



# Full wwPDB NMR Structure Validation Report ⓘ

Nov 20, 2022 – 11:30 am GMT

PDB ID : 5LCB  
EMDB ID : EMD-4033  
BMRB ID : 34012  
Title : In situ atomic-resolution structure of the baseplate antenna complex in *Chlorobaculum tepidum* obtained combining solid-state NMR spectroscopy, cryo electron microscopy and polarization spectroscopy  
Authors : Nielsen, J.T.; Kulminskaya, N.V.; Bjerring, M.; Linnanto, J.M.; Ratsep, M.; Pedersen, M.; Lambrev, P.H.; Dorogi, M.; Garab, G.; Thomsen, K.; Jegerschold, C.; Frigaard, N.U.; Lindahl, M.; Nielsen, N.C.  
Deposited on : 2016-06-20

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

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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>.

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

EMDB validation analysis : **NOT EXECUTED**  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : **NOT EXECUTED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

# 1 Overall quality at a glance

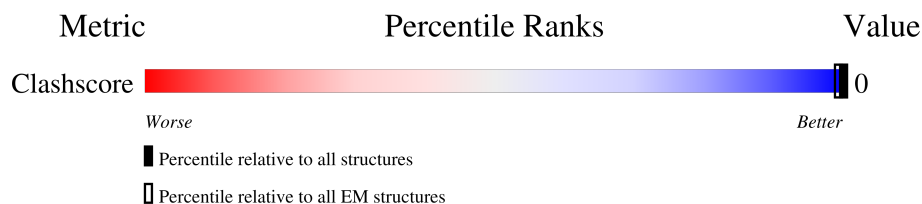
The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY, SOLID-STATE NMR*

The reported resolution of this entry is 26.50 Å.

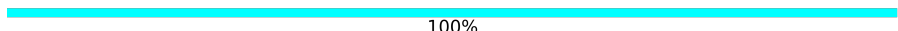
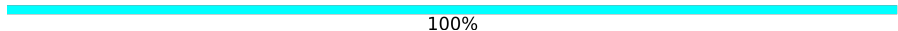
The overall completeness of chemical shifts assignment is 2%.

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)	NMR archive (#Entries)
Clashscore	158937	4297

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	59	 100%
1	B	59	 100%
1	C	59	 100%
1	D	59	 100%
1	E	59	 100%
1	F	59	 100%
1	G	59	 100%
1	H	59	 100%
1	I	59	 100%

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Mol	Chain	Length	Quality of chain
1	J	59	 100%
1	K	59	 100%
1	L	59	 100%
1	M	59	 100%
1	N	59	 100%

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

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	A	BCL	101	1	-
2	B	BCL	101	1	-
2	C	BCL	101	1	-
2	D	BCL	101	1	-
2	E	BCL	101	1	-
2	F	BCL	101	1	-
2	G	BCL	101	1	-
2	H	BCL	101	1	-
2	I	BCL	101	1	-
2	J	BCL	101	1	-
2	K	BCL	101	1	-
2	L	BCL	101	1	-
2	M	BCL	101	1	-
2	N	BCL	101	1	-

## 2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13860 atoms, of which 6930 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 Bacteriochlorophyll c-binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	59	Total 850	C 266	H 421	N 77	O 81	S 5	0	
1	B	59	Total 850	C 266	H 421	N 77	O 81	S 5	0	
1	C	59	Total 850	C 266	H 421	N 77	O 81	S 5	0	
1	D	59	Total 850	C 266	H 421	N 77	O 81	S 5	0	
1	E	59	Total 850	C 266	H 421	N 77	O 81	S 5	0	
1	F	59	Total 850	C 266	H 421	N 77	O 81	S 5	0	
1	G	59	Total 850	C 266	H 421	N 77	O 81	S 5	0	
1	H	59	Total 850	C 266	H 421	N 77	O 81	S 5	0	
1	I	59	Total 850	C 266	H 421	N 77	O 81	S 5	0	
1	J	59	Total 850	C 266	H 421	N 77	O 81	S 5	0	
1	K	59	Total 850	C 266	H 421	N 77	O 81	S 5	0	
1	L	59	Total 850	C 266	H 421	N 77	O 81	S 5	0	
1	M	59	Total 850	C 266	H 421	N 77	O 81	S 5	0	
1	N	59	Total 850	C 266	H 421	N 77	O 81	S 5	0	

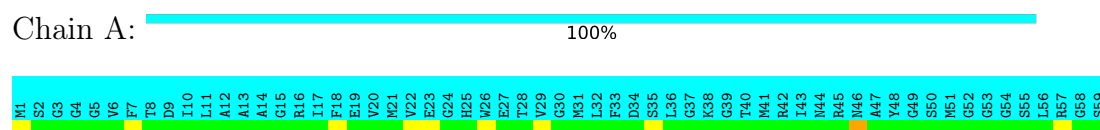
- Molecule 2 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



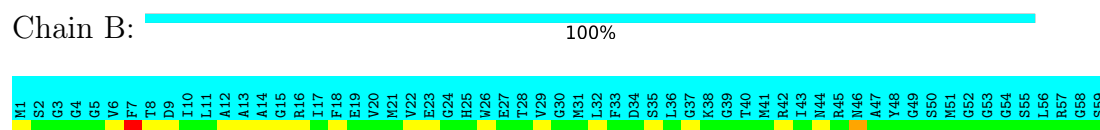
## 4 Residue-property plots

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

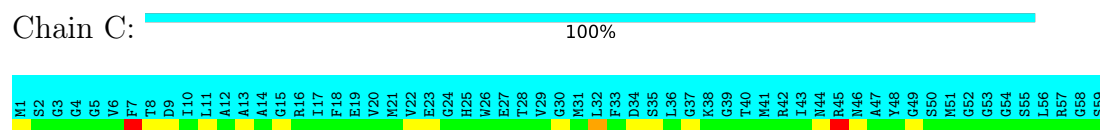
- Molecule 1: Bacteriochlorophyll c-binding protein



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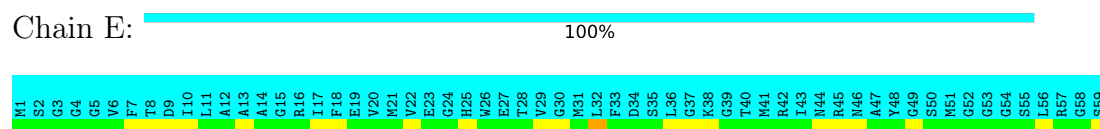
- Molecule 1: Bacteriochlorophyll c-binding protein



