C01	-2.01	107.03	111.79
8	S	102	BCL	CHB-C4A-NA	2.01	127.29	124.51
8	7	101	BCL	CMD-C2D-C3D	-2.00	123.01	127.61

There are no chirality outliers.

All (1301) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	W	101	BCL	C1A-C2A-CAA-CBA
8	W	101	BCL	C4C-C3C-CAC-CBC
8	W	102	BCL	C2-C1-O2A-CGA
8	W	102	BCL	C2C-C3C-CAC-CBC
8	W	102	BCL	C4-C3-C5-C6
8	U	102	BCL	C2C-C3C-CAC-CBC
8	U	102	BCL	C2-C3-C5-C6
8	U	102	BCL	C4-C3-C5-C6
8	S	102	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
8	S	102	BCL	C11-C10-C8-C9
8	S	102	BCL	C11-C12-C13-C15
8	Q	102	BCL	C1A-C2A-CAA-CBA
8	Q	102	BCL	C2C-C3C-CAC-CBC
8	O	102	BCL	C2C-C3C-CAC-CBC
8	O	102	BCL	CBD-CGD-O2D-CED
8	O	102	BCL	C2-C3-C5-C6
8	O	102	BCL	C4-C3-C5-C6
8	K	101	BCL	C4C-C3C-CAC-CBC
8	K	102	BCL	C1A-C2A-CAA-CBA
8	K	102	BCL	C2C-C3C-CAC-CBC
8	K	102	BCL	C4C-C3C-CAC-CBC
8	I	102	BCL	C2C-C3C-CAC-CBC
8	I	102	BCL	C4C-C3C-CAC-CBC
8	G	102	BCL	C1A-C2A-CAA-CBA
8	G	102	BCL	C2C-C3C-CAC-CBC
8	G	102	BCL	C4C-C3C-CAC-CBC
8	G	102	BCL	C2-C3-C5-C6
8	G	102	BCL	C4-C3-C5-C6
8	E	101	BCL	C1A-C2A-CAA-CBA
8	E	101	BCL	C2-C3-C5-C6
8	E	101	BCL	C4-C3-C5-C6
8	E	102	BCL	C2-C3-C5-C6
8	E	102	BCL	C4-C3-C5-C6
8	0	102	BCL	C2C-C3C-CAC-CBC
8	0	102	BCL	C4C-C3C-CAC-CBC
8	0	102	BCL	C2-C3-C5-C6
8	0	102	BCL	C4-C3-C5-C6
8	8	101	BCL	C11-C12-C13-C14
8	8	102	BCL	C2C-C3C-CAC-CBC
8	6	102	BCL	C2C-C3C-CAC-CBC
8	6	102	BCL	C4C-C3C-CAC-CBC
8	6	102	BCL	CBD-CGD-O2D-CED
8	6	102	BCL	C2-C3-C5-C6
8	6	102	BCL	C4-C3-C5-C6
8	4	101	BCL	C4C-C3C-CAC-CBC
8	4	101	BCL	C2-C3-C5-C6
8	4	101	BCL	C4-C3-C5-C6
8	4	101	BCL	C6-C7-C8-C9
8	2	102	BCL	C2C-C3C-CAC-CBC
8	2	102	BCL	C4C-C3C-CAC-CBC
8	2	102	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	L	702	BCL	C1A-C2A-CAA-CBA
8	L	703	BCL	C1A-C2A-CAA-CBA
8	L	703	BCL	C2-C3-C5-C6
8	L	703	BCL	C4-C3-C5-C6
8	H	101	BCL	C2C-C3C-CAC-CBC
8	H	101	BCL	C4C-C3C-CAC-CBC
8	J	102	BCL	C4C-C3C-CAC-CBC
8	T	101	BCL	C2C-C3C-CAC-CBC
8	T	101	BCL	C4C-C3C-CAC-CBC
8	V	101	BCL	C1A-C2A-CAA-CBA
8	V	101	BCL	C3A-C2A-CAA-CBA
8	1	101	BCL	C1A-C2A-CAA-CBA
8	3	103	BCL	C1A-C2A-CAA-CBA
8	5	101	BCL	C11-C12-C13-C14
8	A	102	BCL	C2A-CAA-CBA-CGA
8	D	102	BCL	C1A-C2A-CAA-CBA
8	D	102	BCL	C2C-C3C-CAC-CBC
8	D	102	BCL	C4C-C3C-CAC-CBC
8	F	101	BCL	C1A-C2A-CAA-CBA
8	F	101	BCL	C3A-C2A-CAA-CBA
8	F	101	BCL	C4C-C3C-CAC-CBC
9	U	103	PGV	C03-O11-P-O14
9	U	103	PGV	C04-O12-P-O11
9	U	104	PGV	C03-O11-P-O13
9	U	104	PGV	C04-O12-P-O13
9	U	104	PGV	O01-C02-C03-O11
9	K	103	PGV	O01-C02-C03-O11
9	K	104	PGV	C04-O12-P-O14
9	K	104	PGV	C2-C1-O01-C02
9	I	103	PGV	C04-O12-P-O14
9	E	103	PGV	C03-O11-P-O13
9	E	103	PGV	C04-O12-P-O13
9	E	104	PGV	C04-O12-P-O11
9	E	104	PGV	C04-O12-P-O13
9	0	104	PGV	C03-O11-P-O12
9	0	104	PGV	C03-O11-P-O13
9	0	104	PGV	C04-O12-P-O11
9	0	104	PGV	C04-O12-P-O13
9	6	103	PGV	C2-C1-O01-C02
9	4	102	PGV	C04-O12-P-O11
9	4	102	PGV	C04-O12-P-O13
9	4	102	PGV	O01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
9	M	705	PGV	C04-C05-C06-O06
9	L	706	PGV	C04-O12-P-O13
9	L	711	PGV	C04-O12-P-O14
9	L	712	PGV	C03-O11-P-O14
9	h	102	PGV	C03-O11-P-O12
9	C	506	PGV	C03-O11-P-O12
9	C	506	PGV	C03-O11-P-O13
9	C	506	PGV	C03-O11-P-O14
9	C	506	PGV	O03-C01-C02-O01
10	J	101	U4Z	CAH-CAD-CAJ-CAL
11	M	702	BPH	C4C-C3C-CAC-CBC
11	M	702	BPH	C2C-C3C-CAC-CBC
11	L	701	BPH	C1-C2-C3-C4
11	L	701	BPH	C1-C2-C3-C5
11	L	704	BPH	O2A-C1-C2-C3
11	L	704	BPH	C1-C2-C3-C4
11	L	704	BPH	C1-C2-C3-C5
13	L	705	MQE	CBK-CAX-CAY-CBL
13	L	705	MQE	CBQ-CAX-CAY-CBL
15	M	708	PEF	C1-O3P-P-O1P
15	M	708	PEF	C4-O4P-P-O2P
15	M	708	PEF	C4-O4P-P-O3P
15	L	713	PEF	C11-C10-O2-C2
15	L	713	PEF	O4-C10-O2-C2
15	L	713	PEF	C4-O4P-P-O2P
15	L	717	PEF	C1-O3P-P-O1P
15	h	103	PEF	C1-O3P-P-O1P
15	h	103	PEF	C1-O3P-P-O2P
15	h	103	PEF	C1-O3P-P-O4P
16	M	709	LMT	C2'-C1'-O1'-C1
16	M	709	LMT	O5'-C1'-O1'-C1
18	P	102	CDL	CA2-OA2-PA1-OA4
18	P	102	CDL	CB3-OB5-PB2-OB2
18	P	102	CDL	CB3-OB5-PB2-OB3
18	P	102	CDL	CB3-OB5-PB2-OB4
18	P	102	CDL	C51-CB5-OB6-CB4
19	h	101	LHG	C4-C5-C6-O8
19	h	101	LHG	O7-C5-C6-O8
19	h	101	LHG	C6-C5-O7-C7
19	h	101	LHG	O9-C7-O7-C5
15	M	708	PEF	C11-C10-O2-C2
8	K	102	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	W	102	BCL	CBD-CGD-O2D-CED
8	U	102	BCL	CBD-CGD-O2D-CED
8	Q	102	BCL	CBD-CGD-O2D-CED
8	K	102	BCL	CBD-CGD-O2D-CED
8	I	102	BCL	CBD-CGD-O2D-CED
8	E	102	BCL	CBD-CGD-O2D-CED
8	4	101	BCL	CBD-CGD-O2D-CED
8	2	102	BCL	O1D-CGD-O2D-CED
8	G	101	BCL	CBD-CGD-O2D-CED
8	B	101	BCL	CBD-CGD-O2D-CED
8	8	102	BCL	CBD-CGD-O2D-CED
8	1	101	BCL	CBD-CGD-O2D-CED
15	M	708	PEF	O4-C10-O2-C2
8	6	101	BCL	O1A-CGA-O2A-C1
8	O	102	BCL	O1D-CGD-O2D-CED
8	6	102	BCL	O1D-CGD-O2D-CED
8	E	102	BCL	O1D-CGD-O2D-CED
9	K	104	PGV	O02-C1-O01-C02
9	6	103	PGV	O02-C1-O01-C02
18	P	102	CDL	OB7-CB5-OB6-CB4
8	S	102	BCL	O1A-CGA-O2A-C1
8	W	102	BCL	C3-C5-C6-C7
8	U	101	BCL	C3-C5-C6-C7
8	E	102	BCL	C3-C5-C6-C7
8	B	101	BCL	C3-C5-C6-C7
8	0	102	BCL	C3-C5-C6-C7
8	6	101	BCL	C3-C5-C6-C7
8	6	102	BCL	C3-C5-C6-C7
8	R	102	BCL	C3-C5-C6-C7
8	V	101	BCL	C3-C5-C6-C7
8	5	101	BCL	C3-C5-C6-C7
8	S	101	BCL	CBA-CGA-O2A-C1
9	1	102	PGV	C20-C19-O03-C01
8	U	102	BCL	O1D-CGD-O2D-CED
8	E	101	BCL	CBD-CGD-O2D-CED
8	3	101	BCL	CBD-CGD-O2D-CED
11	L	701	BPH	CBD-CGD-O2D-CED
8	K	102	BCL	C2A-CAA-CBA-CGA
8	Q	101	BCL	O1A-CGA-O2A-C1
8	H	101	BCL	C15-C16-C17-C18
16	H	102	LMT	C3'-C4'-O1B-C1B
8	U	102	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
8	O	102	BCL	C3-C5-C6-C7
8	I	101	BCL	C3-C5-C6-C7
8	G	101	BCL	C3-C5-C6-C7
8	G	102	BCL	C3-C5-C6-C7
8	2	102	BCL	C3-C5-C6-C7
8	T	101	BCL	C3-C5-C6-C7
8	1	101	BCL	C3-C5-C6-C7
8	S	102	BCL	CBA-CGA-O2A-C1
8	Q	101	BCL	CBA-CGA-O2A-C1
8	0	101	BCL	CBA-CGA-O2A-C1
8	6	101	BCL	CBA-CGA-O2A-C1
8	2	101	BCL	CBA-CGA-O2A-C1
8	Q	102	BCL	O1D-CGD-O2D-CED
8	M	701	BCL	CBD-CGD-O2D-CED
16	M	709	LMT	C3'-C4'-O1B-C1B
8	W	102	BCL	O1D-CGD-O2D-CED
8	I	102	BCL	O1D-CGD-O2D-CED
8	W	101	BCL	O1A-CGA-O2A-C1
8	S	101	BCL	O1A-CGA-O2A-C1
8	O	101	BCL	CBD-CGD-O2D-CED
8	L	702	BCL	CBD-CGD-O2D-CED
8	5	101	BCL	CBD-CGD-O2D-CED
8	A	102	BCL	CBD-CGD-O2D-CED
18	P	102	CDL	O1-C1-CB2-OB2
8	3	103	BCL	C3-C5-C6-C7
8	I	102	BCL	CBA-CGA-O2A-C1
8	A	101	BCL	CBA-CGA-O2A-C1
11	L	701	BPH	CBA-CGA-O2A-C1
9	1	102	PGV	O04-C19-O03-C01
8	G	102	BCL	CBD-CGD-O2D-CED
8	V	101	BCL	CBD-CGD-O2D-CED
8	A	101	BCL	CBD-CGD-O2D-CED
11	M	702	BPH	CBD-CGD-O2D-CED
8	0	101	BCL	O1A-CGA-O2A-C1
8	4	101	BCL	O1D-CGD-O2D-CED
11	L	704	BPH	CBD-CGD-O2D-CED
8	8	102	BCL	C3-C5-C6-C7
8	W	101	BCL	CBA-CGA-O2A-C1
8	2	101	BCL	O1A-CGA-O2A-C1
8	V	101	BCL	C4-C3-C5-C6
11	M	702	BPH	C4-C3-C5-C6
13	M	704	MQE	CBA-CAU-CAZ-CBZ

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Mol	Chain	Res	Type	Atoms
8	W	102	BCL	C2-C3-C5-C6
8	V	101	BCL	C2-C3-C5-C6
11	M	702	BPH	C2-C3-C5-C6
13	M	704	MQE	CBA-CAU-CAZ-CBI
11	L	701	BPH	C2A-CAA-CBA-CGA
8	A	101	BCL	O1A-CGA-O2A-C1
11	L	701	BPH	O1A-CGA-O2A-C1
13	M	704	MQE	CAR-CAE-CAL-CBF
8	U	102	BCL	CBA-CGA-O2A-C1
8	8	101	BCL	CBA-CGA-O2A-C1
8	8	102	BCL	O1D-CGD-O2D-CED
8	I	102	BCL	O1A-CGA-O2A-C1
9	O	103	PGV	C2-C1-O01-C02
9	C	506	PGV	C2-C1-O01-C02
9	h	102	PGV	C26-C27-C28-C29
8	U	102	BCL	O1A-CGA-O2A-C1
8	O	102	BCL	O1A-CGA-O2A-C1
8	8	101	BCL	O1A-CGA-O2A-C1
8	Q	102	BCL	C3-C5-C6-C7
8	W	102	BCL	CBA-CGA-O2A-C1
8	O	101	BCL	CBA-CGA-O2A-C1
8	O	102	BCL	CBA-CGA-O2A-C1
8	K	102	BCL	CBA-CGA-O2A-C1
8	8	102	BCL	CBA-CGA-O2A-C1
8	2	102	BCL	CBA-CGA-O2A-C1
8	J	102	BCL	CBD-CGD-O2D-CED
8	G	101	BCL	O1D-CGD-O2D-CED
8	H	101	BCL	C8-C10-C11-C12
8	O	101	BCL	O1A-CGA-O2A-C1
9	0	104	PGV	O01-C02-C03-O11
16	M	709	LMT	C4'-C5'-C6'-O6'
8	1	101	BCL	C10-C11-C12-C13
9	C	506	PGV	O12-C04-C05-O05
8	2	102	BCL	O1A-CGA-O2A-C1
16	M	709	LMT	O5'-C5'-C6'-O6'
8	U	101	BCL	C4-C3-C5-C6
8	U	102	BCL	C11-C10-C8-C9
8	S	102	BCL	C14-C13-C15-C16
8	Q	101	BCL	C11-C12-C13-C14
8	Q	102	BCL	C11-C10-C8-C9
8	Q	102	BCL	C11-C12-C13-C14
8	K	101	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
8	K	101	BCL	C11-C10-C8-C9
8	G	101	BCL	C11-C10-C8-C9
8	E	101	BCL	C11-C10-C8-C9
8	E	101	BCL	C11-C12-C13-C14
8	E	102	BCL	C6-C7-C8-C9
8	E	102	BCL	C11-C12-C13-C14
8	0	102	BCL	C6-C7-C8-C9
8	2	102	BCL	C11-C12-C13-C14
8	2	102	BCL	C14-C13-C15-C16
8	1	101	BCL	C6-C7-C8-C9
8	3	103	BCL	C6-C7-C8-C9
8	3	103	BCL	C11-C12-C13-C14
8	D	102	BCL	C14-C13-C15-C16
8	F	101	BCL	C11-C10-C8-C9
11	M	702	BPH	C11-C10-C8-C9
11	M	702	BPH	C11-C12-C13-C14
11	M	702	BPH	C14-C13-C15-C16
8	1	101	BCL	O1D-CGD-O2D-CED
8	3	103	BCL	C2A-CAA-CBA-CGA
9	K	103	PGV	C19-C20-C21-C22
8	W	102	BCL	O1A-CGA-O2A-C1
8	W	101	BCL	C5-C6-C7-C8
8	B	101	BCL	C5-C6-C7-C8
8	M	701	BCL	C15-C16-C17-C18
8	7	101	BCL	C5-C6-C7-C8
8	B	101	BCL	O1D-CGD-O2D-CED
8	I	101	BCL	CBD-CGD-O2D-CED
8	K	102	BCL	C3-C5-C6-C7
8	4	101	BCL	C3-C5-C6-C7
8	3	101	BCL	C3-C5-C6-C7
8	4	101	BCL	CBA-CGA-O2A-C1
8	Q	101	BCL	C8-C10-C11-C12
8	I	101	BCL	C15-C16-C17-C18
8	E	101	BCL	C10-C11-C12-C13
8	P	101	BCL	C8-C10-C11-C12
8	A	101	BCL	C10-C11-C12-C13
8	F	101	BCL	C15-C16-C17-C18
16	T	102	LMT	C3'-C4'-O1B-C1B
8	U	101	BCL	C10-C11-C12-C13
8	S	102	BCL	C10-C11-C12-C13
8	K	102	BCL	C15-C16-C17-C18
8	E	101	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
8	6	101	BCL	C10-C11-C12-C13
8	6	102	BCL	C13-C15-C16-C17
8	L	703	BCL	C15-C16-C17-C18
8	1	101	BCL	C5-C6-C7-C8
8	3	101	BCL	C13-C15-C16-C17
8	A	102	BCL	C13-C15-C16-C17
8	D	102	BCL	C15-C16-C17-C18
9	I	103	PGV	C19-C20-C21-C22
9	4	102	PGV	C19-C20-C21-C22
9	C	506	PGV	C1-C2-C3-C4
8	I	102	BCL	C10-C11-C12-C13
8	E	101	BCL	C8-C10-C11-C12
8	8	101	BCL	C13-C15-C16-C17
8	2	102	BCL	C13-C15-C16-C17
8	N	101	BCL	C10-C11-C12-C13
8	3	101	BCL	C15-C16-C17-C18
8	F	101	BCL	C5-C6-C7-C8
8	F	101	BCL	C8-C10-C11-C12
11	M	702	BPH	C13-C15-C16-C17
14	L	715	BGL	O2-C1'-C2'-C3'
15	h	103	PEF	C35-C36-C37-C38
9	O	103	PGV	O02-C1-O01-C02
9	C	506	PGV	O02-C1-O01-C02
8	G	101	BCL	C8-C10-C11-C12
8	E	102	BCL	C15-C16-C17-C18
8	8	102	BCL	C5-C6-C7-C8
8	H	101	BCL	C5-C6-C7-C8
8	G	102	BCL	C8-C10-C11-C12
8	Q	101	BCL	C11-C10-C8-C7
8	Q	102	BCL	C6-C7-C8-C10
8	I	102	BCL	C11-C10-C8-C7
8	E	102	BCL	C11-C10-C8-C7
8	2	102	BCL	C11-C10-C8-C7
8	D	102	BCL	C6-C7-C8-C10
8	D	102	BCL	C3-C5-C6-C7
8	K	102	BCL	O1A-CGA-O2A-C1
8	4	101	BCL	O1A-CGA-O2A-C1
16	T	102	LMT	C5'-C4'-O1B-C1B
8	W	101	BCL	C2A-CAA-CBA-CGA
8	E	101	BCL	C2A-CAA-CBA-CGA
8	2	101	BCL	C2A-CAA-CBA-CGA
8	J	102	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
8	9	101	BCL	C2A-CAA-CBA-CGA
8	W	101	BCL	C15-C16-C17-C18
8	Q	102	BCL	C13-C15-C16-C17
8	0	102	BCL	C15-C16-C17-C18
8	5	101	BCL	C13-C15-C16-C17
8	9	101	BCL	CBD-CGD-O2D-CED
16	D	104	LMT	O5'-C1'-O1'-C1
8	P	101	BCL	C13-C15-C16-C17
8	E	102	BCL	C5-C6-C7-C8
8	6	102	BCL	C8-C10-C11-C12
8	2	101	BCL	C5-C6-C7-C8
8	2	101	BCL	C10-C11-C12-C13
8	M	701	BCL	C10-C11-C12-C13
8	M	701	BCL	C13-C15-C16-C17
8	5	101	BCL	C10-C11-C12-C13
11	L	704	BPH	C10-C11-C12-C13
16	1	104	LMT	C5'-C4'-O1B-C1B
8	W	101	BCL	C8-C10-C11-C12
8	U	101	BCL	C13-C15-C16-C17
8	G	101	BCL	C5-C6-C7-C8
8	N	101	BCL	C8-C10-C11-C12
8	8	102	BCL	O1A-CGA-O2A-C1
8	3	101	BCL	O1D-CGD-O2D-CED
8	Q	102	BCL	C10-C11-C12-C13
8	0	101	BCL	C10-C11-C12-C13
8	6	101	BCL	C13-C15-C16-C17
9	U	103	PGV	C03-O11-P-O12
9	S	103	PGV	C04-O12-P-O11
9	O	103	PGV	C03-O11-P-O12
9	O	103	PGV	C04-O12-P-O11
9	K	103	PGV	C03-O11-P-O12
9	K	103	PGV	C04-O12-P-O11
9	K	104	PGV	C03-O11-P-O12
9	K	104	PGV	C04-O12-P-O11
9	I	103	PGV	C04-O12-P-O11
9	4	102	PGV	C03-O11-P-O12
9	L	711	PGV	C03-O11-P-O12
9	L	711	PGV	C04-O12-P-O11
15	M	708	PEF	C1-O3P-P-O4P
15	h	103	PEF	C4-O4P-P-O3P
18	P	102	CDL	CA2-OA2-PA1-OA5
8	O	101	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
8	I	101	BCL	CBA-CGA-O2A-C1
8	G	102	BCL	CBA-CGA-O2A-C1
8	0	101	BCL	C15-C16-C17-C18
11	L	701	BPH	O1D-CGD-O2D-CED
8	E	101	BCL	O1D-CGD-O2D-CED
8	U	102	BCL	C5-C6-C7-C8
8	U	102	BCL	C15-C16-C17-C18
8	I	102	BCL	C8-C10-C11-C12
8	G	102	BCL	C10-C11-C12-C13
8	E	102	BCL	C10-C11-C12-C13
8	P	101	BCL	C5-C6-C7-C8
8	5	101	BCL	C5-C6-C7-C8
8	8	102	BCL	C16-C17-C18-C19
8	A	101	BCL	C16-C17-C18-C20
8	3	103	BCL	CBA-CGA-O2A-C1
18	P	102	CDL	C71-CB7-OB8-CB6
9	1	102	PGV	C2-C1-O01-C02
8	2	101	BCL	C3-C5-C6-C7
9	h	102	PGV	C27-C28-C29-C30
16	D	104	LMT	C5-C6-C7-C8
8	G	102	BCL	C16-C17-C18-C20
8	B	101	BCL	C16-C17-C18-C20
8	N	101	BCL	C16-C17-C18-C19
18	P	102	CDL	CB6-CB4-OB6-CB5
9	0	105	PGV	C2-C3-C4-C5
9	O	103	PGV	C20-C21-C22-C23
9	I	103	PGV	O12-C04-C05-O05
9	0	105	PGV	O12-C04-C05-O05
9	S	103	PGV	C5-C6-C7-C8
8	J	102	BCL	CBA-CGA-O2A-C1
16	1	104	LMT	C3'-C4'-O1B-C1B
8	I	101	BCL	O1A-CGA-O2A-C1
8	I	101	BCL	C16-C17-C18-C19
8	L	702	BCL	C16-C17-C18-C19
8	H	101	BCL	C16-C17-C18-C19
8	M	701	BCL	O1D-CGD-O2D-CED
8	5	101	BCL	O1D-CGD-O2D-CED
9	O	103	PGV	C29-C30-C31-C32
9	K	103	PGV	C29-C30-C31-C32
9	8	103	PGV	C6-C7-C8-C9
9	h	102	PGV	C24-C25-C26-C27
16	M	709	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
8	W	101	BCL	C11-C12-C13-C14
8	S	102	BCL	C11-C12-C13-C14
8	I	102	BCL	C11-C12-C13-C14
8	0	101	BCL	C11-C10-C8-C9
8	8	101	BCL	C11-C10-C8-C9
8	H	101	BCL	C6-C7-C8-C9
8	T	101	BCL	C11-C10-C8-C9
8	3	101	BCL	C11-C10-C8-C9
9	U	103	PGV	C27-C28-C29-C30
9	C	506	PGV	C20-C21-C22-C23
19	h	101	LHG	C33-C34-C35-C36
9	K	104	PGV	C04-C05-C06-O06
9	L	706	PGV	C04-C05-C06-O06
9	1	102	PGV	O02-C1-O01-C02
8	S	101	BCL	C10-C11-C12-C13
9	U	104	PGV	C29-C30-C31-C32
9	8	103	PGV	C20-C21-C22-C23
14	Y	103	BGL	C4'-C5'-C6'-C7'
15	L	717	PEF	C17-C18-C19-C20
9	E	103	PGV	C1-C2-C3-C4
9	8	103	PGV	C1-C2-C3-C4
16	1	104	LMT	C3-C4-C5-C6
16	D	104	LMT	C3-C4-C5-C6
8	Q	102	BCL	C16-C17-C18-C20
8	8	102	BCL	C16-C17-C18-C20
8	L	702	BCL	C16-C17-C18-C20
8	H	101	BCL	C16-C17-C18-C20
8	3	103	BCL	C16-C17-C18-C19
8	W	102	BCL	C5-C6-C7-C8
8	O	101	BCL	C10-C11-C12-C13
9	U	104	PGV	C20-C21-C22-C23
9	E	104	PGV	C6-C7-C8-C9
9	O	103	PGV	C28-C29-C30-C31
15	L	713	PEF	C37-C38-C39-C40
19	h	101	LHG	C32-C33-C34-C35
19	h	101	LHG	C23-C24-C25-C26
8	Q	102	BCL	C8-C10-C11-C12
8	A	102	BCL	C10-C11-C12-C13
9	0	105	PGV	C27-C28-C29-C30
9	C	506	PGV	C22-C23-C24-C25
16	H	102	LMT	O5B-C5B-C6B-O6B
8	G	101	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
8	S	102	BCL	C3A-C2A-CAA-CBA
8	Q	102	BCL	C3A-C2A-CAA-CBA
8	I	102	BCL	C3A-C2A-CAA-CBA
8	G	102	BCL	C3A-C2A-CAA-CBA
8	E	102	BCL	C3A-C2A-CAA-CBA
8	B	101	BCL	C3A-C2A-CAA-CBA
8	L	702	BCL	C3A-C2A-CAA-CBA
8	L	703	BCL	C3A-C2A-CAA-CBA
8	J	102	BCL	C3A-C2A-CAA-CBA
8	P	101	BCL	C3A-C2A-CAA-CBA
8	1	101	BCL	C3A-C2A-CAA-CBA
8	3	103	BCL	C3A-C2A-CAA-CBA
8	9	101	BCL	C3A-C2A-CAA-CBA
8	D	102	BCL	C3A-C2A-CAA-CBA
11	L	701	BPH	C3A-C2A-CAA-CBA
8	H	101	BCL	C13-C15-C16-C17
8	T	101	BCL	C15-C16-C17-C18
14	Y	103	BGL	C1'-C2'-C3'-C4'
15	h	103	PEF	C33-C34-C35-C36
8	A	102	BCL	O1D-CGD-O2D-CED
8	I	101	BCL	C16-C17-C18-C20
8	B	101	BCL	C16-C17-C18-C19
8	N	101	BCL	C16-C17-C18-C20
8	D	102	BCL	C16-C17-C18-C19
8	O	101	BCL	O1D-CGD-O2D-CED
9	I	103	PGV	C25-C26-C27-C28
8	S	101	BCL	O2A-C1-C2-C3
8	L	702	BCL	C3-C5-C6-C7
8	G	102	BCL	O1A-CGA-O2A-C1
8	B	101	BCL	C4-C3-C5-C6
8	U	101	BCL	C2-C3-C5-C6
8	B	101	BCL	C2-C3-C5-C6
18	P	102	CDL	C11-CA5-OA6-CA4
9	K	104	PGV	O05-C05-C06-O06
9	M	705	PGV	O05-C05-C06-O06
9	I	103	PGV	C6-C7-C8-C9
9	E	104	PGV	C27-C28-C29-C30
9	L	706	PGV	C21-C22-C23-C24
8	J	102	BCL	O1A-CGA-O2A-C1
8	3	103	BCL	O1A-CGA-O2A-C1
8	W	102	BCL	C8-C10-C11-C12
8	0	102	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
8	V	101	BCL	C13-C15-C16-C17
8	V	101	BCL	C15-C16-C17-C18
8	S	101	BCL	C3-C5-C6-C7
16	D	104	LMT	O5'-C5'-C6'-O6'
18	P	102	CDL	OA7-CA5-OA6-CA4
9	U	103	PGV	C22-C23-C24-C25
18	P	102	CDL	OB9-CB7-OB8-CB6
8	V	101	BCL	C16-C17-C18-C20
9	L	712	PGV	C19-C20-C21-C22
10	0	103	U4Z	CAH-CAD-CAJ-CAL
10	J	101	U4Z	CAB-CAD-CAJ-CAL
10	R	101	U4Z	CAH-CAD-CAJ-CAL
10	3	102	U4Z	CAB-CAD-CAJ-CAL
10	3	102	U4Z	CAH-CAD-CAJ-CAL
10	D	101	U4Z	CAB-CAD-CAJ-CAL
10	D	101	U4Z	CAH-CAD-CAJ-CAL
9	0	104	PGV	C20-C21-C22-C23
15	L	717	PEF	C15-C16-C17-C18
8	G	102	BCL	O1D-CGD-O2D-CED
8	S	102	BCL	C5-C6-C7-C8
8	O	101	BCL	C8-C10-C11-C12
8	K	101	BCL	C10-C11-C12-C13
8	K	102	BCL	C5-C6-C7-C8
8	R	102	BCL	C10-C11-C12-C13
8	T	101	BCL	C13-C15-C16-C17
11	M	702	BPH	C10-C11-C12-C13
9	E	103	PGV	C28-C29-C30-C31
9	0	105	PGV	C1-C2-C3-C4
8	Q	101	BCL	C4-C3-C5-C6
11	L	704	BPH	C4-C3-C5-C6
8	W	101	BCL	C6-C7-C8-C10
8	W	101	BCL	C11-C12-C13-C15
8	S	102	BCL	C11-C10-C8-C7
8	K	101	BCL	C6-C7-C8-C10
8	K	101	BCL	C11-C12-C13-C15
8	I	102	BCL	C11-C12-C13-C15
8	G	102	BCL	C11-C10-C8-C7
8	E	102	BCL	C12-C13-C15-C16
8	0	101	BCL	C11-C10-C8-C7
8	0	102	BCL	C6-C7-C8-C10
8	8	101	BCL	C11-C10-C8-C7
8	6	102	BCL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
8	2	101	BCL	C6-C7-C8-C10
8	H	101	BCL	C6-C7-C8-C10
8	T	101	BCL	C11-C10-C8-C7
8	V	101	BCL	C11-C10-C8-C7
8	1	101	BCL	C6-C7-C8-C10
8	1	101	BCL	C11-C12-C13-C15
8	3	101	BCL	C11-C10-C8-C7
11	L	704	BPH	C2-C3-C5-C6
11	L	704	BPH	C11-C10-C8-C7
8	G	101	BCL	O1A-CGA-O2A-C1
8	6	102	BCL	C5-C6-C7-C8
11	M	702	BPH	O1D-CGD-O2D-CED
9	S	103	PGV	C28-C29-C30-C31
8	I	101	BCL	C2A-CAA-CBA-CGA
8	N	101	BCL	C15-C16-C17-C18
8	9	101	BCL	C8-C10-C11-C12
8	V	101	BCL	O1D-CGD-O2D-CED
8	0	102	BCL	C13-C15-C16-C17
8	V	101	BCL	C5-C6-C7-C8
8	4	101	BCL	C16-C17-C18-C19
8	O	102	BCL	C5-C6-C7-C8
8	R	102	BCL	C8-C10-C11-C12
8	A	101	BCL	O1D-CGD-O2D-CED
9	U	104	PGV	C26-C27-C28-C29
15	h	103	PEF	C34-C35-C36-C37
9	E	103	PGV	O01-C02-C03-O11
8	Q	101	BCL	C10-C11-C12-C13
8	3	103	BCL	C5-C6-C7-C8
8	7	101	BCL	C15-C16-C17-C18
19	h	101	LHG	C25-C26-C27-C28
9	6	103	PGV	C30-C31-C32-C33
8	A	102	BCL	C15-C16-C17-C18
15	L	713	PEF	O2-C2-C3-O3
9	K	103	PGV	C30-C31-C32-C33
9	C	506	PGV	C2-C3-C4-C5
8	Q	102	BCL	C16-C17-C18-C19
8	G	102	BCL	C16-C17-C18-C19
16	H	102	LMT	C5'-C4'-O1B-C1B
8	N	101	BCL	C5-C6-C7-C8
9	E	103	PGV	C19-C20-C21-C22
8	Q	101	BCL	C2-C3-C5-C6
8	Q	101	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
8	K	101	BCL	C11-C12-C13-C14
8	I	102	BCL	C11-C10-C8-C9
8	G	102	BCL	C11-C10-C8-C9
8	E	102	BCL	C11-C10-C8-C9
8	6	102	BCL	C14-C13-C15-C16
8	2	101	BCL	C6-C7-C8-C9
8	M	701	BCL	C6-C7-C8-C9
8	V	101	BCL	C11-C10-C8-C9
8	3	101	BCL	C14-C13-C15-C16
8	A	101	BCL	C11-C10-C8-C9
8	D	102	BCL	C6-C7-C8-C9
11	L	704	BPH	C11-C10-C8-C9
9	U	104	PGV	C23-C24-C25-C26
8	I	102	BCL	C2A-CAA-CBA-CGA
8	8	101	BCL	C2A-CAA-CBA-CGA
8	J	102	BCL	O1D-CGD-O2D-CED
8	8	101	BCL	C10-C11-C12-C13
9	O	103	PGV	C5-C6-C7-C8
8	S	102	BCL	C1A-C2A-CAA-CBA
8	O	102	BCL	C1A-C2A-CAA-CBA
8	I	102	BCL	C1A-C2A-CAA-CBA
8	E	102	BCL	C1A-C2A-CAA-CBA
8	B	101	BCL	C1A-C2A-CAA-CBA
8	0	102	BCL	C1A-C2A-CAA-CBA
8	J	102	BCL	C1A-C2A-CAA-CBA
8	P	101	BCL	C1A-C2A-CAA-CBA
8	9	101	BCL	C1A-C2A-CAA-CBA
8	4	101	BCL	C16-C17-C18-C20
8	V	101	BCL	C16-C17-C18-C19
9	L	706	PGV	C2-C1-O01-C02
11	L	704	BPH	O1D-CGD-O2D-CED
8	B	101	BCL	C8-C10-C11-C12
9	U	104	PGV	C03-O11-P-O12
9	E	103	PGV	C04-O12-P-O11
9	L	712	PGV	C03-O11-P-O12
14	L	708	BGL	O5-C5-C6-O6
14	L	714	BGL	O5-C5-C6-O6
11	L	701	BPH	C13-C15-C16-C17
9	L	711	PGV	C20-C19-O03-C01
9	L	712	PGV	C20-C19-O03-C01
9	0	104	PGV	C01-C02-C03-O11
9	C	506	PGV	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
15	L	713	PEF	O3P-C1-C2-C3
9	L	712	PGV	C22-C23-C24-C25
8	6	102	BCL	C15-C16-C17-C18
18	P	102	CDL	CA2-C1-CB2-OB2
8	W	101	BCL	C2C-C3C-CAC-CBC
8	S	102	BCL	C2C-C3C-CAC-CBC
8	4	101	BCL	C2C-C3C-CAC-CBC
8	J	102	BCL	C2C-C3C-CAC-CBC
8	R	102	BCL	C2C-C3C-CAC-CBC
8	5	101	BCL	C2C-C3C-CAC-CBC
8	9	101	BCL	C2C-C3C-CAC-CBC
8	F	101	BCL	C2C-C3C-CAC-CBC
9	K	104	PGV	C24-C25-C26-C27
8	A	101	BCL	C16-C17-C18-C19
8	N	101	BCL	C3-C5-C6-C7
8	2	102	BCL	C10-C11-C12-C13
14	L	708	BGL	C4'-C5'-C6'-C7'
8	L	702	BCL	O1D-CGD-O2D-CED
8	Q	102	BCL	C5-C6-C7-C8
8	I	102	BCL	C13-C15-C16-C17
9	8	103	PGV	C5-C6-C7-C8
8	W	101	BCL	C13-C15-C16-C17
14	Y	103	BGL	O5-C5-C6-O6
8	U	102	BCL	C10-C11-C12-C13
14	H	103	BGL	O5-C5-C6-O6
14	Y	101	BGL	O5-C5-C6-O6
16	H	102	LMT	O5'-C5'-C6'-O6'
8	W	101	BCL	C4-C3-C5-C6
8	I	102	BCL	C4-C3-C5-C6
8	G	101	BCL	C4-C3-C5-C6
8	U	102	BCL	C8-C10-C11-C12
15	h	103	PEF	C11-C12-C13-C14
8	I	101	BCL	O1D-CGD-O2D-CED
16	T	102	LMT	O5'-C5'-C6'-O6'
8	Q	102	BCL	C15-C16-C17-C18
8	P	101	BCL	C15-C16-C17-C18
9	1	102	PGV	C03-O11-P-O13
9	h	102	PGV	C03-O11-P-O13
9	O	103	PGV	O01-C02-C03-O11
8	9	101	BCL	O1D-CGD-O2D-CED
8	9	101	BCL	C5-C6-C7-C8
8	K	101	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	N	101	BCL	C4-C3-C5-C6
8	F	101	BCL	C4-C3-C5-C6
10	D	101	U4Z	CAT-CAS-CAW-CAZ
13	M	704	MQE	CAL-CAE-CAR-CBV
8	W	101	BCL	C2-C3-C5-C6
8	U	101	BCL	C6-C7-C8-C10
8	U	102	BCL	C11-C10-C8-C7
8	S	101	BCL	C11-C12-C13-C15
8	S	102	BCL	C12-C13-C15-C16
8	O	101	BCL	C11-C10-C8-C7
8	K	102	BCL	C11-C10-C8-C7
8	I	102	BCL	C6-C7-C8-C10
8	G	101	BCL	C2-C3-C5-C6
8	E	102	BCL	C6-C7-C8-C10
8	2	102	BCL	C6-C7-C8-C10
8	2	102	BCL	C12-C13-C15-C16
8	M	701	BCL	C6-C7-C8-C10
8	L	702	BCL	C11-C10-C8-C7
8	H	101	BCL	C11-C10-C8-C7
8	N	101	BCL	C2-C3-C5-C6
8	V	101	BCL	C6-C7-C8-C10
8	3	101	BCL	C12-C13-C15-C16
8	3	103	BCL	C6-C7-C8-C10
8	9	101	BCL	C6-C7-C8-C10
8	A	101	BCL	C11-C10-C8-C7
8	F	101	BCL	C11-C10-C8-C7
11	M	702	BPH	C11-C12-C13-C15
11	M	702	BPH	C12-C13-C15-C16
13	M	704	MQE	CAL-CAE-CAR-CBD
19	h	101	LHG	C34-C35-C36-C37
8	U	102	BCL	C11-C12-C13-C14
8	S	101	BCL	C14-C13-C15-C16
8	O	101	BCL	C11-C10-C8-C9
8	O	102	BCL	C6-C7-C8-C9
8	K	102	BCL	C11-C10-C8-C9
8	I	102	BCL	C6-C7-C8-C9
8	B	101	BCL	C14-C13-C15-C16
8	0	102	BCL	C11-C12-C13-C14
8	6	102	BCL	C6-C7-C8-C9
8	2	102	BCL	C6-C7-C8-C9
8	L	702	BCL	C14-C13-C15-C16
8	H	101	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
8	V	101	BCL	C6-C7-C8-C9
8	5	101	BCL	C11-C10-C8-C9
8	9	101	BCL	C6-C7-C8-C9
9	O	103	PGV	C19-C20-C21-C22
9	U	103	PGV	C7-C8-C9-C10
16	T	102	LMT	C6-C7-C8-C9
8	U	101	BCL	C16-C17-C18-C19
9	C	506	PGV	C19-C20-C21-C22
9	K	104	PGV	C4-C5-C6-C7
9	h	102	PGV	C20-C21-C22-C23
9	U	104	PGV	C01-C02-C03-O11
9	E	103	PGV	C01-C02-C03-O11
9	L	712	PGV	C01-C02-C03-O11
18	P	102	CDL	OB5-CB3-CB4-CB6
9	0	104	PGV	C1-C2-C3-C4
16	M	709	LMT	C7-C8-C9-C10
8	L	702	BCL	C13-C15-C16-C17
9	L	712	PGV	C27-C28-C29-C30
8	A	101	BCL	C4-C3-C5-C6
8	K	101	BCL	C2-C3-C5-C6
8	F	101	BCL	C2-C3-C5-C6
10	D	101	U4Z	CAT-CAS-CAW-CBA
9	E	104	PGV	C2-C3-C4-C5
9	L	712	PGV	O04-C19-O03-C01
8	M	701	BCL	C16-C17-C18-C19
11	M	702	BPH	C16-C17-C18-C19
8	2	102	BCL	C15-C16-C17-C18
8	F	101	BCL	CBA-CGA-O2A-C1
8	M	701	BCL	C3A-C2A-CAA-CBA
8	H	101	BCL	C3A-C2A-CAA-CBA
8	G	102	BCL	C13-C15-C16-C17
9	0	104	PGV	C26-C27-C28-C29
16	M	709	LMT	C2-C1-O1'-C1'
8	L	702	BCL	C15-C16-C17-C18
16	T	102	LMT	C11-C10-C9-C8
8	D	102	BCL	C16-C17-C18-C20
8	0	102	BCL	CBA-CGA-O2A-C1
11	M	702	BPH	CBA-CGA-O2A-C1
8	G	101	BCL	C15-C16-C17-C18
9	O	103	PGV	O03-C01-C02-C03
9	8	103	PGV	O03-C01-C02-C03
9	6	103	PGV	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
9	L	712	PGV	O03-C01-C02-C03
15	L	713	PEF	C1-C2-C3-O3
18	P	102	CDL	CA3-CA4-CA6-OA8
9	L	706	PGV	O02-C1-O01-C02
9	L	711	PGV	O04-C19-O03-C01
8	G	101	BCL	C10-C11-C12-C13
8	U	101	BCL	C16-C17-C18-C20
11	M	702	BPH	C16-C17-C18-C20
8	A	101	BCL	C2-C3-C5-C6
9	8	103	PGV	C03-O11-P-O12
15	L	717	PEF	C4-O4P-P-O3P
9	h	102	PGV	O01-C02-C03-O11
15	h	103	PEF	O3P-C1-C2-O2
16	T	102	LMT	C5-C6-C7-C8
8	3	103	BCL	C16-C17-C18-C20
9	L	711	PGV	C24-C25-C26-C27
19	h	101	LHG	C27-C28-C29-C30
9	K	103	PGV	C7-C8-C9-C10
9	O	103	PGV	O03-C01-C02-O01
9	L	712	PGV	O03-C01-C02-O01
18	P	102	CDL	OA6-CA4-CA6-OA8
8	7	101	BCL	C2-C1-O2A-CGA
11	L	704	BPH	C2-C1-O2A-CGA
8	B	101	BCL	C10-C11-C12-C13
8	S	101	BCL	C11-C12-C13-C14
8	G	102	BCL	C14-C13-C15-C16
8	2	101	BCL	C11-C12-C13-C14
11	M	702	BPH	C6-C7-C8-C9
9	0	104	PGV	C27-C28-C29-C30
9	I	103	PGV	C27-C28-C29-C30
9	1	102	PGV	C2-C3-C4-C5
8	U	102	BCL	C4C-C3C-CAC-CBC
8	O	102	BCL	C4C-C3C-CAC-CBC
8	G	101	BCL	C4C-C3C-CAC-CBC
8	8	102	BCL	C4C-C3C-CAC-CBC
8	L	702	BCL	C4C-C3C-CAC-CBC
8	R	102	BCL	C4C-C3C-CAC-CBC
8	5	101	BCL	C4C-C3C-CAC-CBC
8	9	101	BCL	C4C-C3C-CAC-CBC
8	E	102	BCL	C13-C15-C16-C17
9	S	103	PGV	C19-C20-C21-C22
14	Y	101	BGL	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
8	E	102	BCL	C16-C17-C18-C19
8	J	102	BCL	C8-C10-C11-C12
9	K	103	PGV	C01-C02-C03-O11
9	L	706	PGV	C01-C02-C03-O11
9	L	711	PGV	C01-C02-C03-O11
9	h	102	PGV	C01-C02-C03-O11
8	W	102	BCL	C6-C7-C8-C10
8	U	102	BCL	C6-C7-C8-C10
8	U	102	BCL	C11-C12-C13-C15
8	S	101	BCL	C6-C7-C8-C10
8	S	101	BCL	C12-C13-C15-C16
8	Q	102	BCL	C11-C12-C13-C15
8	O	102	BCL	C6-C7-C8-C10
8	I	102	BCL	C2-C3-C5-C6
8	G	101	BCL	C11-C10-C8-C7
8	G	102	BCL	C12-C13-C15-C16
8	B	101	BCL	C12-C13-C15-C16
8	0	101	BCL	C12-C13-C15-C16
8	0	102	BCL	C11-C12-C13-C15
8	6	102	BCL	C6-C7-C8-C10
8	4	101	BCL	C6-C7-C8-C10
8	2	101	BCL	C11-C12-C13-C15
8	L	702	BCL	C12-C13-C15-C16
8	P	101	BCL	C6-C7-C8-C10
8	7	101	BCL	C11-C10-C8-C7
11	M	702	BPH	C6-C7-C8-C10
11	M	702	BPH	C11-C10-C8-C7
8	0	102	BCL	C8-C10-C11-C12
8	S	102	BCL	C16-C17-C18-C20
9	8	103	PGV	C31-C32-C33-C34
8	H	101	BCL	C10-C11-C12-C13
8	E	101	BCL	C5-C6-C7-C8
15	L	717	PEF	C13-C14-C15-C16
9	U	104	PGV	C19-C20-C21-C22
8	M	701	BCL	C16-C17-C18-C20
8	L	703	BCL	C8-C10-C11-C12
8	6	102	BCL	CBA-CGA-O2A-C1
19	h	101	LHG	C30-C31-C32-C33
9	6	103	PGV	C20-C21-C22-C23
14	M	706	BGL	C3'-C4'-C5'-C6'
8	W	102	BCL	CAD-CBD-CGD-O2D
8	U	102	BCL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
8	E	102	BCL	CAD-CBD-CGD-O2D
8	8	102	BCL	CAD-CBD-CGD-O2D
8	4	101	BCL	CAD-CBD-CGD-O2D
11	M	702	BPH	CAD-CBD-CGD-O2D
11	L	701	BPH	CAD-CBD-CGD-O2D
9	0	104	PGV	C19-C20-C21-C22
11	M	702	BPH	O1A-CGA-O2A-C1
15	L	713	PEF	C31-C30-O3-C3
9	K	104	PGV	C27-C28-C29-C30
8	K	101	BCL	CBD-CGD-O2D-CED
9	L	706	PGV	O01-C02-C03-O11
9	L	711	PGV	O01-C02-C03-O11
9	C	506	PGV	O01-C02-C03-O11
15	L	713	PEF	O3P-C1-C2-O2
9	U	103	PGV	C23-C24-C25-C26
16	H	102	LMT	C5-C6-C7-C8
8	7	101	BCL	C16-C17-C18-C19
9	I	103	PGV	O12-C04-C05-C06
18	P	102	CDL	CB2-C1-CA2-OA2
8	S	102	BCL	CHA-CBD-CGD-O1D
8	S	102	BCL	CHA-CBD-CGD-O2D
8	P	101	BCL	C3-C5-C6-C7
8	0	102	BCL	O1A-CGA-O2A-C1
8	F	101	BCL	O1A-CGA-O2A-C1
14	L	714	BGL	C1'-C2'-C3'-C4'
8	J	102	BCL	C13-C15-C16-C17
9	L	706	PGV	O03-C01-C02-O01
8	V	101	BCL	C8-C10-C11-C12
8	T	101	BCL	CBA-CGA-O2A-C1
8	P	101	BCL	C6-C7-C8-C9
8	R	102	BCL	C11-C10-C8-C9
8	V	101	BCL	C11-C12-C13-C14
9	I	103	PGV	C24-C25-C26-C27
15	h	103	PEF	C30-C31-C32-C33
15	L	713	PEF	C18-C19-C20-C21
8	2	101	BCL	CBD-CGD-O2D-CED
8	6	102	BCL	O1A-CGA-O2A-C1
8	7	101	BCL	C3-C5-C6-C7
9	K	103	PGV	C5-C6-C7-C8
9	0	104	PGV	C30-C31-C32-C33
15	h	103	PEF	C38-C39-C40-C41
8	H	101	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	4	101	BCL	C5-C6-C7-C8
15	L	713	PEF	O5-C30-O3-C3
9	U	104	PGV	C04-O12-P-O11
9	I	103	PGV	C03-O11-P-O12
9	E	104	PGV	C03-O11-P-O12
9	0	105	PGV	C03-O11-P-O12
9	L	706	PGV	C04-O12-P-O11
9	N	102	PGV	C03-O11-P-O12
15	L	713	PEF	C4-O4P-P-O3P
16	D	104	LMT	O1'-C1-C2-C3
9	8	103	PGV	C11-C10-C9-C8
9	0	105	PGV	C30-C31-C32-C33
9	U	103	PGV	C04-O12-P-O14
9	S	103	PGV	C04-O12-P-O13
9	O	103	PGV	C03-O11-P-O13
9	O	103	PGV	C04-O12-P-O13
9	K	103	PGV	C03-O11-P-O13
9	K	103	PGV	C04-O12-P-O13
9	K	104	PGV	C03-O11-P-O14
9	4	102	PGV	C03-O11-P-O13
9	L	712	PGV	C03-O11-P-O13
15	M	708	PEF	C1-O3P-P-O2P
15	M	708	PEF	C4-O4P-P-O1P
15	L	713	PEF	C4-O4P-P-O1P
15	L	717	PEF	C1-O3P-P-O2P
15	h	103	PEF	C4-O4P-P-O1P
18	P	102	CDL	CB2-OB2-PB2-OB3
8	O	101	BCL	C16-C17-C18-C20
8	6	102	BCL	C16-C17-C18-C20
8	F	101	BCL	C16-C17-C18-C20
9	4	102	PGV	C01-C02-C03-O11
15	h	103	PEF	O3P-C1-C2-C3
9	U	104	PGV	C24-C25-C26-C27
9	1	102	PGV	C22-C23-C24-C25
8	M	701	BCL	CAD-CBD-CGD-O1D
8	0	101	BCL	C13-C15-C16-C17
8	R	102	BCL	C15-C16-C17-C18
9	U	103	PGV	C6-C7-C8-C9
9	U	104	PGV	C1-C2-C3-C4
15	L	717	PEF	C30-C31-C32-C33
9	C	506	PGV	O12-C04-C05-C06
9	0	104	PGV	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
9	8	103	PGV	C4-C5-C6-C7
16	M	709	LMT	C6-C7-C8-C9
8	Q	101	BCL	C16-C17-C18-C19
8	O	102	BCL	C16-C17-C18-C19
10	3	102	U4Z	CAT-CAS-CAW-CAZ
8	W	102	BCL	C11-C12-C13-C15
8	G	102	BCL	C11-C12-C13-C15
8	2	102	BCL	C11-C12-C13-C15
8	L	703	BCL	C2C-C3C-CAC-CBC
8	L	703	BCL	C12-C13-C15-C16
8	J	102	BCL	C11-C10-C8-C7
8	N	101	BCL	C12-C13-C15-C16
8	P	101	BCL	C2C-C3C-CAC-CBC
8	R	102	BCL	C11-C10-C8-C7
8	T	101	BCL	C6-C7-C8-C10
8	V	101	BCL	C11-C12-C13-C15
8	7	101	BCL	C12-C13-C15-C16
8	F	101	BCL	C6-C7-C8-C10
9	L	712	PGV	O01-C02-C03-O11
9	1	102	PGV	C1-C2-C3-C4
11	L	701	BPH	C6-C7-C8-C10
8	T	101	BCL	O1A-CGA-O2A-C1
16	M	709	LMT	O1'-C1-C2-C3
9	U	103	PGV	C1-C2-C3-C4
9	C	506	PGV	O03-C01-C02-C03
9	6	103	PGV	O03-C01-C02-O01
8	S	102	BCL	C16-C17-C18-C19
14	M	706	BGL	C2'-C3'-C4'-C5'
8	1	101	BCL	C4-C3-C5-C6
8	7	101	BCL	C4-C3-C5-C6
9	E	104	PGV	C4-C5-C6-C7
9	h	102	PGV	C25-C26-C27-C28
8	U	101	BCL	C6-C7-C8-C9
8	S	101	BCL	C6-C7-C8-C9
8	Q	102	BCL	C6-C7-C8-C9
8	0	101	BCL	C14-C13-C15-C16
8	2	102	BCL	C11-C10-C8-C9
8	N	101	BCL	C11-C10-C8-C9
8	5	101	BCL	C6-C7-C8-C9
8	7	101	BCL	C11-C10-C8-C9
8	E	102	BCL	C16-C17-C18-C20
13	M	704	MQE	CBM-CBJ-CBO-CCB