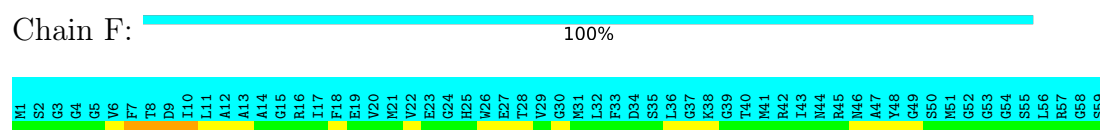
- Molecule 1: Bacteriochlorophyll c-binding protein



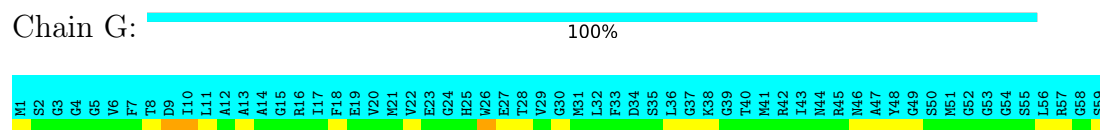
- Molecule 1: Bacteriochlorophyll c-binding protein



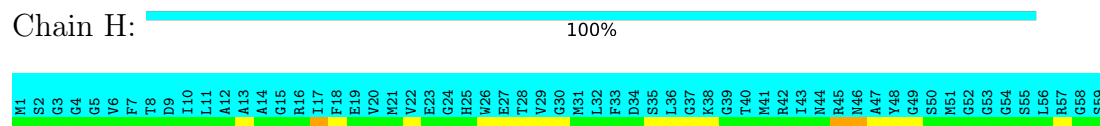
- Molecule 1: Bacteriochlorophyll c-binding protein



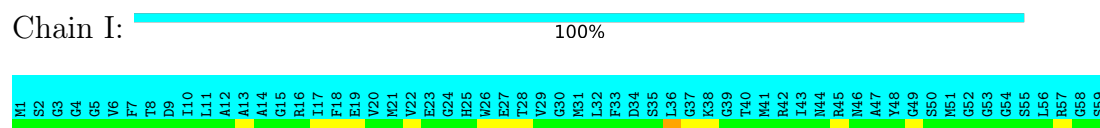
- Molecule 1: Bacteriochlorophyll c-binding protein



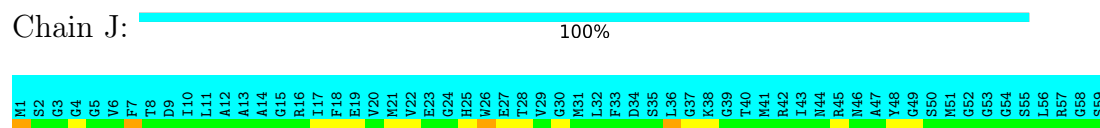
- Molecule 1: Bacteriochlorophyll c-binding protein



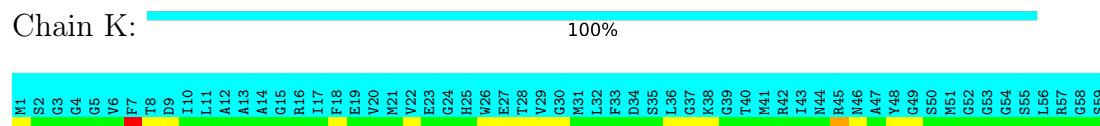
- Molecule 1: Bacteriochlorophyll c-binding protein



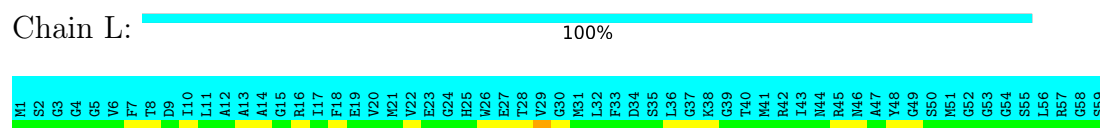
- Molecule 1: Bacteriochlorophyll c-binding protein



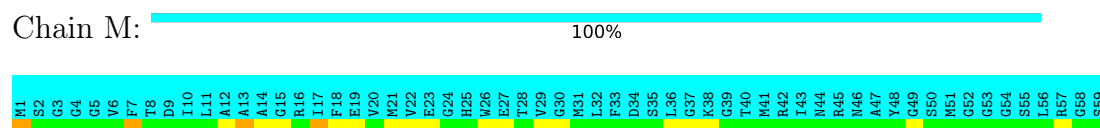
- Molecule 1: Bacteriochlorophyll c-binding protein



- Molecule 1: Bacteriochlorophyll c-binding protein



- Molecule 1: Bacteriochlorophyll c-binding protein



- Molecule 1: Bacteriochlorophyll c-binding protein





M1	S2	G3	G4	G5	V6	F7	T8	D9	I10	L11	A12	A13	A14	G15	R16	I17	F18	E19	V20	M21	V22	E23	G24	H25	W26	E27	T28	V29	G30	M31	L32	F33	D34	S35	L36	G37	K38	G39	T40	M41	R42	I43	N44	R45	N46	A47	Y48	G49	S50	M51	G52	G53	G54	S55	L56	R57	G58	S59
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## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 80 calculated structures, 1 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
Xplor-NIH	refinement	2.33
GASyCS	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	207
Number of shifts mapped to atoms	207
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	2%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
BCL

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	0	0	0	0
1	B	0	0	0	0
1	C	0	0	0	0
1	D	0	0	0	0
1	E	0	0	0	0
1	F	0	0	0	0
1	G	0	0	0	0
1	H	0	0	0	0
1	I	0	0	0	0
1	J	0	0	0	0
1	K	0	0	0	0
1	L	0	0	0	0
1	M	0	0	0	0
1	N	0	0	0	0
2	A	66	74	0	0
2	B	66	74	0	0
2	C	66	74	0	0
2	D	66	74	0	0
2	E	66	74	0	0
2	F	66	74	0	0
2	G	66	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
2	H	66	74	0	0
2	I	66	74	0	0
2	J	66	74	0	0
2	K	66	74	0	0
2	L	66	74	0	0
2	M	66	74	0	0
2	N	66	74	0	0
All	All	924	1036	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 -.

There are no clashes.