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Mol	Chain	Res	Type	Atoms
9	0	104	PGV	C25-C26-C27-C28
8	D	102	BCL	C13-C15-C16-C17
9	U	104	PGV	C25-C26-C27-C28
9	S	103	PGV	C3-C4-C5-C6
9	0	105	PGV	C4-C5-C6-C7
9	0	104	PGV	C21-C22-C23-C24
8	Q	102	BCL	O1A-CGA-O2A-C1
8	S	101	BCL	C15-C16-C17-C18
8	T	101	BCL	C16-C17-C18-C20
8	S	101	BCL	C13-C15-C16-C17
9	O	103	PGV	C01-C02-C03-O11
8	O	101	BCL	C2-C1-O2A-CGA
8	6	101	BCL	C2-C1-O2A-CGA
8	M	701	BCL	C2-C1-O2A-CGA
8	L	703	BCL	C2-C1-O2A-CGA
8	A	101	BCL	C2-C1-O2A-CGA
9	0	105	PGV	C23-C24-C25-C26
8	Q	102	BCL	CBA-CGA-O2A-C1
8	R	102	BCL	O1A-CGA-O2A-C1
18	P	102	CDL	OB5-CB3-CB4-OB6
8	F	101	BCL	C16-C17-C18-C19
8	H	101	BCL	C3-C5-C6-C7
8	N	101	BCL	O1A-CGA-O2A-C1
8	9	101	BCL	C3-C5-C6-C7
8	F	101	BCL	C10-C11-C12-C13
8	R	102	BCL	CBA-CGA-O2A-C1
9	S	103	PGV	C03-O11-P-O12
9	E	103	PGV	C03-O11-P-O12
9	0	105	PGV	C04-O12-P-O11
9	8	103	PGV	C04-O12-P-O11
9	6	103	PGV	C03-O11-P-O12
9	6	103	PGV	C04-O12-P-O11
9	M	705	PGV	C03-O11-P-O12
9	M	705	PGV	C04-O12-P-O11
9	L	706	PGV	C03-O11-P-O12
9	N	102	PGV	C04-O12-P-O11
9	C	506	PGV	C04-O12-P-O11
9	L	706	PGV	C4-C5-C6-C7
8	R	102	BCL	C16-C17-C18-C20
8	2	101	BCL	O1D-CGD-O2D-CED
9	S	103	PGV	C27-C28-C29-C30
9	L	711	PGV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
8	N	101	BCL	CBA-CGA-O2A-C1
10	J	101	U4Z	CAT-CAS-CAW-CAZ
13	L	705	MQE	CAJ-CAD-CAQ-CBU
8	6	101	BCL	C12-C13-C15-C16
8	D	102	BCL	C12-C13-C15-C16
8	I	102	BCL	C3-C5-C6-C7
8	W	102	BCL	C11-C12-C13-C14
8	U	102	BCL	C6-C7-C8-C9
8	L	702	BCL	C11-C10-C8-C9
8	L	703	BCL	C14-C13-C15-C16
8	N	101	BCL	C14-C13-C15-C16
8	F	101	BCL	C6-C7-C8-C9
8	U	102	BCL	C16-C17-C18-C20
16	T	102	LMT	C4B-C5B-C6B-O6B
8	8	101	BCL	C15-C16-C17-C18
8	8	102	BCL	C8-C10-C11-C12
9	M	705	PGV	C5-C6-C7-C8
8	O	102	BCL	C16-C17-C18-C20
8	E	101	BCL	C15-C16-C17-C18
14	C	507	BGL	C3'-C4'-C5'-C6'
9	L	706	PGV	O05-C05-C06-O06
8	S	101	BCL	C16-C17-C18-C20
8	O	101	BCL	C16-C17-C18-C19
8	6	102	BCL	C16-C17-C18-C19
8	2	102	BCL	C16-C17-C18-C19
8	K	101	BCL	CBA-CGA-O2A-C1
9	6	103	PGV	C20-C19-O03-C01
9	4	102	PGV	C20-C19-O03-C01
8	K	101	BCL	O1A-CGA-O2A-C1
9	8	103	PGV	C30-C31-C32-C33
9	4	102	PGV	C4-C5-C6-C7
14	M	710	BGL	C4-C5-C6-O6
9	0	105	PGV	O01-C02-C03-O11
9	8	103	PGV	O01-C02-C03-O11
9	6	103	PGV	O01-C02-C03-O11
8	0	101	BCL	C16-C17-C18-C19
9	4	102	PGV	C20-C21-C22-C23
13	M	704	MQE	CAI-CAC-CAP-CBT
8	Q	101	BCL	C2-C1-O2A-CGA
8	B	101	BCL	C2-C1-O2A-CGA
8	T	101	BCL	C2-C1-O2A-CGA
8	9	101	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
8	K	102	BCL	C10-C11-C12-C13
13	M	704	MQE	CAU-CBA-CBN-CBM
8	E	101	BCL	C3A-C2A-CAA-CBA
20	C	504	HEC	C3D-CAD-CBD-CGD
9	6	103	PGV	C31-C32-C33-C34
13	L	705	MQE	CAK-CAF-CAT-CBW
9	S	103	PGV	C24-C25-C26-C27
8	7	101	BCL	C2-C3-C5-C6
9	O	103	PGV	C26-C27-C28-C29
9	6	103	PGV	C29-C30-C31-C32
8	E	102	BCL	C14-C13-C15-C16
8	N	101	BCL	C11-C12-C13-C14
8	T	101	BCL	C6-C7-C8-C9
15	L	717	PEF	C19-C20-C21-C22
9	K	104	PGV	O03-C01-C02-C03
9	E	103	PGV	O03-C01-C02-C03
9	U	103	PGV	C25-C26-C27-C28
8	W	101	BCL	O2A-C1-C2-C3
11	M	702	BPH	O2A-C1-C2-C3
8	O	102	BCL	C10-C11-C12-C13
8	4	101	BCL	C1A-C2A-CAA-CBA
8	M	701	BCL	C1A-C2A-CAA-CBA
8	R	102	BCL	C16-C17-C18-C19
8	O	102	BCL	C12-C13-C15-C16
8	K	102	BCL	C6-C7-C8-C10
8	8	101	BCL	C11-C12-C13-C15
8	M	701	BCL	C11-C10-C8-C7
8	L	703	BCL	C11-C12-C13-C15
8	3	103	BCL	C11-C12-C13-C15
8	5	101	BCL	C11-C12-C13-C15
8	F	101	BCL	C12-C13-C15-C16
9	E	104	PGV	C1-C2-C3-C4
9	E	103	PGV	C6-C7-C8-C9
8	F	101	BCL	C2A-CAA-CBA-CGA
8	N	101	BCL	C13-C15-C16-C17
9	6	103	PGV	C21-C22-C23-C24
8	6	102	BCL	C10-C11-C12-C13
8	A	102	BCL	C5-C6-C7-C8
9	C	506	PGV	C4-C5-C6-C7
14	H	103	BGL	C4'-C5'-C6'-C7'
8	M	701	BCL	C4-C3-C5-C6
8	2	102	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	Q	101	BCL	CBD-CGD-O2D-CED
16	H	102	LMT	C2-C3-C4-C5
8	0	102	BCL	O1D-CGD-O2D-CED
9	8	103	PGV	O03-C01-C02-O01
9	M	705	PGV	O03-C01-C02-O01
20	C	504	HEC	CAA-CBA-CGA-O2A
8	A	101	BCL	C8-C10-C11-C12
8	Q	101	BCL	C16-C17-C18-C20
8	L	703	BCL	C16-C17-C18-C20
9	K	104	PGV	C29-C30-C31-C32
9	E	103	PGV	C3-C4-C5-C6
9	L	706	PGV	O12-C04-C05-C06
8	K	101	BCL	O1D-CGD-O2D-CED
8	8	101	BCL	C4-C3-C5-C6
8	E	102	BCL	C2-C1-O2A-CGA
13	L	705	MQE	CAJ-CAD-CAQ-CBE
13	L	705	MQE	CAK-CAF-CAT-CBG
9	4	102	PGV	O04-C19-O03-C01
19	h	101	LHG	O10-C23-O8-C6
19	h	101	LHG	C29-C30-C31-C32
8	A	102	BCL	C14-C13-C15-C16
11	L	701	BPH	C1A-C2A-CAA-CBA
8	A	101	BCL	C2A-CAA-CBA-CGA
9	6	103	PGV	O04-C19-O03-C01
10	0	103	U4Z	CAB-CAD-CAJ-CAL
10	R	101	U4Z	CAB-CAD-CAJ-CAL
15	L	717	PEF	C14-C15-C16-C17
9	1	102	PGV	C5-C6-C7-C8
8	L	703	BCL	C4C-C3C-CAC-CBC
8	T	101	BCL	C16-C17-C18-C19
8	1	101	BCL	C2-C3-C5-C6
10	J	101	U4Z	CAT-CAS-CAW-CBA
10	3	102	U4Z	CAT-CAS-CAW-CBA
13	M	704	MQE	CAI-CAC-CAP-CBC
9	C	506	PGV	C25-C26-C27-C28
8	E	101	BCL	C3-C5-C6-C7
8	7	101	BCL	C2A-CAA-CBA-CGA
16	T	102	LMT	O1'-C1-C2-C3
20	C	504	HEC	CAA-CBA-CGA-O1A
10	R	101	U4Z	CAT-CAS-CAW-CAZ
9	M	705	PGV	C2-C3-C4-C5
8	5	101	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
9	E	104	PGV	C20-C19-O03-C01
9	S	103	PGV	C29-C30-C31-C32
9	O	103	PGV	C4-C5-C6-C7
11	M	702	BPH	C1-C2-C3-C4
9	K	103	PGV	C1-C2-C3-C4
19	h	101	LHG	O8-C23-C24-C25
14	M	707	BGL	C3'-C4'-C5'-C6'
14	L	708	BGL	C5'-C6'-C7'-C8'
16	D	104	LMT	C4-C5-C6-C7
8	T	101	BCL	C5-C6-C7-C8
9	S	103	PGV	C4-C5-C6-C7
8	8	101	BCL	C2-C3-C5-C6
10	R	101	U4Z	CAT-CAS-CAW-CBA
9	4	102	PGV	C6-C7-C8-C9
8	W	101	BCL	C6-C7-C8-C9
8	W	102	BCL	C6-C7-C8-C9
8	O	102	BCL	C14-C13-C15-C16
8	K	102	BCL	C6-C7-C8-C9
8	I	101	BCL	C6-C7-C8-C9
8	G	102	BCL	C11-C12-C13-C14
8	8	101	BCL	C6-C7-C8-C9
8	6	101	BCL	C11-C10-C8-C9
8	6	101	BCL	C14-C13-C15-C16
8	J	102	BCL	C11-C10-C8-C9
8	1	101	BCL	C11-C12-C13-C14
8	7	101	BCL	C14-C13-C15-C16
8	A	101	BCL	C6-C7-C8-C9
11	L	701	BPH	C6-C7-C8-C9
8	W	101	BCL	C3A-C2A-CAA-CBA
9	M	705	PGV	O01-C1-C2-C3
8	S	101	BCL	C16-C17-C18-C19
8	2	101	BCL	C2-C1-O2A-CGA
8	I	102	BCL	CAA-CBA-CGA-O2A
9	L	712	PGV	C28-C29-C30-C31
8	6	101	BCL	C4-C3-C5-C6
9	C	506	PGV	C28-C29-C30-C31
8	L	703	BCL	C13-C15-C16-C17
8	M	701	BCL	C2-C3-C5-C6
8	K	101	BCL	CAA-CBA-CGA-O2A
15	h	103	PEF	C31-C32-C33-C34
9	E	103	PGV	C25-C26-C27-C28
19	h	101	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
9	L	706	PGV	O03-C01-C02-C03
8	A	102	BCL	C8-C10-C11-C12
15	L	717	PEF	O3-C30-C31-C32
9	K	104	PGV	C25-C26-C27-C28
8	B	101	BCL	O2A-C1-C2-C3
8	J	102	BCL	C15-C16-C17-C18
9	1	102	PGV	O03-C19-C20-C21
9	h	102	PGV	C11-C12-C13-C14
8	U	102	BCL	C16-C17-C18-C19
9	4	102	PGV	C30-C31-C32-C33
9	L	706	PGV	O12-C04-C05-O05
8	G	102	BCL	CHA-CBD-CGD-O2D
8	0	102	BCL	CHA-CBD-CGD-O1D
8	0	102	BCL	CHA-CBD-CGD-O2D
8	M	701	BCL	CHA-CBD-CGD-O1D
8	T	101	BCL	CHA-CBD-CGD-O1D
8	T	101	BCL	CHA-CBD-CGD-O2D
8	5	101	BCL	CHA-CBD-CGD-O2D
8	7	101	BCL	CHA-CBD-CGD-O1D
8	7	101	BCL	CHA-CBD-CGD-O2D
8	D	102	BCL	CHA-CBD-CGD-O2D
9	8	103	PGV	C01-C02-C03-O11
15	L	717	PEF	C11-C12-C13-C14
19	h	101	LHG	C24-C25-C26-C27
11	L	701	BPH	C16-C17-C18-C19
8	S	101	BCL	CAA-CBA-CGA-O2A
15	h	103	PEF	C40-C41-C42-C43
9	h	102	PGV	O03-C01-C02-O01
8	3	101	BCL	CAA-CBA-CGA-O2A
15	L	713	PEF	C16-C17-C18-C19
8	4	101	BCL	C10-C11-C12-C13
8	U	101	BCL	CAA-CBA-CGA-O2A
8	E	102	BCL	C11-C12-C13-C15
8	S	102	BCL	CAA-CBA-CGA-O2A
8	L	703	BCL	C11-C12-C13-C14
18	P	102	CDL	O1-C1-CA2-OA2
9	E	104	PGV	O04-C19-O03-C01
18	P	102	CDL	C51-C52-C53-C54
8	0	101	BCL	C16-C17-C18-C20
8	L	703	BCL	C16-C17-C18-C19
19	h	101	LHG	C24-C23-O8-C6
8	2	102	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
9	E	104	PGV	C3-C4-C5-C6
9	L	706	PGV	C2-C3-C4-C5
8	K	102	BCL	CAA-CBA-CGA-O2A
8	5	101	BCL	C1A-C2A-CAA-CBA
8	A	102	BCL	C1A-C2A-CAA-CBA
15	L	717	PEF	O5-C30-C31-C32
14	M	706	BGL	O2-C1'-C2'-C3'
15	h	103	PEF	O5-C30-O3-C3
9	M	705	PGV	C3-C4-C5-C6
8	I	102	BCL	CAA-CBA-CGA-O1A
9	K	103	PGV	C6-C7-C8-C9
8	K	101	BCL	CAA-CBA-CGA-O1A
19	h	101	LHG	O10-C23-C24-C25
9	4	102	PGV	C23-C24-C25-C26
18	P	102	CDL	CB5-C51-C52-C53
8	W	102	BCL	C10-C11-C12-C13
9	8	103	PGV	C04-O12-P-O13
9	6	103	PGV	C04-O12-P-O13
9	M	705	PGV	C03-O11-P-O13
9	L	711	PGV	C03-O11-P-O14
9	C	506	PGV	C04-O12-P-O13
8	3	101	BCL	CAA-CBA-CGA-O1A
9	M	705	PGV	O02-C1-C2-C3
9	1	102	PGV	O04-C19-C20-C21
8	3	103	BCL	C10-C11-C12-C13
15	h	103	PEF	C32-C33-C34-C35
20	C	501	HEC	CAA-CBA-CGA-O2A
9	I	103	PGV	C20-C21-C22-C23
8	2	101	BCL	C13-C15-C16-C17
9	K	104	PGV	C20-C21-C22-C23
8	G	101	BCL	C16-C17-C18-C20
8	S	101	BCL	CAA-CBA-CGA-O1A
16	D	104	LMT	C5'-C4'-O1B-C1B
9	6	103	PGV	C22-C23-C24-C25
8	0	102	BCL	CBD-CGD-O2D-CED
16	M	709	LMT	C3-C4-C5-C6
9	4	102	PGV	C22-C23-C24-C25
8	B	101	BCL	CAD-CBD-CGD-O1D
8	7	101	BCL	CAD-CBD-CGD-O1D
19	h	101	LHG	C4-C5-O7-C7
16	M	709	LMT	O5B-C1B-O1B-C4'
9	L	712	PGV	O01-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	D	102	BCL	C5-C6-C7-C8
8	U	102	BCL	C14-C13-C15-C16
8	M	701	BCL	C11-C12-C13-C14
8	A	102	BCL	C11-C10-C8-C9
8	F	101	BCL	C14-C13-C15-C16
8	L	703	BCL	O1A-CGA-O2A-C1
13	M	704	MQE	CAD-CAJ-CBC-CAP
13	M	704	MQE	CAH-CAO-CBI-CAZ
9	L	711	PGV	O12-C04-C05-C06
9	E	103	PGV	C26-C27-C28-C29
9	E	103	PGV	C21-C22-C23-C24
8	Q	101	BCL	C11-C12-C13-C15
8	M	701	BCL	C11-C12-C13-C15
8	N	101	BCL	C2C-C3C-CAC-CBC
8	5	101	BCL	C12-C13-C15-C16
8	A	102	BCL	C2C-C3C-CAC-CBC
8	A	102	BCL	C11-C10-C8-C7
9	U	103	PGV	O01-C02-C03-O11
8	Q	101	BCL	O1D-CGD-O2D-CED
8	G	101	BCL	CAA-CBA-CGA-O2A
15	h	103	PEF	C12-C13-C14-C15
8	8	101	BCL	C8-C10-C11-C12
8	U	101	BCL	CAA-CBA-CGA-O1A
13	M	704	MQE	CAZ-CAU-CBA-CBN
20	C	501	HEC	CAA-CBA-CGA-O1A
8	7	101	BCL	CAA-CBA-CGA-O2A
9	L	712	PGV	C24-C25-C26-C27
8	K	102	BCL	CAA-CBA-CGA-O1A
8	M	701	BCL	C2A-CAA-CBA-CGA
8	N	101	BCL	C2A-CAA-CBA-CGA
8	R	102	BCL	C2A-CAA-CBA-CGA
9	0	105	PGV	C21-C22-C23-C24

There are no ring outliers.

77 monomers are involved in 178 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	101	BCL	3	0
20	C	501	HEC	2	0
8	2	102	BCL	10	0
10	3	102	U4Z	2	0
9	I	103	PGV	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	704	MQE	1	0
16	1	104	LMT	1	0
8	0	101	BCL	1	0
16	H	102	LMT	2	0
8	4	101	BCL	7	0
11	L	704	BPH	2	0
8	3	101	BCL	1	0
14	L	715	BGL	1	0
8	S	102	BCL	5	0
18	P	102	CDL	2	0
8	O	102	BCL	3	0
8	W	102	BCL	3	0
11	M	702	BPH	2	0
8	L	703	BCL	2	0
8	U	101	BCL	4	0
8	F	101	BCL	3	0
20	C	504	HEC	3	0
8	G	101	BCL	1	0
15	L	717	PEF	2	0
8	1	101	BCL	3	0
8	8	101	BCL	2	0
9	0	104	PGV	2	0
8	I	101	BCL	2	0
16	M	709	LMT	2	0
8	K	102	BCL	1	0
8	E	101	BCL	8	0
8	M	701	BCL	2	0
20	C	503	HEC	2	0
8	H	101	BCL	1	0
8	A	102	BCL	3	0
8	U	102	BCL	4	0
9	8	103	PGV	1	0
8	K	101	BCL	1	0
8	B	101	BCL	2	0
8	V	101	BCL	8	0
8	P	101	BCL	2	0
8	O	101	BCL	1	0
9	K	104	PGV	1	0
9	L	711	PGV	2	0
8	5	101	BCL	2	0
8	G	102	BCL	2	0
9	O	103	PGV	1	0

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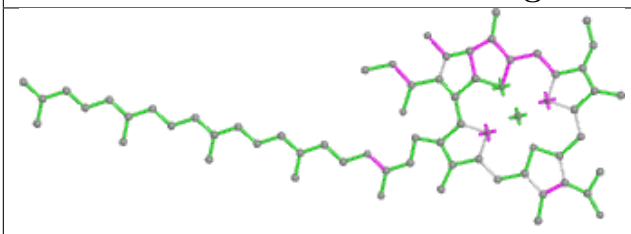
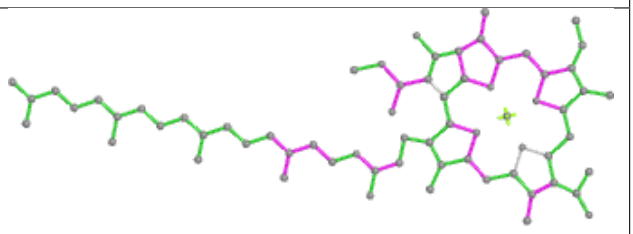
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	S	103	PGV	1	0
16	D	104	LMT	3	0
8	S	101	BCL	1	0
8	Q	102	BCL	2	0
8	A	101	BCL	1	0
8	W	101	BCL	4	0
8	0	102	BCL	8	0
9	6	103	PGV	1	0
8	Q	101	BCL	3	0
9	C	506	PGV	1	0
9	M	705	PGV	5	0
8	L	702	BCL	1	0
8	2	101	BCL	1	0
14	M	710	BGL	2	0
9	K	103	PGV	2	0
16	T	102	LMT	1	0
15	L	713	PEF	2	0
9	E	103	PGV	2	0
8	6	102	BCL	3	0
8	8	102	BCL	4	0
10	R	101	U4Z	1	0
8	I	102	BCL	4	0
8	6	101	BCL	2	0
9	1	102	PGV	1	0
8	R	102	BCL	3	0
9	4	102	PGV	1	0
8	7	101	BCL	1	0
8	D	102	BCL	3	0
9	U	103	PGV	2	0
8	E	102	BCL	3	0

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

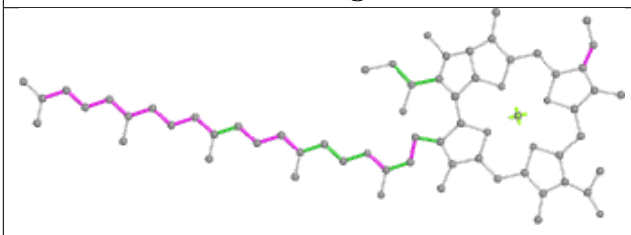
Ligand BCL N 101



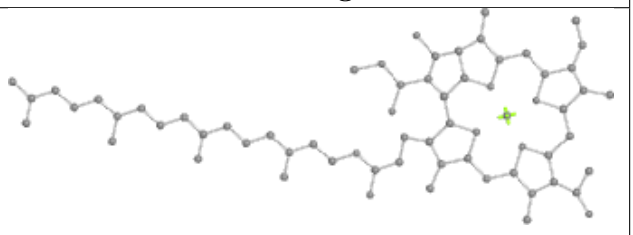
Bond lengths



Bond angles

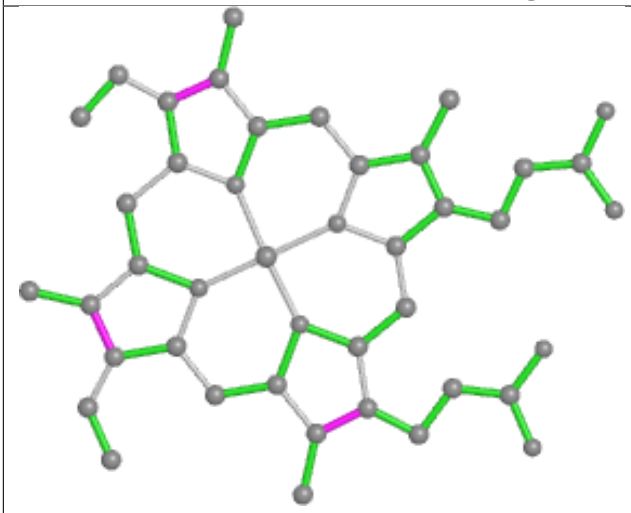


Torsions

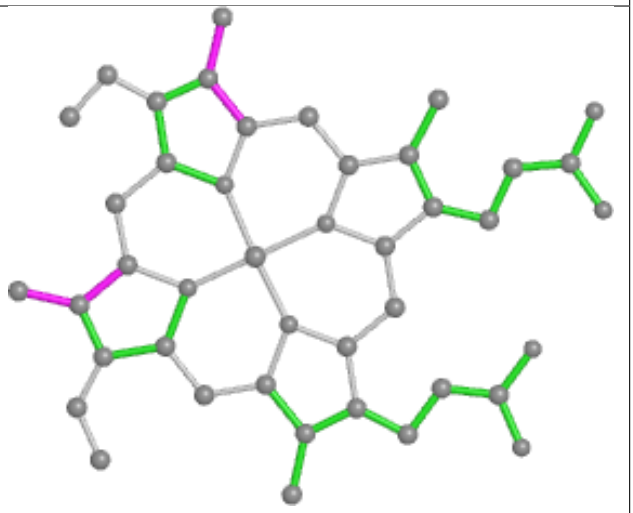


Rings

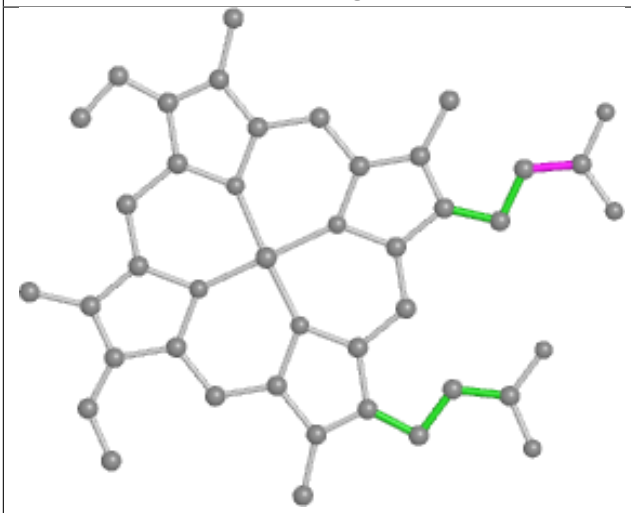
Ligand HEC C 501



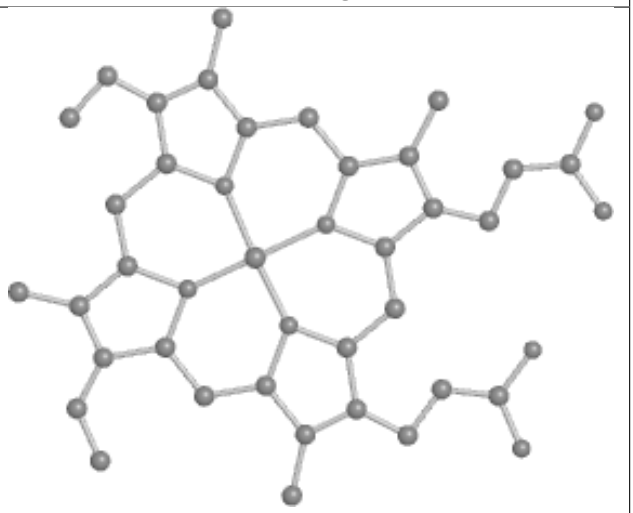
Bond lengths



Bond angles

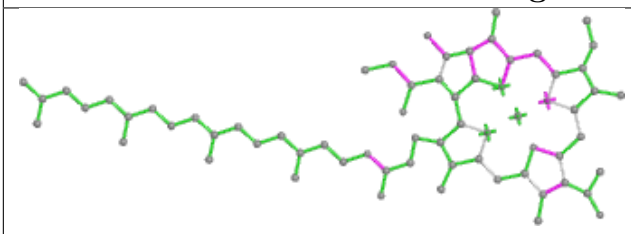


Torsions



Rings

Ligand BCL 2 102



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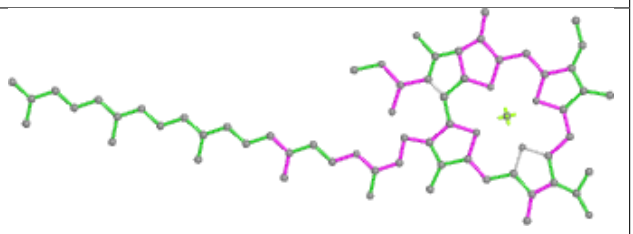
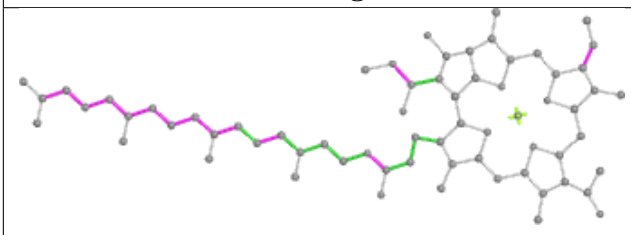
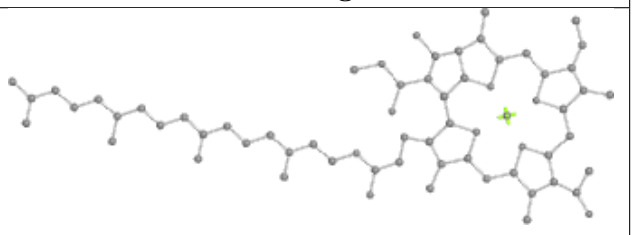


Bond angles

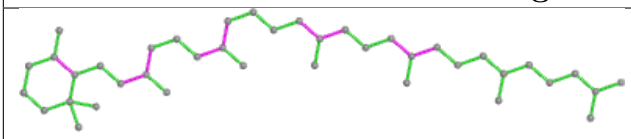


Torsions



Rings

Ligand U4Z 3 102



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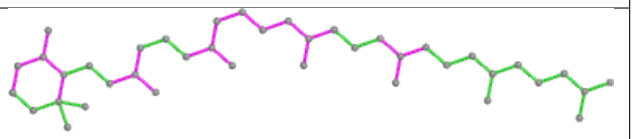
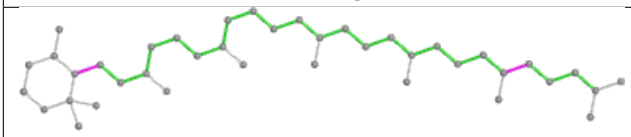


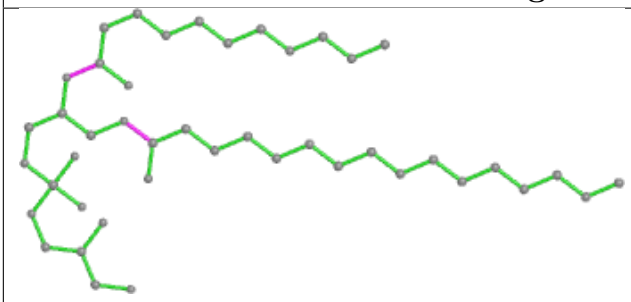
Bond angles



Torsions

Rings

Ligand PGV I 103



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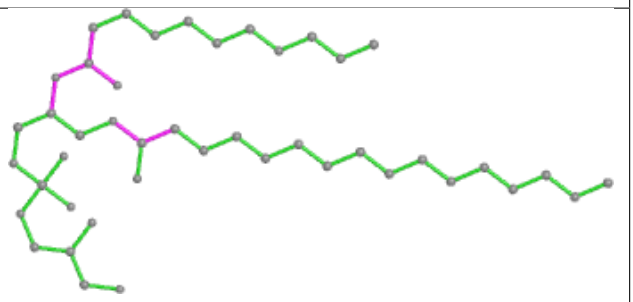

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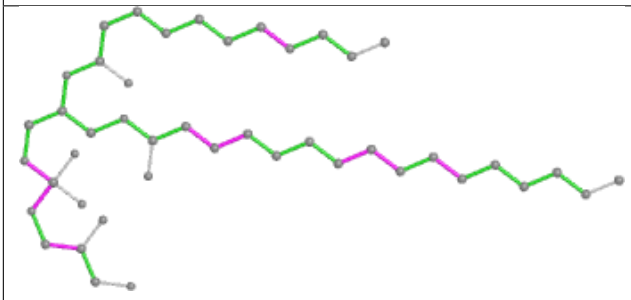
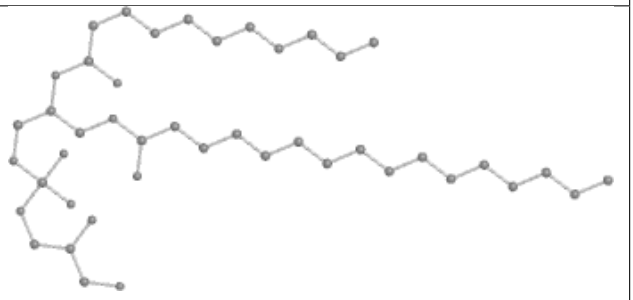
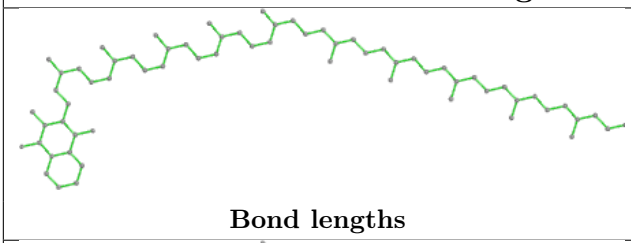


Torsions



Rings

Ligand MQE M 704



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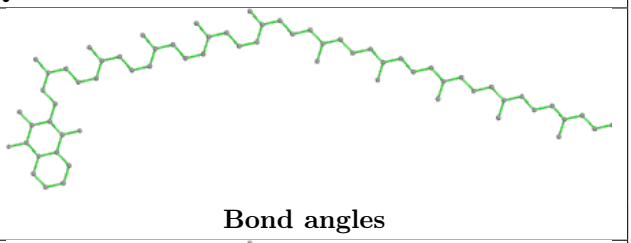

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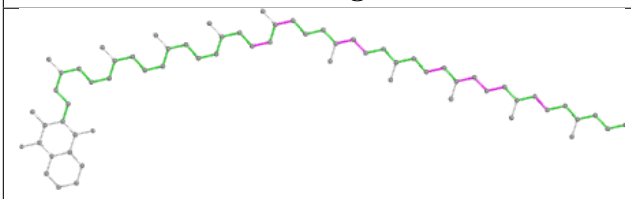

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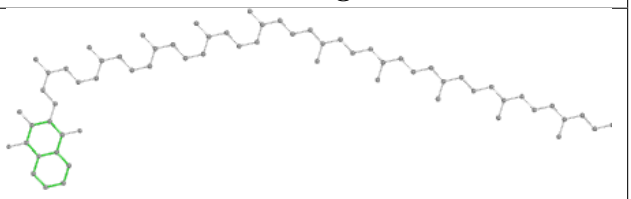
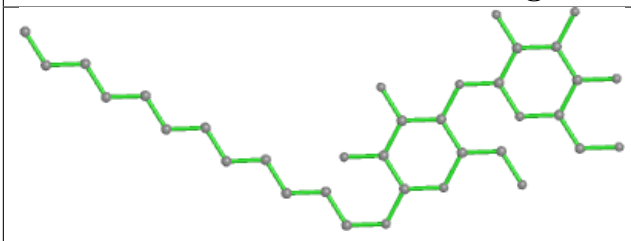


Rings

Ligand LMT 1 104



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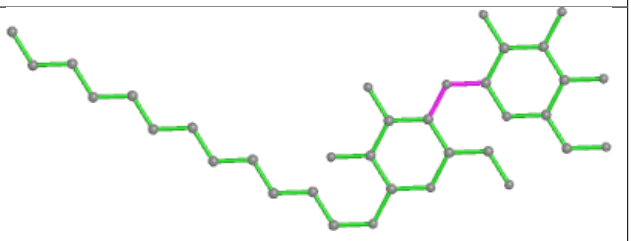