## 6.3 Torsion angles [i](#)

### 6.3.1 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 NMR 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	A	0	-	-	-	-
1	B	0	-	-	-	-
1	C	0	-	-	-	-
1	D	0	-	-	-	-
1	E	0	-	-	-	-
1	F	0	-	-	-	-
1	G	0	-	-	-	-
1	H	0	-	-	-	-
1	I	0	-	-	-	-
1	J	0	-	-	-	-
1	K	0	-	-	-	-
1	L	0	-	-	-	-
1	M	0	-	-	-	-
1	N	0	-	-	-	-
All	All	0	-	-	-	-

There are no Ramachandran outliers.

### 6.3.2 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 NMR 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	A	0	-	-	-
1	B	0	-	-	-
1	C	0	-	-	-
1	D	0	-	-	-
1	E	0	-	-	-
1	F	0	-	-	-
1	G	0	-	-	-
1	H	0	-	-	-
1	I	0	-	-	-
1	J	0	-	-	-
1	K	0	-	-	-
1	L	0	-	-	-
1	M	0	-	-	-
1	N	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	BCL	D	101	1	58,74,74	1.40	11 (18%)
2	BCL	J	101	1	58,74,74	1.72	9 (15%)
2	BCL	M	101	1	58,74,74	1.64	11 (18%)
2	BCL	H	101	1	58,74,74	1.46	12 (20%)
2	BCL	C	101	1	58,74,74	1.43	10 (17%)
2	BCL	A	101	1	58,74,74	1.57	10 (17%)
2	BCL	E	101	1	58,74,74	1.48	12 (20%)
2	BCL	L	101	1	58,74,74	1.54	11 (18%)
2	BCL	I	101	1	58,74,74	1.73	11 (18%)
2	BCL	K	101	1	58,74,74	1.59	11 (18%)
2	BCL	F	101	1	58,74,74	1.69	11 (18%)
2	BCL	B	101	1	58,74,74	1.58	10 (17%)
2	BCL	N	101	1	58,74,74	1.65	10 (17%)
2	BCL	G	101	1	58,74,74	1.60	10 (17%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	BCL	D	101	1	69,115,115	1.92	13 (18%)
2	BCL	J	101	1	69,115,115	1.81	13 (18%)
2	BCL	M	101	1	69,115,115	1.93	16 (23%)
2	BCL	H	101	1	69,115,115	1.91	12 (17%)
2	BCL	C	101	1	69,115,115	1.98	14 (20%)
2	BCL	A	101	1	69,115,115	1.95	12 (17%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	BCL	E	101	1	69,115,115	1.91	14 (20%)
2	BCL	L	101	1	69,115,115	1.87	12 (17%)
2	BCL	I	101	1	69,115,115	1.89	14 (20%)
2	BCL	K	101	1	69,115,115	1.87	13 (18%)
2	BCL	F	101	1	69,115,115	1.83	13 (18%)
2	BCL	B	101	1	69,115,115	1.95	13 (18%)
2	BCL	N	101	1	69,115,115	1.97	13 (18%)
2	BCL	G	101	1	69,115,115	1.86	13 (18%)

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
2	BCL	D	101	1	1,1,25,25	1,37,137,137	-
2	BCL	J	101	1	1,1,25,25	0,37,137,137	-
2	BCL	M	101	1	1,1,25,25	1,37,137,137	-
2	BCL	H	101	1	1,1,25,25	1,37,137,137	-
2	BCL	C	101	1	1,1,25,25	0,37,137,137	-
2	BCL	A	101	1	1,1,25,25	0,37,137,137	-
2	BCL	E	101	1	1,1,25,25	0,37,137,137	-
2	BCL	L	101	1	1,1,25,25	0,37,137,137	-
2	BCL	I	101	1	1,1,25,25	1,37,137,137	-
2	BCL	K	101	1	1,1,25,25	0,37,137,137	-
2	BCL	F	101	1	1,1,25,25	0,37,137,137	-
2	BCL	B	101	1	1,1,25,25	0,37,137,137	-
2	BCL	N	101	1	1,1,25,25	0,37,137,137	-
2	BCL	G	101	1	1,1,25,25	1,37,137,137	-

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	101	BCL	C3C-C4C	8.63	1.62	1.51
2	F	101	BCL	C3C-C4C	7.87	1.61	1.51
2	J	101	BCL	C3C-C4C	7.82	1.61	1.51
2	N	101	BCL	C3C-C4C	7.55	1.61	1.51
2	M	101	BCL	C3C-C4C	7.24	1.60	1.51
2	G	101	BCL	C3C-C4C	6.55	1.59	1.51
2	K	101	BCL	C3C-C4C	6.31	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	101	BCL	C3C-C4C	5.93	1.59	1.51
2	B	101	BCL	C3C-C4C	5.29	1.58	1.51
2	A	101	BCL	C3C-C4C	4.86	1.57	1.51
2	E	101	BCL	C3C-C4C	4.43	1.57	1.51
2	H	101	BCL	C3C-C4C	4.35	1.57	1.51
2	A	101	BCL	O2D-CGD	3.90	1.42	1.33
2	C	101	BCL	C3C-C4C	3.71	1.56	1.51
2	D	101	BCL	C3C-C4C	3.58	1.56	1.51
2	J	101	BCL	O2D-CGD	3.47	1.41	1.33
2	B	101	BCL	O2D-CGD	3.29	1.41	1.33
2	B	101	BCL	C3B-CAB	3.29	1.40	1.49
2	B	101	BCL	C3D-CAD	3.09	1.38	1.46
2	J	101	BCL	C3B-CAB	3.09	1.41	1.49
2	J	101	BCL	C3D-CAD	3.07	1.38	1.46
2	A	101	BCL	C3D-CAD	3.04	1.38	1.46
2	N	101	BCL	O2D-CGD	3.00	1.40	1.33
2	A	101	BCL	C3B-CAB	2.95	1.41	1.49
2	M	101	BCL	C3B-CAB	2.95	1.41	1.49
2	N	101	BCL	C3B-CAB	2.95	1.41	1.49
2	D	101	BCL	O2D-CGD	2.91	1.40	1.33
2	J	101	BCL	CAA-C2A	2.90	1.59	1.54
2	C	101	BCL	C5-C3	2.89	1.57	1.51
2	H	101	BCL	O2D-CGD	2.88	1.40	1.33
2	E	101	BCL	O2D-CGD	2.86	1.40	1.33
2	I	101	BCL	C3D-CAD	2.83	1.38	1.46
2	L	101	BCL	O2D-CGD	2.82	1.40	1.33
2	F	101	BCL	C3B-CAB	2.81	1.41	1.49
2	D	101	BCL	C3B-CAB	2.79	1.41	1.49
2	D	101	BCL	CAA-C2A	2.78	1.59	1.54
2	L	101	BCL	C3B-CAB	2.78	1.41	1.49
2	F	101	BCL	CAA-C2A	2.78	1.59	1.54
2	K	101	BCL	O2D-CGD	2.77	1.40	1.33
2	N	101	BCL	C3D-CAD	2.76	1.39	1.46
2	D	101	BCL	C5-C3	2.76	1.57	1.51
2	C	101	BCL	C3B-CAB	2.75	1.41	1.49
2	A	101	BCL	C5-C3	2.75	1.57	1.51
2	K	101	BCL	C3B-CAB	2.75	1.41	1.49
2	H	101	BCL	C2A-C1A	2.74	1.58	1.52
2	E	101	BCL	C3B-CAB	2.74	1.41	1.49
2	E	101	BCL	C3D-CAD	2.73	1.39	1.46
2	C	101	BCL	C3D-CAD	2.72	1.39	1.46
2	K	101	BCL	C2A-C1A	2.71	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	101	BCL	C3B-CAB	2.71	1.42	1.49
2	G	101	BCL	C3D-CAD	2.70	1.39	1.46
2	K	101	BCL	C3D-CAD	2.69	1.39	1.46
2	N	101	BCL	CAA-C2A	2.69	1.59	1.54
2	G	101	BCL	CAA-C2A	2.68	1.59	1.54
2	M	101	BCL	C3D-CAD	2.67	1.39	1.46
2	A	101	BCL	CAA-C2A	2.66	1.59	1.54
2	L	101	BCL	C3D-CAD	2.66	1.39	1.46
2	E	101	BCL	CAA-C2A	2.66	1.59	1.54
2	B	101	BCL	O2A-CGA	2.65	1.41	1.33
2	L	101	BCL	C2A-C1A	2.65	1.58	1.52
2	D	101	BCL	C2A-C1A	2.65	1.58	1.52
2	F	101	BCL	C3D-CAD	2.65	1.39	1.46
2	C	101	BCL	O2D-CGD	2.64	1.39	1.33
2	G	101	BCL	O2D-CGD	2.63	1.39	1.33
2	A	101	BCL	O2D-CED	2.63	1.39	1.45
2	C	101	BCL	C2A-C1A	2.63	1.58	1.52
2	H	101	BCL	C3B-CAB	2.62	1.42	1.49
2	C	101	BCL	CAA-C2A	2.61	1.58	1.54
2	B	101	BCL	O2D-CED	2.58	1.39	1.45
2	E	101	BCL	C5-C3	2.58	1.56	1.51
2	M	101	BCL	O2D-CGD	2.57	1.39	1.33
2	E	101	BCL	C2A-C1A	2.57	1.58	1.52
2	B	101	BCL	C5-C3	2.56	1.56	1.51
2	G	101	BCL	C3B-CAB	2.56	1.42	1.49
2	K	101	BCL	CAA-C2A	2.55	1.58	1.54
2	H	101	BCL	C3D-CAD	2.54	1.39	1.46
2	F	101	BCL	O2A-CGA	2.52	1.40	1.33
2	D	101	BCL	C3D-CAD	2.52	1.39	1.46
2	L	101	BCL	CAA-C2A	2.51	1.58	1.54
2	J	101	BCL	C2A-C1A	2.50	1.57	1.52
2	M	101	BCL	C5-C3	2.49	1.56	1.51
2	B	101	BCL	CAA-C2A	2.47	1.58	1.54
2	I	101	BCL	O2D-CGD	2.46	1.39	1.33
2	A	101	BCL	O2A-CGA	2.46	1.40	1.33
2	E	101	BCL	O2A-CGA	2.46	1.40	1.33
2	J	101	BCL	C5-C3	2.45	1.56	1.51
2	I	101	BCL	C5-C3	2.43	1.56	1.51
2	M	101	BCL	CAA-C2A	2.42	1.58	1.54
2	I	101	BCL	C2A-C1A	2.41	1.57	1.52
2	F	101	BCL	O2D-CGD	2.40	1.39	1.33
2	H	101	BCL	CAA-C2A	2.40	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	BCL	C2A-C1A	2.40	1.57	1.52
2	D	101	BCL	O2D-CED	2.39	1.39	1.45
2	H	101	BCL	O2A-CGA	2.39	1.40	1.33
2	G	101	BCL	C5-C3	2.38	1.56	1.51
2	F	101	BCL	C5-C3	2.37	1.56	1.51
2	N	101	BCL	C5-C3	2.35	1.56	1.51
2	I	101	BCL	O2A-CGA	2.32	1.40	1.33
2	C	101	BCL	O2A-CGA	2.30	1.40	1.33
2	C	101	BCL	O2D-CED	2.29	1.39	1.45
2	L	101	BCL	O2D-CED	2.29	1.39	1.45
2	H	101	BCL	O2D-CED	2.28	1.39	1.45
2	H	101	BCL	C5-C3	2.28	1.56	1.51
2	M	101	BCL	O2A-CGA	2.28	1.40	1.33
2	K	101	BCL	C5-C3	2.27	1.56	1.51
2	L	101	BCL	C5-C3	2.26	1.56	1.51
2	K	101	BCL	O2D-CED	2.26	1.40	1.45
2	F	101	BCL	C2A-C1A	2.24	1.57	1.52
2	K	101	BCL	O2A-CGA	2.24	1.39	1.33
2	M	101	BCL	C2A-C1A	2.23	1.57	1.52
2	G	101	BCL	C1B-NB	2.23	1.37	1.35
2	E	101	BCL	O2D-CED	2.23	1.40	1.45
2	N	101	BCL	O2D-CED	2.20	1.40	1.45
2	G	101	BCL	CAC-C3C	2.19	1.58	1.54
2	M	101	BCL	O2A-C1	2.19	1.40	1.46
2	M	101	BCL	CAC-C3C	2.18	1.58	1.54
2	G	101	BCL	O2D-CED	2.17	1.40	1.45
2	H	101	BCL	O2A-C1	2.17	1.40	1.46
2	I	101	BCL	CAC-C3C	2.17	1.58	1.54
2	K	101	BCL	O2A-C1	2.17	1.40	1.46
2	J	101	BCL	C1B-NB	2.16	1.37	1.35
2	B	101	BCL	C1-C2	2.15	1.55	1.49
2	D	101	BCL	O2A-CGA	2.15	1.39	1.33
2	F	101	BCL	O2A-C1	2.15	1.40	1.46
2	I	101	BCL	CAA-C2A	2.14	1.58	1.54
2	E	101	BCL	C1-C2	2.14	1.55	1.49
2	H	101	BCL	CAC-C3C	2.14	1.58	1.54
2	N	101	BCL	C4B-NB	2.14	1.37	1.35
2	L	101	BCL	O2A-CGA	2.11	1.39	1.33
2	F	101	BCL	C1-C2	2.11	1.55	1.49
2	E	101	BCL	O2A-C1	2.11	1.40	1.46
2	N	101	BCL	CAC-C3C	2.10	1.58	1.54
2	J	101	BCL	O2A-C1	2.09	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	101	BCL	O2A-C1	2.09	1.40	1.46
2	M	101	BCL	O2D-CED	2.08	1.40	1.45
2	A	101	BCL	C1-C2	2.07	1.55	1.49
2	N	101	BCL	O2A-C1	2.06	1.40	1.46
2	F	101	BCL	C2-C3	2.04	1.37	1.33
2	G	101	BCL	C2A-C1A	2.04	1.56	1.52
2	I	101	BCL	C1-C2	2.04	1.55	1.49
2	D	101	BCL	C2-C3	2.03	1.37	1.33
2	C	101	BCL	O2A-C1	2.03	1.40	1.46
2	L	101	BCL	C1B-NB	2.03	1.37	1.35
2	D	101	BCL	C1-C2	2.02	1.55	1.49
2	H	101	BCL	C1-C2	2.02	1.55	1.49
2	I	101	BCL	O2D-CED	2.02	1.40	1.45
2	E	101	BCL	C1B-NB	2.00	1.37	1.35
2	K	101	BCL	C4-C3	2.01	1.55	1.50
2	A	101	BCL	C2-C3	2.00	1.37	1.33