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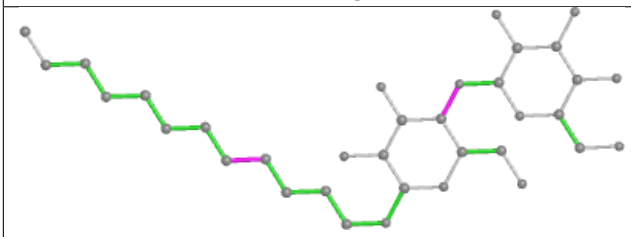

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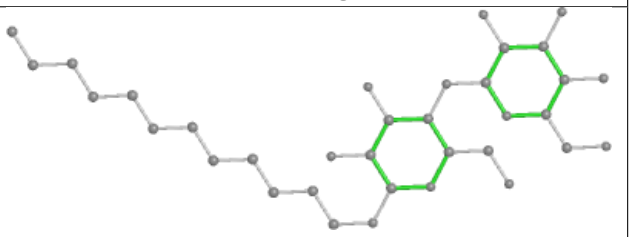
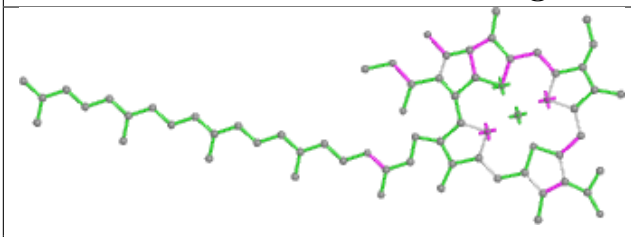
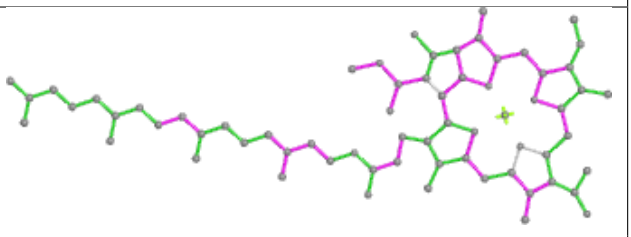


Rings

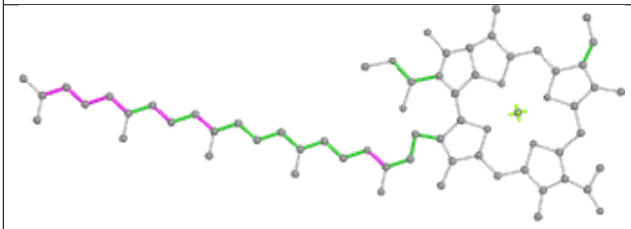
Ligand BCL 0 101



Bond lengths



Bond angles



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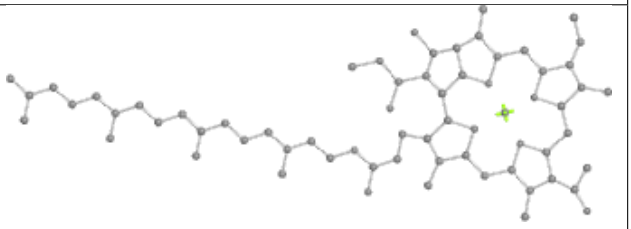
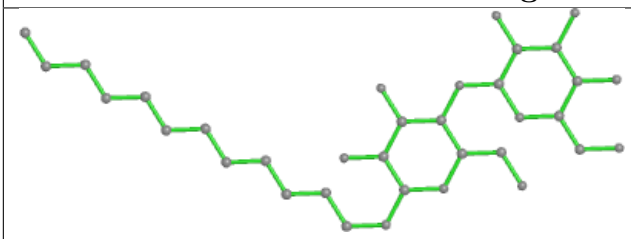
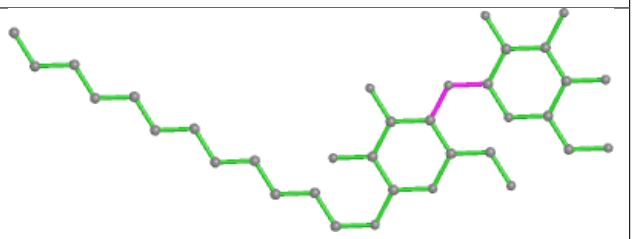


Rings

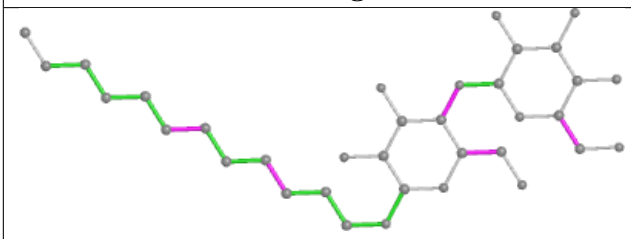
Ligand LMT H 102



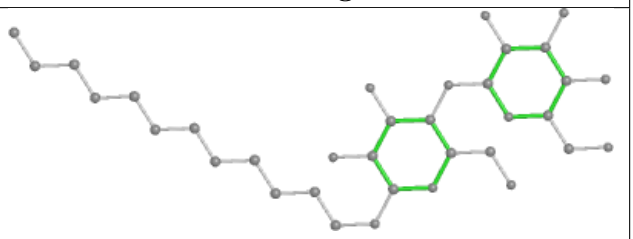
Bond lengths



Bond angles

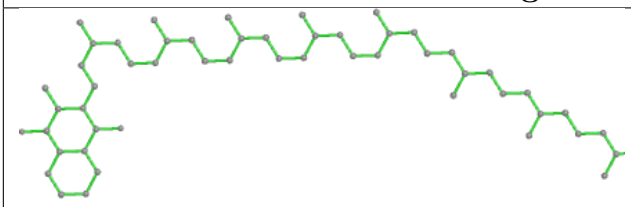


Torsions



Rings

Ligand MQE L 705



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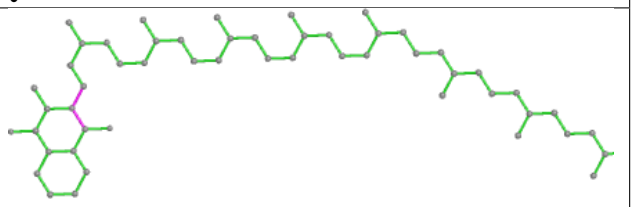
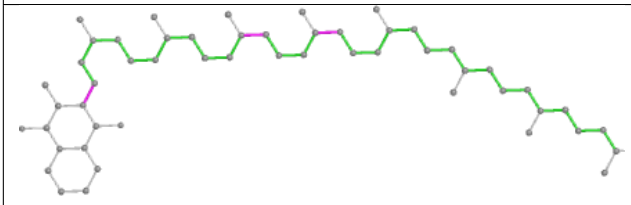


Bond angles



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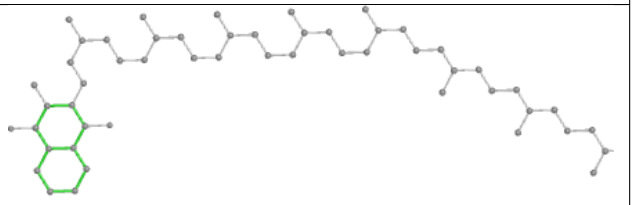
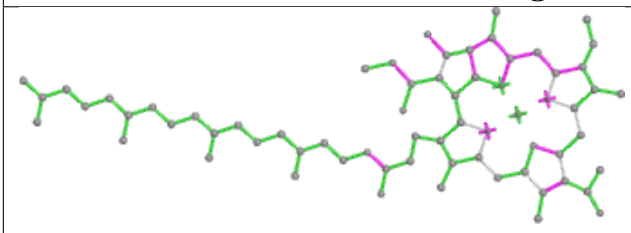


Rings

Ligand BCL 4 101



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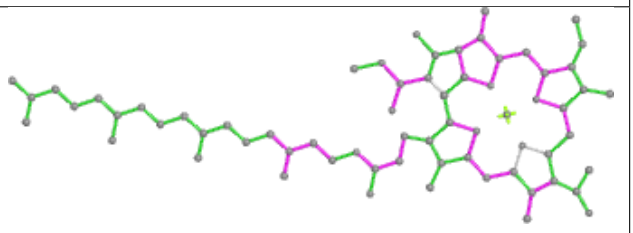

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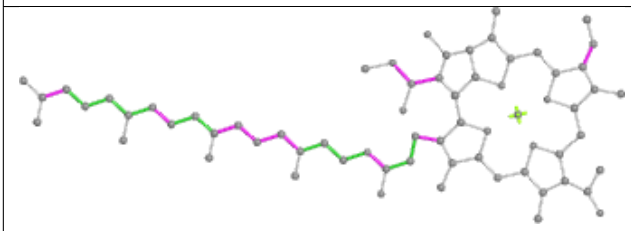

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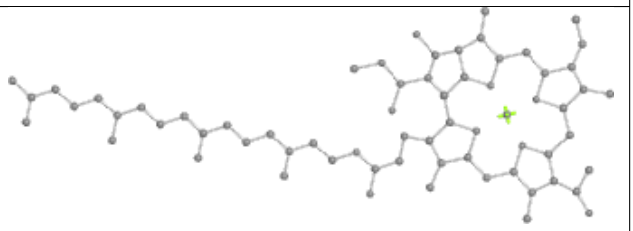
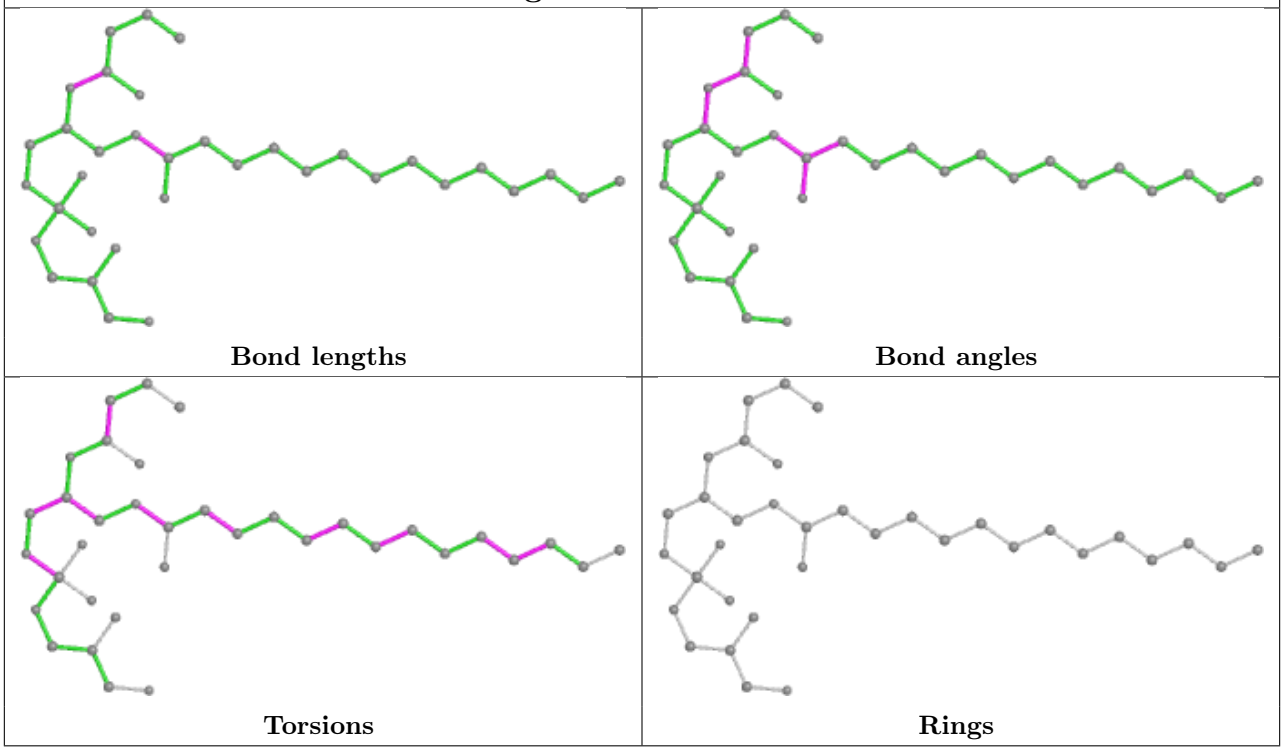
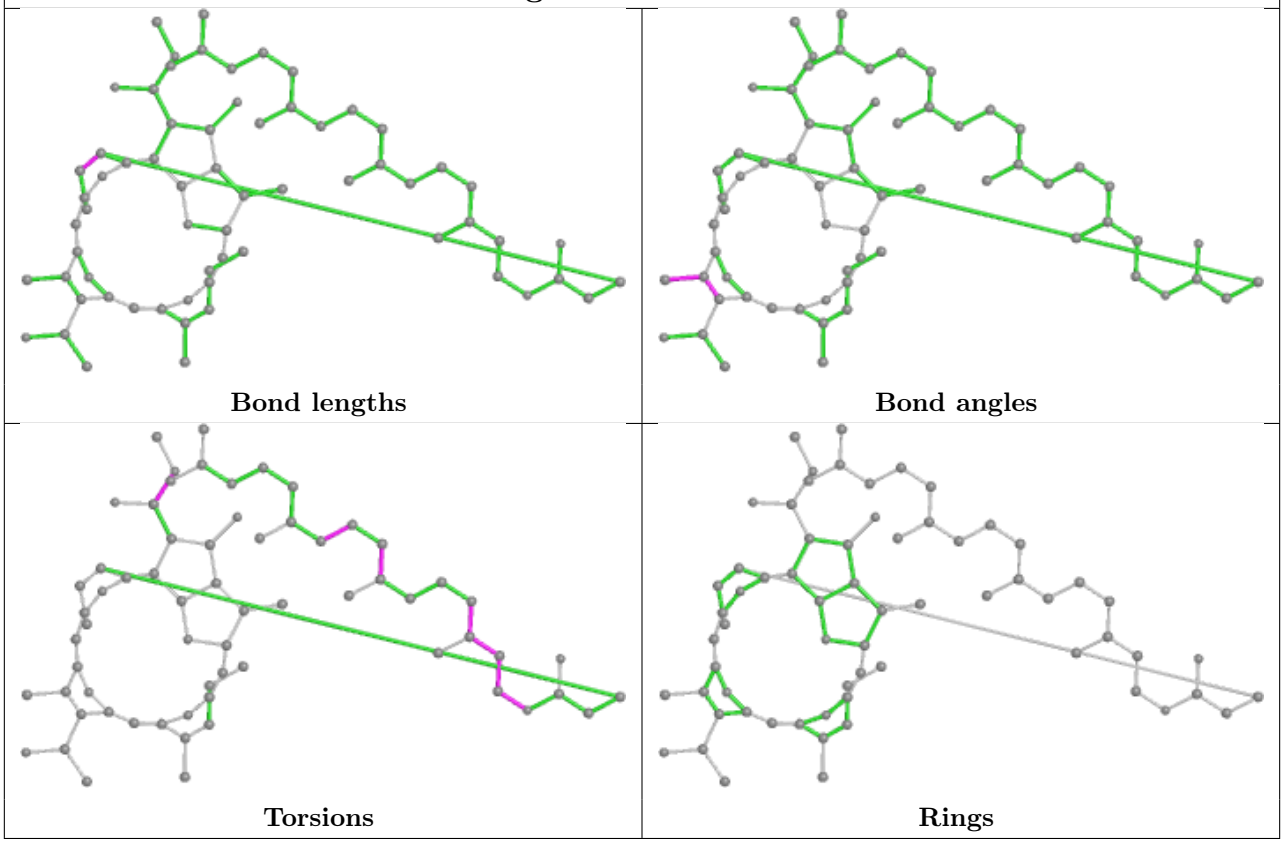


Rings

Ligand PGV L 712



Ligand BPH L 704



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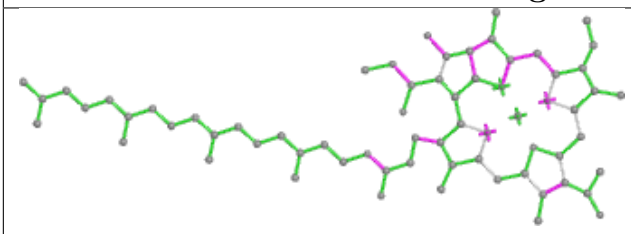
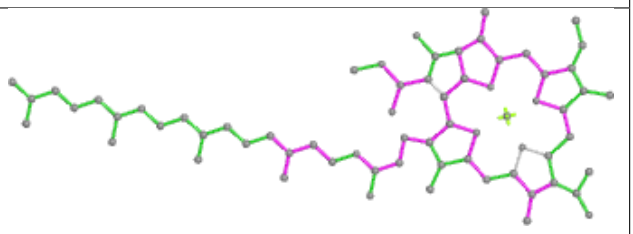
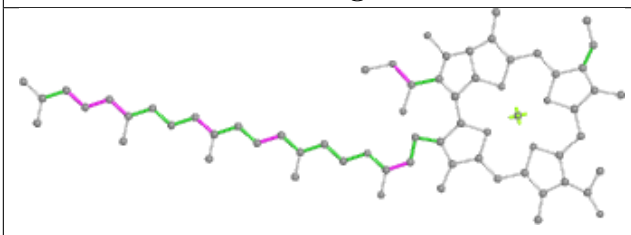


Bond lengths



Bond angles



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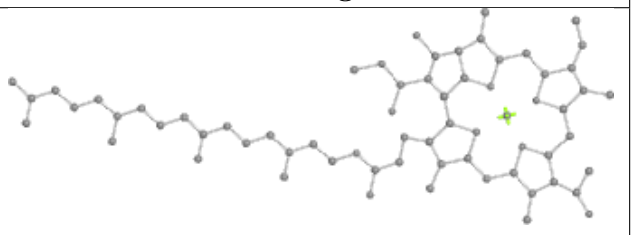
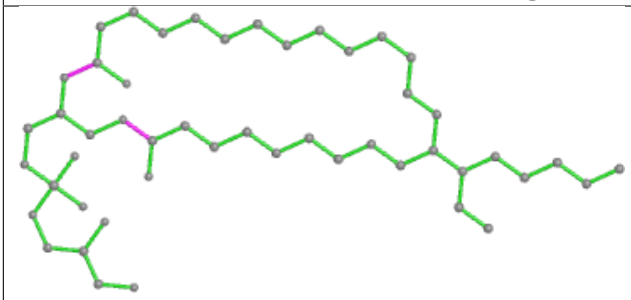
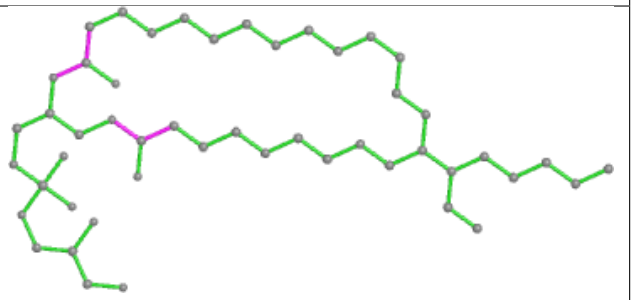


Rings

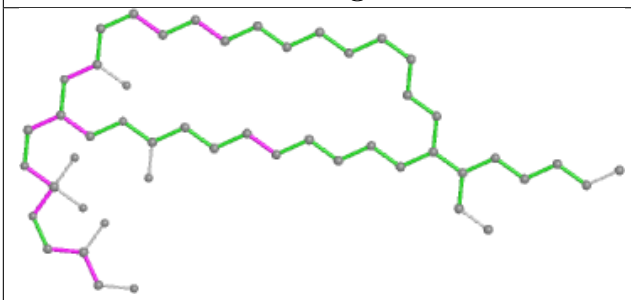
Ligand PGV L 706



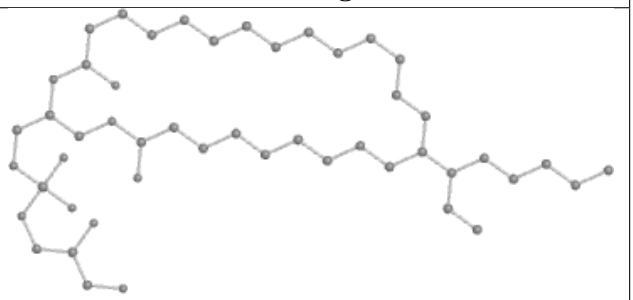
Bond lengths



Bond angles

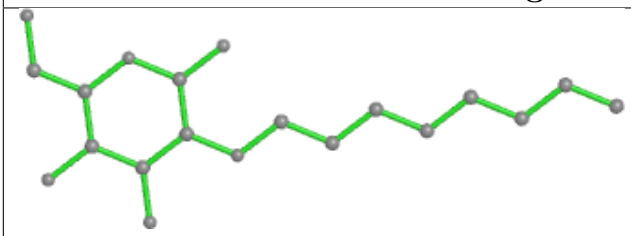


Torsions

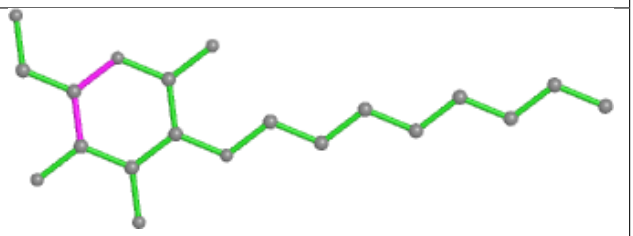


Rings

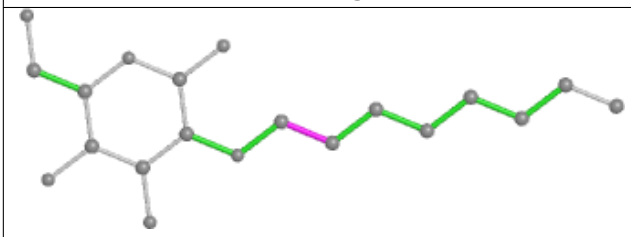
Ligand BGL L 715



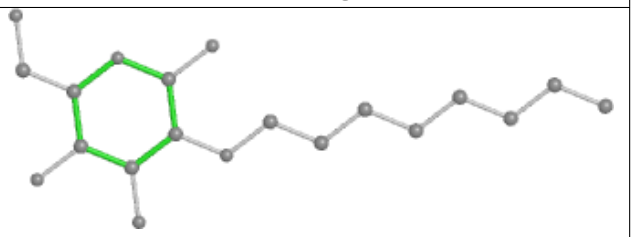
Bond lengths



Bond angles

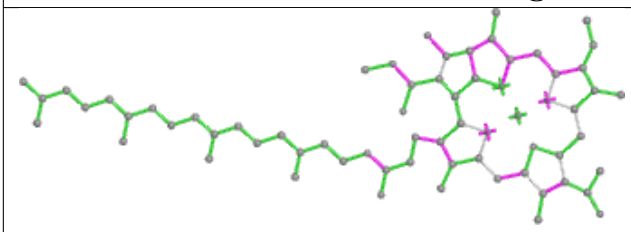


Torsions

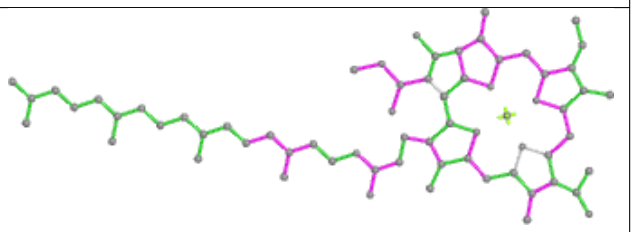


Rings

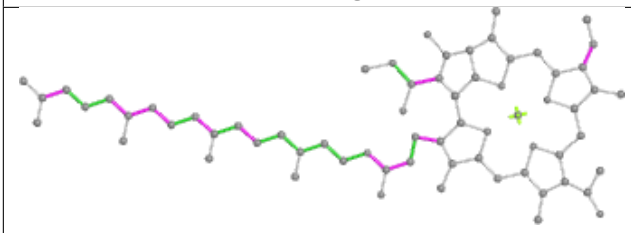
Ligand BCL S 102



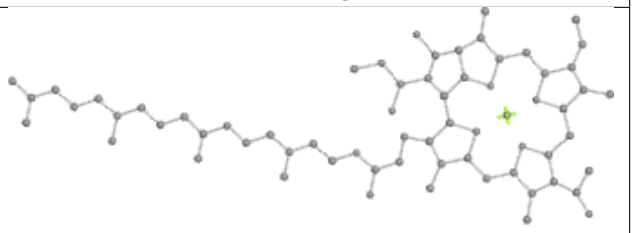
Bond lengths



Bond angles

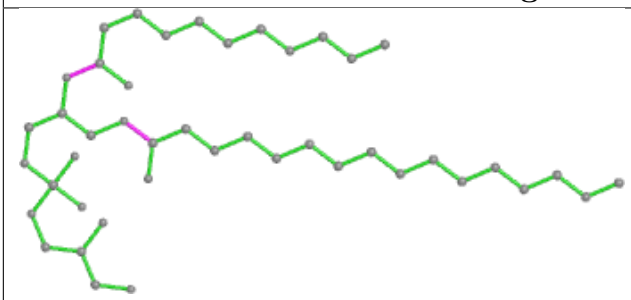


Torsions



Rings

Ligand PGV U 104



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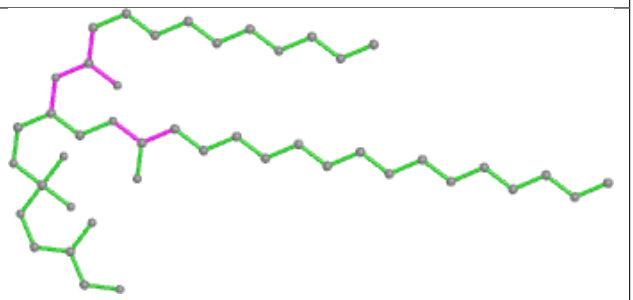
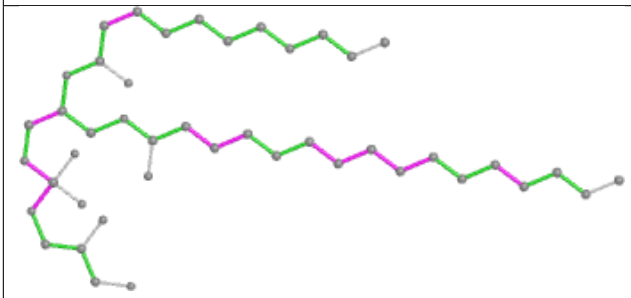
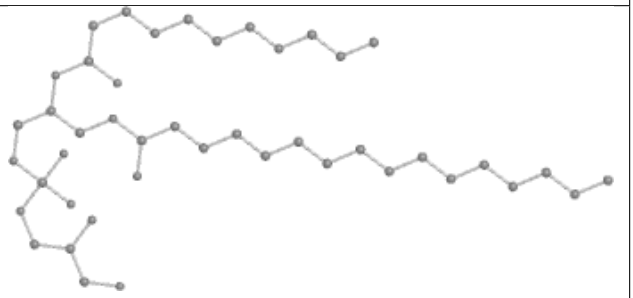


Bond angles

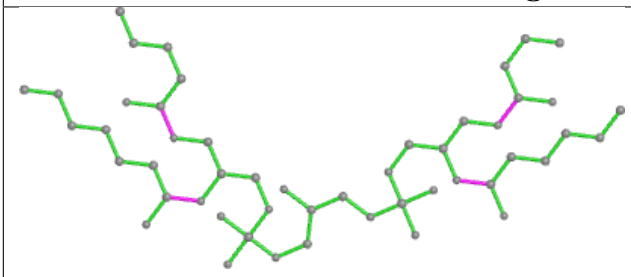


Torsions

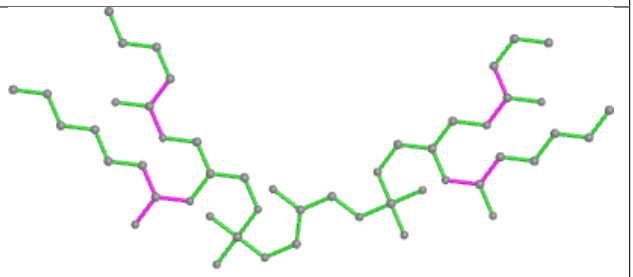


Rings

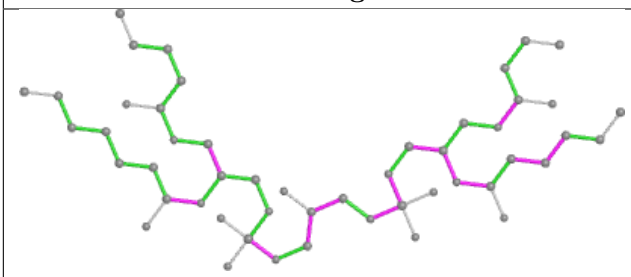
Ligand CDL P 102



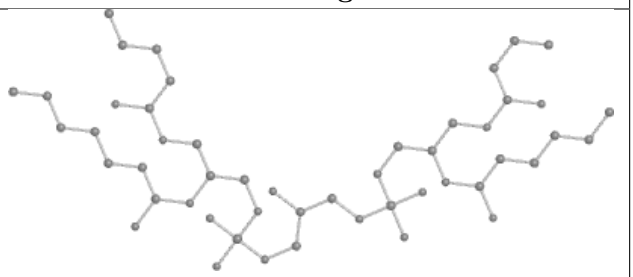
Bond lengths



Bond angles

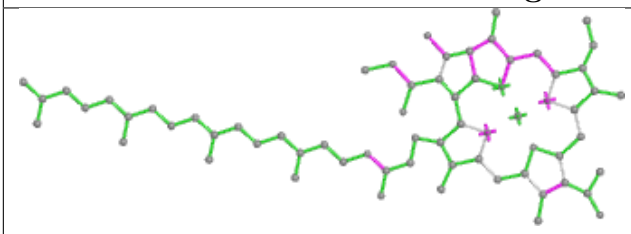


Torsions



Rings

Ligand BCL O 102



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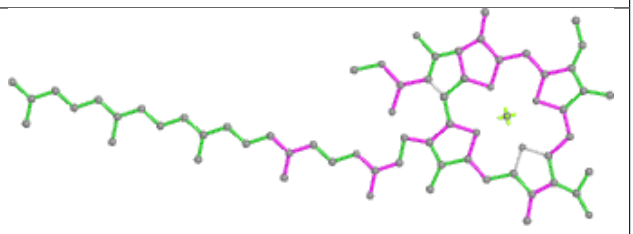
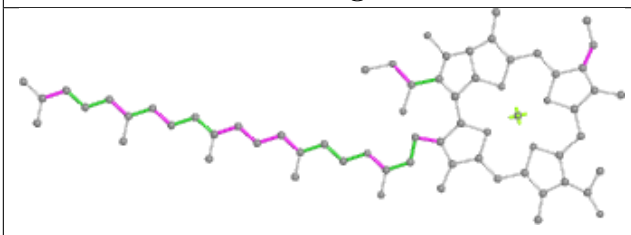


Bond angles



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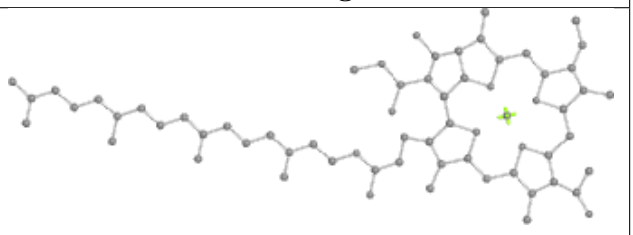
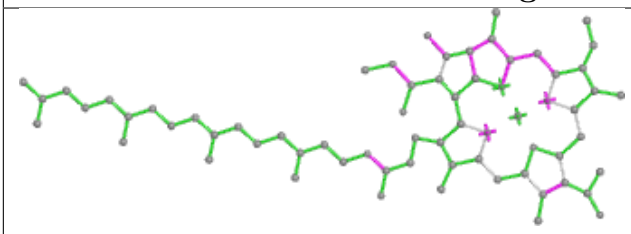


Rings

Ligand BCL W 102



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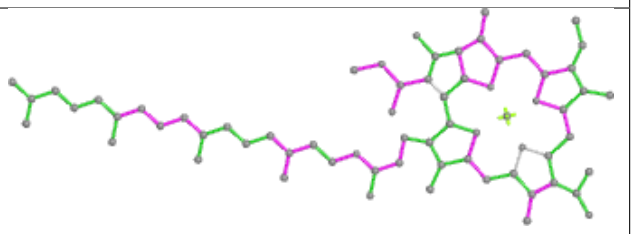
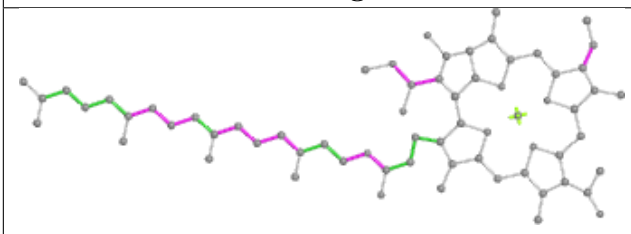
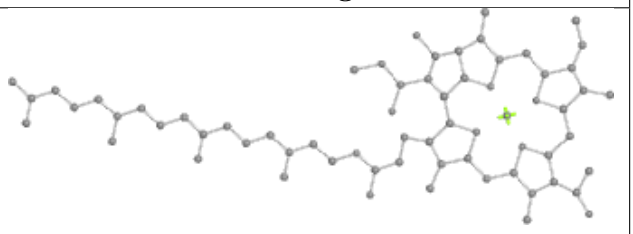


Bond angles

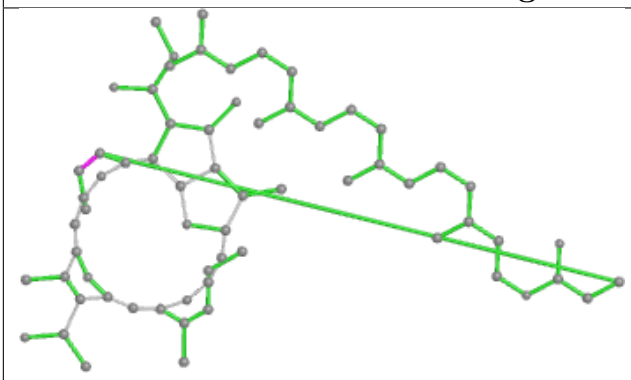


Torsions



Rings

Ligand BPH M 702



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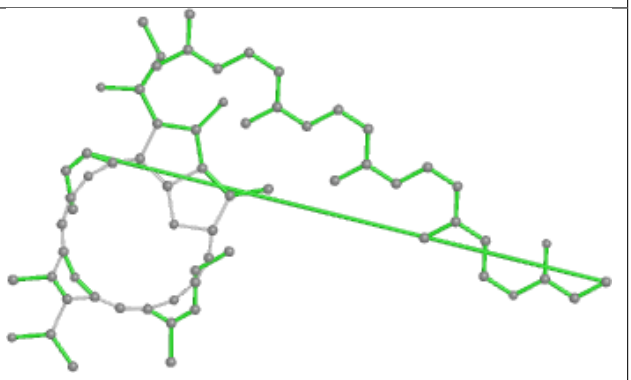
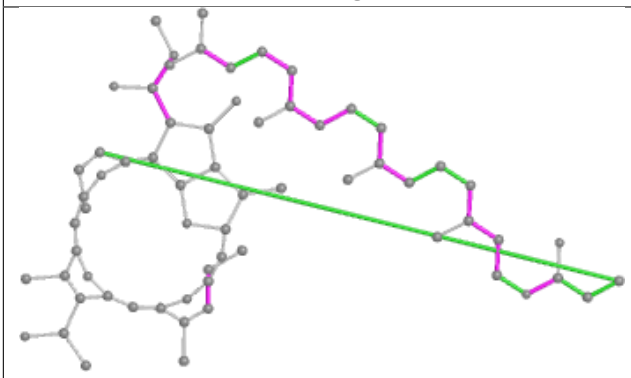


Bond angles



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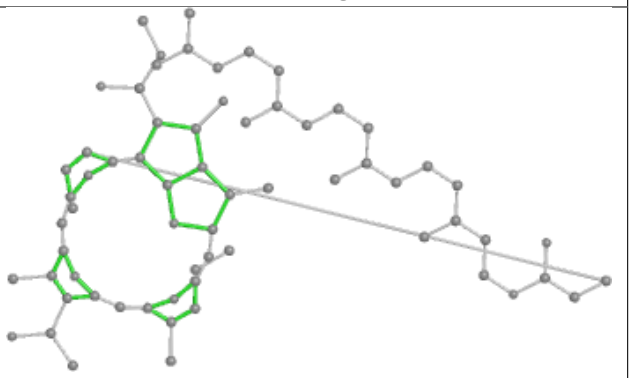
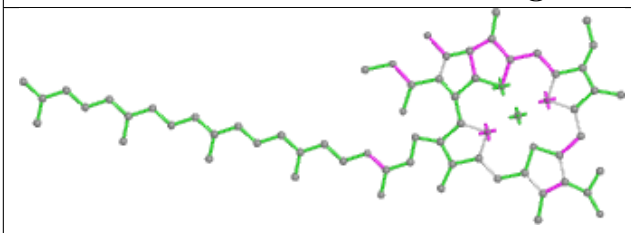
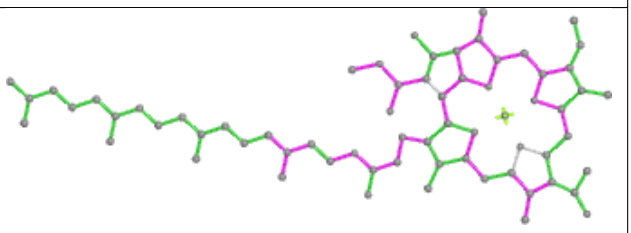


Rings

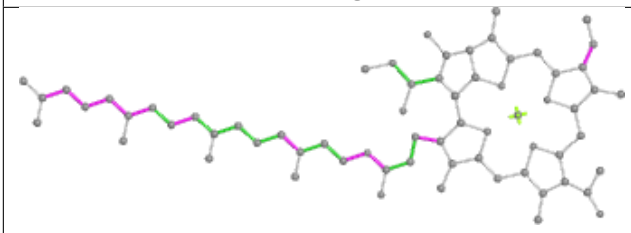
Ligand BCL L 703



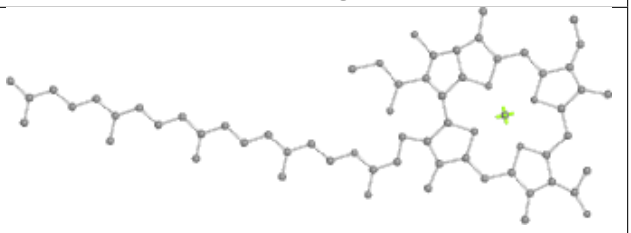
Bond lengths



Bond angles

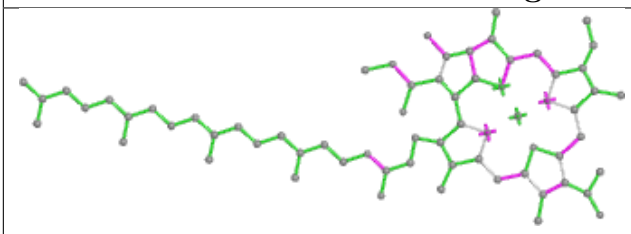


Torsions

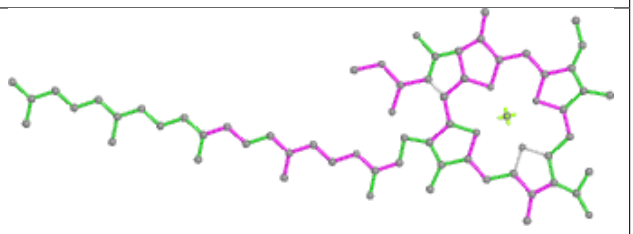


Rings

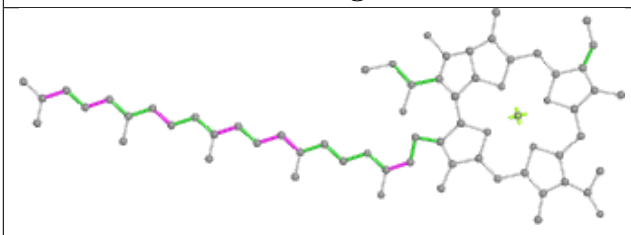
Ligand BCL U 101



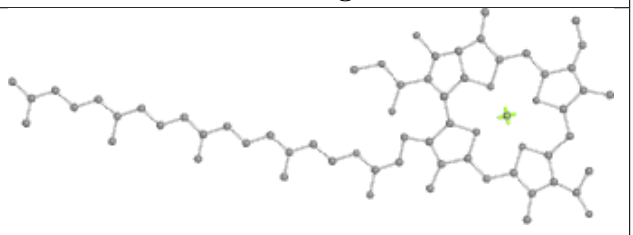
Bond lengths



Bond angles

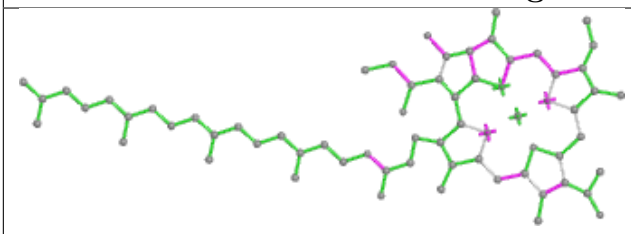


Torsions

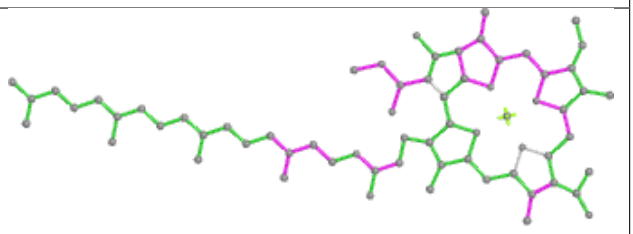


Rings

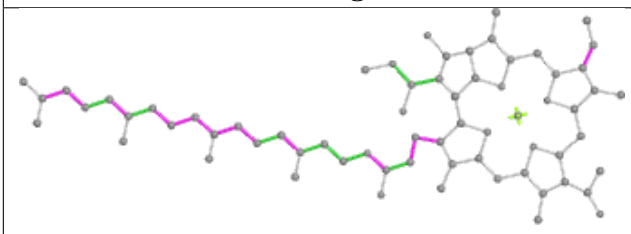
Ligand BCL F 101



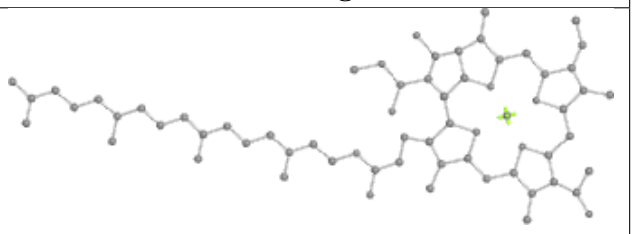
Bond lengths



Bond angles

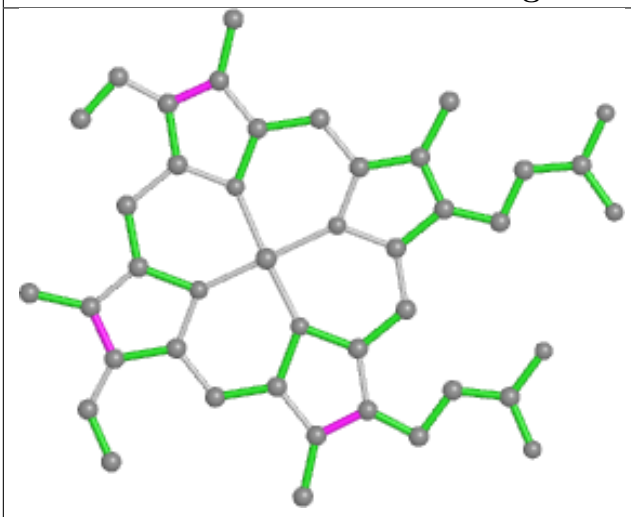


Torsions



Rings

Ligand HEC C 504



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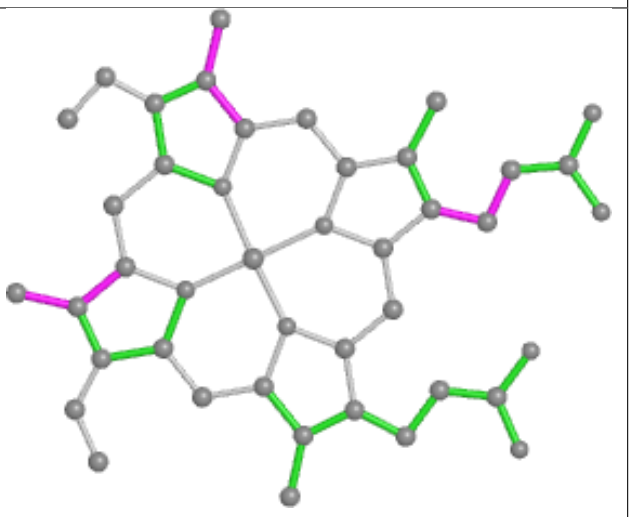
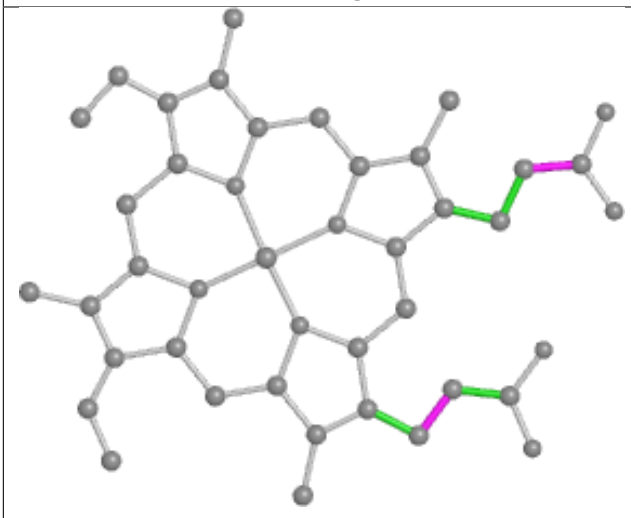