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	101	BCL	C4A-NA-C1A	9.70	111.07	106.71
2	M	101	BCL	C4A-NA-C1A	9.42	110.94	106.71
2	C	101	BCL	C4A-NA-C1A	9.30	110.89	106.71
2	A	101	BCL	C4A-NA-C1A	9.23	110.86	106.71
2	E	101	BCL	C4A-NA-C1A	8.80	110.66	106.71
2	H	101	BCL	C4A-NA-C1A	8.69	110.61	106.71
2	G	101	BCL	C4A-NA-C1A	8.65	110.60	106.71
2	B	101	BCL	C4A-NA-C1A	8.57	110.56	106.71
2	K	101	BCL	C4A-NA-C1A	8.48	110.52	106.71
2	I	101	BCL	C4A-NA-C1A	8.45	110.50	106.71
2	F	101	BCL	C4A-NA-C1A	8.42	110.49	106.71
2	L	101	BCL	C4A-NA-C1A	8.28	110.43	106.71
2	D	101	BCL	C4A-NA-C1A	8.23	110.41	106.71
2	J	101	BCL	C4A-NA-C1A	7.45	110.06	106.71
2	A	101	BCL	CAD-C3D-C4D	6.08	105.08	108.47
2	B	101	BCL	OBB-CAB-C3B	5.55	129.85	119.99
2	J	101	BCL	OBB-CAB-C3B	5.52	129.79	119.99
2	D	101	BCL	CAD-C3D-C4D	5.30	105.51	108.47
2	B	101	BCL	CAD-C3D-C4D	5.29	105.52	108.47
2	H	101	BCL	OBB-CAB-C3B	5.19	129.20	119.99
2	C	101	BCL	CAD-C3D-C4D	5.18	105.58	108.47
2	K	101	BCL	OBB-CAB-C3B	5.13	129.09	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	101	BCL	OBB-CAB-C3B	5.13	129.09	119.99
2	I	101	BCL	OBB-CAB-C3B	5.12	129.08	119.99
2	L	101	BCL	OBB-CAB-C3B	5.08	129.00	119.99
2	N	101	BCL	OBB-CAB-C3B	5.03	128.91	119.99
2	A	101	BCL	OBB-CAB-C3B	4.92	128.73	119.99
2	F	101	BCL	OBB-CAB-C3B	4.90	128.69	119.99
2	G	101	BCL	OBB-CAB-C3B	4.87	128.64	119.99
2	E	101	BCL	OBB-CAB-C3B	4.87	128.63	119.99
2	D	101	BCL	OBB-CAB-C3B	4.83	128.57	119.99
2	C	101	BCL	OBB-CAB-C3B	4.76	128.44	119.99
2	L	101	BCL	CAD-C3D-C4D	4.66	105.87	108.47
2	H	101	BCL	CAD-C3D-C4D	4.64	105.88	108.47
2	N	101	BCL	CAD-C3D-C4D	4.50	105.96	108.47
2	E	101	BCL	CAD-C3D-C4D	4.44	106.00	108.47
2	D	101	BCL	C1C-NC-C4C	4.36	108.67	106.71
2	H	101	BCL	C1C-NC-C4C	4.35	108.66	106.71
2	G	101	BCL	C1C-NC-C4C	4.16	108.58	106.71
2	E	101	BCL	C1C-NC-C4C	4.08	108.54	106.71
2	K	101	BCL	CAD-C3D-C4D	4.05	106.21	108.47
2	G	101	BCL	CAD-C3D-C4D	3.86	106.32	108.47
2	K	101	BCL	C1C-NC-C4C	3.85	108.44	106.71
2	I	101	BCL	CAD-C3D-C4D	3.80	106.35	108.47
2	B	101	BCL	C1C-NC-C4C	3.71	108.37	106.71
2	L	101	BCL	C1C-NC-C4C	3.54	108.30	106.71
2	J	101	BCL	CAD-C3D-C4D	3.49	106.52	108.47
2	F	101	BCL	CAD-C3D-C4D	3.47	106.53	108.47
2	C	101	BCL	C1C-NC-C4C	3.41	108.24	106.71
2	I	101	BCL	C1C-NC-C4C	3.37	108.22	106.71
2	J	101	BCL	CBB-CAB-C3B	3.37	110.33	120.34
2	C	101	BCL	C6-C5-C3	3.29	104.82	113.45
2	B	101	BCL	C6-C5-C3	3.27	104.89	113.45
2	M	101	BCL	CAD-C3D-C4D	3.26	106.65	108.47
2	I	101	BCL	C6-C5-C3	3.26	104.92	113.45
2	D	101	BCL	C6-C5-C3	3.23	104.99	113.45
2	E	101	BCL	C6-C5-C3	3.23	104.99	113.45
2	A	101	BCL	C6-C5-C3	3.22	105.01	113.45
2	N	101	BCL	C6-C5-C3	3.22	105.02	113.45
2	F	101	BCL	C6-C5-C3	3.20	105.06	113.45
2	L	101	BCL	C6-C5-C3	3.20	105.08	113.45
2	M	101	BCL	C6-C5-C3	3.19	105.08	113.45
2	H	101	BCL	C6-C5-C3	3.19	105.08	113.45
2	K	101	BCL	C6-C5-C3	3.19	105.09	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	101	BCL	C6-C5-C3	3.19	105.10	113.45
2	G	101	BCL	C6-C5-C3	3.16	105.18	113.45
2	J	101	BCL	C1C-NC-C4C	3.15	108.12	106.71
2	A	101	BCL	C1C-NC-C4C	3.13	108.11	106.71
2	C	101	BCL	C4B-CHC-C1C	3.13	123.93	130.12
2	M	101	BCL	CBB-CAB-C3B	3.05	111.29	120.34
2	B	101	BCL	C4B-CHC-C1C	3.05	124.09	130.12
2	I	101	BCL	CBB-CAB-C3B	3.04	111.33	120.34
2	B	101	BCL	CBB-CAB-C3B	3.01	111.39	120.34
2	M	101	BCL	C4B-CHC-C1C	3.01	124.15	130.12
2	N	101	BCL	CBB-CAB-C3B	3.00	111.43	120.34
2	L	101	BCL	CBB-CAB-C3B	2.98	111.48	120.34
2	K	101	BCL	CBB-CAB-C3B	2.98	111.50	120.34
2	H	101	BCL	CBB-CAB-C3B	2.97	111.52	120.34
2	N	101	BCL	C4B-CHC-C1C	2.97	124.24	130.12
2	F	101	BCL	C4B-CHC-C1C	2.95	124.28	130.12
2	F	101	BCL	O2D-CGD-CBD	2.90	116.42	111.27
2	L	101	BCL	C4B-CHC-C1C	2.88	124.40	130.12
2	N	101	BCL	O2D-CGD-CBD	2.87	116.36	111.27
2	K	101	BCL	C4B-CHC-C1C	2.86	124.45	130.12
2	M	101	BCL	O2D-CGD-CBD	2.85	116.33	111.27
2	L	101	BCL	OBD-CAD-CBD	2.84	121.84	125.89
2	F	101	BCL	CBB-CAB-C3B	2.83	111.94	120.34
2	A	101	BCL	C4B-CHC-C1C	2.81	124.55	130.12
2	H	101	BCL	OBD-CAD-CBD	2.80	121.89	125.89
2	D	101	BCL	CBB-CAB-C3B	2.80	112.04	120.34
2	J	101	BCL	CMB-C2B-C1B	2.80	124.17	128.46
2	D	101	BCL	OBD-CAD-CBD	2.79	121.90	125.89
2	G	101	BCL	C4B-CHC-C1C	2.79	124.59	130.12
2	M	101	BCL	OBD-CAD-CBD	2.78	121.93	125.89
2	J	101	BCL	C4B-CHC-C1C	2.77	124.64	130.12
2	A	101	BCL	CBB-CAB-C3B	2.77	112.13	120.34
2	F	101	BCL	OBD-CAD-CBD	2.76	121.95	125.89
2	G	101	BCL	OBD-CAD-CBD	2.76	121.95	125.89
2	C	101	BCL	CBB-CAB-C3B	2.74	112.19	120.34
2	M	101	BCL	C1C-NC-C4C	2.74	107.94	106.71
2	E	101	BCL	CBB-CAB-C3B	2.73	112.23	120.34
2	F	101	BCL	C1C-NC-C4C	2.72	107.93	106.71
2	K	101	BCL	OBD-CAD-CBD	2.72	122.01	125.89
2	N	101	BCL	C1C-NC-C4C	2.72	107.93	106.71
2	J	101	BCL	CMB-C2B-C3B	2.71	129.76	124.68
2	I	101	BCL	C4B-CHC-C1C	2.70	124.77	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	101	BCL	O2D-CGD-CBD	2.69	116.05	111.27
2	G	101	BCL	CBB-CAB-C3B	2.68	112.38	120.34
2	N	101	BCL	OBD-CAD-CBD	2.68	122.06	125.89
2	N	101	BCL	CMB-C2B-C3B	2.67	129.68	124.68
2	I	101	BCL	CMB-C2B-C3B	2.67	129.67	124.68
2	E	101	BCL	OBD-CAD-CBD	2.66	122.09	125.89
2	I	101	BCL	OBD-CAD-CBD	2.66	122.10	125.89
2	J	101	BCL	O2D-CGD-CBD	2.66	115.99	111.27
2	I	101	BCL	O2D-CGD-CBD	2.65	115.98	111.27
2	C	101	BCL	O2D-CGD-CBD	2.64	115.95	111.27
2	K	101	BCL	CMA-C3A-C4A	2.57	104.86	111.77
2	D	101	BCL	C4B-CHC-C1C	2.55	125.07	130.12
2	L	101	BCL	CMA-C3A-C4A	2.55	104.92	111.77
2	L	101	BCL	O2D-CGD-CBD	2.55	115.79	111.27
2	E	101	BCL	C4B-CHC-C1C	2.53	125.10	130.12
2	B	101	BCL	O2D-CGD-CBD	2.53	115.77	111.27
2	K	101	BCL	O2D-CGD-CBD	2.52	115.75	111.27
2	C	101	BCL	CMB-C2B-C3B	2.52	129.39	124.68
2	C	101	BCL	OBD-CAD-CBD	2.51	122.31	125.89
2	E	101	BCL	CMB-C2B-C3B	2.51	129.37	124.68
2	I	101	BCL	CMB-C2B-C1B	2.51	124.61	128.46
2	M	101	BCL	CMB-C2B-C3B	2.50	129.36	124.68
2	G	101	BCL	O2D-CGD-CBD	2.48	115.68	111.27
2	D	101	BCL	O2D-CGD-CBD	2.47	115.67	111.27
2	B	101	BCL	C4B-C3B-CAB	2.47	122.36	127.13
2	I	101	BCL	C2C-C3C-C4C	2.46	97.65	101.34
2	H	101	BCL	CMA-C3A-C4A	2.45	105.19	111.77
2	K	101	BCL	CMB-C2B-C3B	2.45	129.25	124.68
2	D	101	BCL	CMB-C2B-C3B	2.44	129.25	124.68
2	A	101	BCL	CMB-C2B-C3B	2.43	129.23	124.68
2	C	101	BCL	CMA-C3A-C4A	2.43	105.24	111.77
2	E	101	BCL	CMA-C3A-C4A	2.43	105.25	111.77
2	L	101	BCL	CMB-C2B-C3B	2.41	129.18	124.68
2	H	101	BCL	O2D-CGD-CBD	2.41	115.54	111.27
2	E	101	BCL	CMB-C2B-C1B	2.40	124.77	128.46
2	A	101	BCL	CMB-C2B-C1B	2.40	124.78	128.46
2	D	101	BCL	CMA-C3A-C4A	2.39	105.35	111.77
2	N	101	BCL	CMA-C3A-C4A	2.38	105.39	111.77
2	H	101	BCL	C4B-CHC-C1C	2.36	125.45	130.12
2	J	101	BCL	OBD-CAD-CBD	2.35	122.53	125.89
2	H	101	BCL	CMB-C2B-C3B	2.34	129.06	124.68
2	B	101	BCL	CMB-C2B-C3B	2.33	129.04	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	101	BCL	CMA-C3A-C4A	2.32	105.55	111.77
2	A	101	BCL	C4B-C3B-CAB	2.28	122.72	127.13
2	M	101	BCL	C2A-C3A-C4A	2.28	105.55	101.87
2	I	101	BCL	CMA-C3A-C4A	2.27	105.68	111.77
2	D	101	BCL	C4B-C3B-CAB	2.25	122.78	127.13
2	M	101	BCL	CMA-C3A-C4A	2.24	105.76	111.77
2	N	101	BCL	C2C-C3C-C4C	2.23	98.01	101.34
2	E	101	BCL	C4B-C3B-CAB	2.22	122.84	127.13
2	F	101	BCL	CMB-C2B-C1B	2.21	125.06	128.46
2	M	101	BCL	C2A-C1A-CHA	2.20	120.01	123.86
2	G	101	BCL	C4B-C3B-CAB	2.20	122.88	127.13
2	F	101	BCL	CMB-C2B-C3B	2.20	128.79	124.68
2	K	101	BCL	CMB-C2B-C1B	2.17	125.13	128.46
2	A	101	BCL	OBD-CAD-CBD	2.16	122.81	125.89
2	H	101	BCL	C1B-CHB-C4A	2.16	125.84	130.12
2	B	101	BCL	CMB-C2B-C1B	2.15	125.16	128.46
2	B	101	BCL	CMC-C2C-C1C	2.15	105.98	111.77
2	C	101	BCL	C1B-CHB-C4A	2.15	125.86	130.12
2	D	101	BCL	C1B-CHB-C4A	2.14	125.87	130.12
2	J	101	BCL	C4B-C3B-CAB	2.12	123.02	127.13
2	A	101	BCL	O2D-CGD-CBD	2.11	115.02	111.27
2	B	101	BCL	OBD-CAD-CBD	2.11	122.89	125.89
2	C	101	BCL	CMB-C2B-C1B	2.10	125.23	128.46
2	N	101	BCL	O1D-CGD-CBD	2.10	120.18	124.48
2	F	101	BCL	C4B-C3B-CAB	2.09	123.09	127.13
2	L	101	BCL	C1B-CHB-C4A	2.09	125.98	130.12
2	G	101	BCL	CMB-C2B-C1B	2.08	125.27	128.46
2	G	101	BCL	CMB-C2B-C3B	2.07	128.56	124.68
2	E	101	BCL	C1B-CHB-C4A	2.06	126.03	130.12
2	M	101	BCL	C1B-CHB-C4A	2.05	126.05	130.12
2	M	101	BCL	O1D-CGD-CBD	2.04	120.30	124.48
2	C	101	BCL	C4B-C3B-CAB	2.04	123.19	127.13
2	K	101	BCL	C1B-CHB-C4A	2.04	126.08	130.12
2	G	101	BCL	CMA-C3A-C4A	2.02	106.34	111.77
2	F	101	BCL	CMA-C3A-C4A	2.00	106.39	111.77
2	I	101	BCL	C1B-CHB-C4A	2.00	126.15	130.12
2	M	101	BCL	CMB-C2B-C1B	2.00	125.39	128.46