Bond angles



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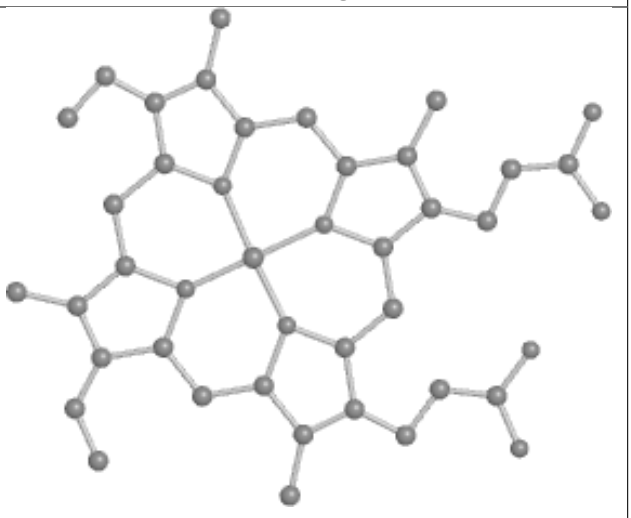
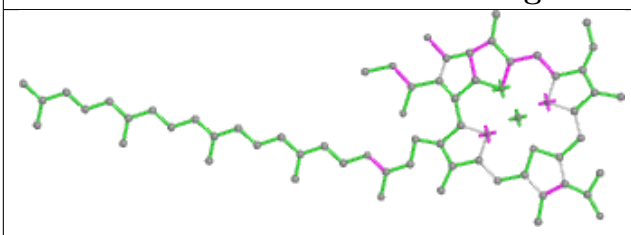
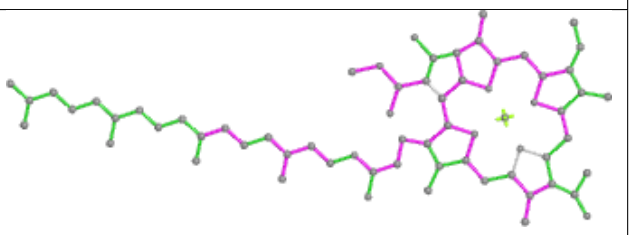


Rings

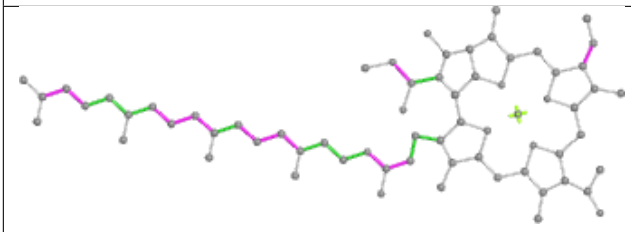
Ligand BCL G 101



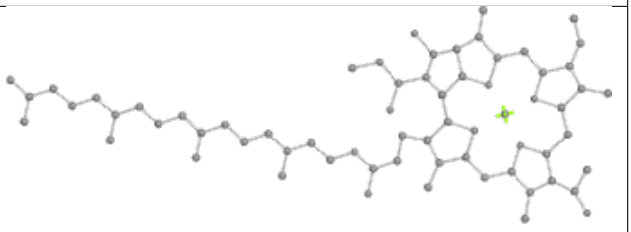
Bond lengths



Bond angles

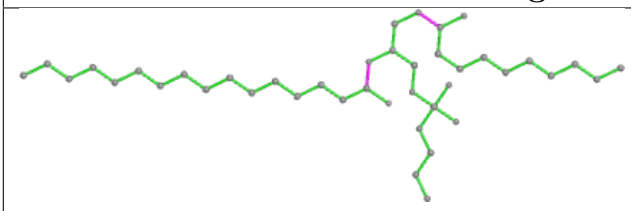


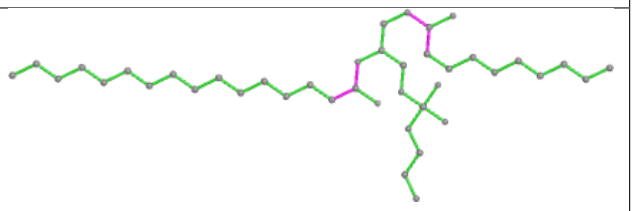
Torsions

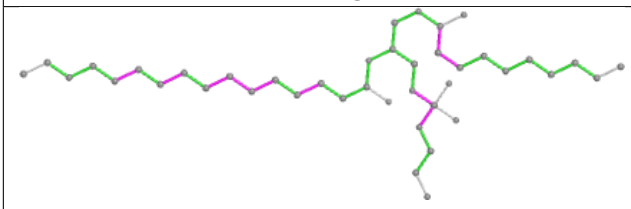


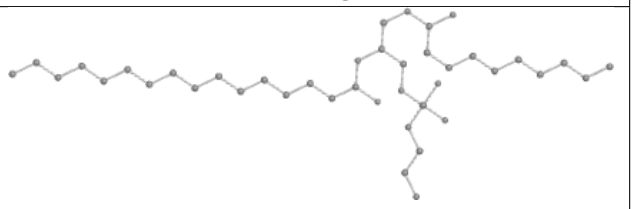
Rings

Ligand PEF L 717

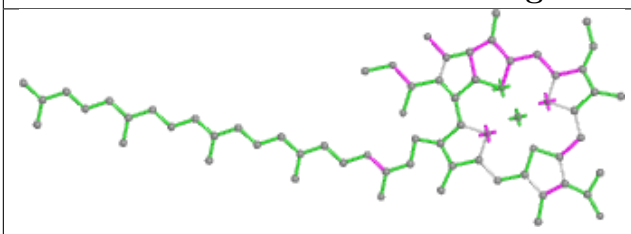

Bond lengths

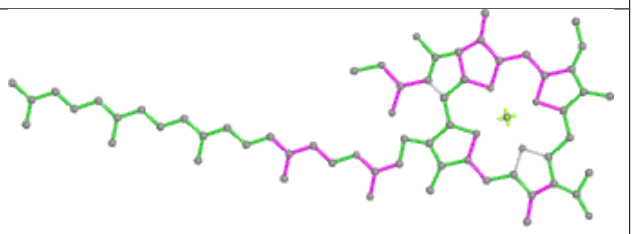

Bond angles

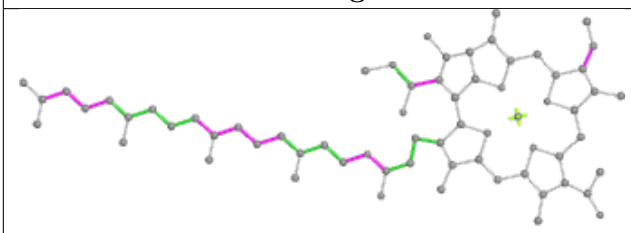

Torsions

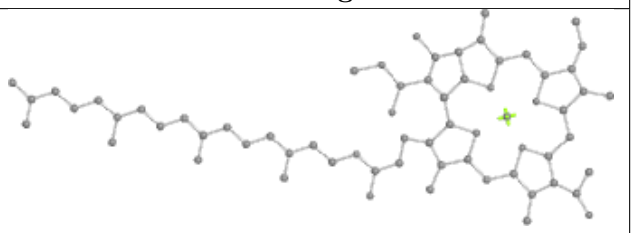

Rings

Ligand BCL T 101

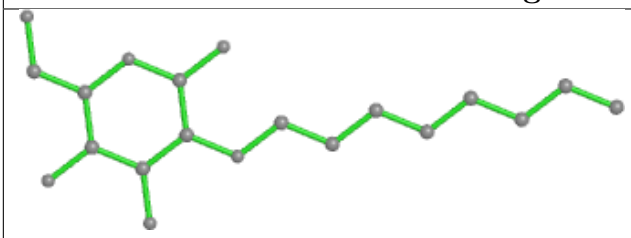

Bond lengths

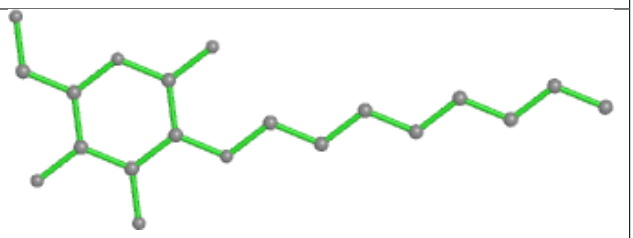

Bond angles

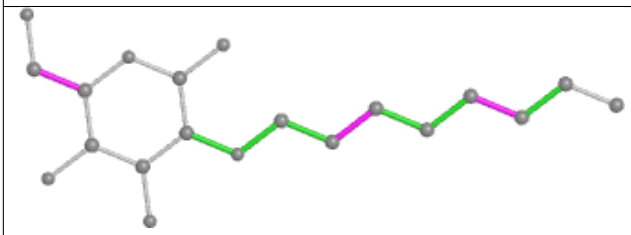

Torsions

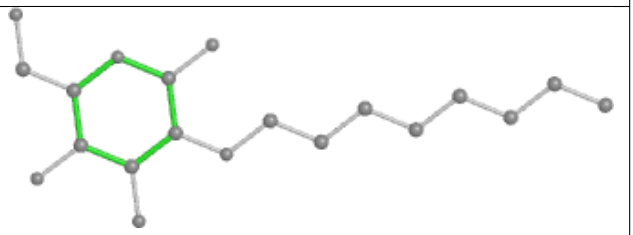

Rings

Ligand BGL Y 103

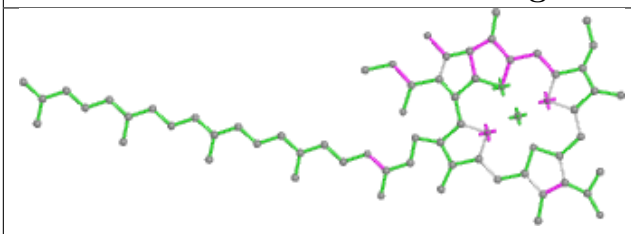

Bond lengths


Bond angles


Torsions


Rings

Ligand BCL 1 101



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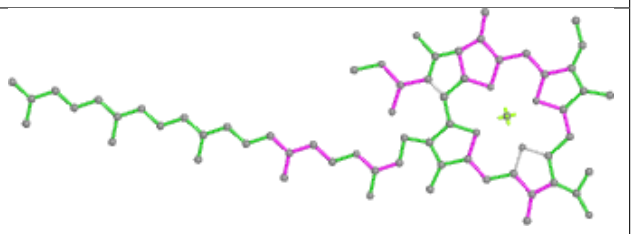
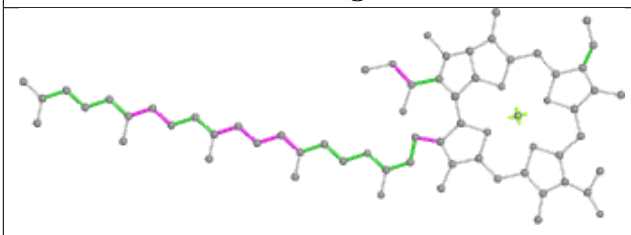


Bond angles



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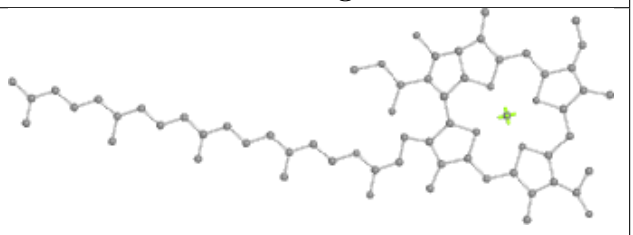
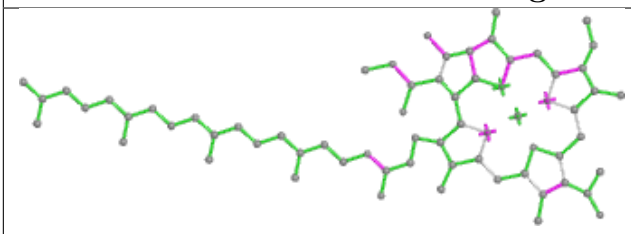
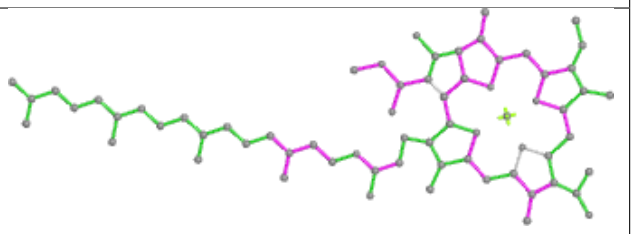


Rings

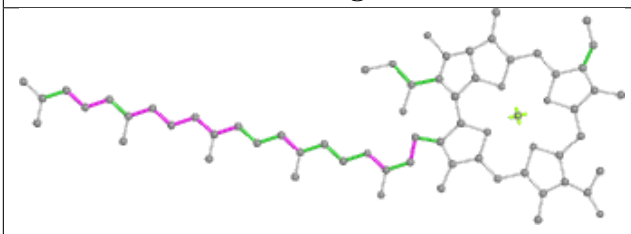
Ligand BCL 8 101



Bond lengths



Bond angles



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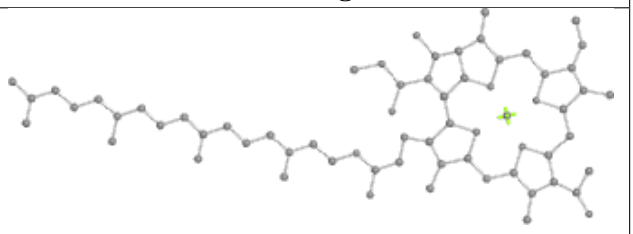
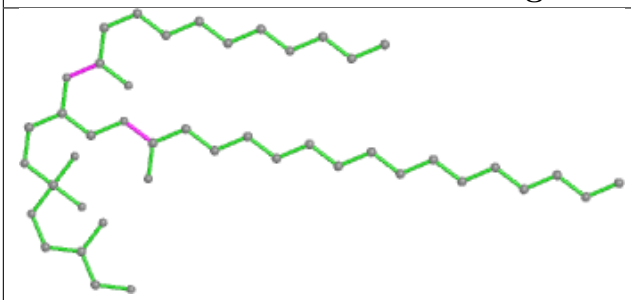
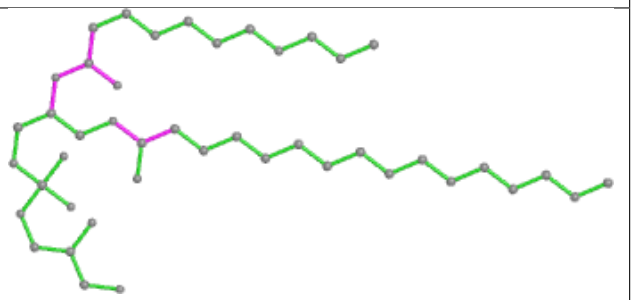


Rings

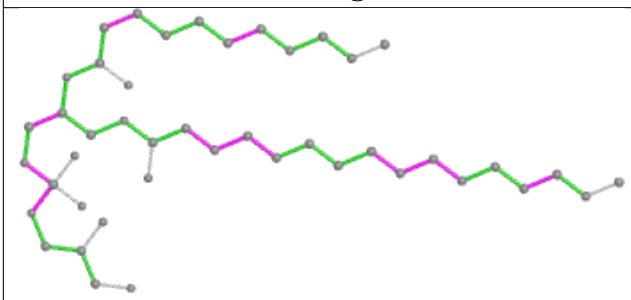
Ligand PGV 0 104



Bond lengths



Bond angles



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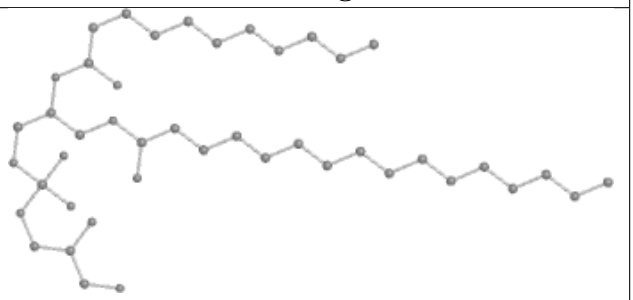
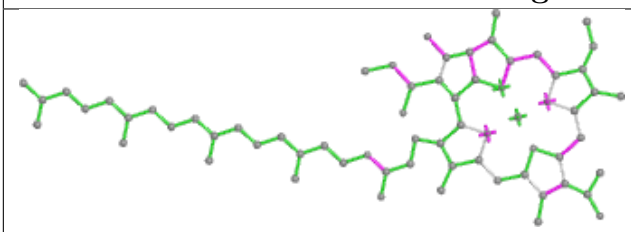


Rings

Ligand BCL I 101



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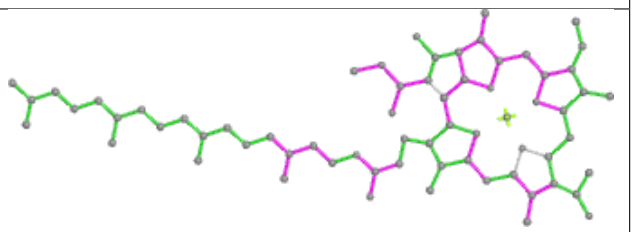
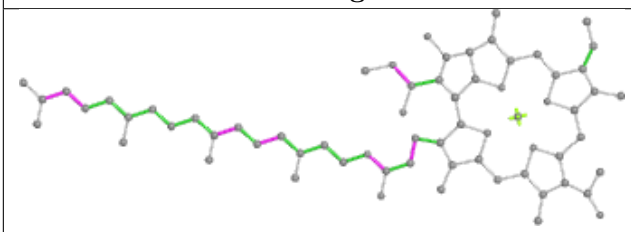


Bond angles



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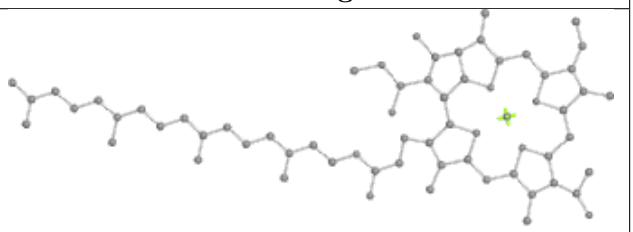
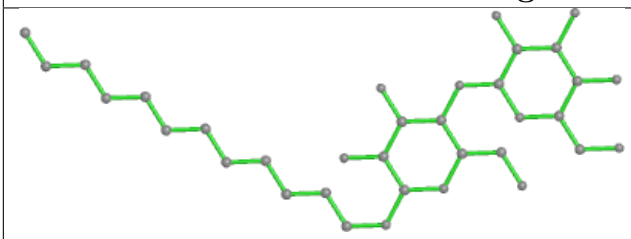


Rings

Ligand LMT M 709



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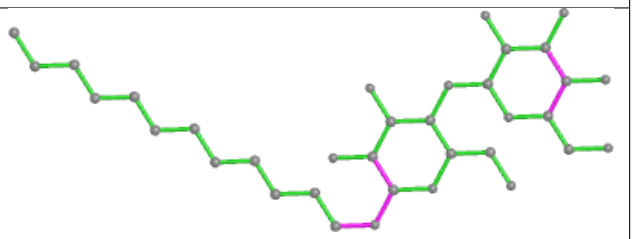

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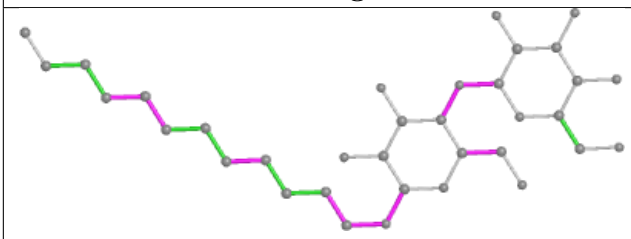

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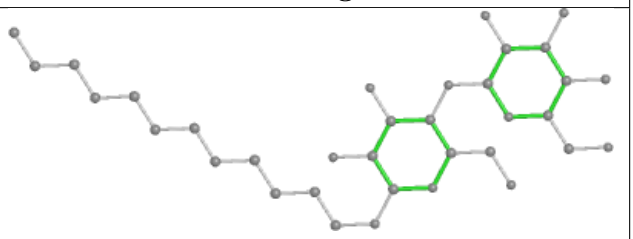
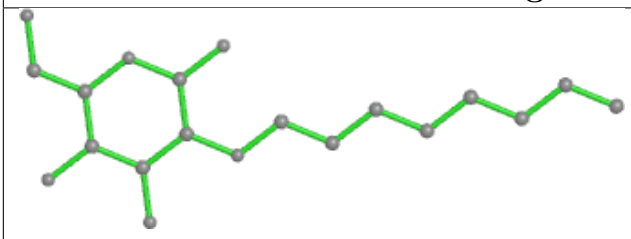


Rings

Ligand BGL L 708



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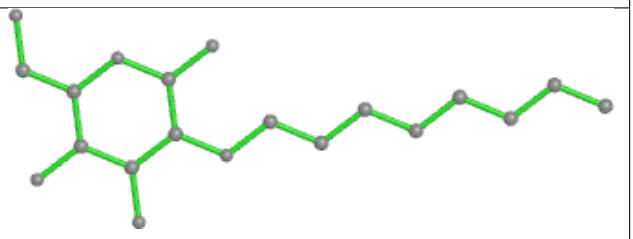
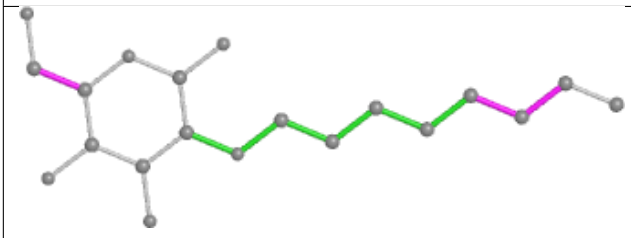


Bond angles



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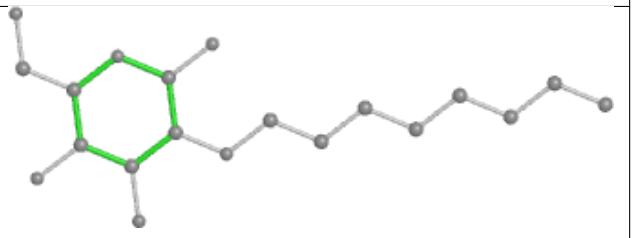
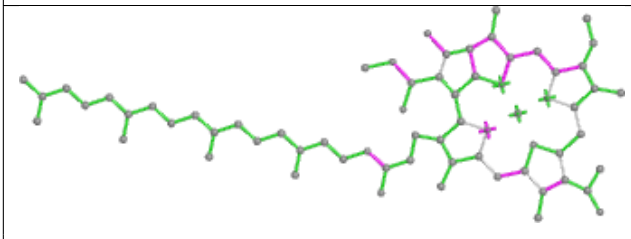
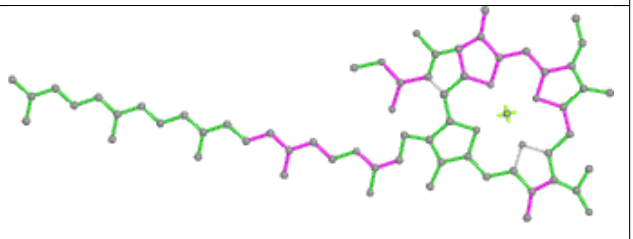


Rings

Ligand BCL 3 103



Bond lengths



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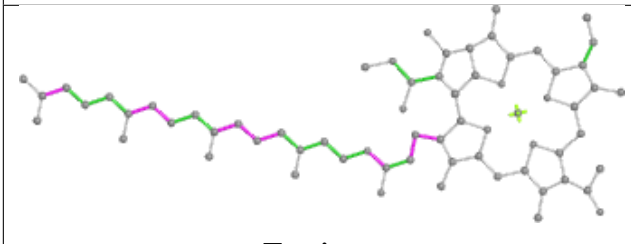

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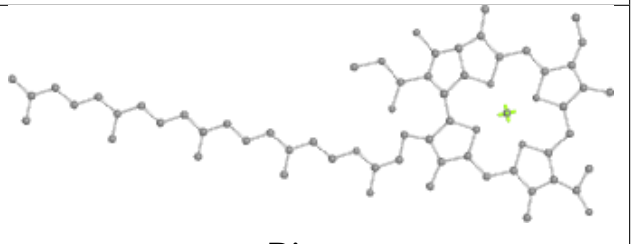
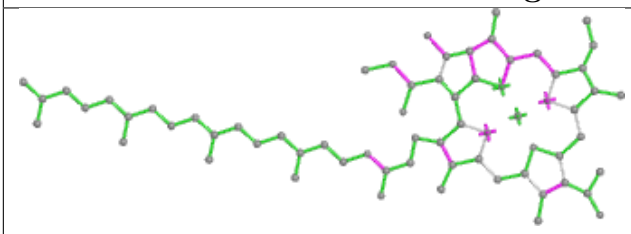


Rings

Ligand BCL K 102



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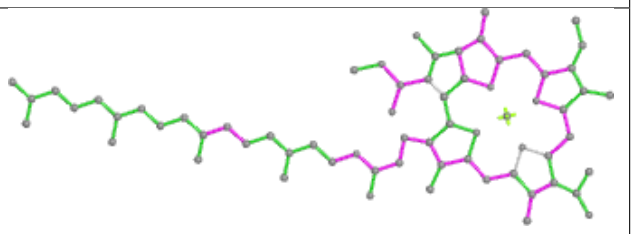
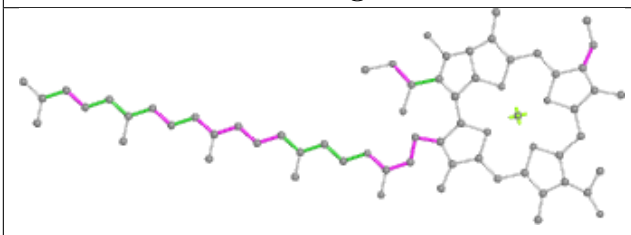


Bond angles



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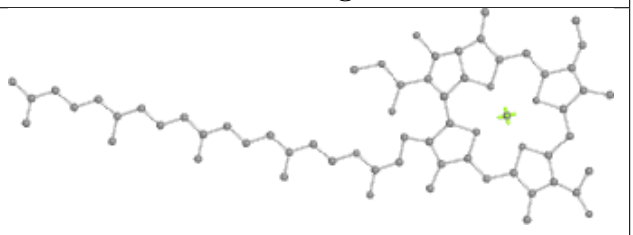
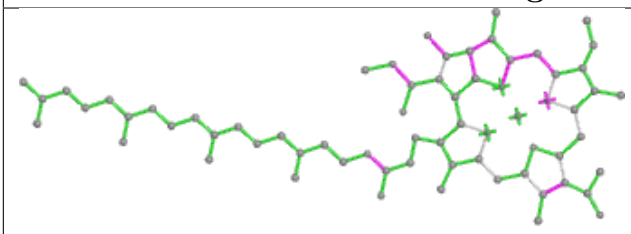
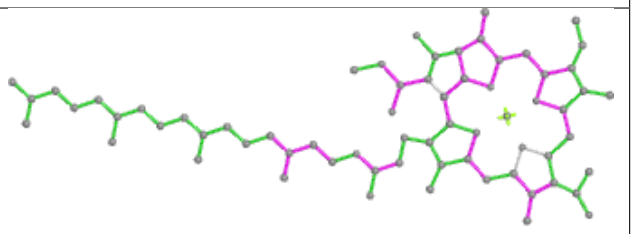


Rings

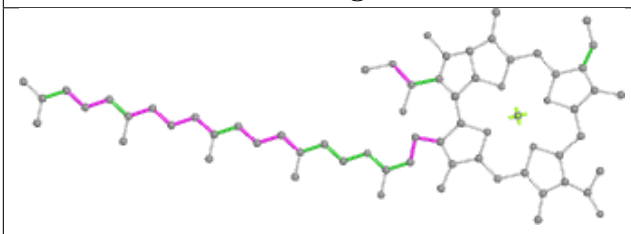
Ligand BCL E 101



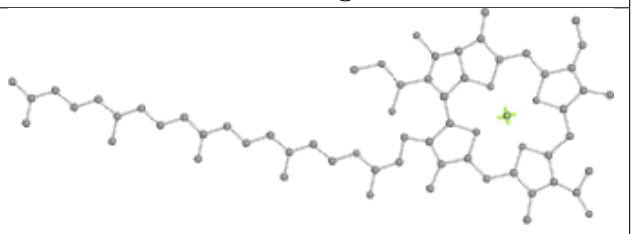
Bond lengths



Bond angles

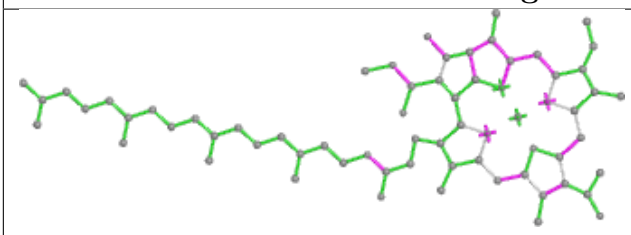


Torsions

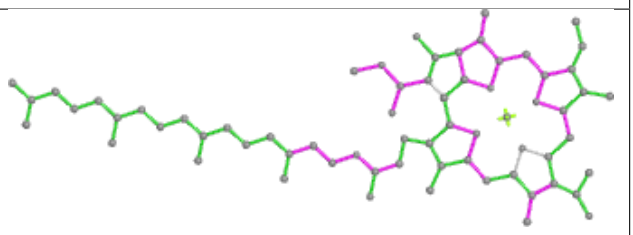


Rings

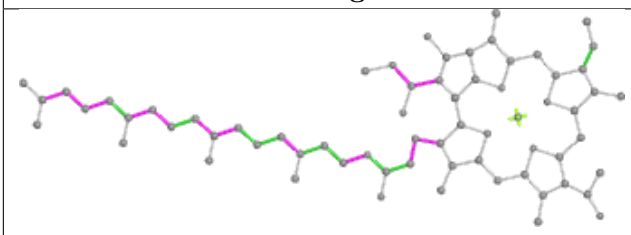
Ligand BCL M 701



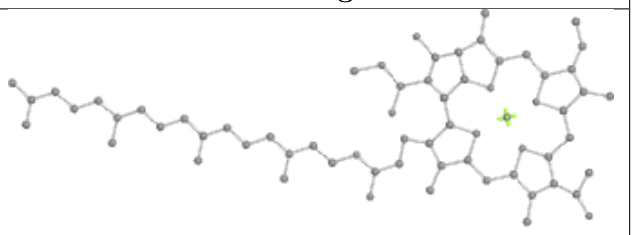
Bond lengths



Bond angles

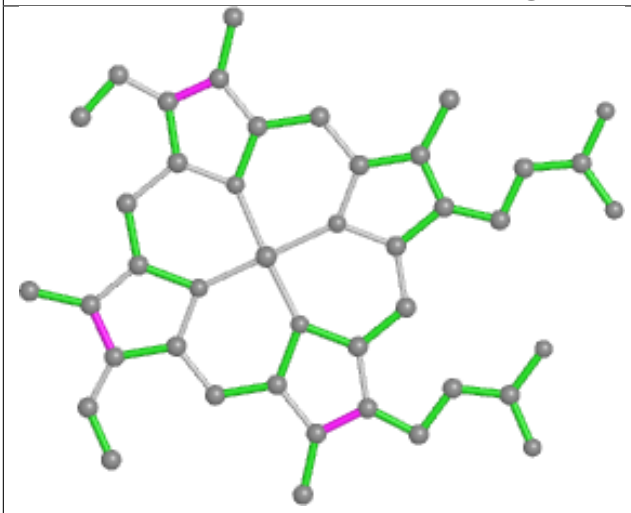


Torsions



Rings

Ligand HEC C 503



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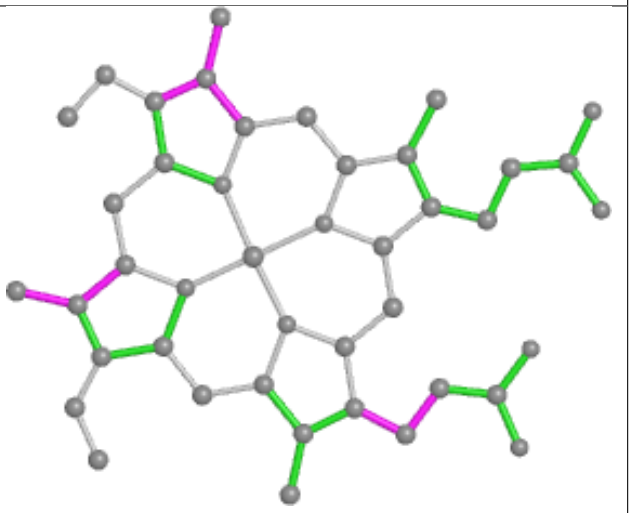
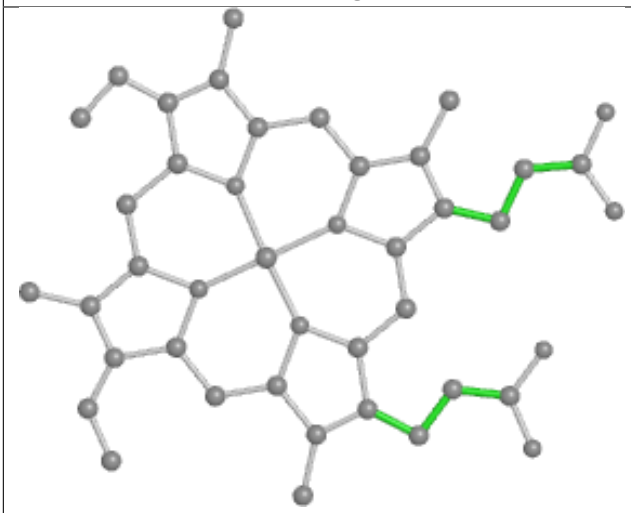


Bond angles



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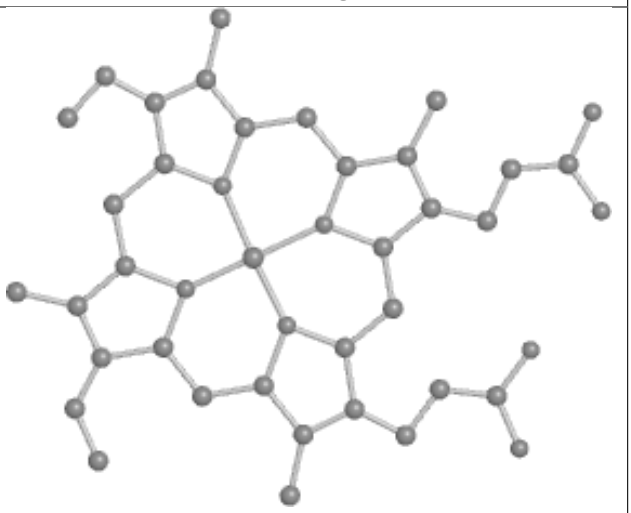
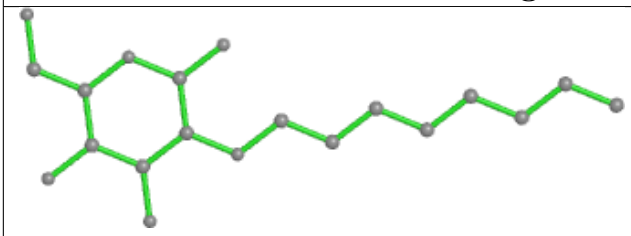


Rings

Ligand BGL M 706



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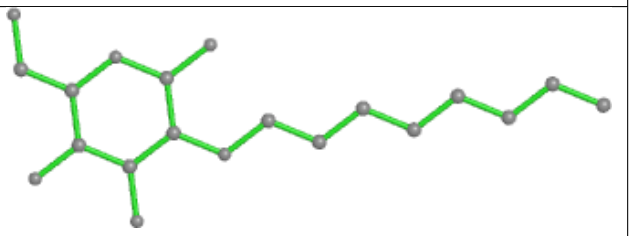
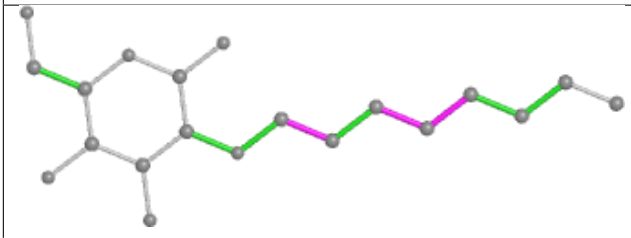


Bond angles



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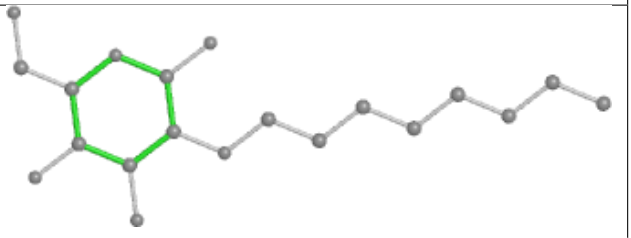
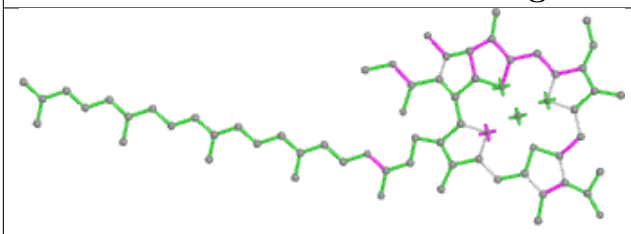
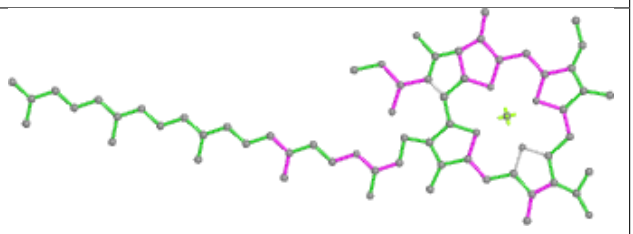


Rings

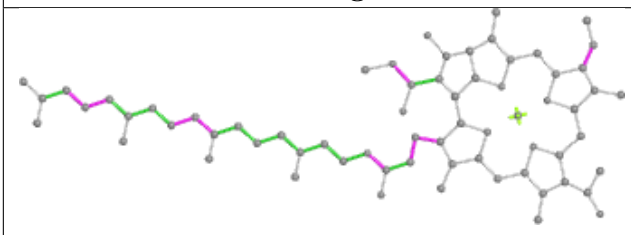
Ligand BCL J 102



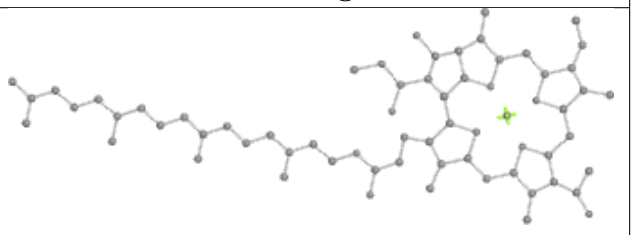
Bond lengths



Bond angles

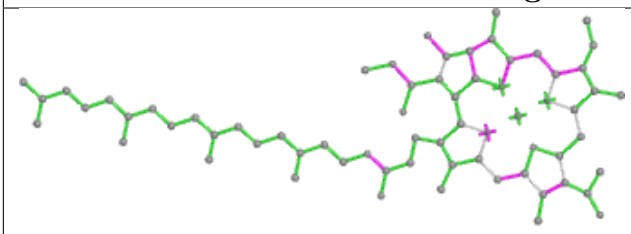


Torsions

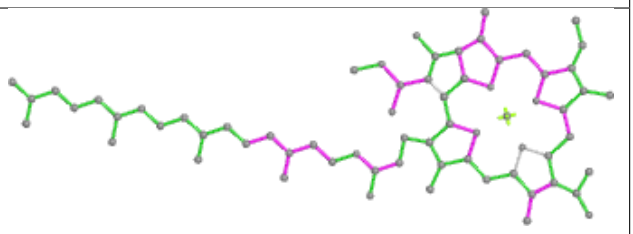


Rings

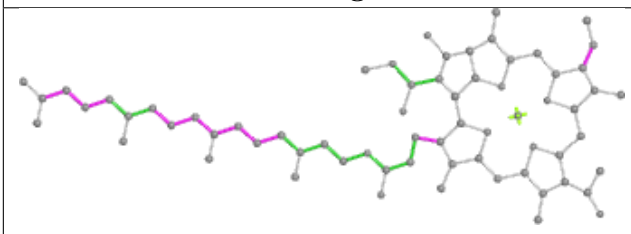
Ligand BCL H 101



Bond lengths



Bond angles



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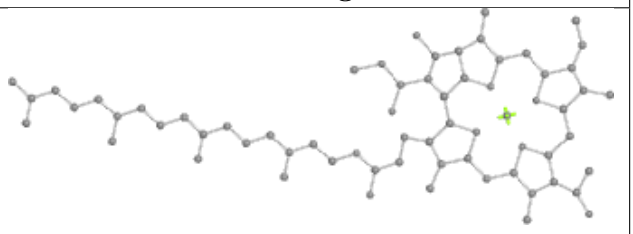
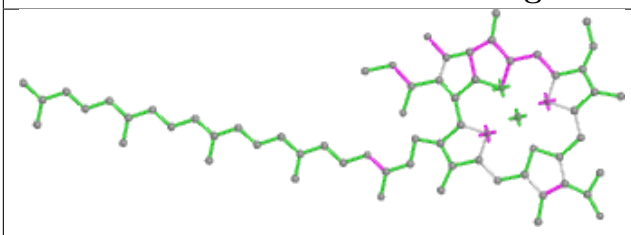
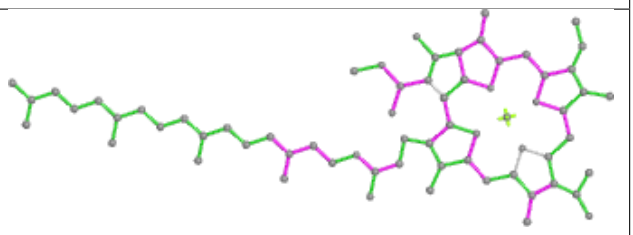


Rings

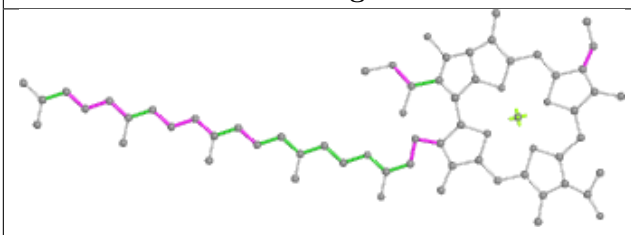
Ligand BCL A 102



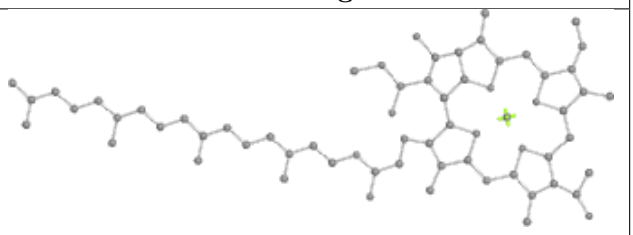
Bond lengths



Bond angles

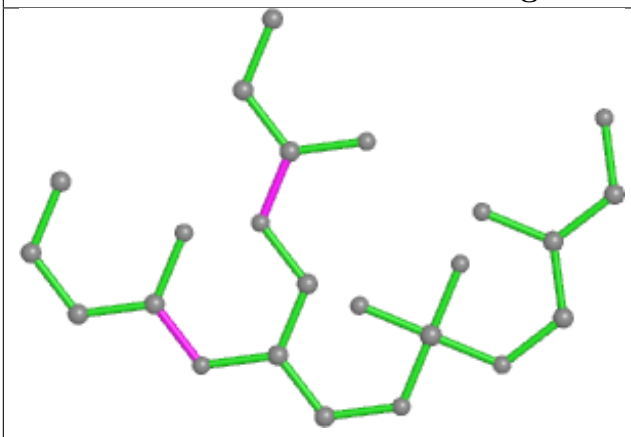


Torsions



Rings

Ligand PGV N 102



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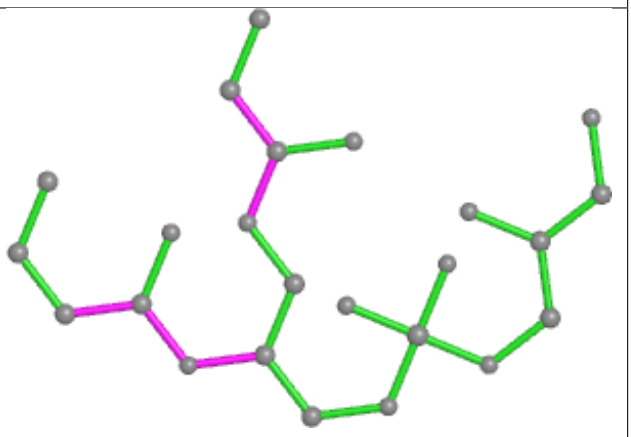

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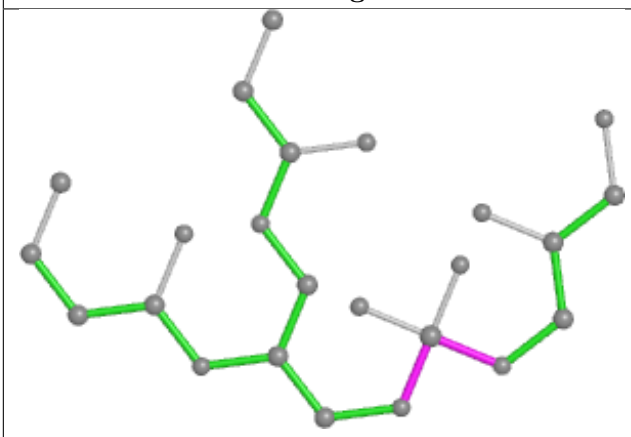

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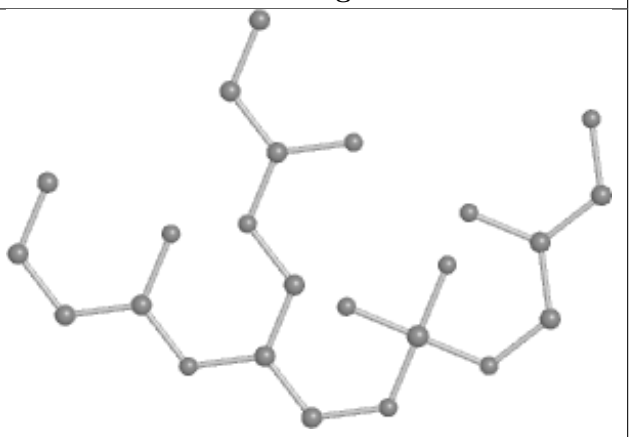
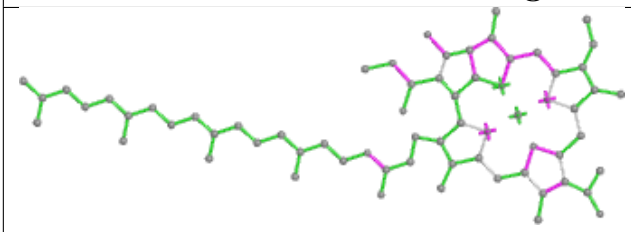


Rings

Ligand BCL U 102



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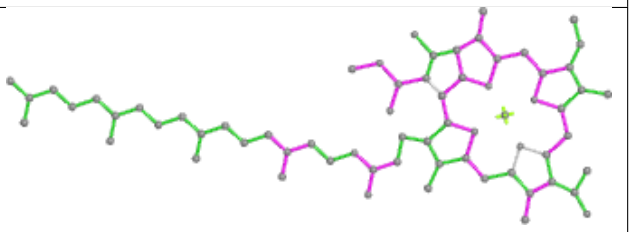

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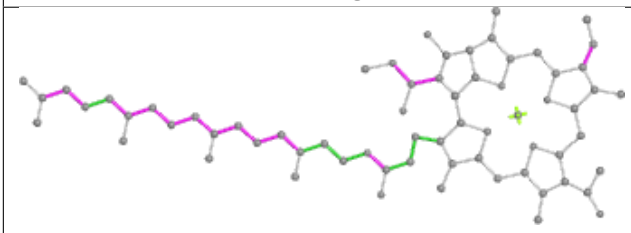

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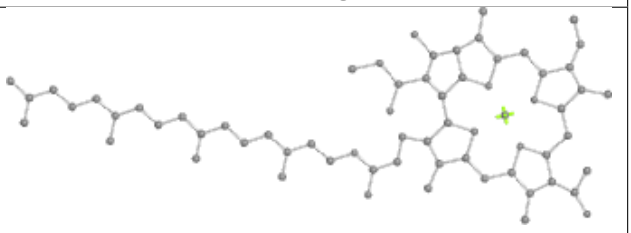
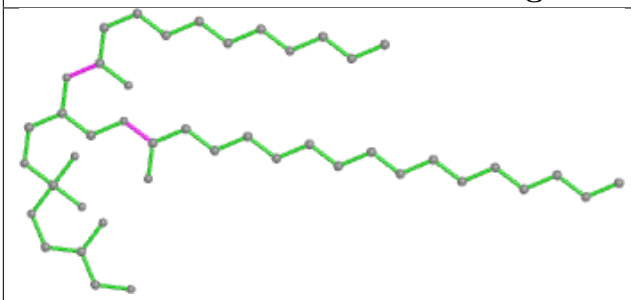


Rings

Ligand PGV 8 103



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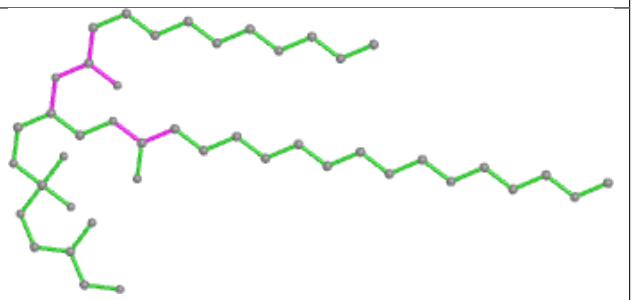
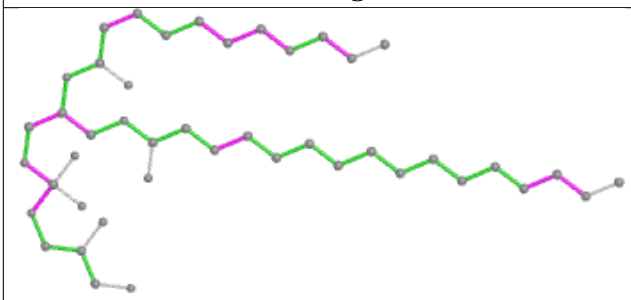


Bond angles



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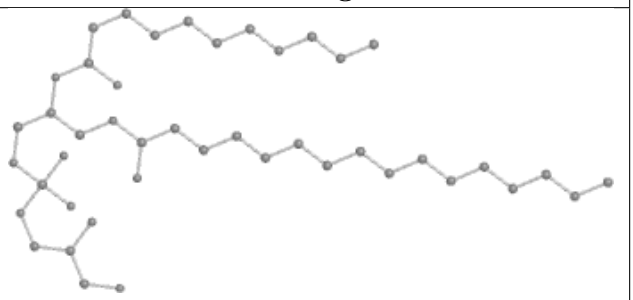
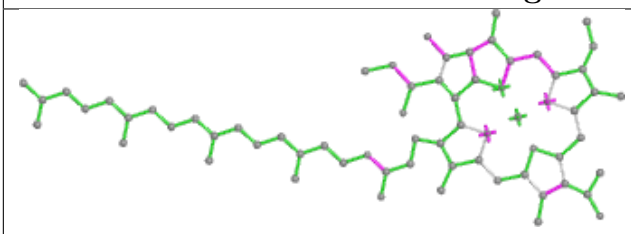


Rings

Ligand BCL K 101



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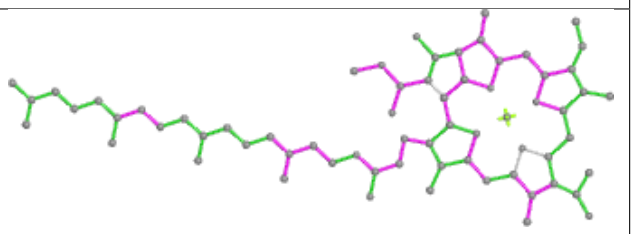

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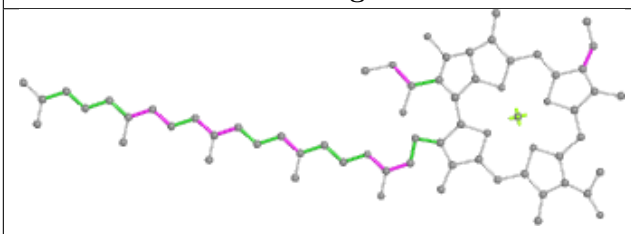

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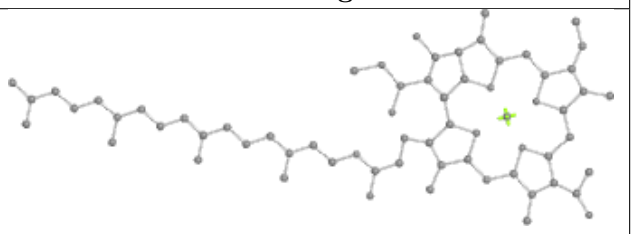
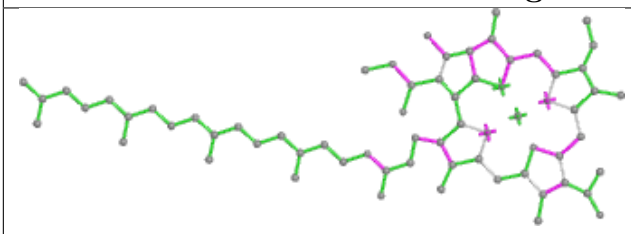


Rings

Ligand BCL B 101



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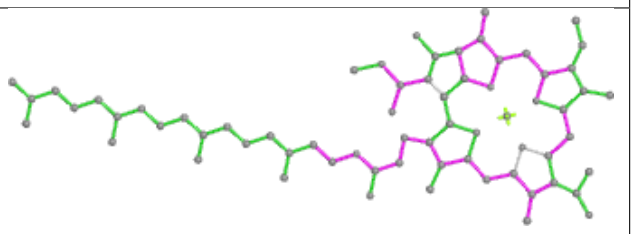
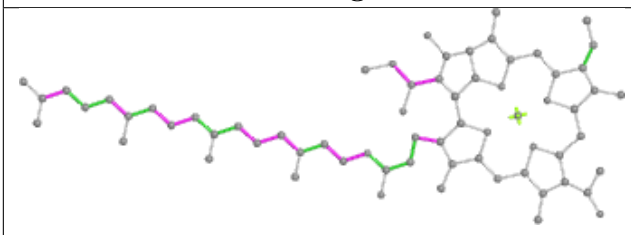


Bond angles



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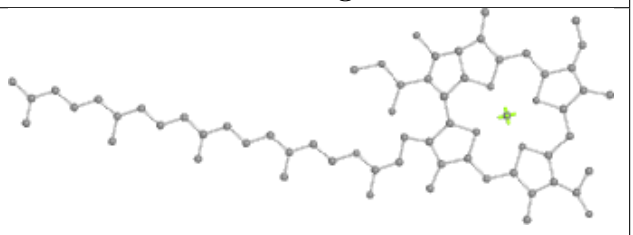
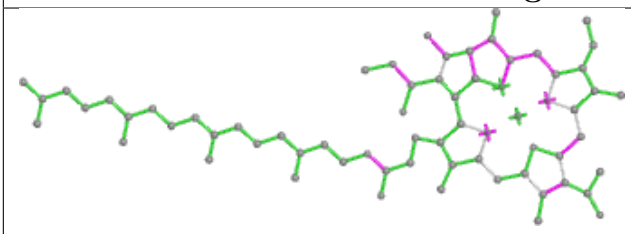


Rings

Ligand BCL V 101



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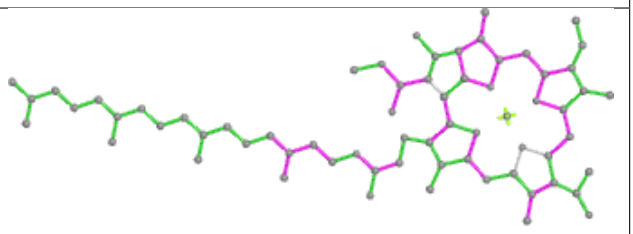
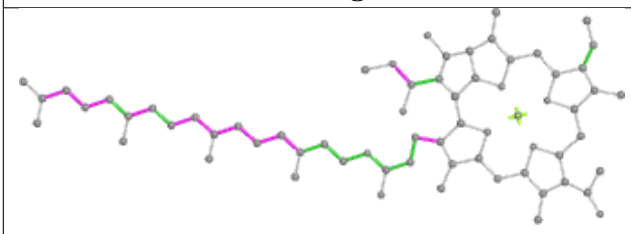


Bond angles



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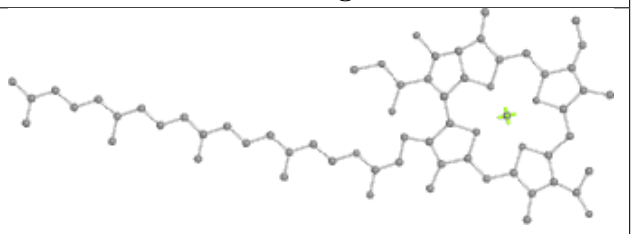
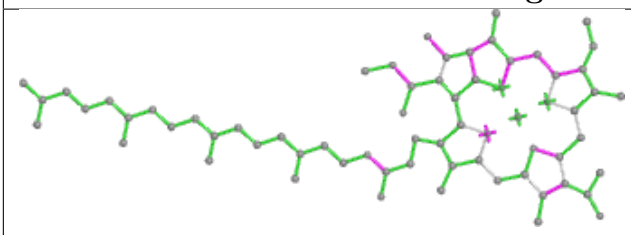


Rings

Ligand BCL P 101



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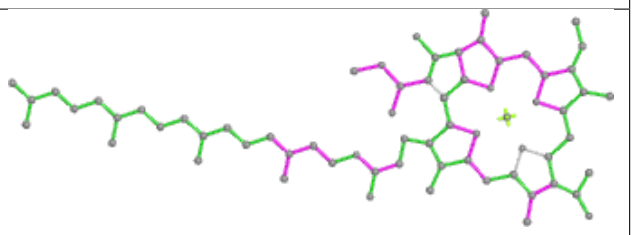

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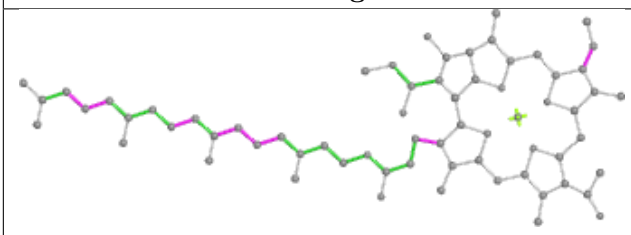

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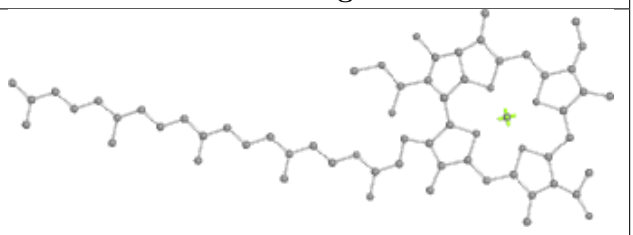
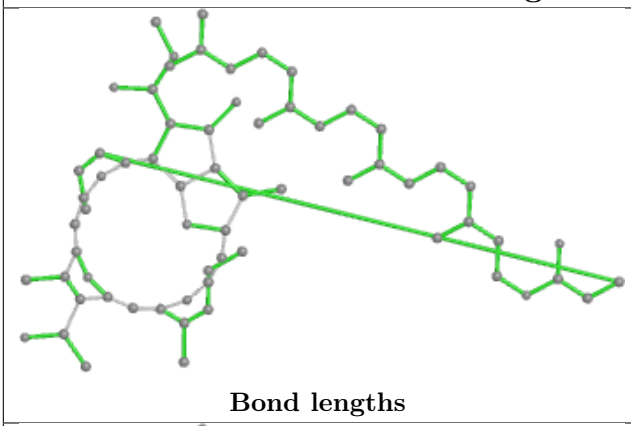
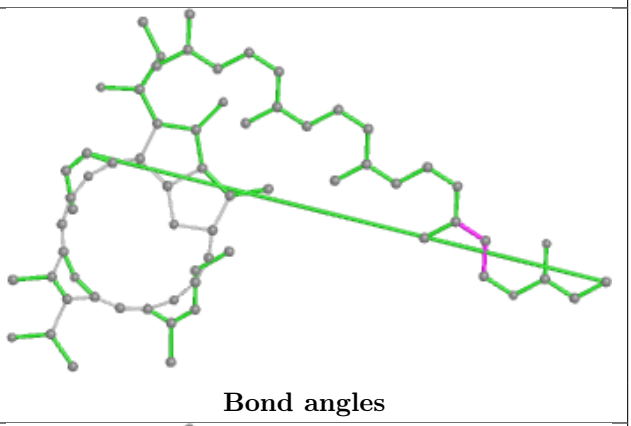


Rings

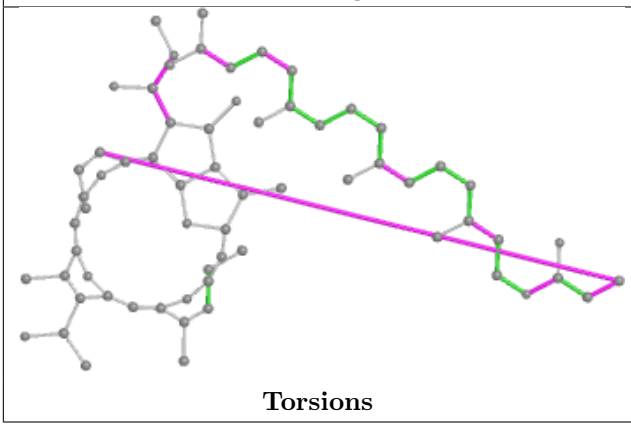
Ligand BPH L 701



Bond lengths



Bond angles



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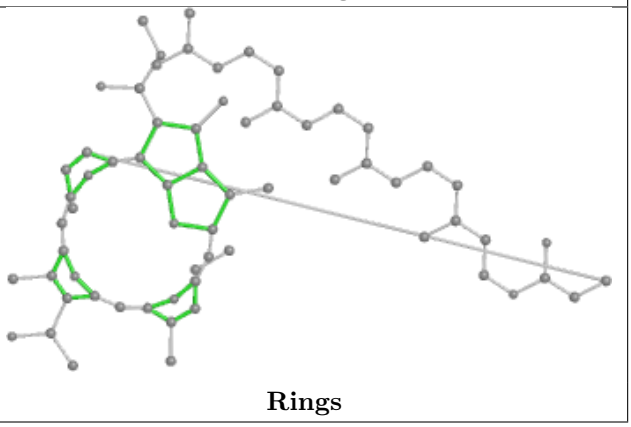
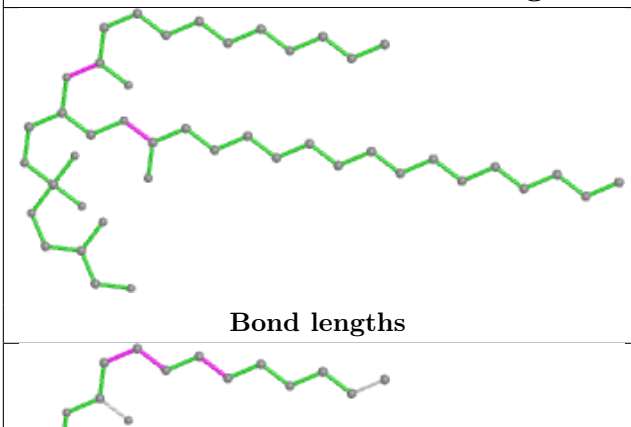


Rings

Ligand PGV 0 105



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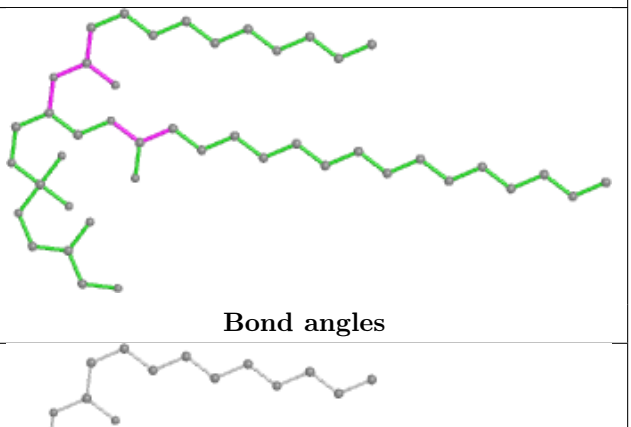
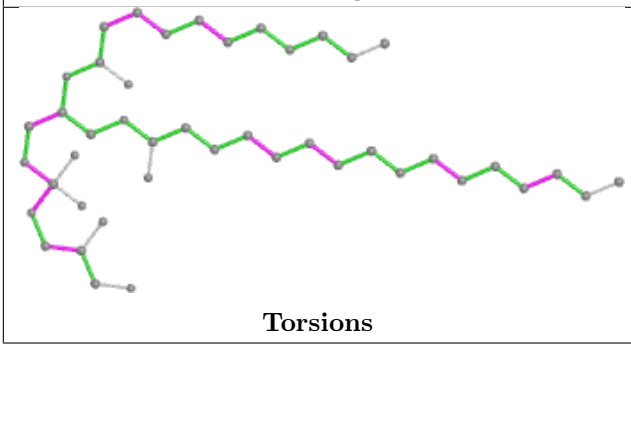


Bond angles



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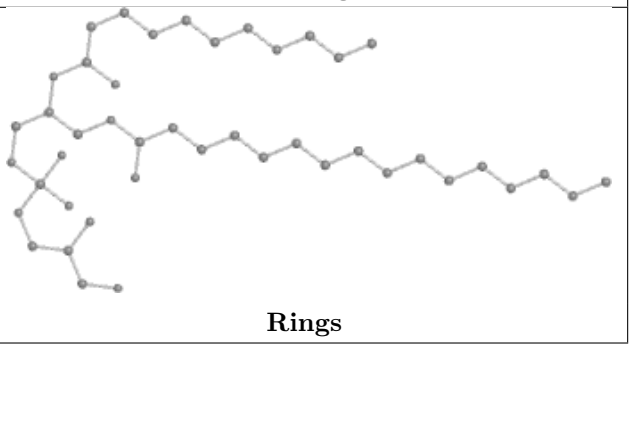
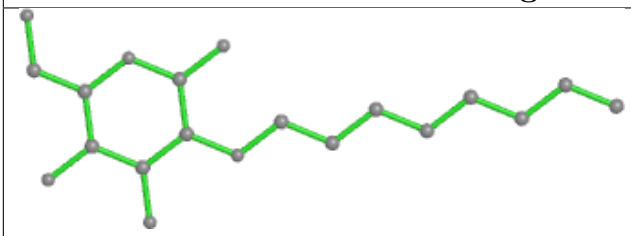


Rings

Ligand BGL M 707



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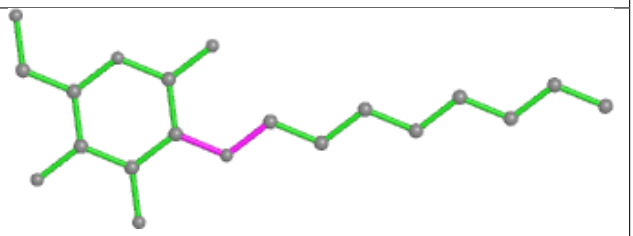
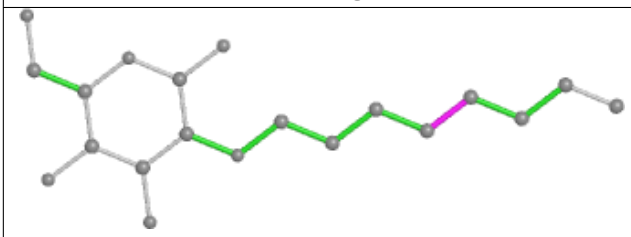


Bond angles



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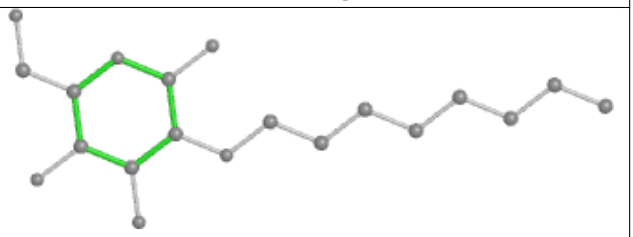
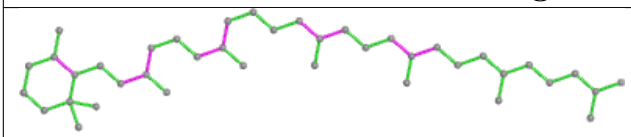


Rings

Ligand U4Z 0 103



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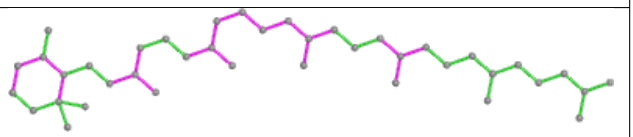
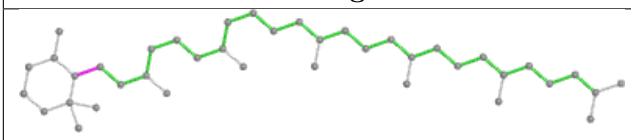


Bond angles



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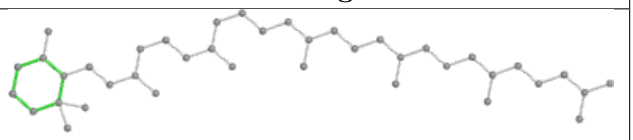
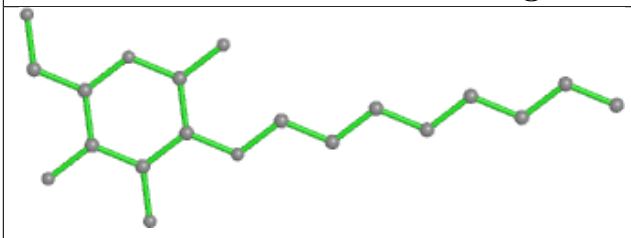
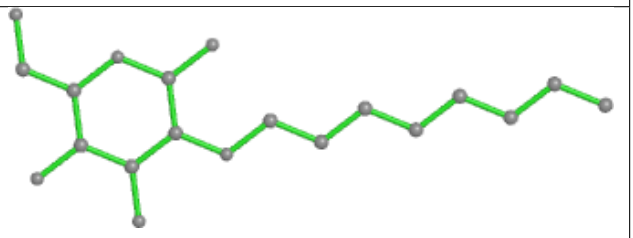


Rings

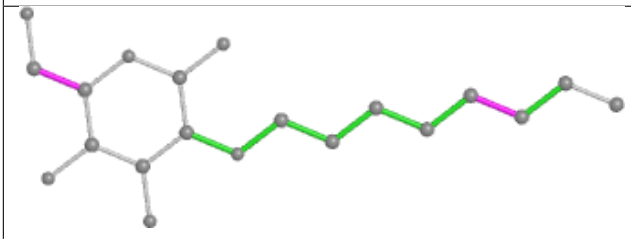
Ligand BGL H 103



Bond lengths



Bond angles



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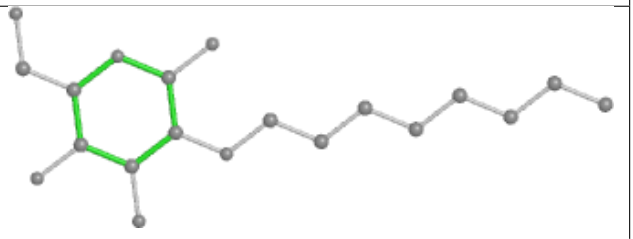
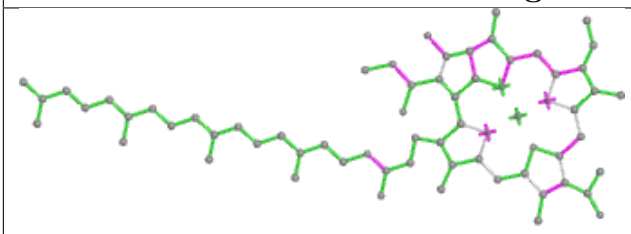


Rings

Ligand BCL O 101



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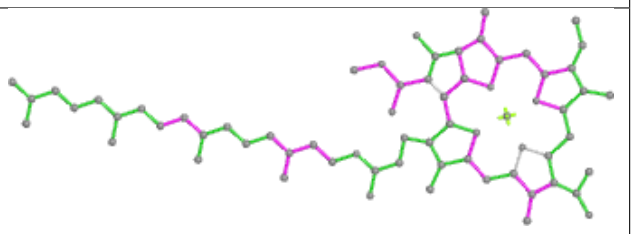
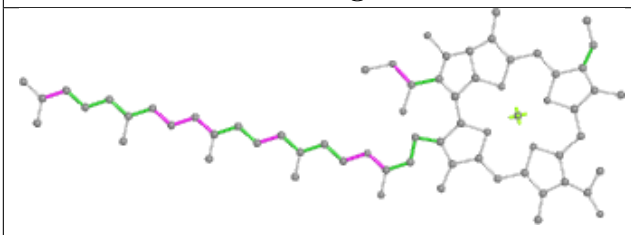


Bond angles



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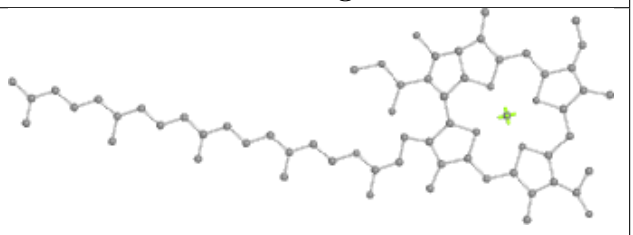
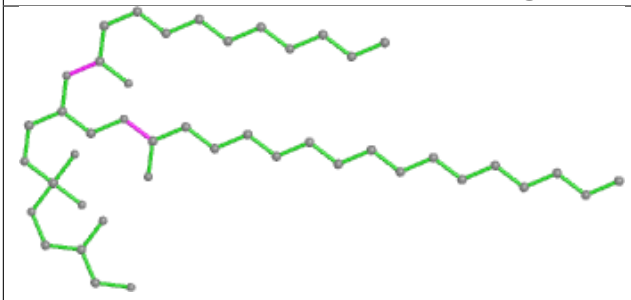


Rings

Ligand PGV K 104



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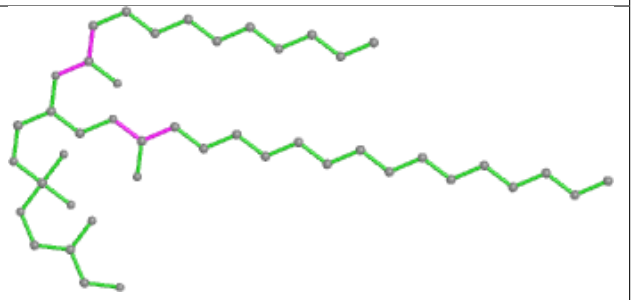
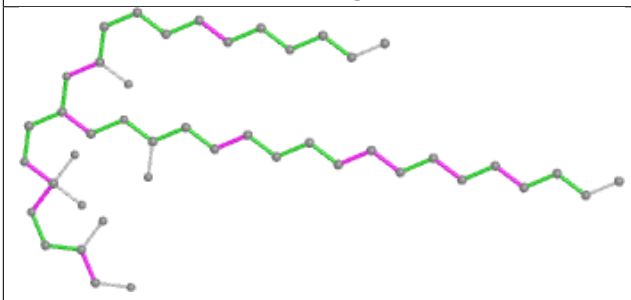


Bond angles



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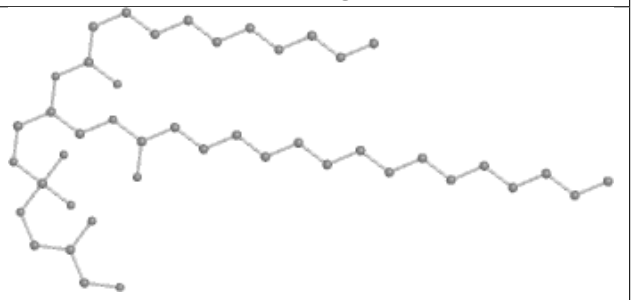
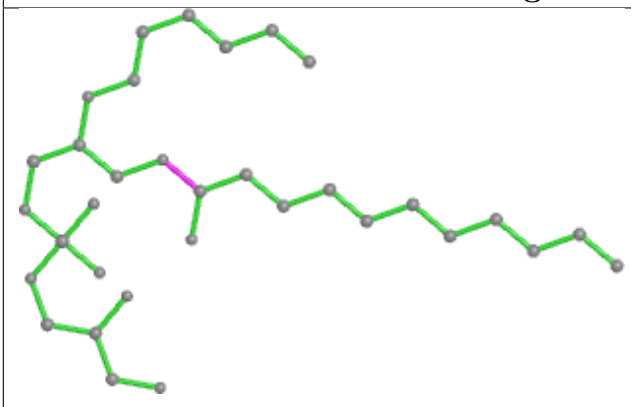
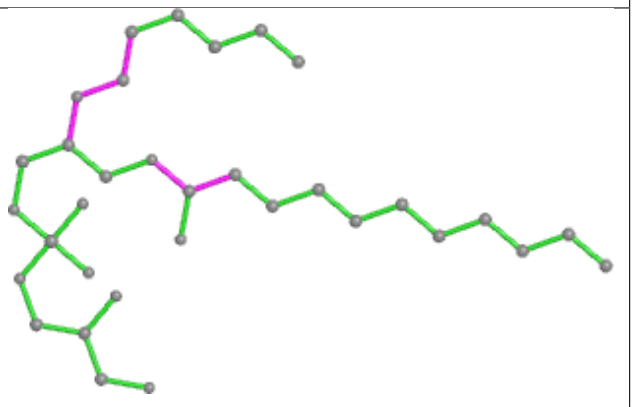


Rings

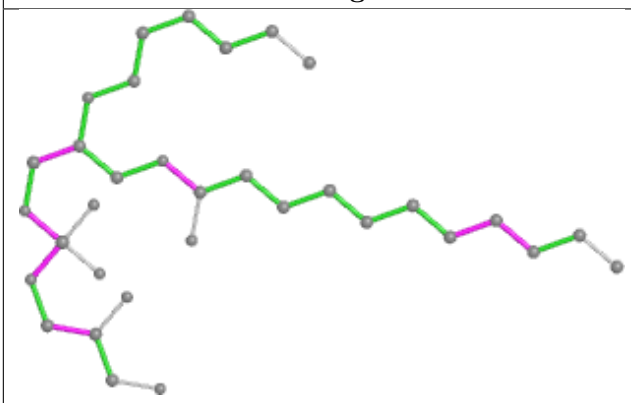
Ligand PGV L 711



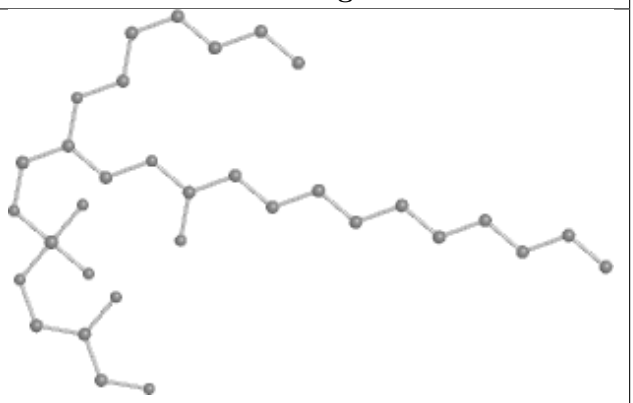
Bond lengths



Bond angles

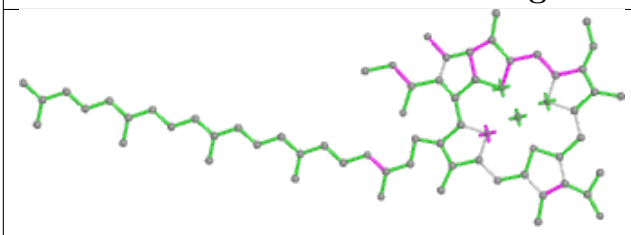


Torsions

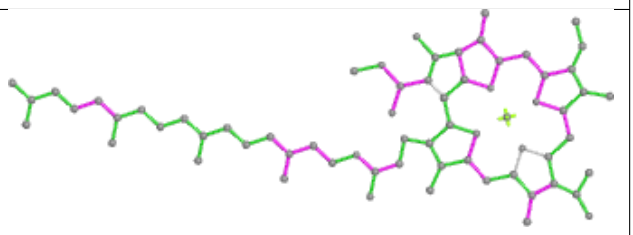


Rings

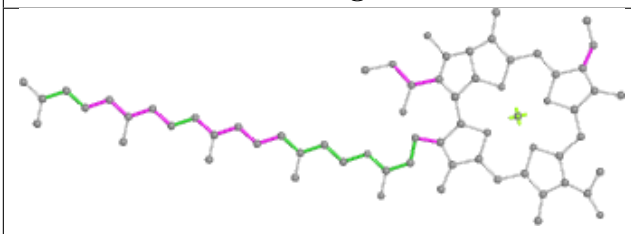
Ligand BCL 5 101



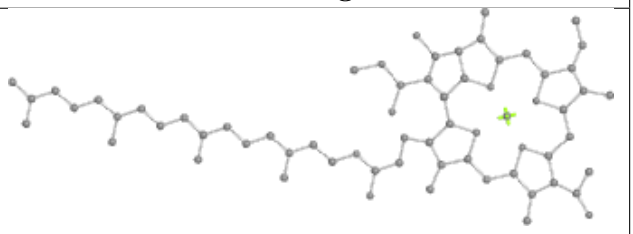
Bond lengths



Bond angles

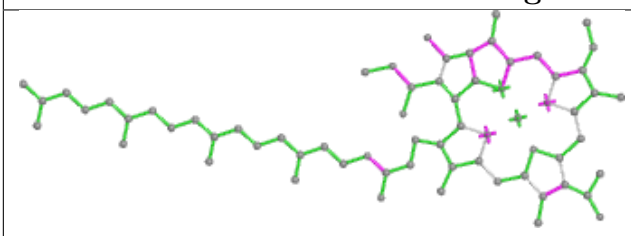


Torsions

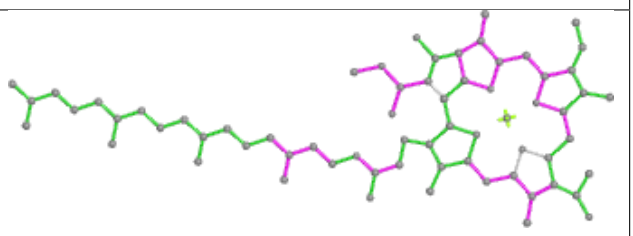


Rings

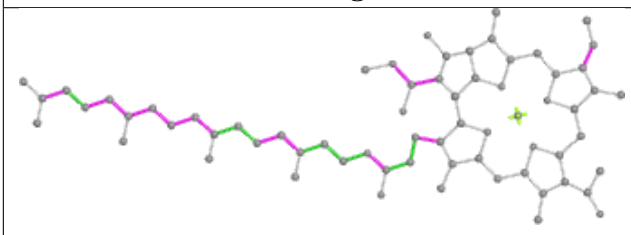
Ligand BCL G 102



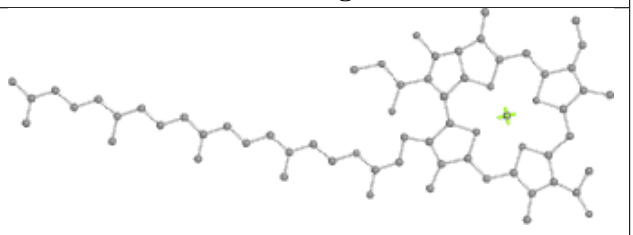
Bond lengths



Bond angles

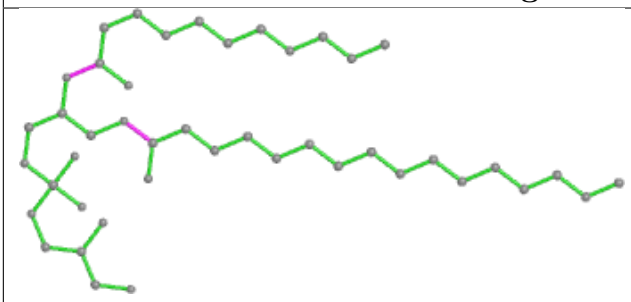


Torsions

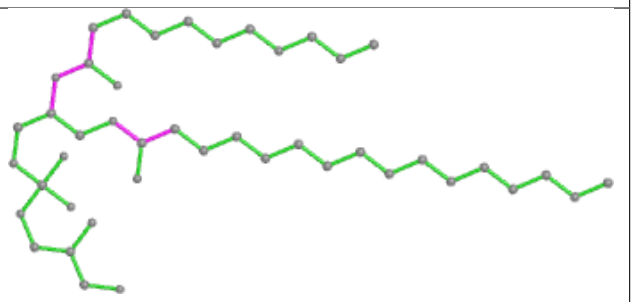


Rings

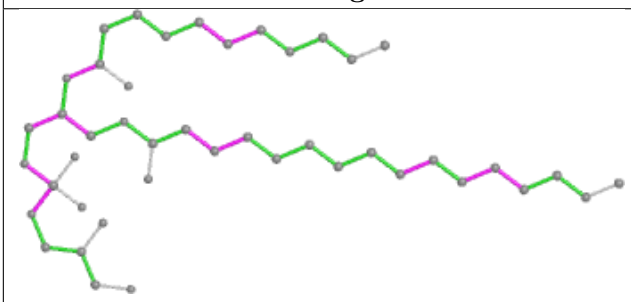
Ligand PGV O 103



Bond lengths



Bond angles



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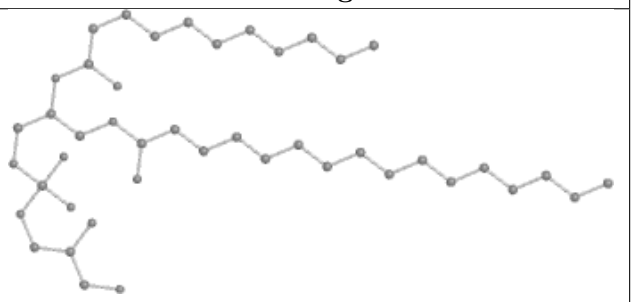
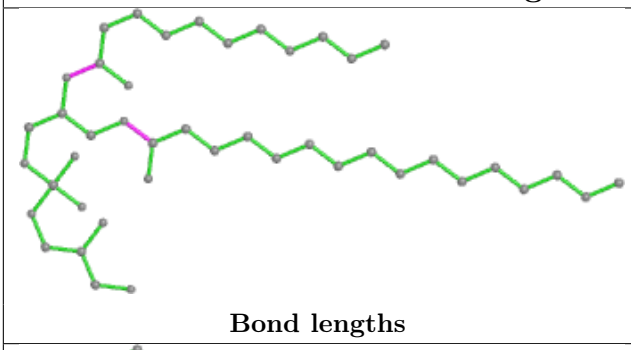