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
2	A	101	BCL	C8
2	B	101	BCL	C8

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Mol	Chain	Res	Type	Atoms
2	C	101	BCL	C8
2	D	101	BCL	C8
2	E	101	BCL	C8
2	F	101	BCL	C8
2	G	101	BCL	C8
2	H	101	BCL	C8
2	I	101	BCL	C8
2	J	101	BCL	C8
2	K	101	BCL	C8
2	L	101	BCL	C8
2	M	101	BCL	C8
2	N	101	BCL	C8

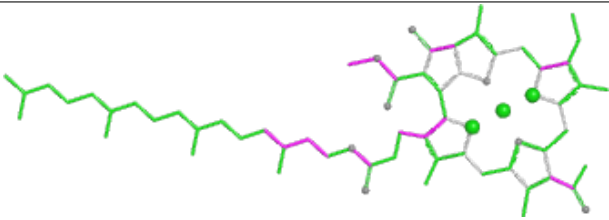
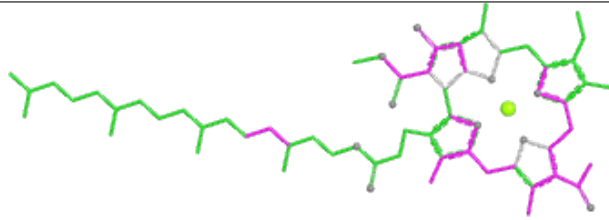
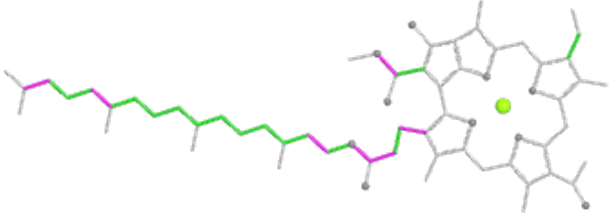
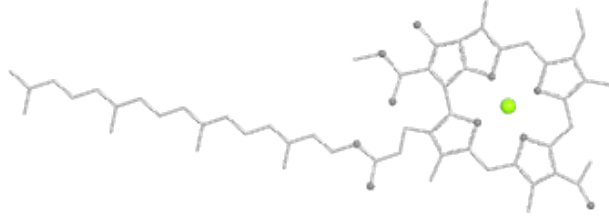
All torsion outliers are listed below.