Rings

Ligand PGV S 103



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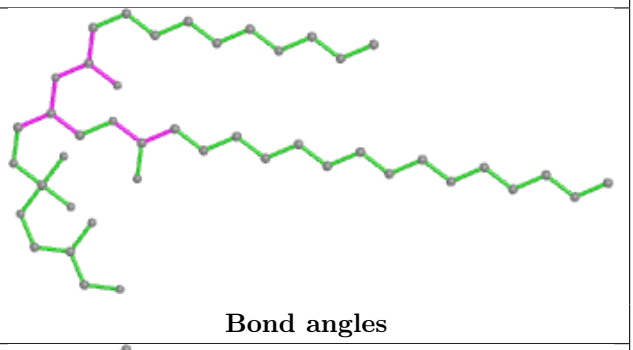
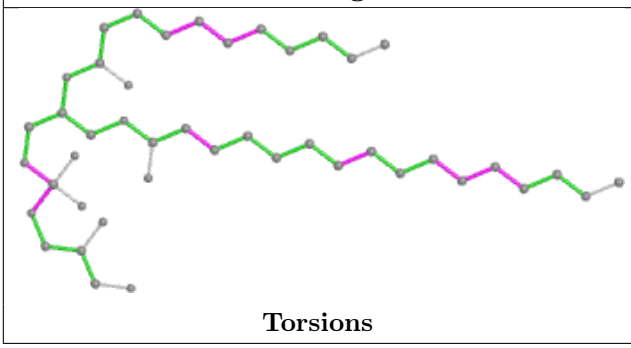


Bond angles



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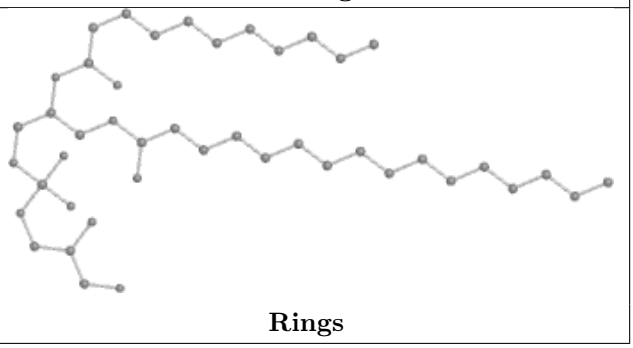
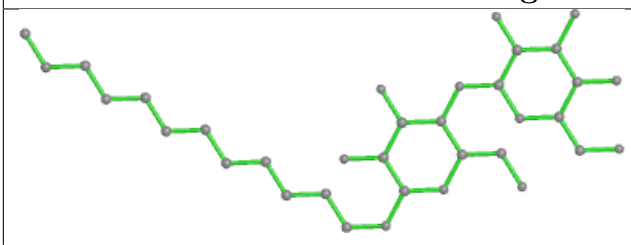
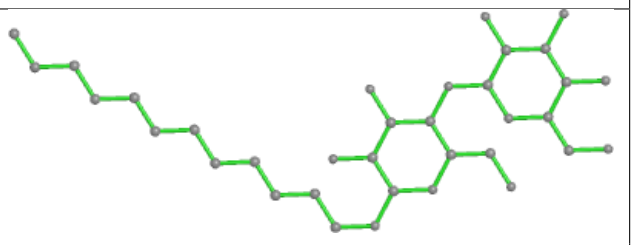


Rings

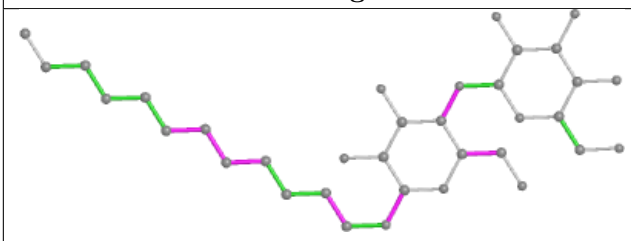
Ligand LMT D 104



Bond lengths



Bond angles



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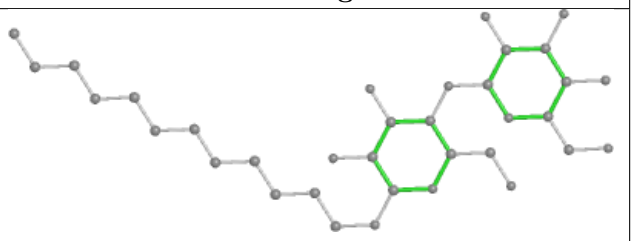
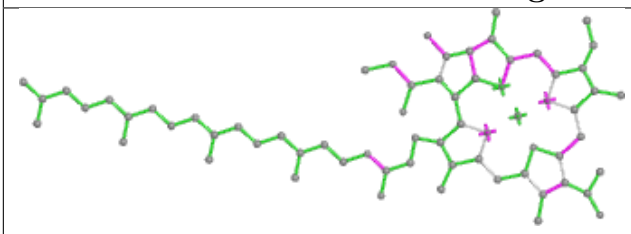


Rings

Ligand BCL S 101



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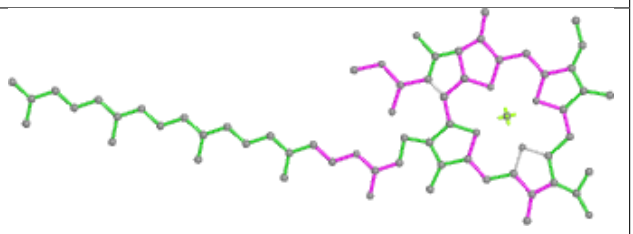
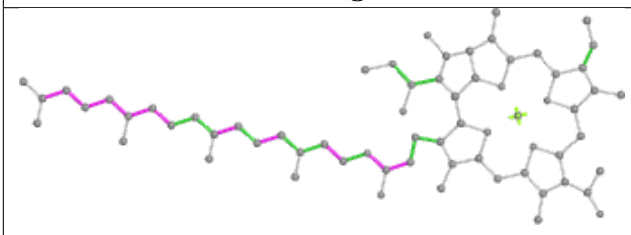


Bond angles



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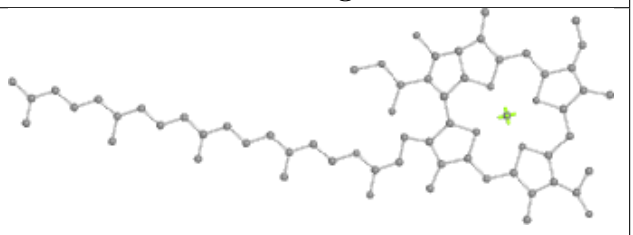
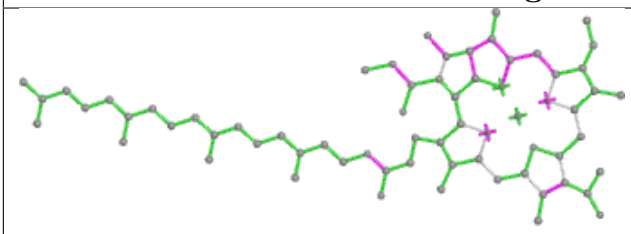


Rings

Ligand BCL Q 102



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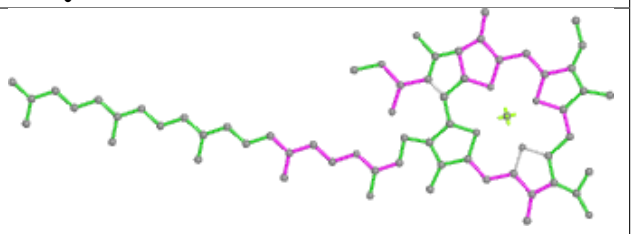
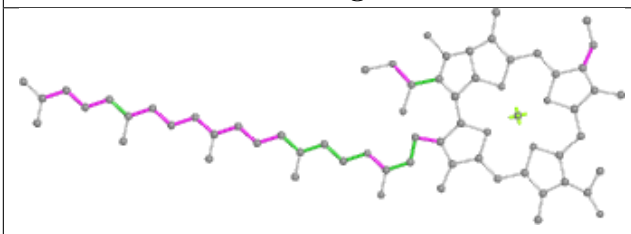
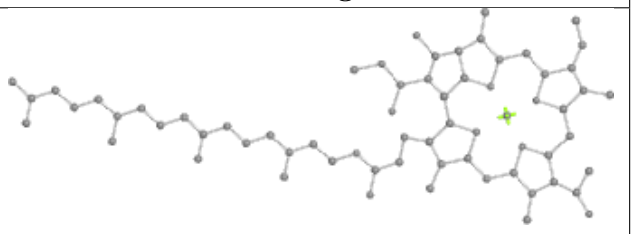


Bond angles

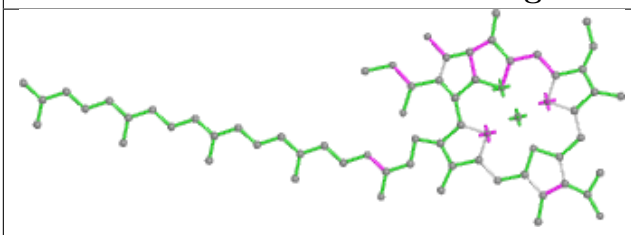


Torsions



Rings

Ligand BCL A 101



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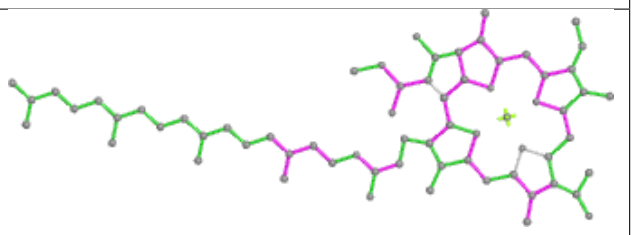
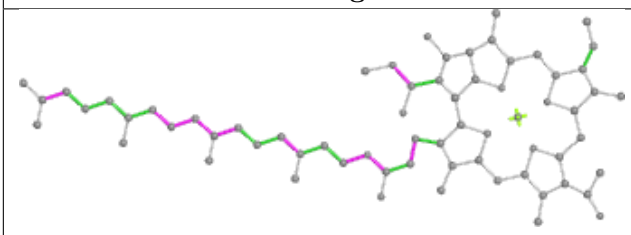
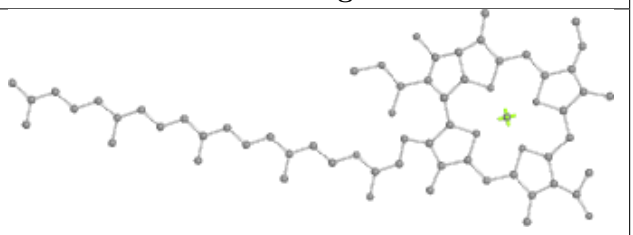


Bond angles

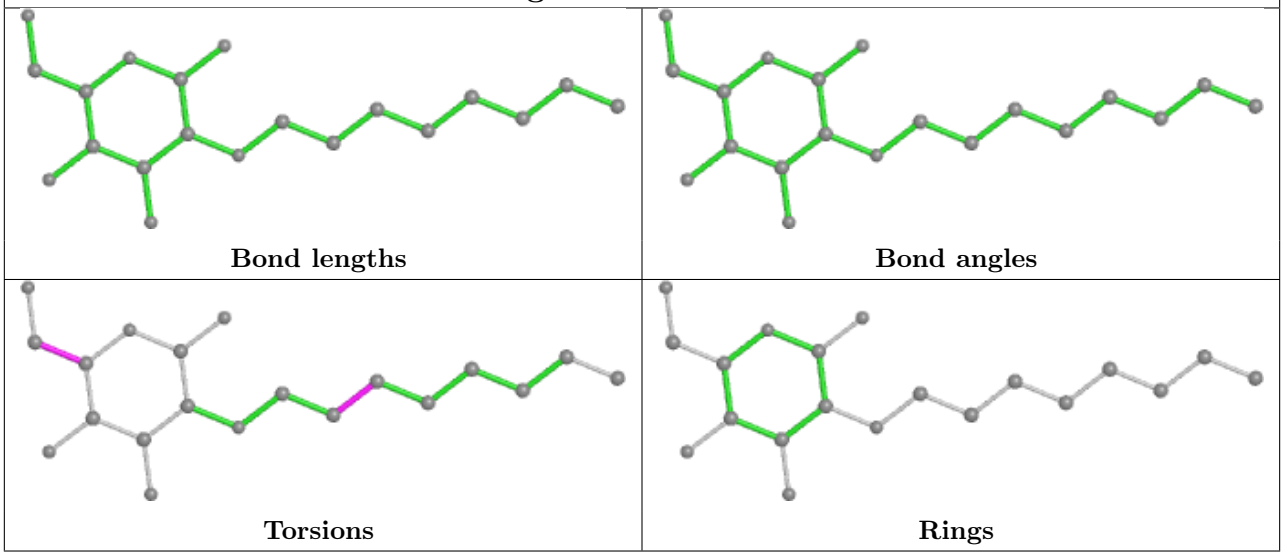


Torsions

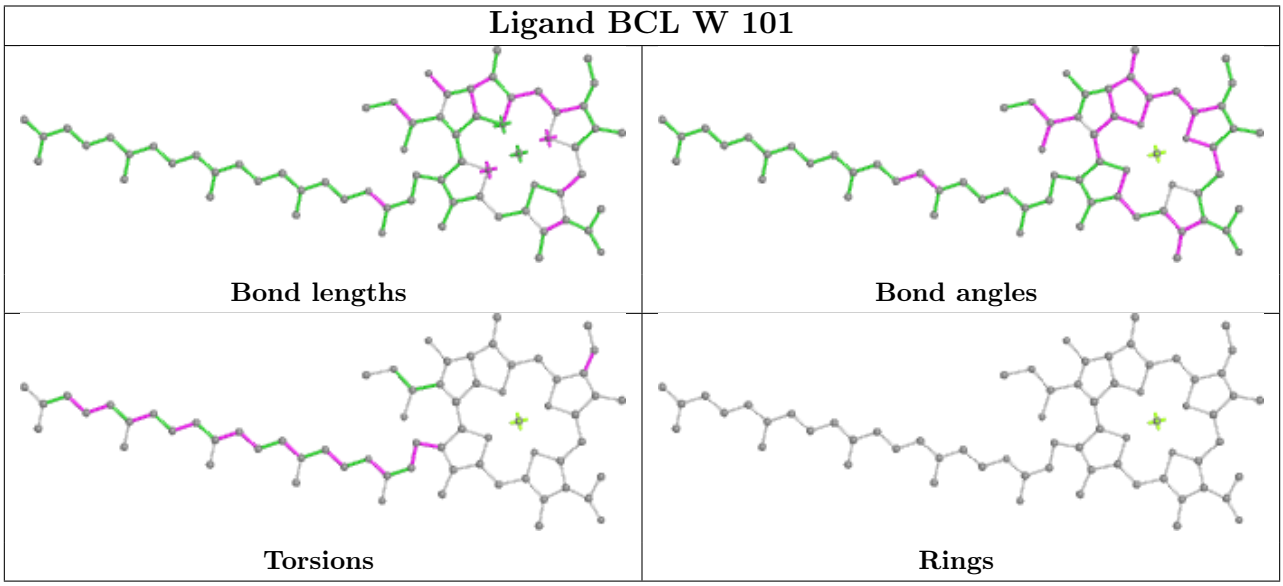


Rings

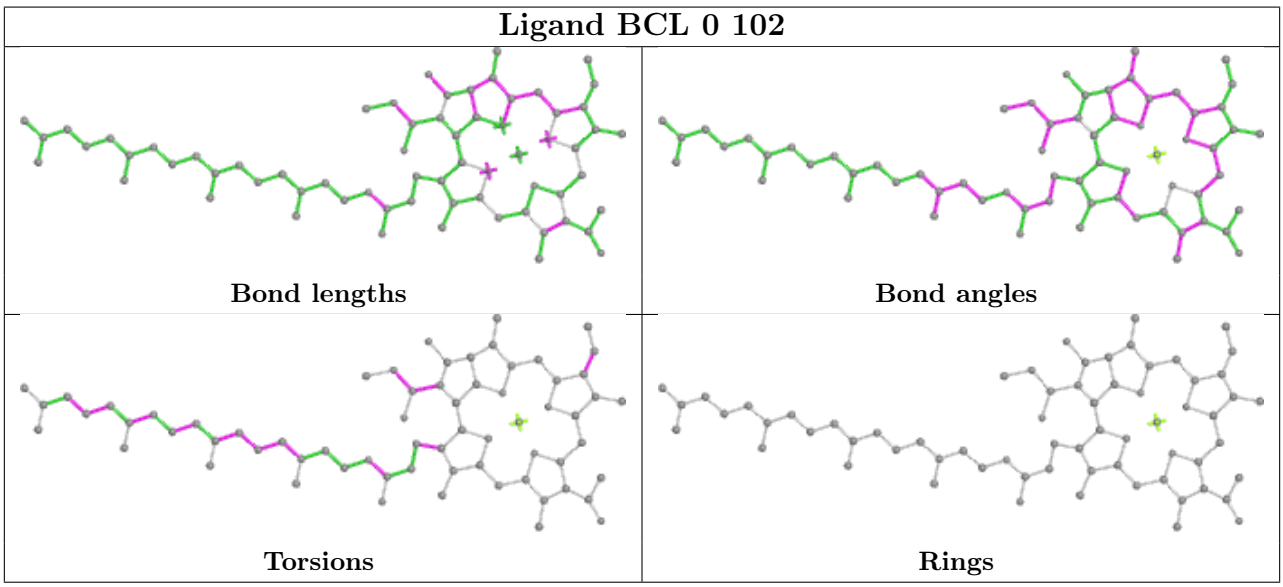
Ligand BGL L 714



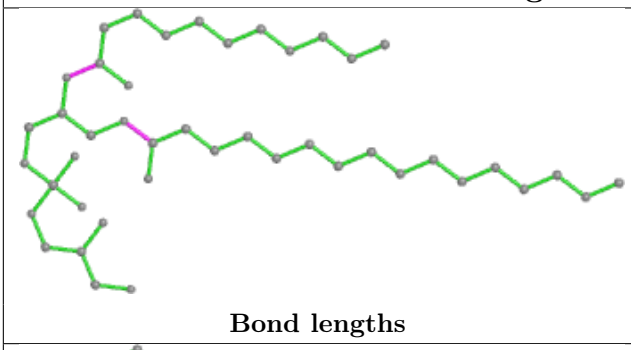
Ligand BCL W 101



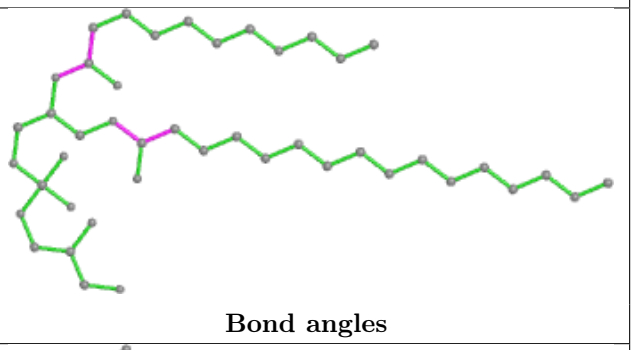
Ligand BCL 0 102



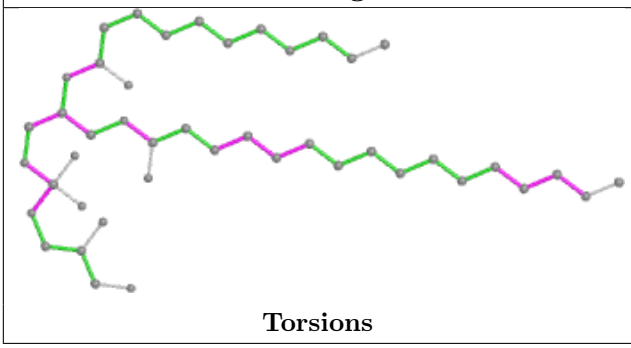
Ligand PGV 6 103



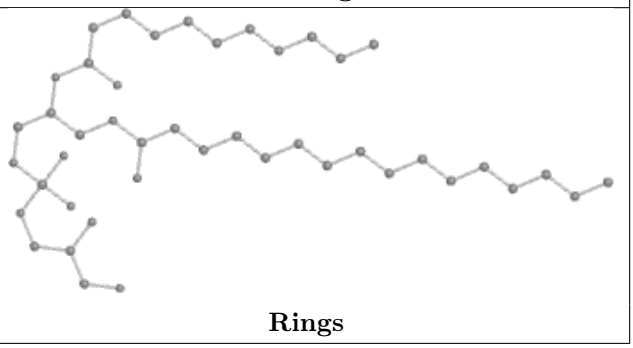
Bond lengths



Bond angles

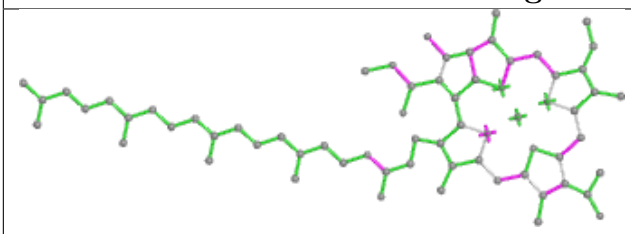


Torsions

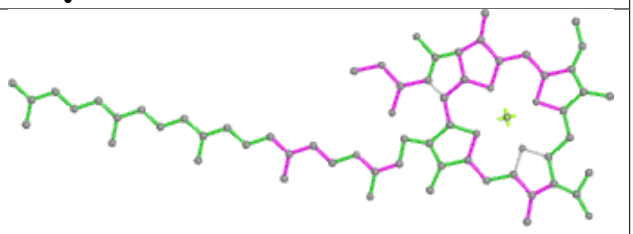


Rings

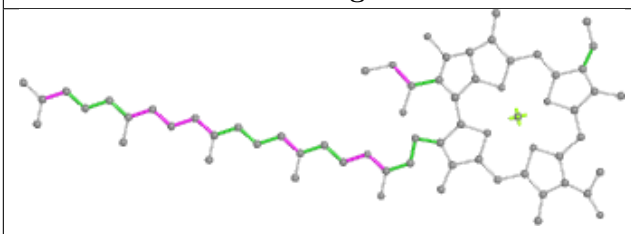
Ligand BCL Q 101



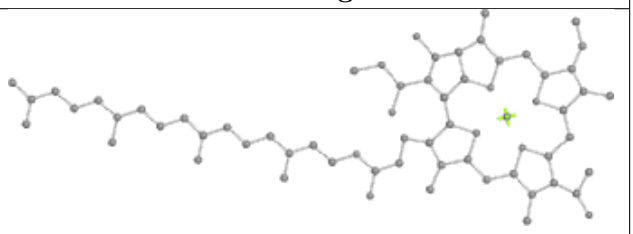
Bond lengths



Bond angles

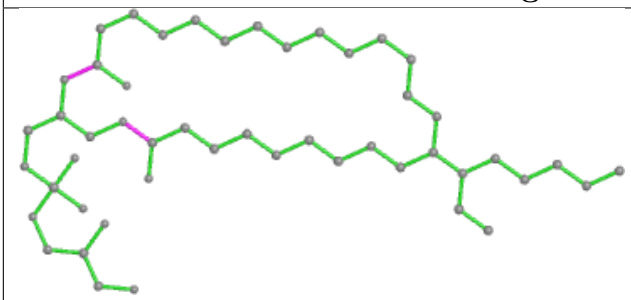


Torsions

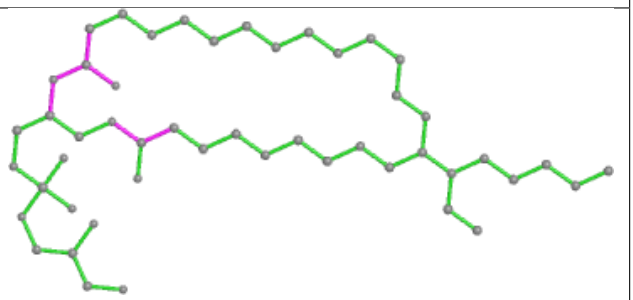


Rings

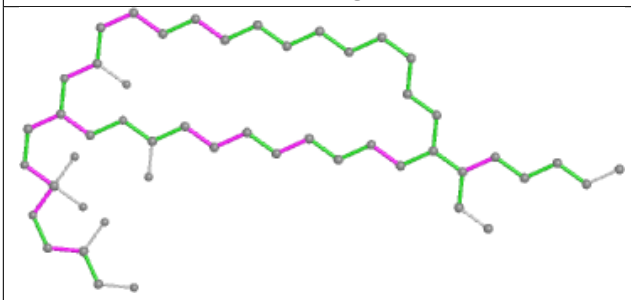
Ligand PGV C 506



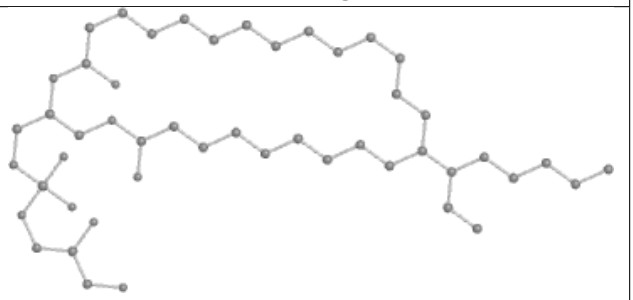
Bond lengths



Bond angles

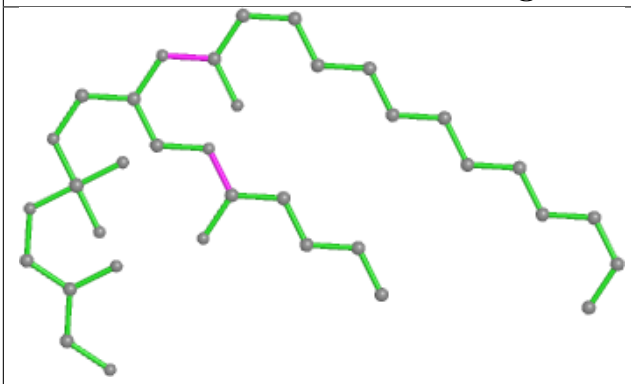


Torsions

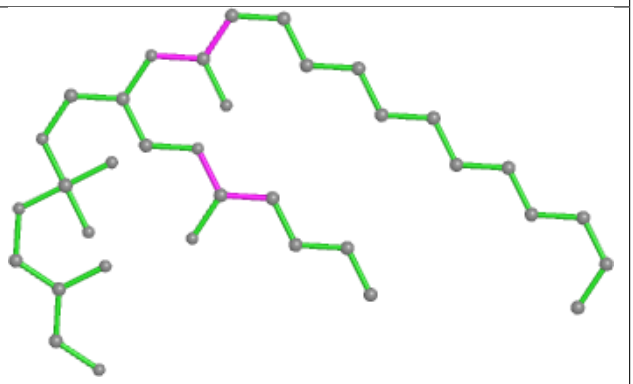


Rings

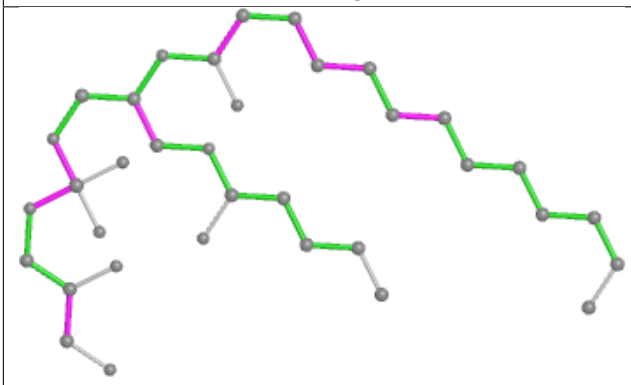
Ligand PGV M 705



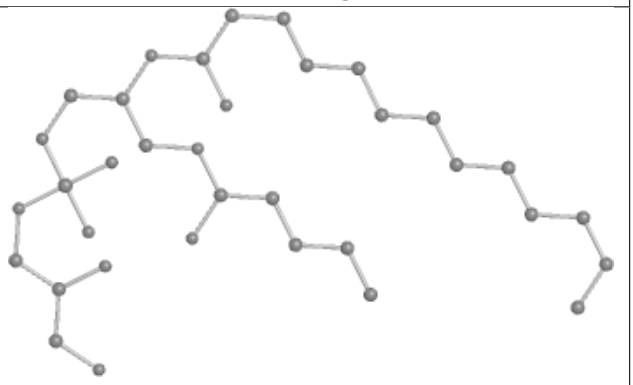
Bond lengths



Bond angles

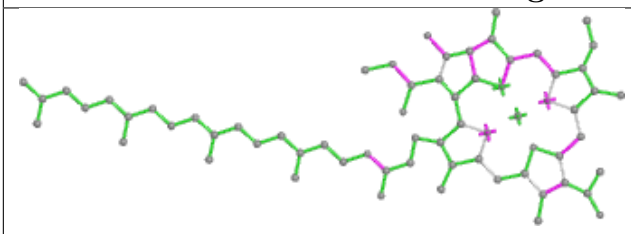


Torsions

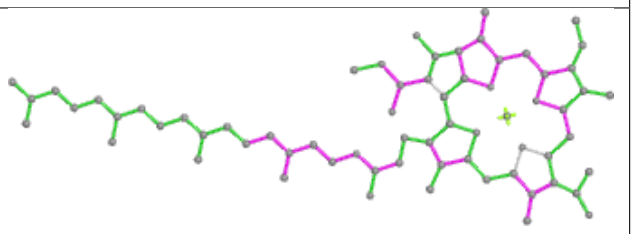


Rings

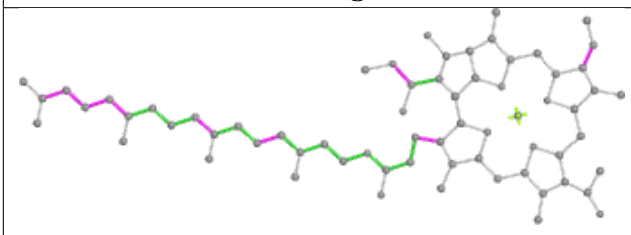
Ligand BCL L 702



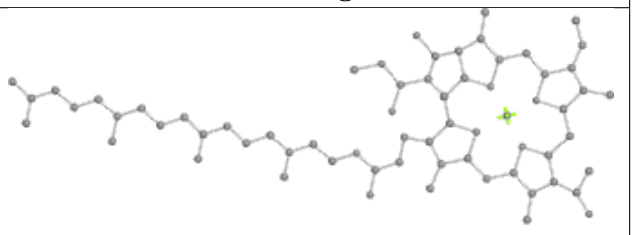
Bond lengths



Bond angles

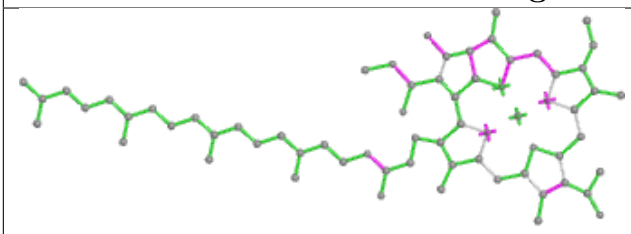


Torsions

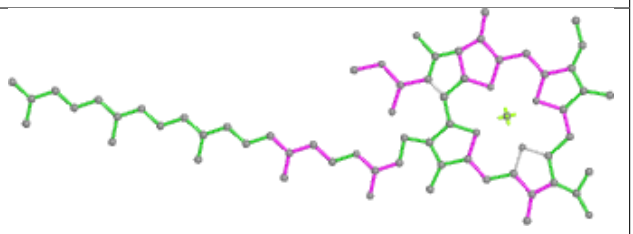


Rings

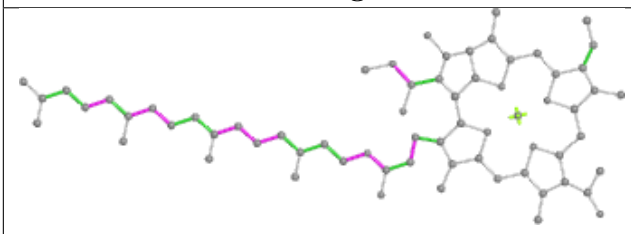
Ligand BCL 2 101



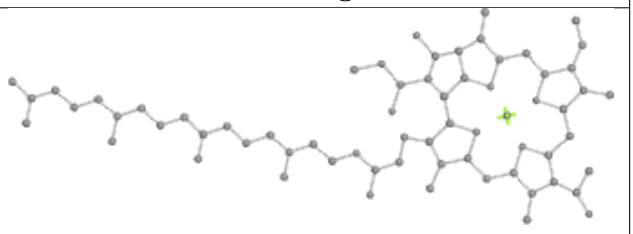
Bond lengths



Bond angles

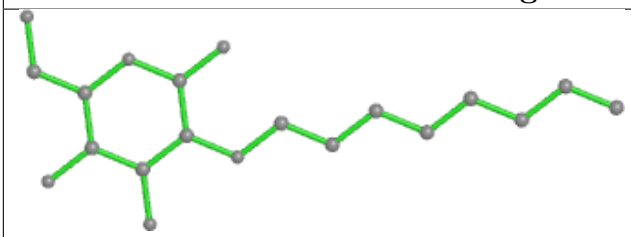


Torsions



Rings

Ligand BGL M 710



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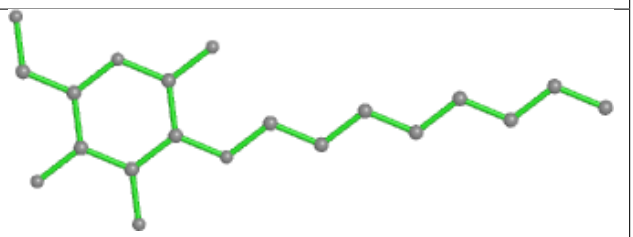
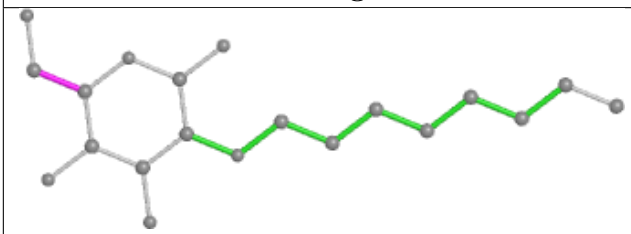
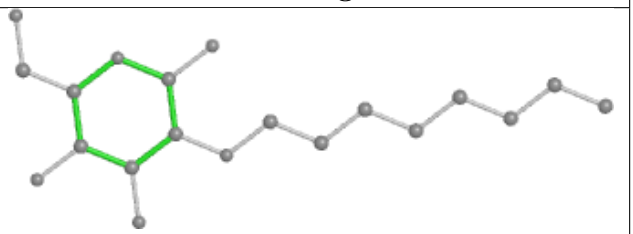


Bond angles

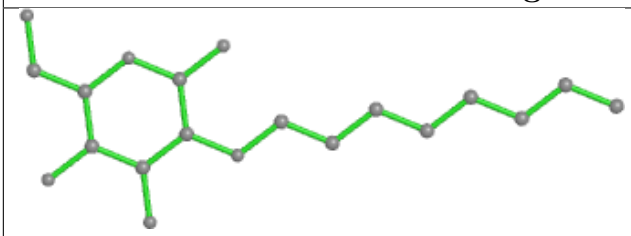


Torsions

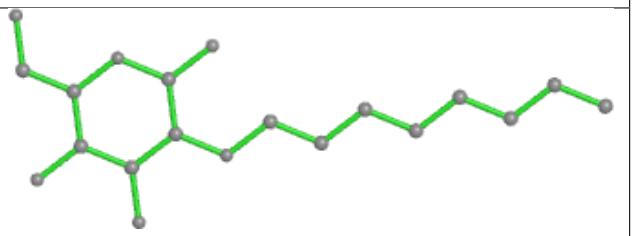


Rings

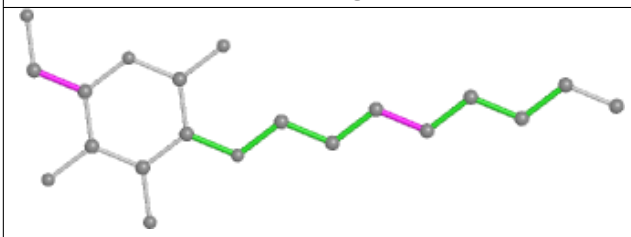
Ligand BGL Y 101



Bond lengths



Bond angles



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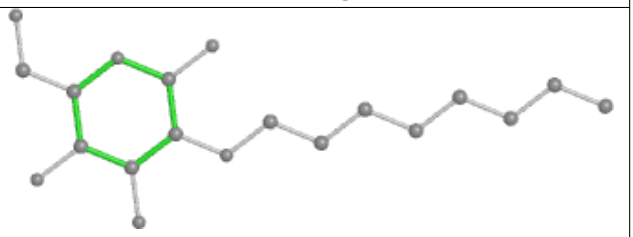
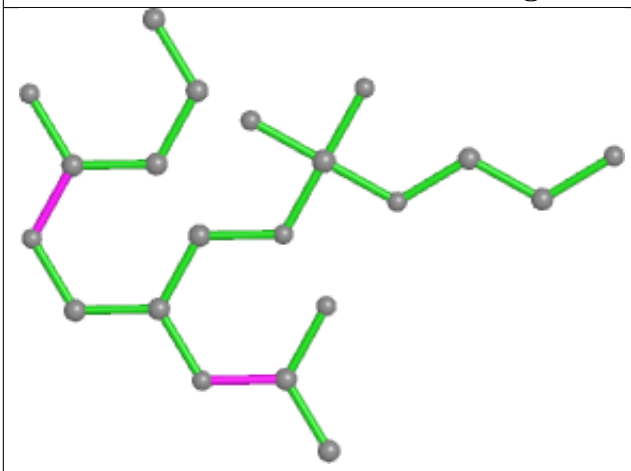
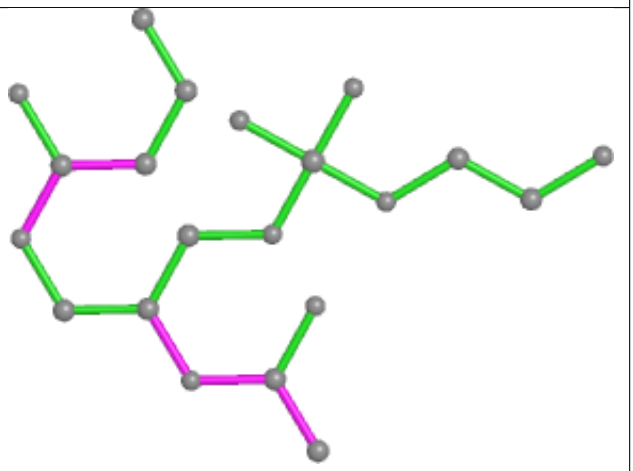


Rings

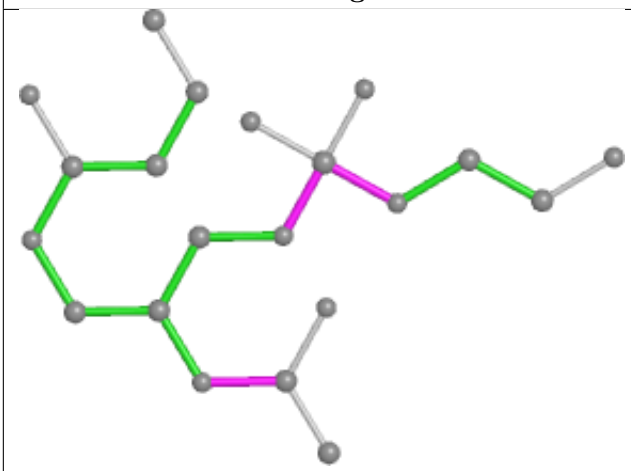
Ligand PEF M 708



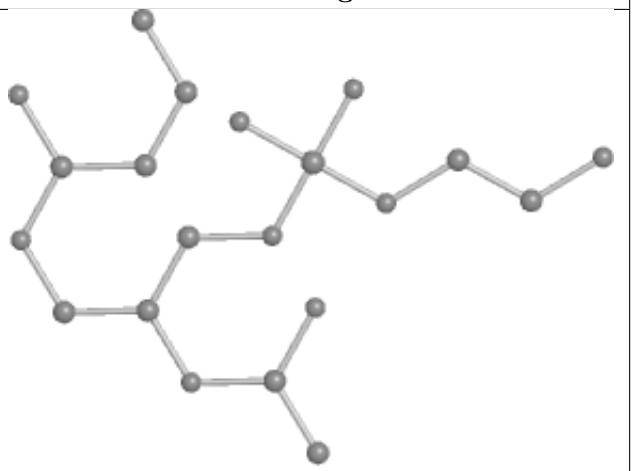
Bond lengths



Bond angles

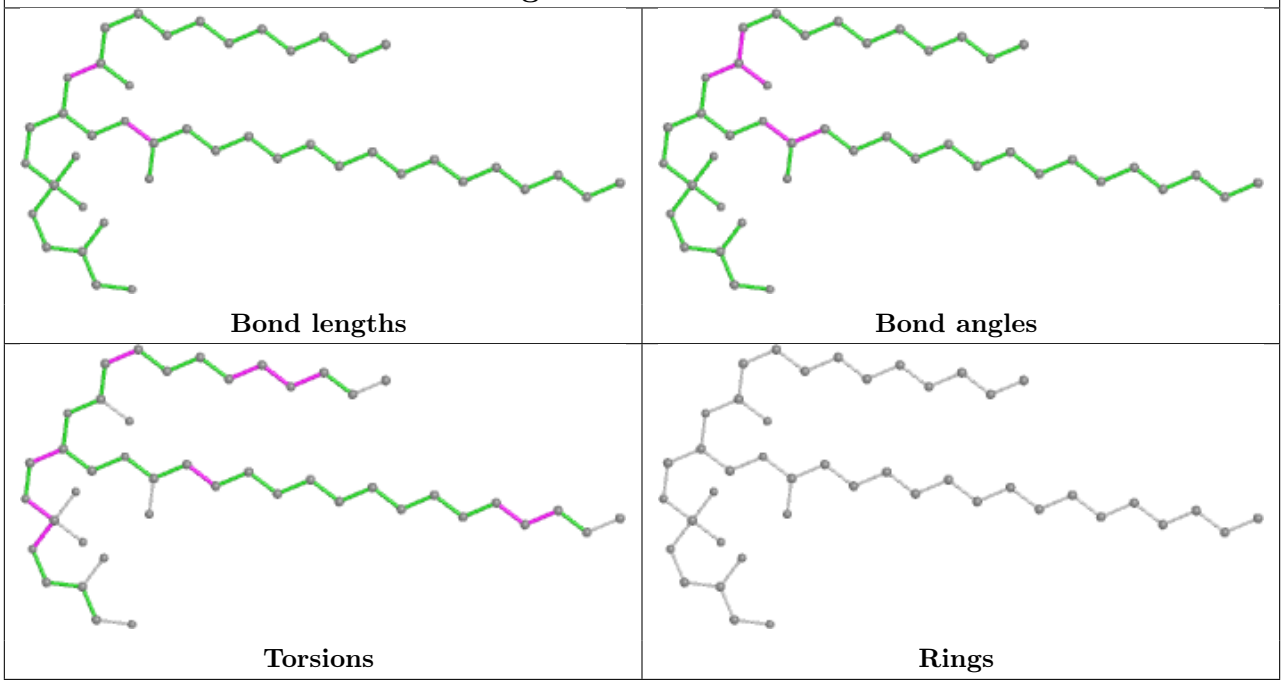


Torsions

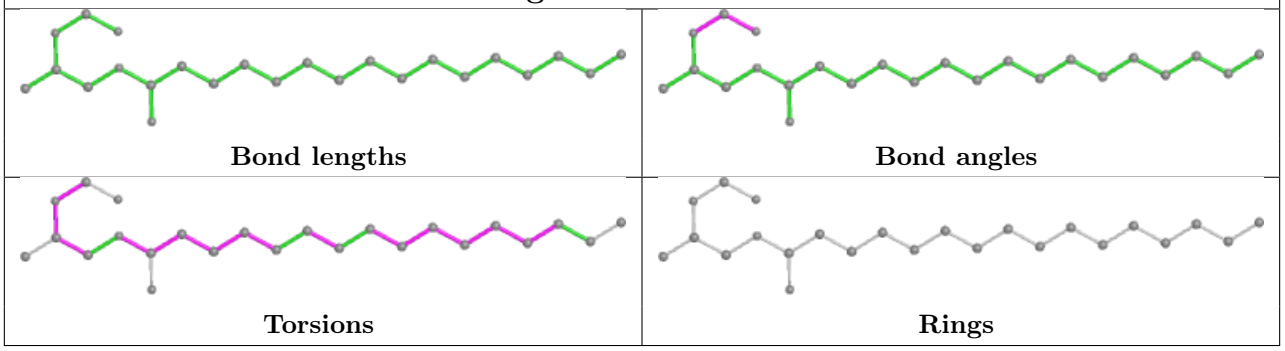


Rings

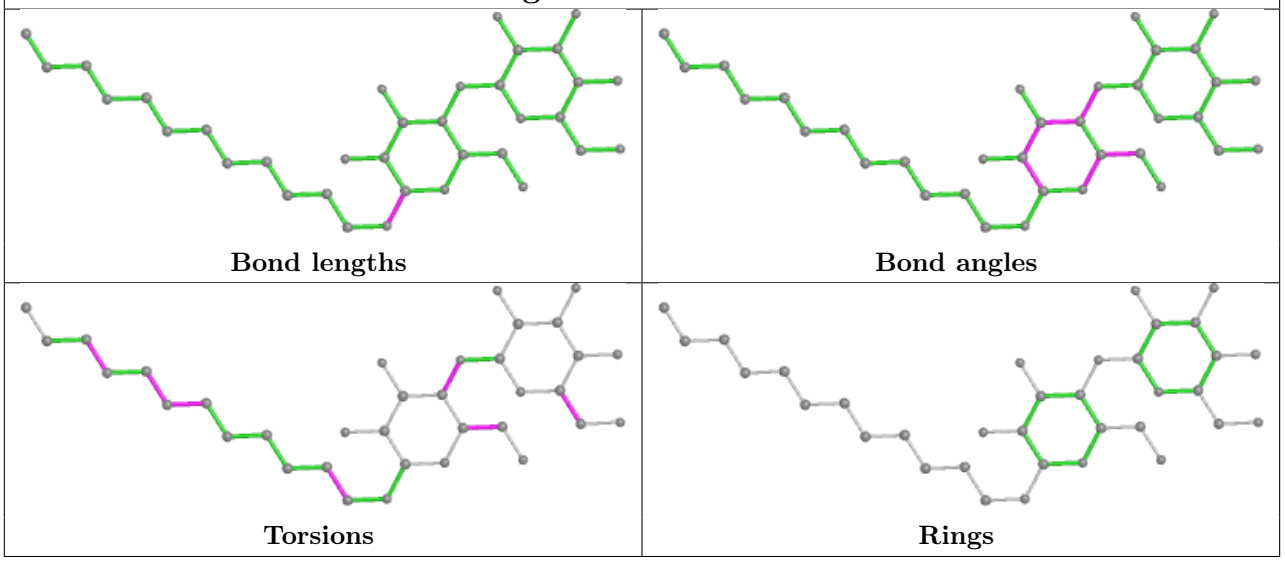
Ligand PGV K 103



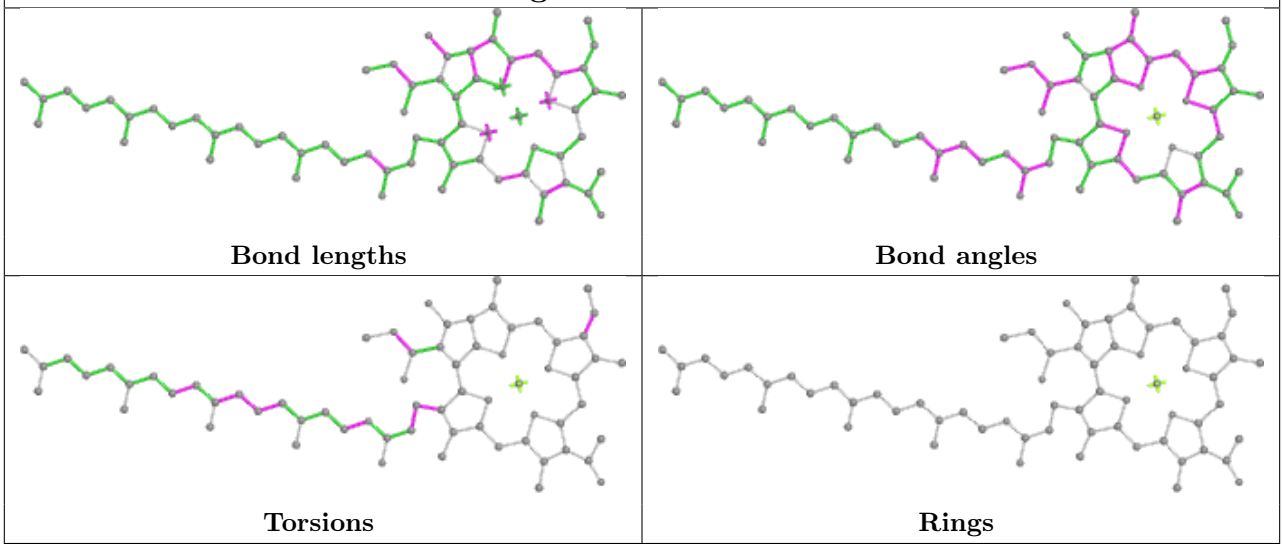
Ligand LHG h 101



Ligand LMT T 102



Ligand BCL 9 101



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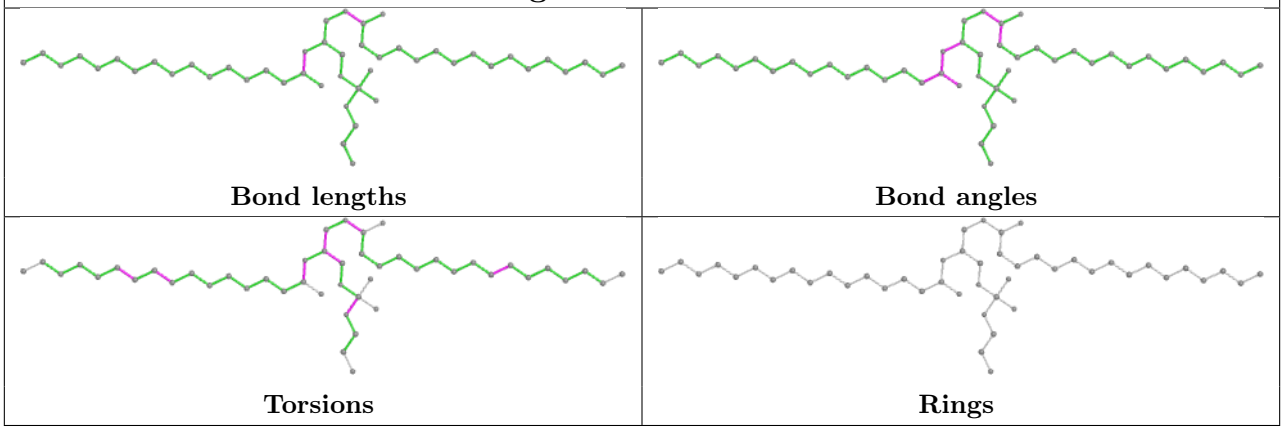

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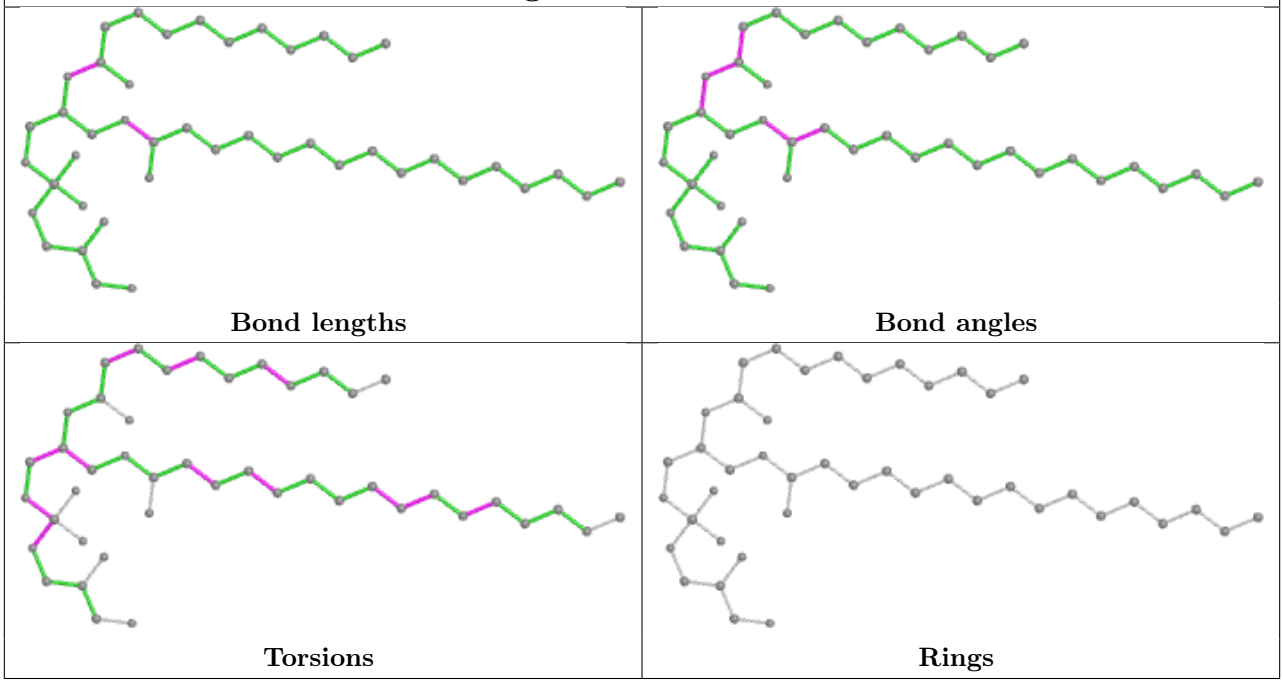

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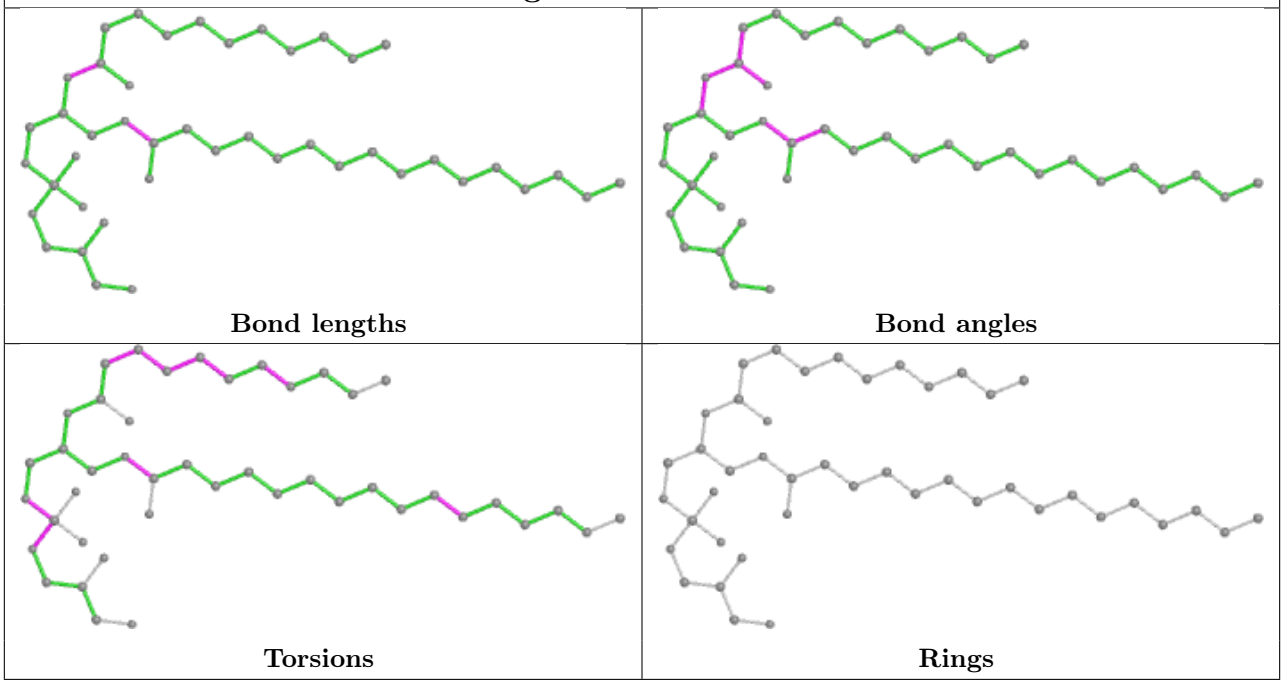
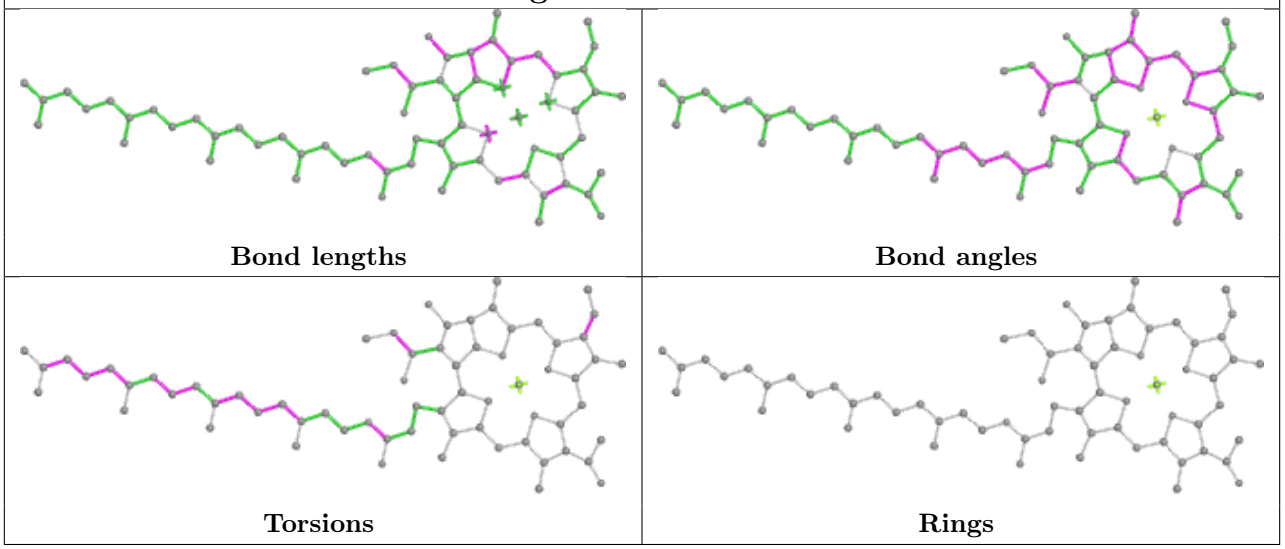
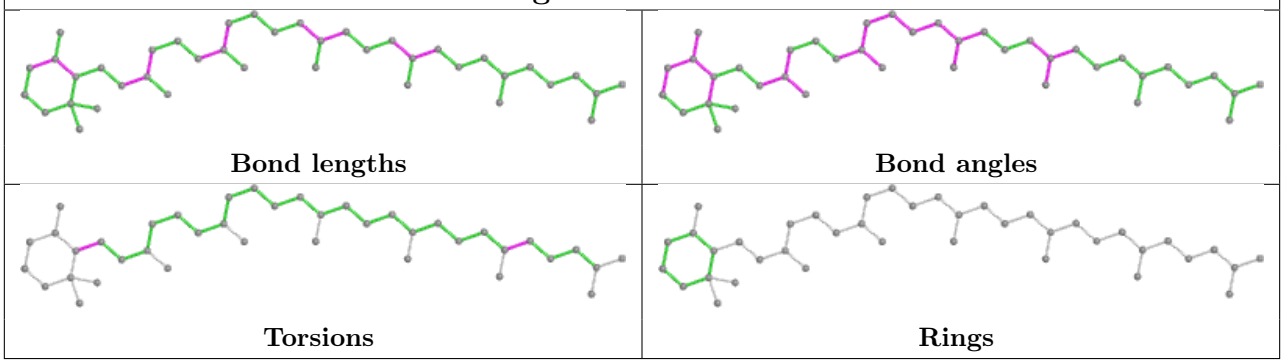


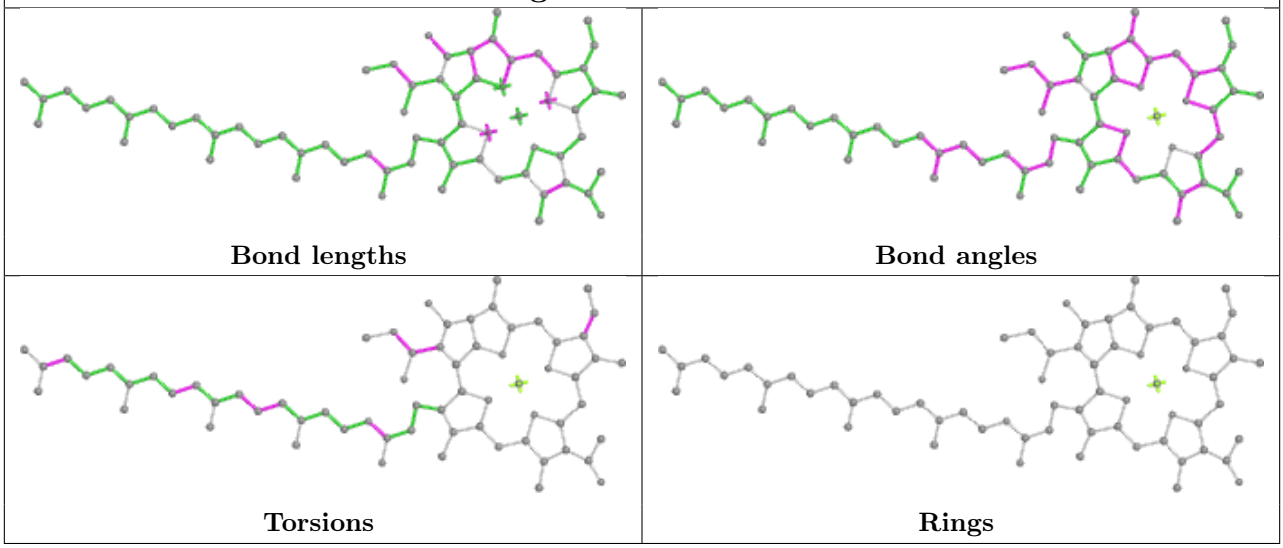
Ligand BCL 6 102



Ligand U4Z J 101

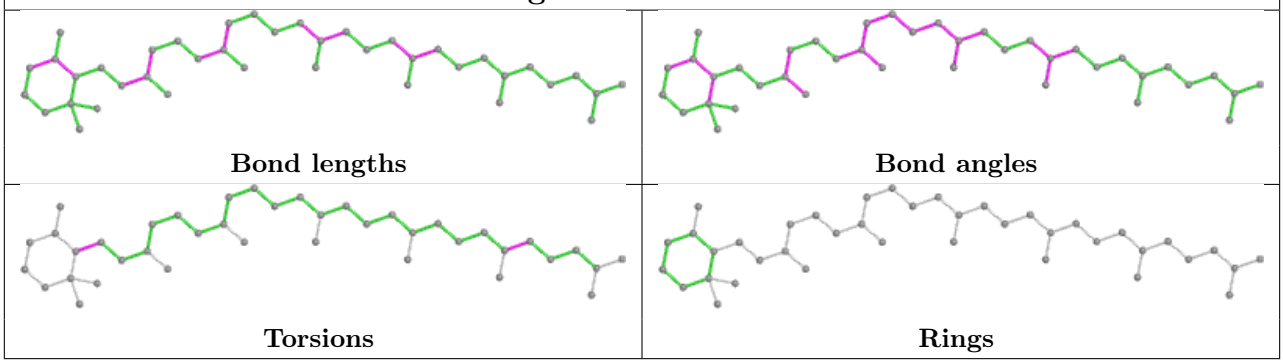


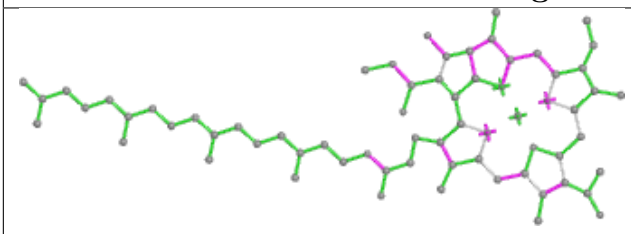
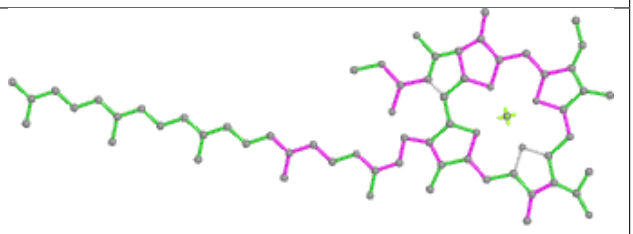
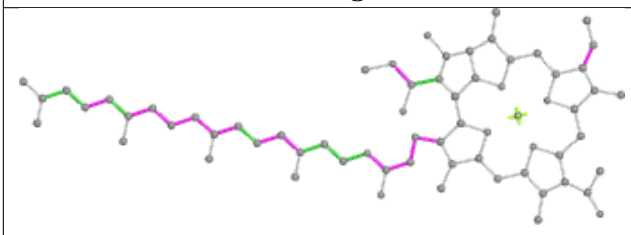
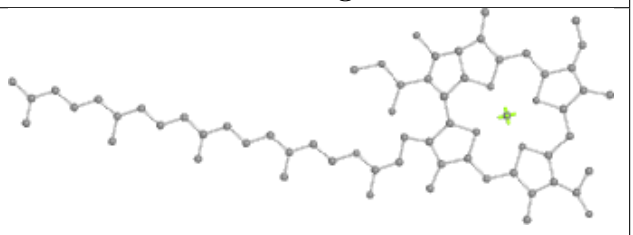
Ligand BCL 8 102

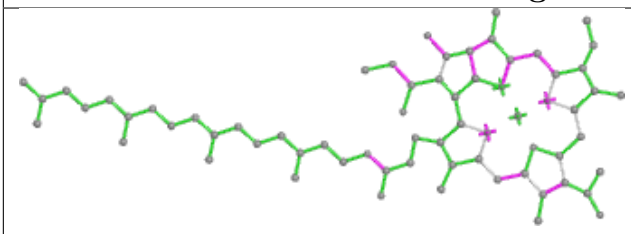
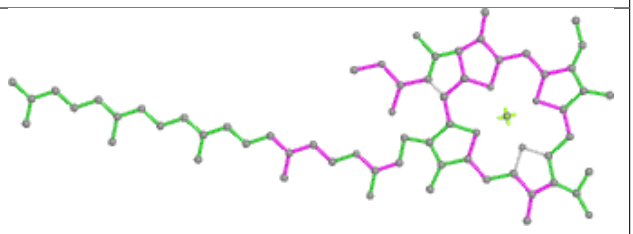
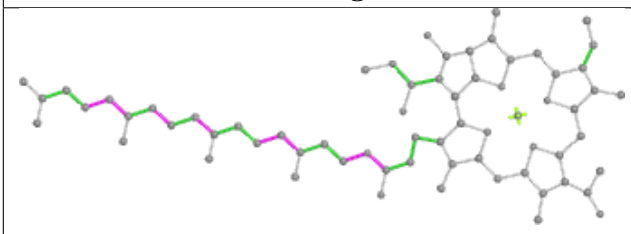
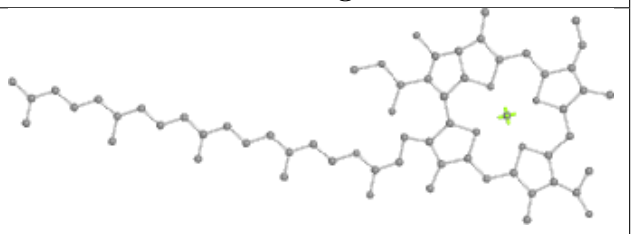


Ligand U4Z R 101

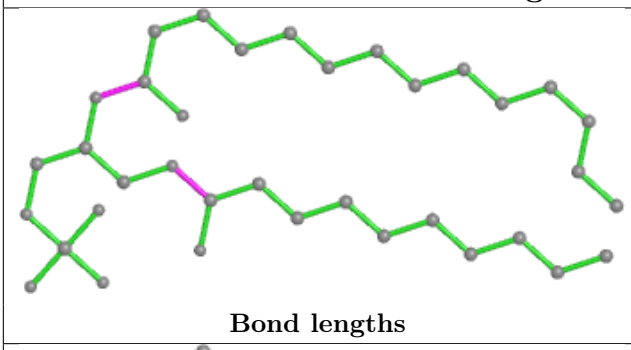
Ligand U4Z D 101



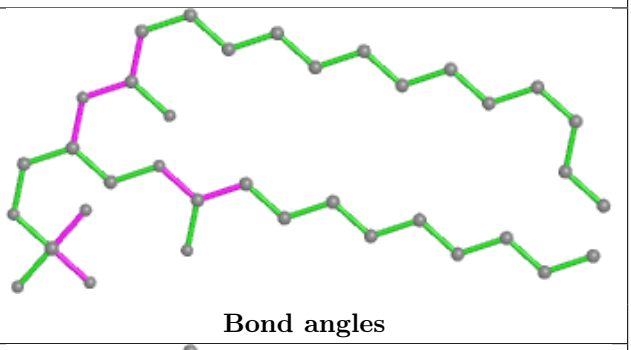
Ligand BCL I 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL 6 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

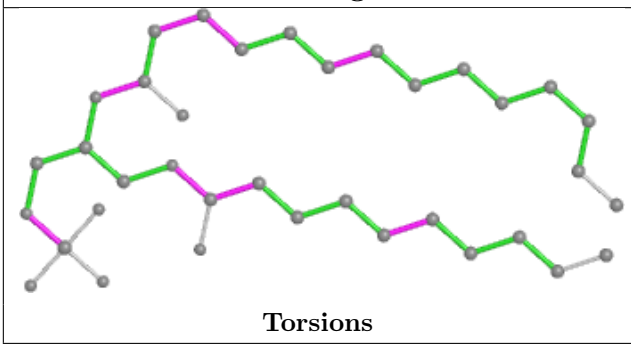
Ligand PGV 1 102



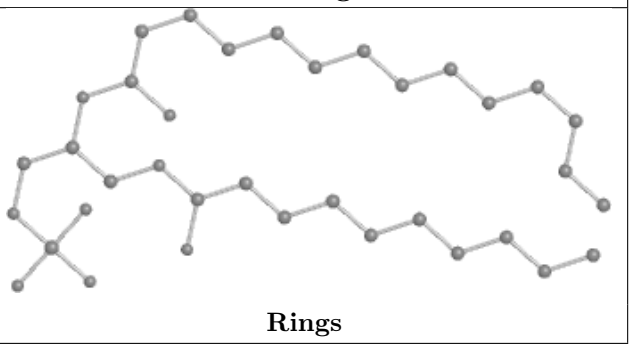
Bond lengths



Bond angles

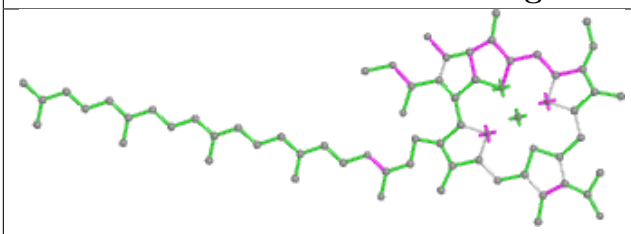


Torsions

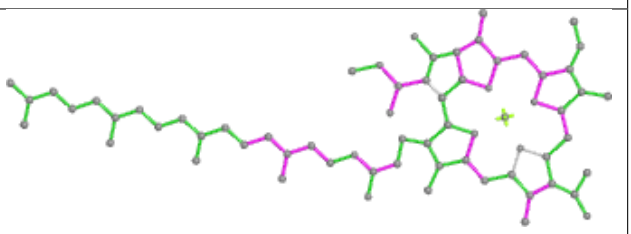


Rings

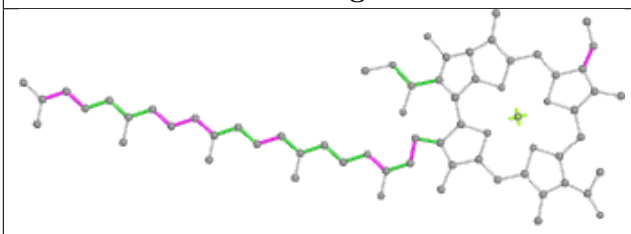
Ligand BCL R 102



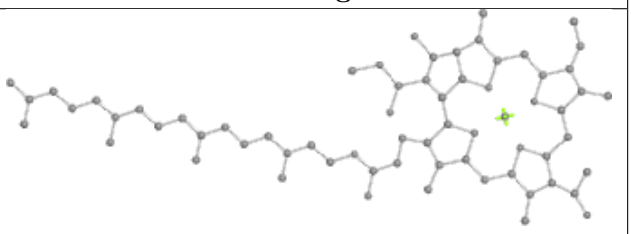
Bond lengths



Bond angles

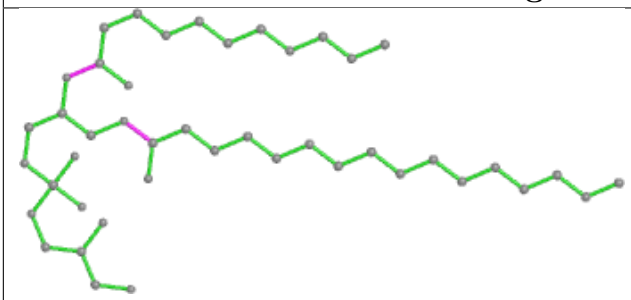


Torsions

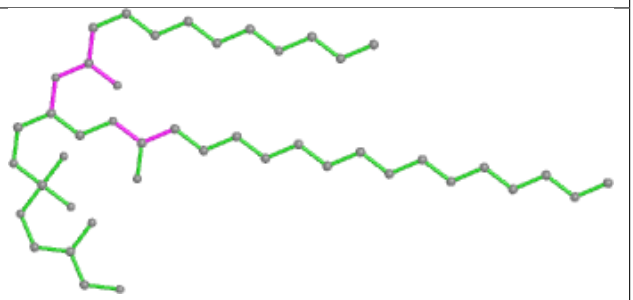


Rings

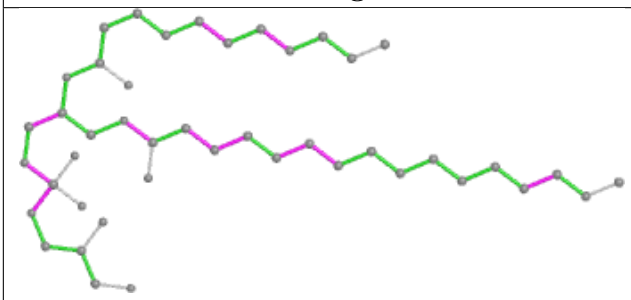
Ligand PGV 4 102



Bond lengths



Bond angles



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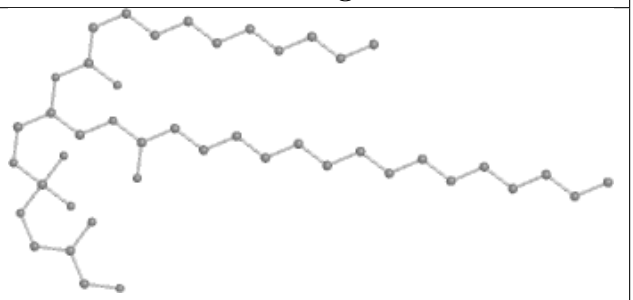
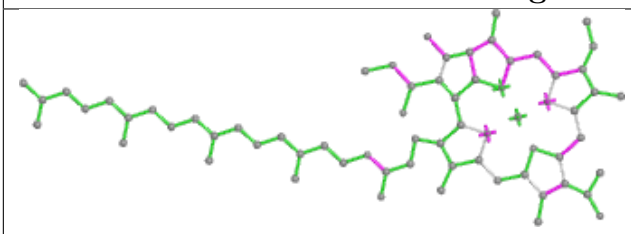
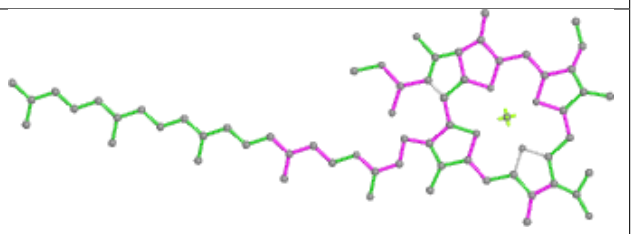


Rings

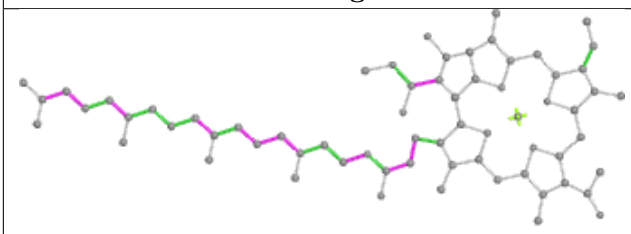
Ligand BCL 7 101



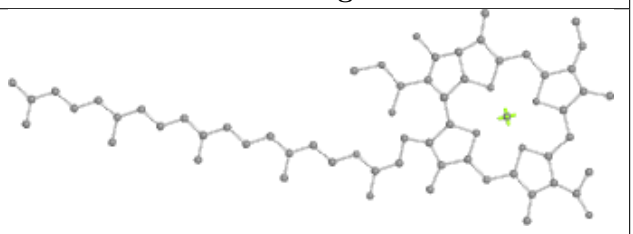
Bond lengths



Bond angles

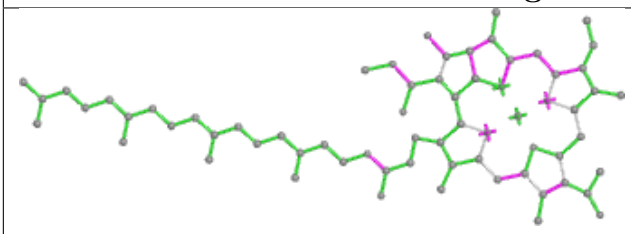


Torsions

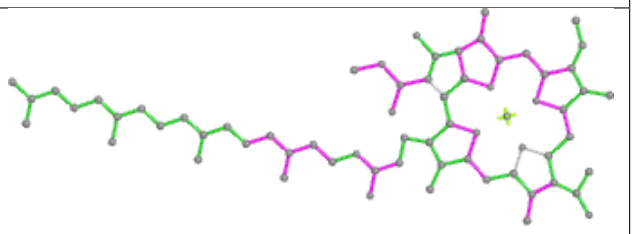


Rings

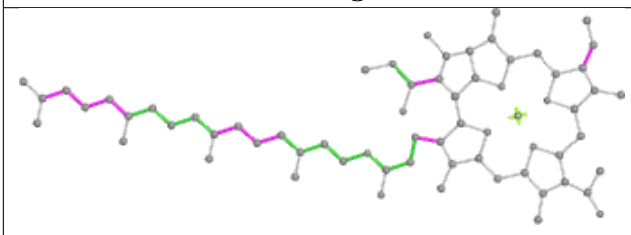
Ligand BCL D 102



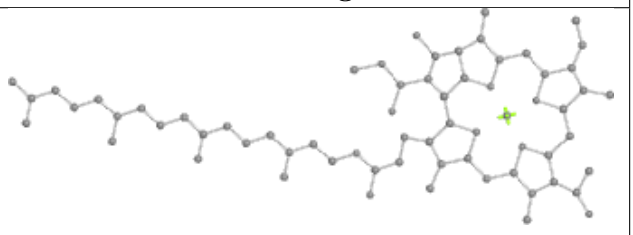
Bond lengths



Bond angles

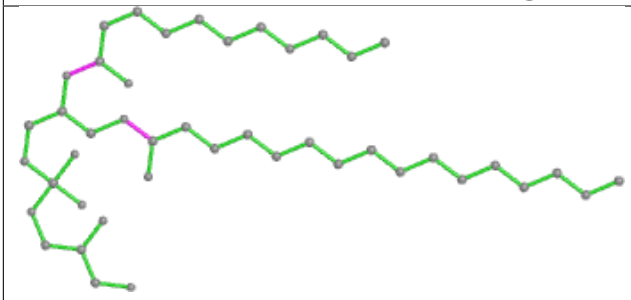


Torsions

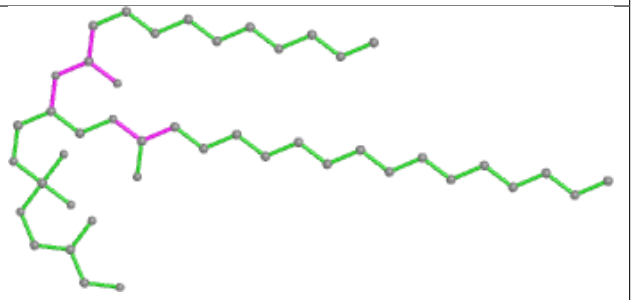


Rings

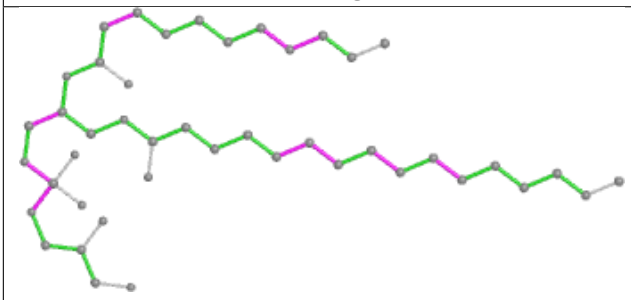
Ligand PGV U 103



Bond lengths



Bond angles



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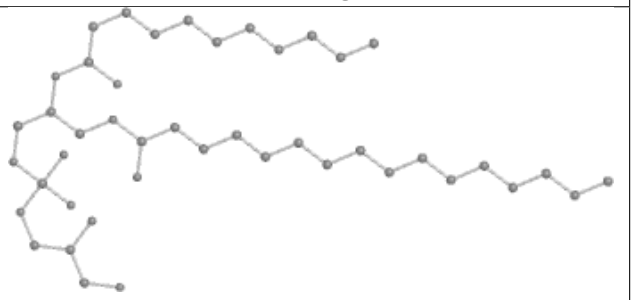
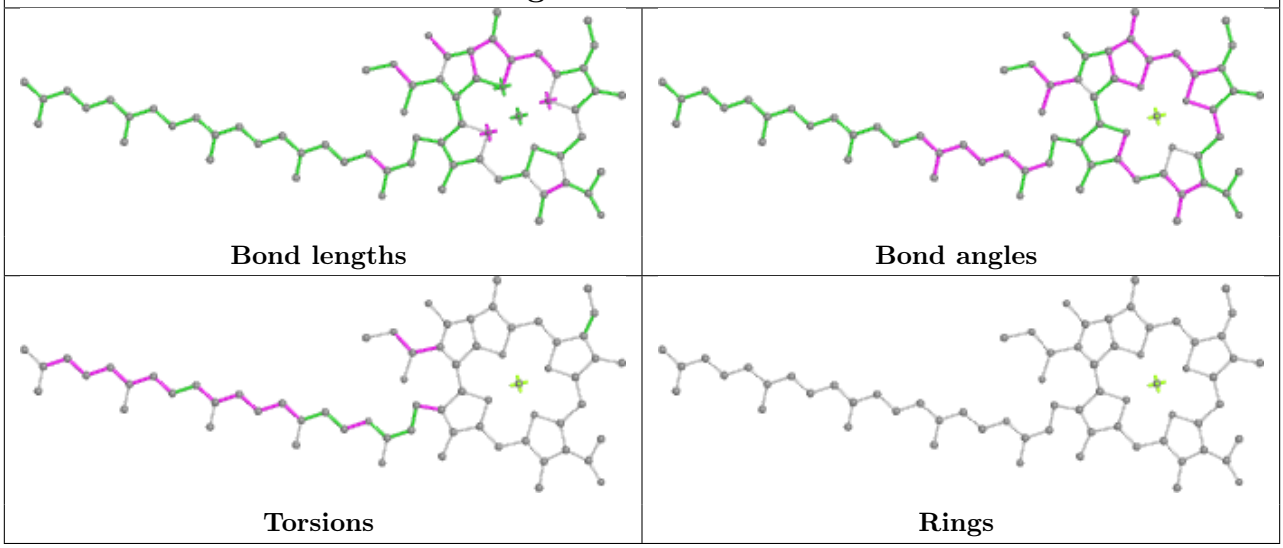
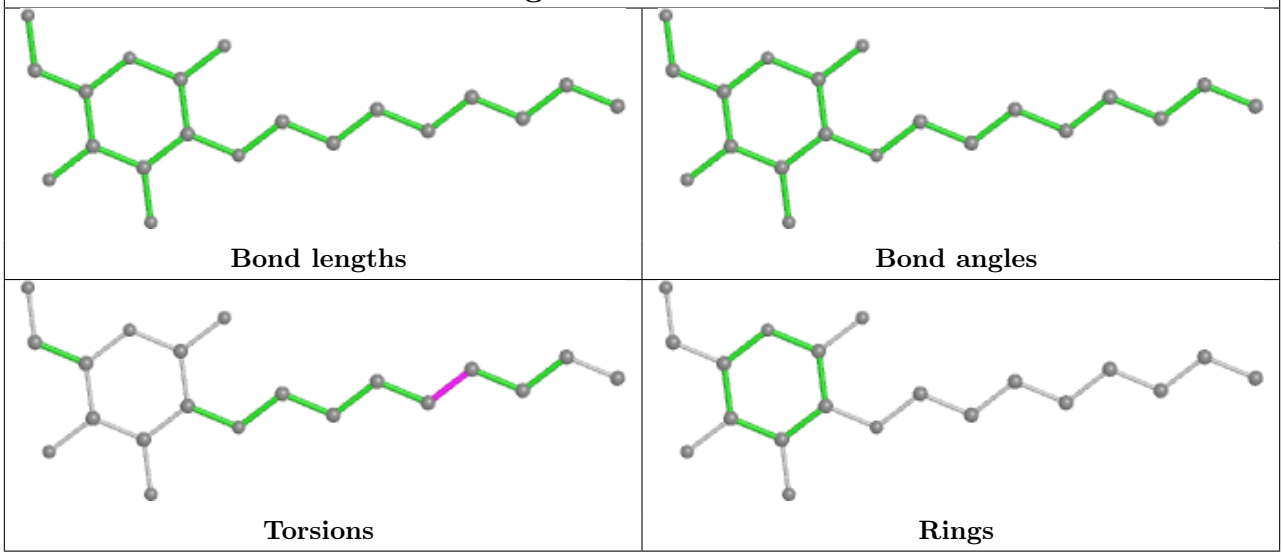


Rings

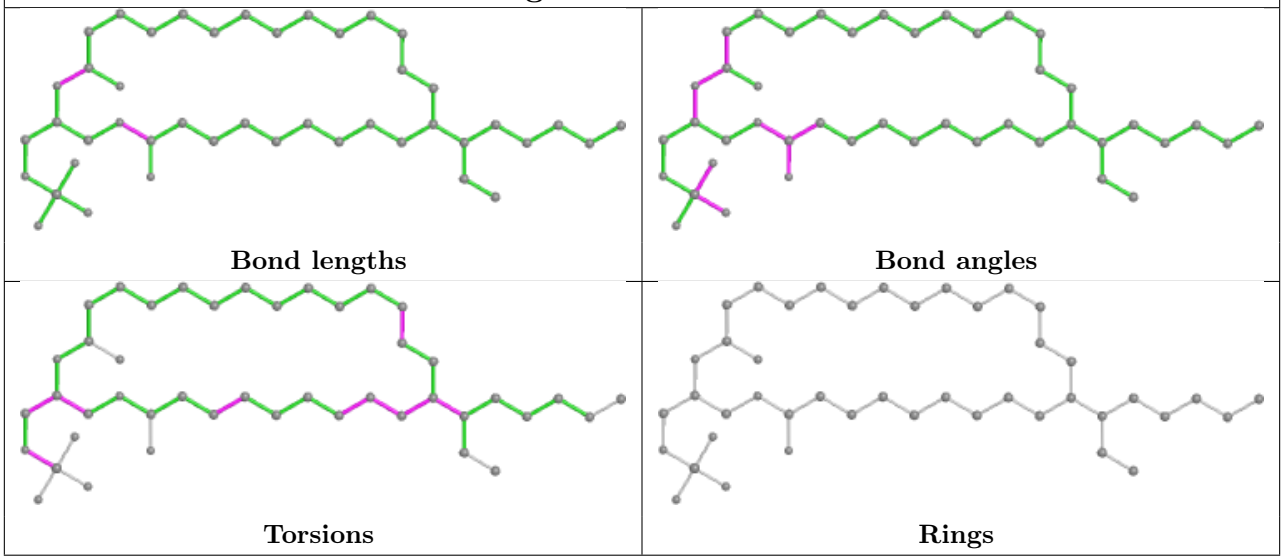
Ligand BCL E 102



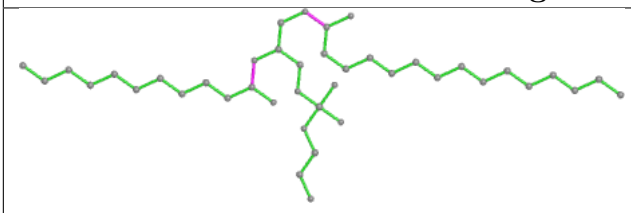
Ligand BGL C 507



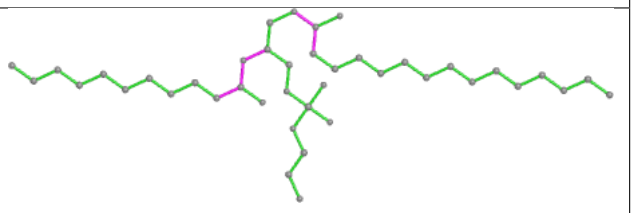
Ligand PGV h 102



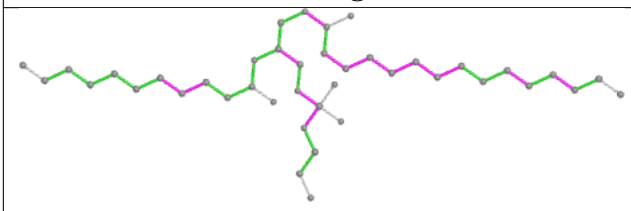
Ligand PEF h 103



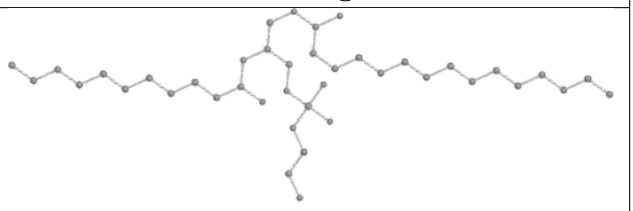
Bond lengths



Bond angles

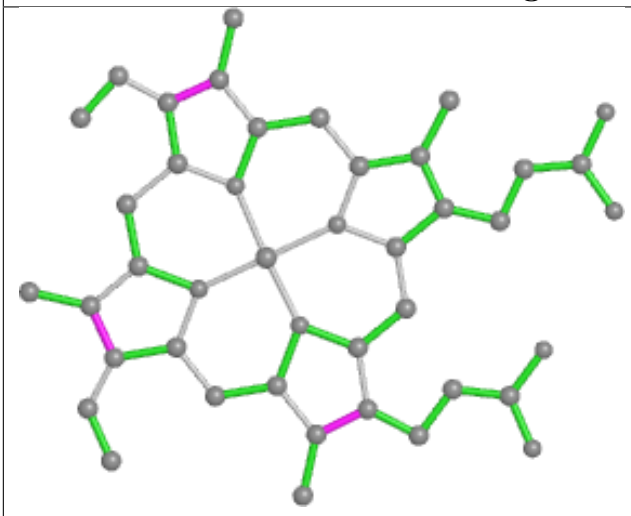


Torsions

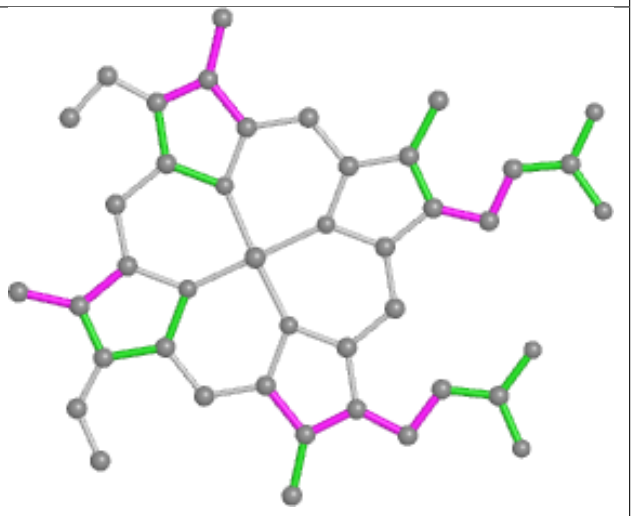


Rings

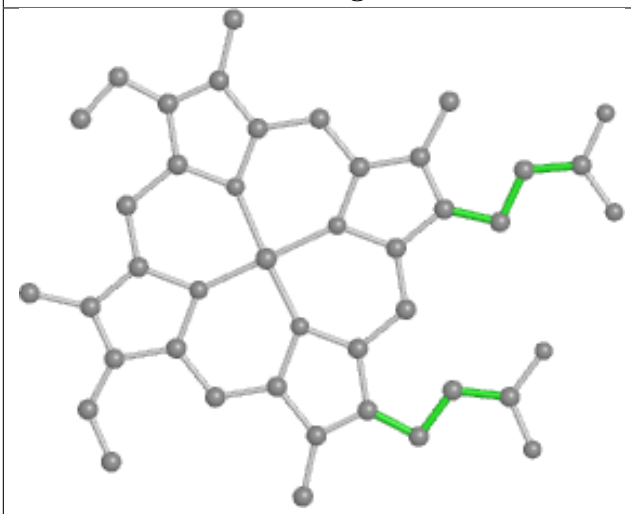
Ligand HEC C 502



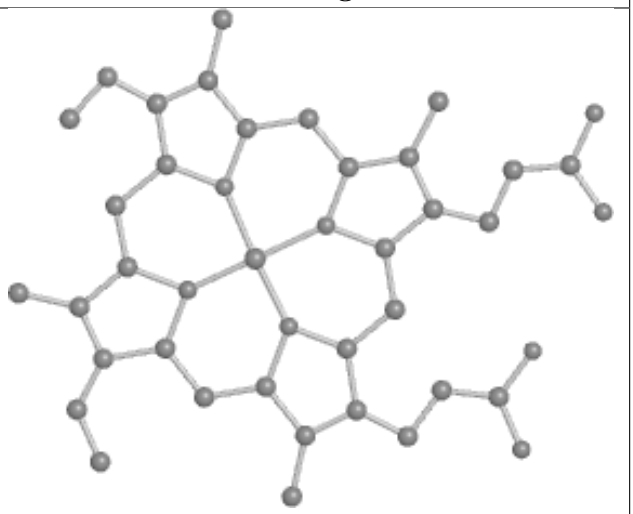
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

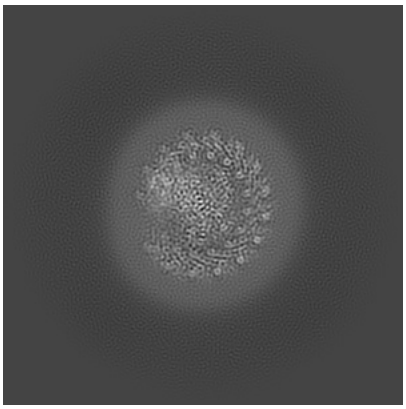
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35727. These allow visual inspection of the internal detail of the map and identification of artifacts.

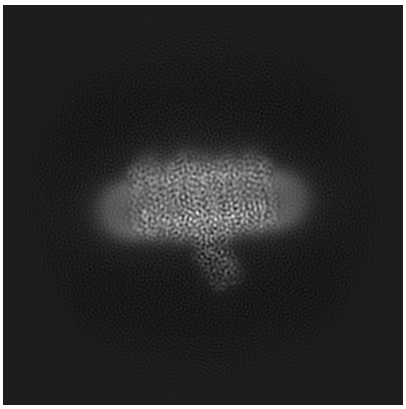
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



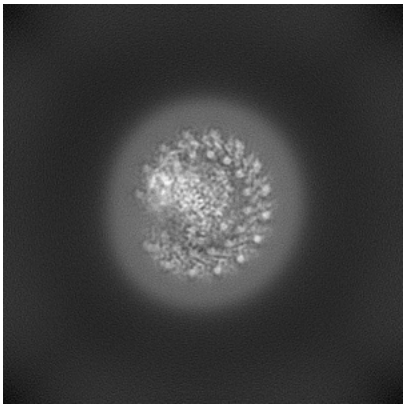
X



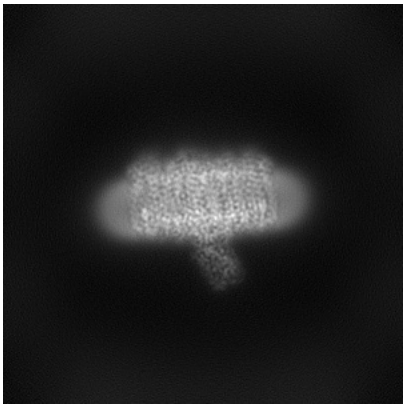
Y

Z

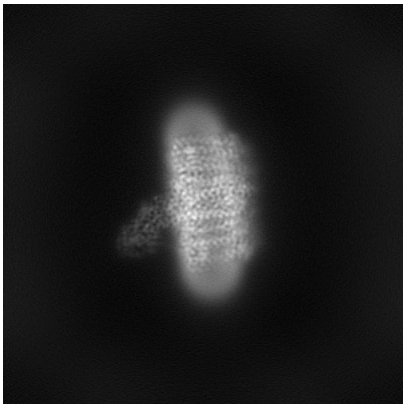
6.1.2 Raw map



X



Y

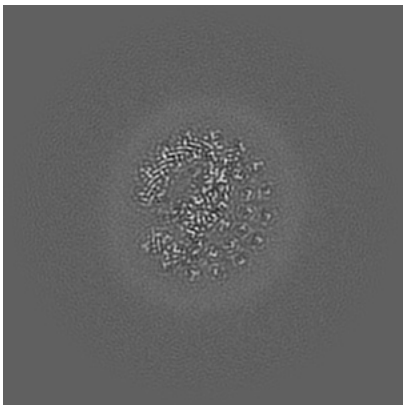


Z

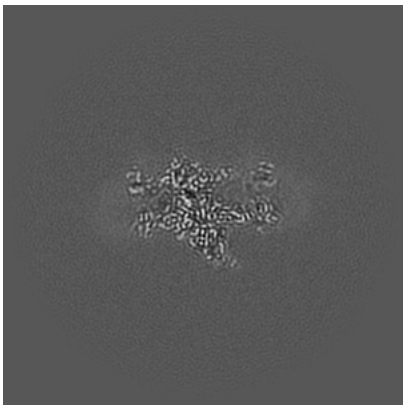
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

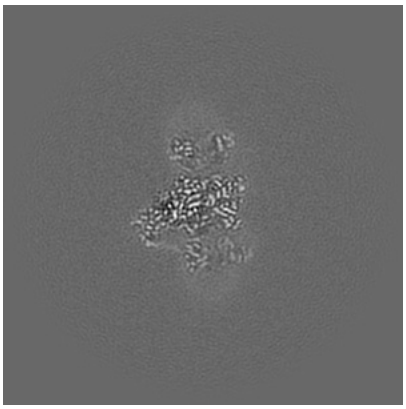
6.2.1 Primary map



X Index: 180

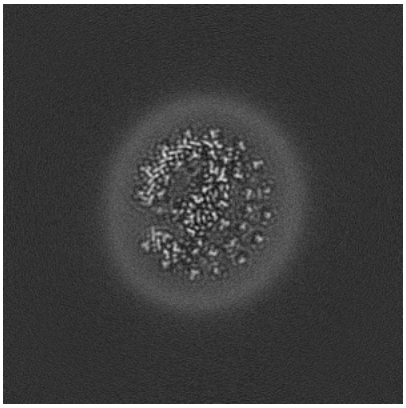


Y Index: 180

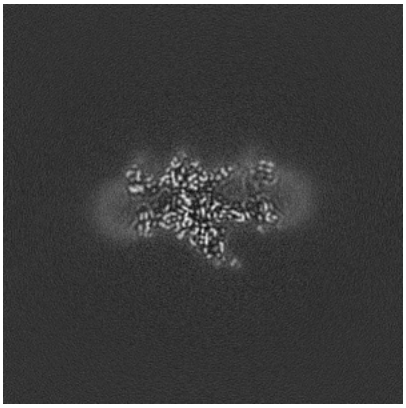


Z Index: 180

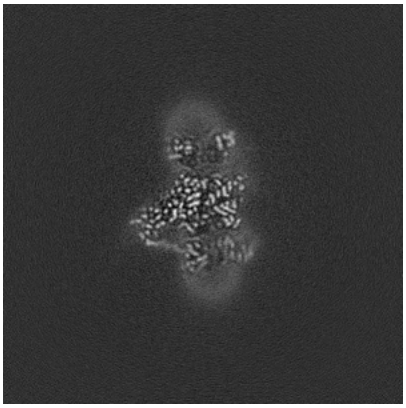
6.2.2 Raw map



X Index: 180



Y Index: 180

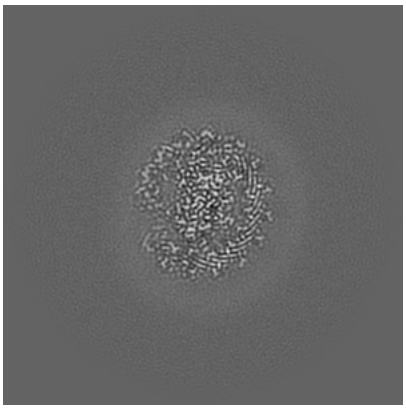


Z Index: 180

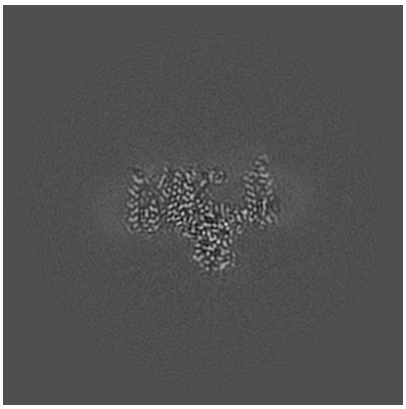
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

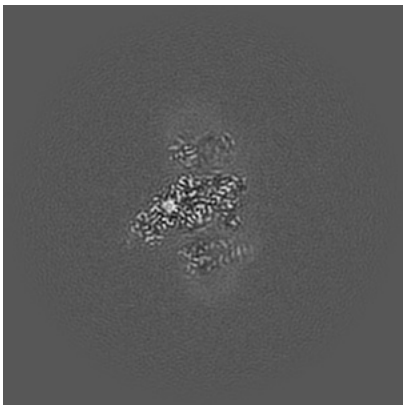
6.3.1 Primary map



X Index: 168

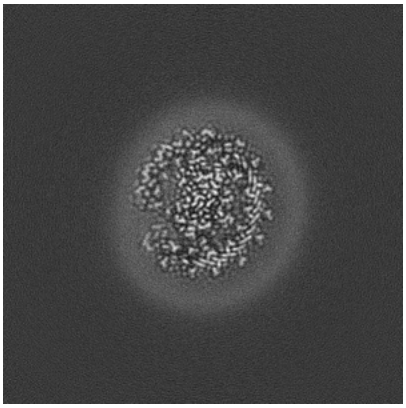


Y Index: 170

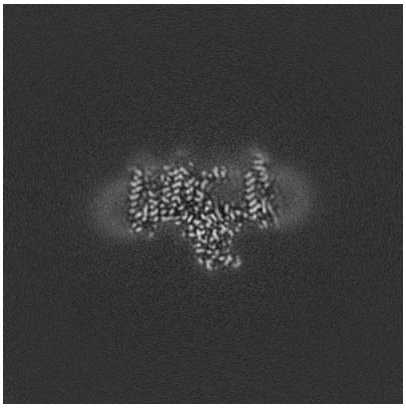


Z Index: 183

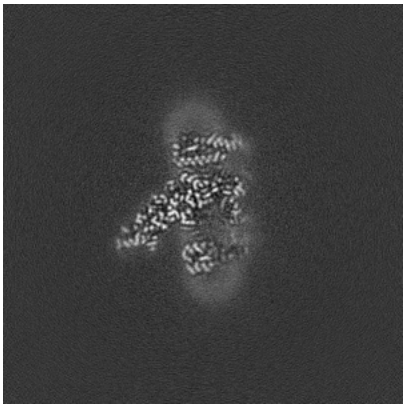
6.3.2 Raw map



X Index: 168



Y Index: 172

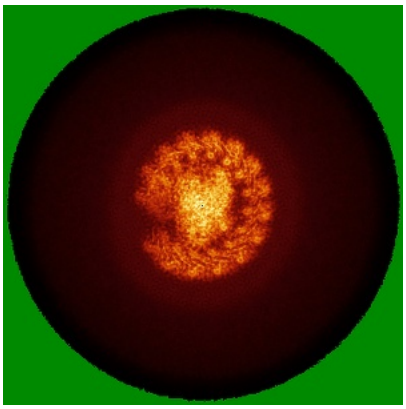


Z Index: 190

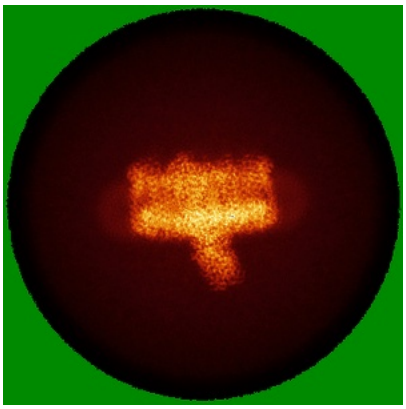
The images above show the largest variance slices of the map in three orthogonal directions.

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

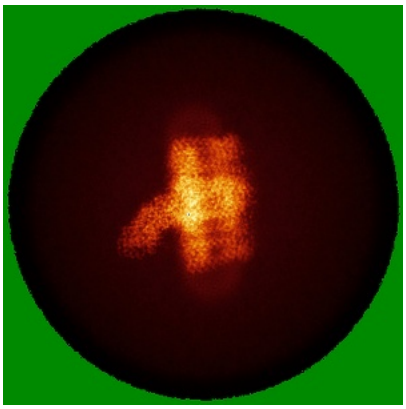
6.4.1 Primary map



X

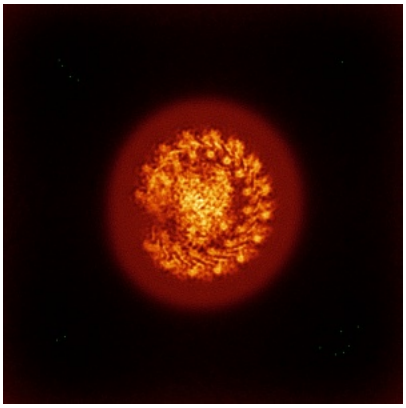


Y

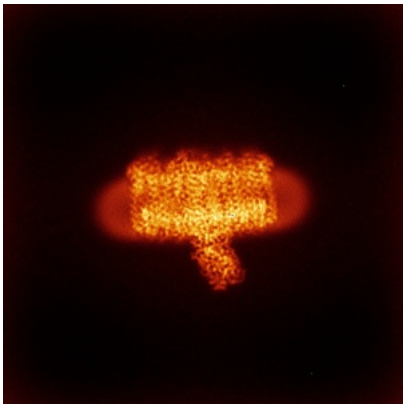


Z

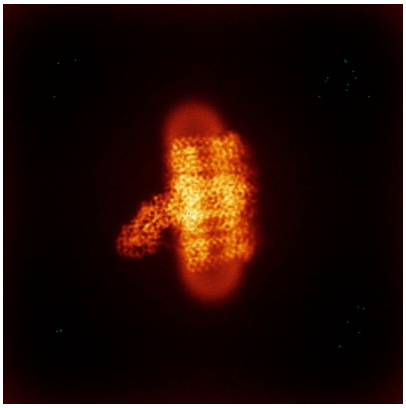
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.307. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

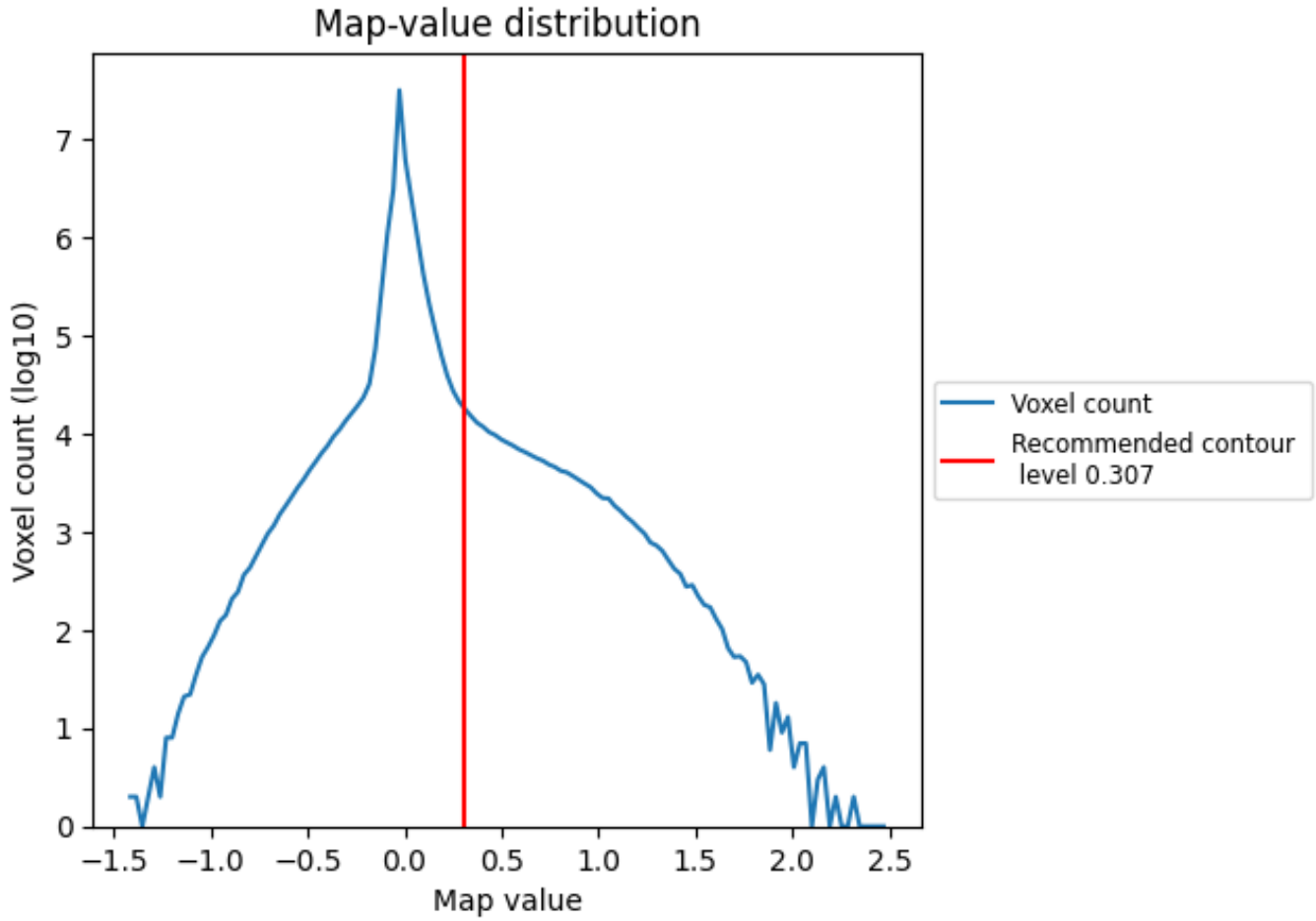
6.6 Mask visualisation (i)

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

7 Map analysis

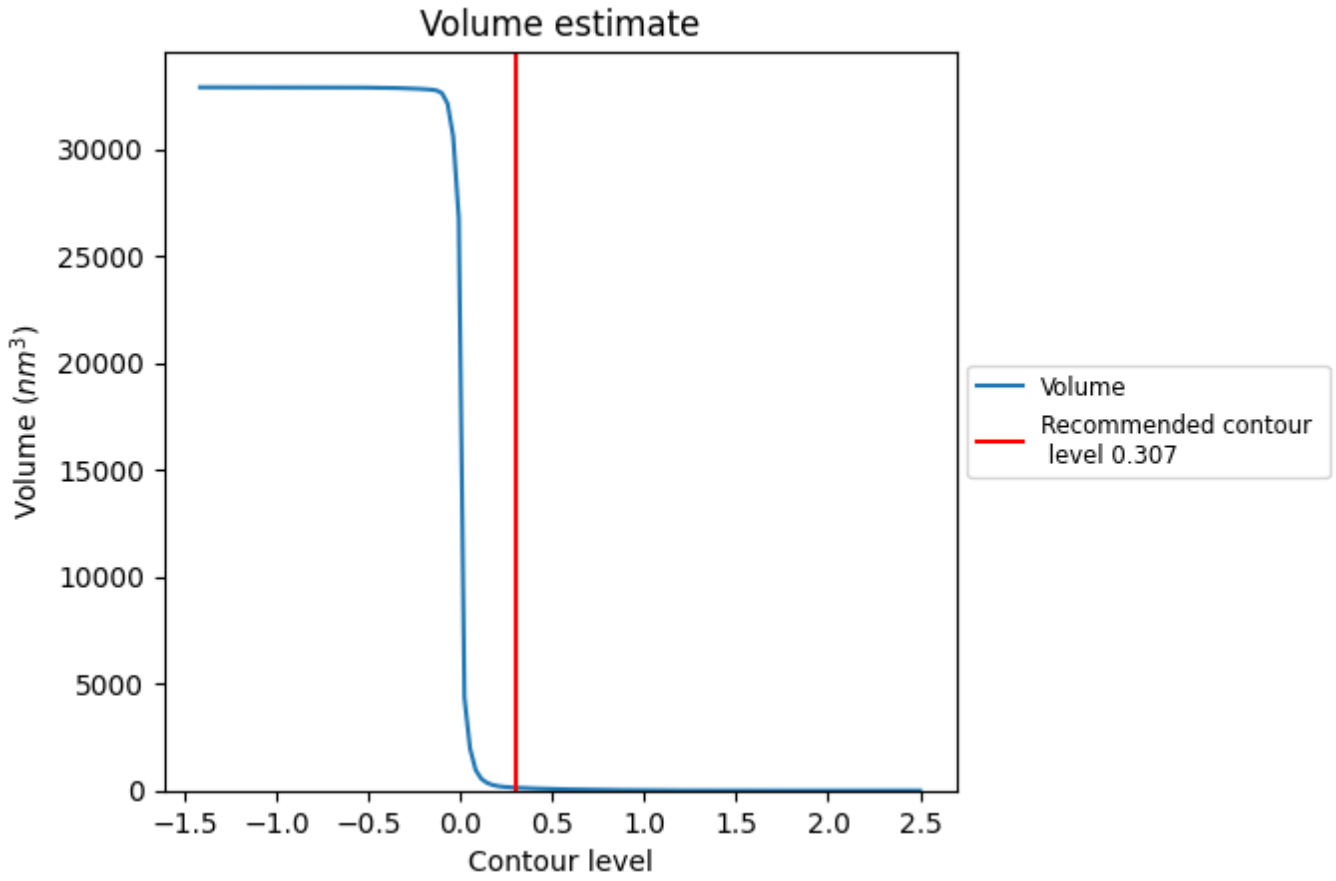
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

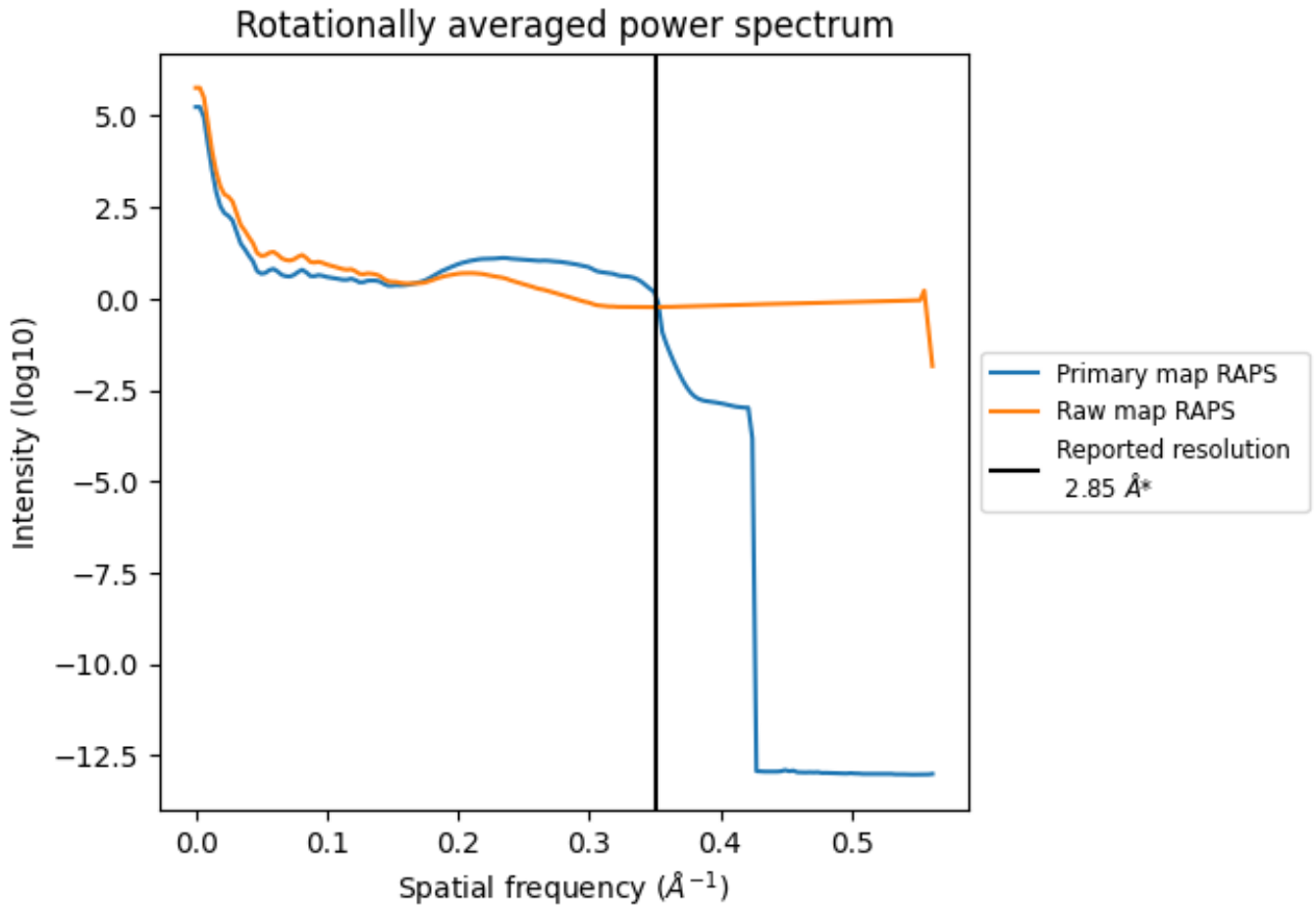
7.2 Volume estimate



The volume at the recommended contour level is 131 nm^3; this corresponds to an approximate mass of 118 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

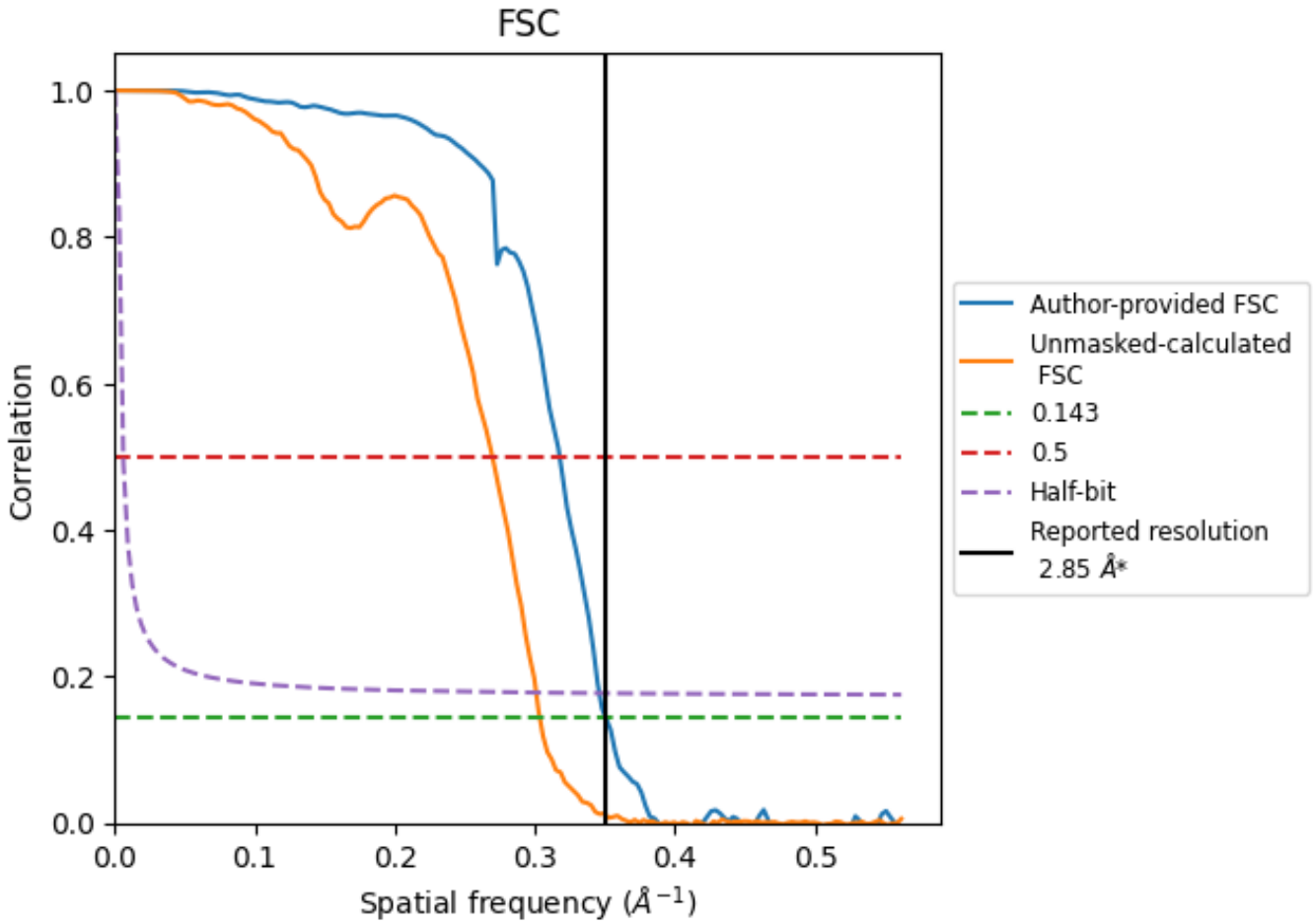


*Reported resolution corresponds to spatial frequency of 0.351 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.351 Å^{-1}

8.2 Resolution estimates (i)

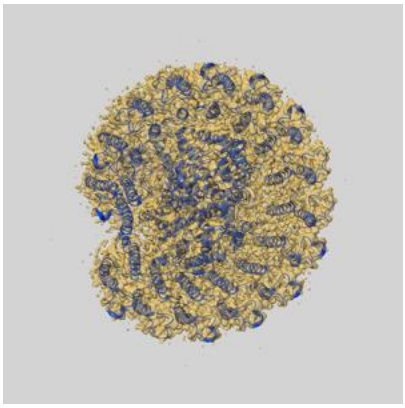
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.85	3.15	2.89
Unmasked-calculated*	3.29	3.71	3.32

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.29 differs from the reported value 2.85 by more than 10 %

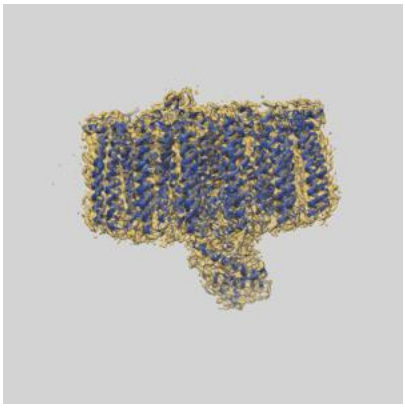
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35727 and PDB model 8IUN. Per-residue inclusion information can be found in section 3 on page 20.

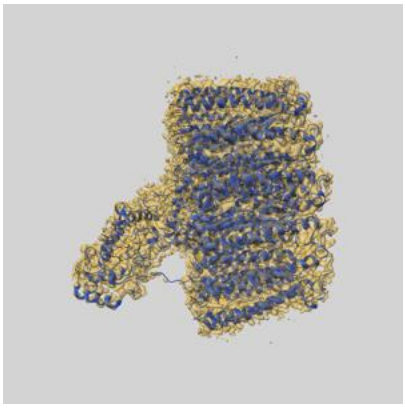
9.1 Map-model overlay



X



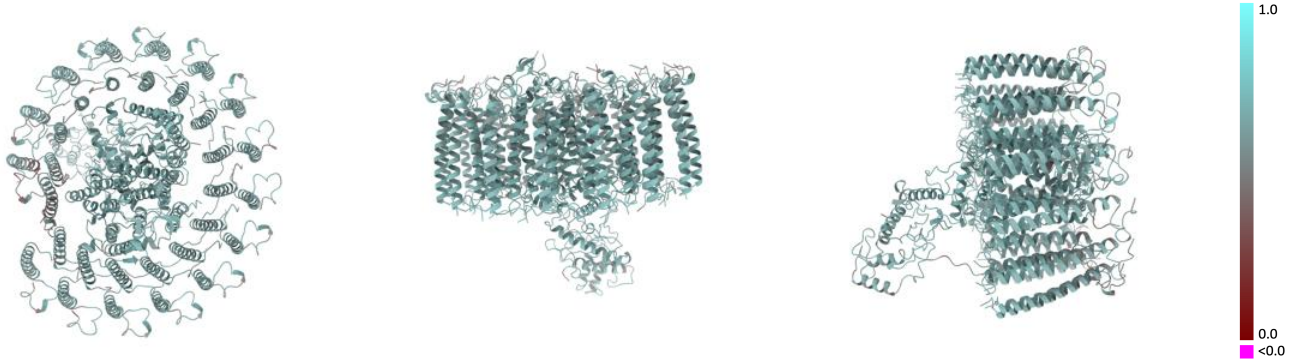
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.307 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

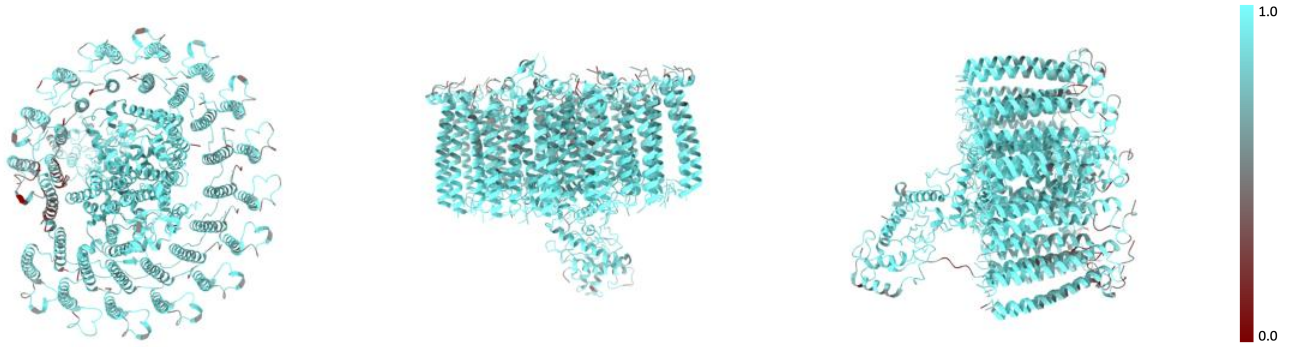
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

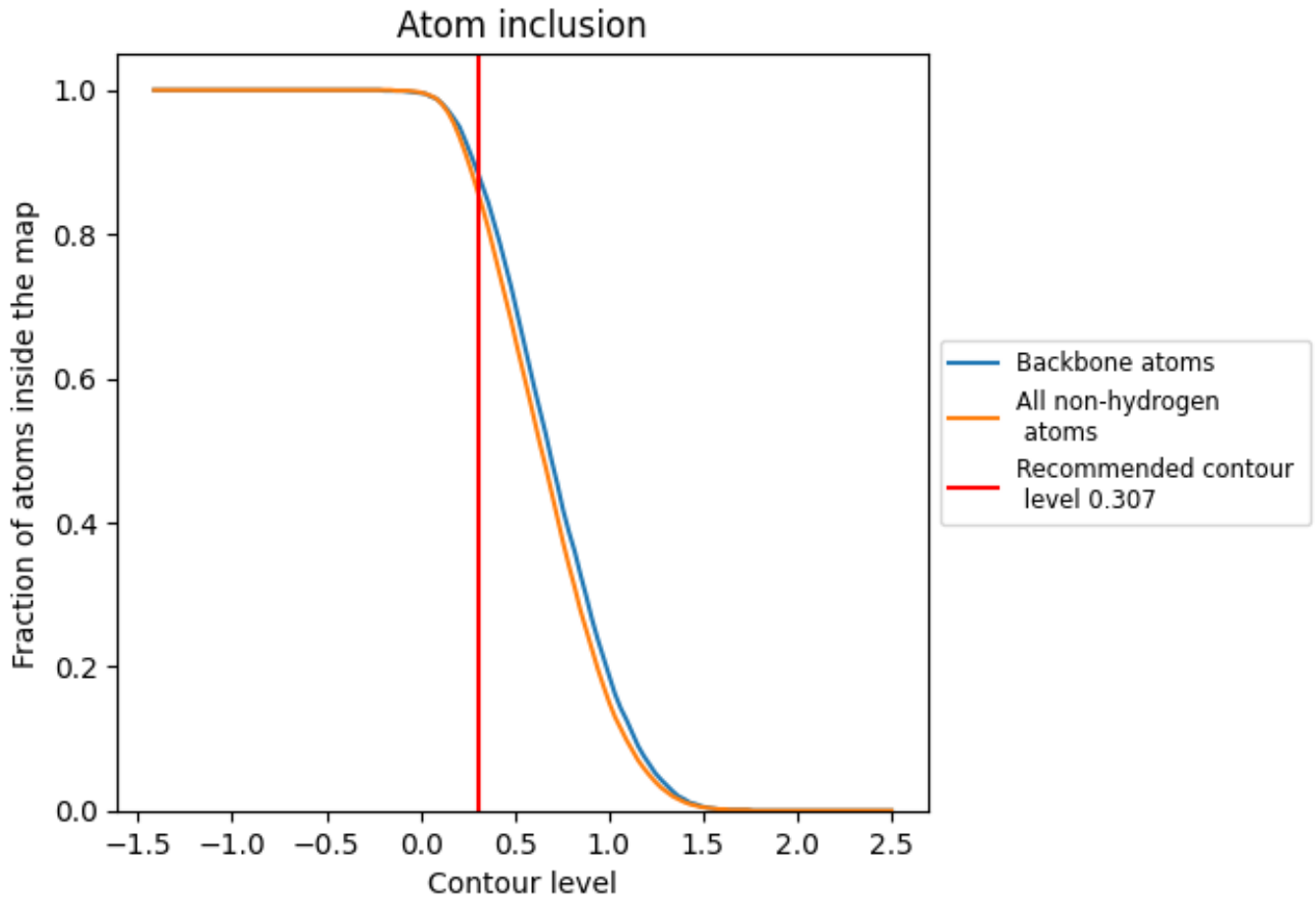
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.307).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.307) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8560	0.6130
0	0.8280	0.6020
1	0.6870	0.5670
2	0.6600	0.5410
3	0.7690	0.5950
4	0.7800	0.5820
5	0.8130	0.5950
6	0.8250	0.6050
7	0.8320	0.6040
8	0.8370	0.6020
9	0.8410	0.5980
A	0.9260	0.6340
B	0.8940	0.6170
C	0.8680	0.6150
D	0.8570	0.6190
E	0.8290	0.6040
F	0.8300	0.6040
G	0.8440	0.6080
H	0.7660	0.5880
I	0.8210	0.5970
J	0.8530	0.6170
K	0.8160	0.6020
L	0.9320	0.6380
M	0.9460	0.6440
N	0.8450	0.6170
O	0.8350	0.6090
P	0.8690	0.6180
Q	0.8500	0.6080
R	0.8900	0.6280
S	0.8440	0.6070
T	0.8620	0.6050
U	0.8240	0.6010
V	0.7400	0.5740
W	0.7860	0.5940
Y	0.8450	0.6080

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Z	0.9610	0.6370
h	0.8750	0.6210