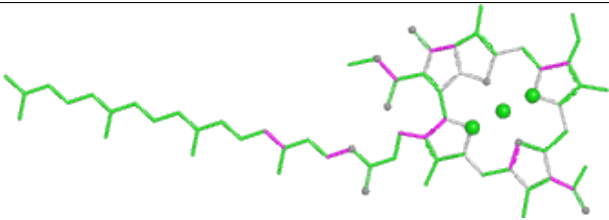
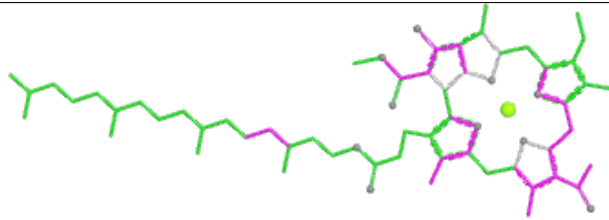
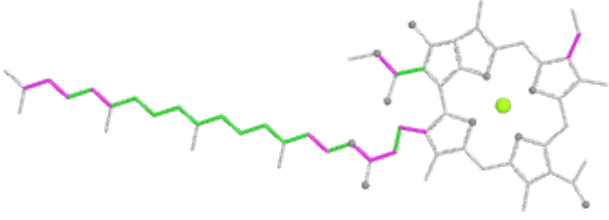
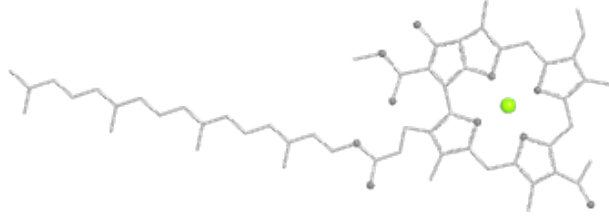
Mol	Chain	Res	Type	Atoms
2	D	101	BCL	O2A-C1-C2-C3
2	G	101	BCL	O2A-C1-C2-C3
2	H	101	BCL	O2A-C1-C2-C3
2	I	101	BCL	O2A-C1-C2-C3
2	M	101	BCL	O2A-C1-C2-C3

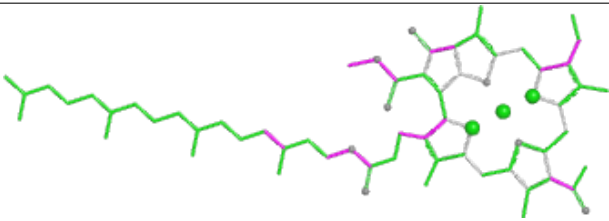
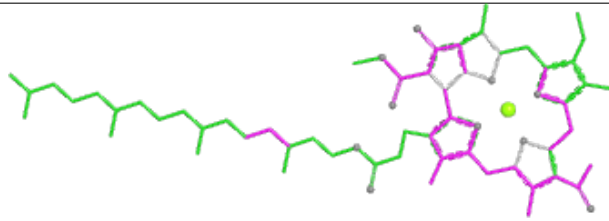
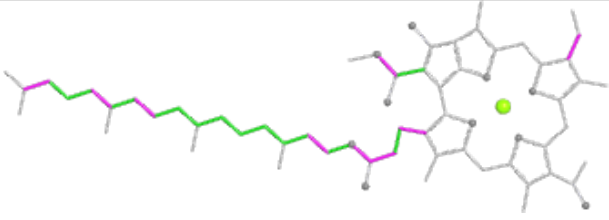
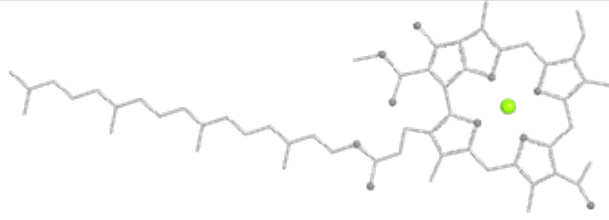
There are no ring outliers.

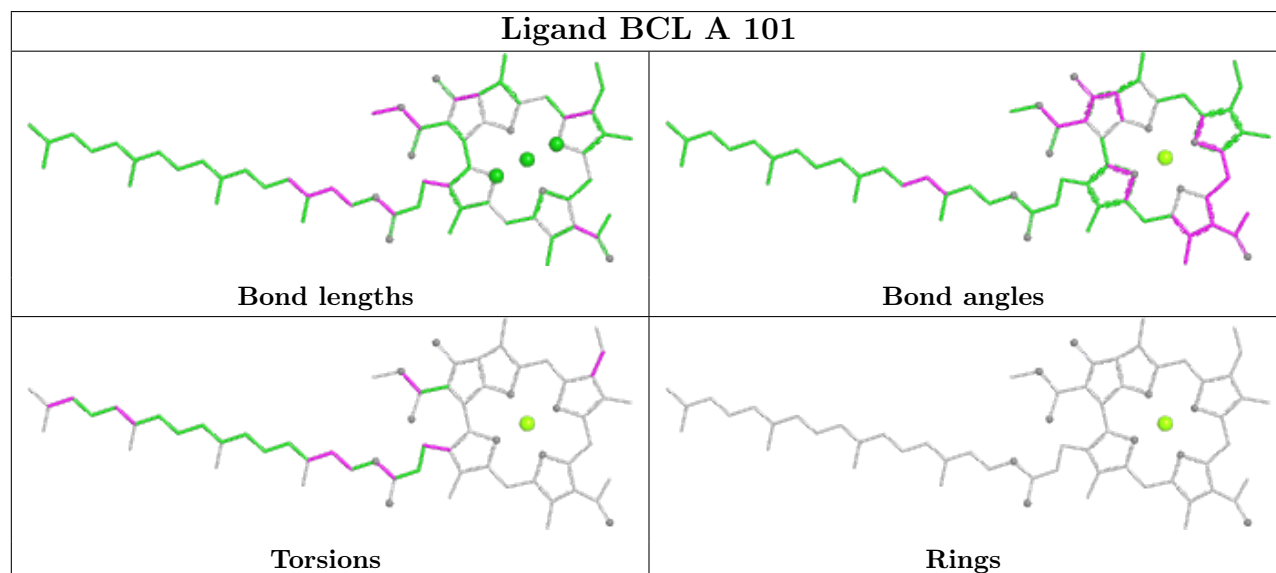
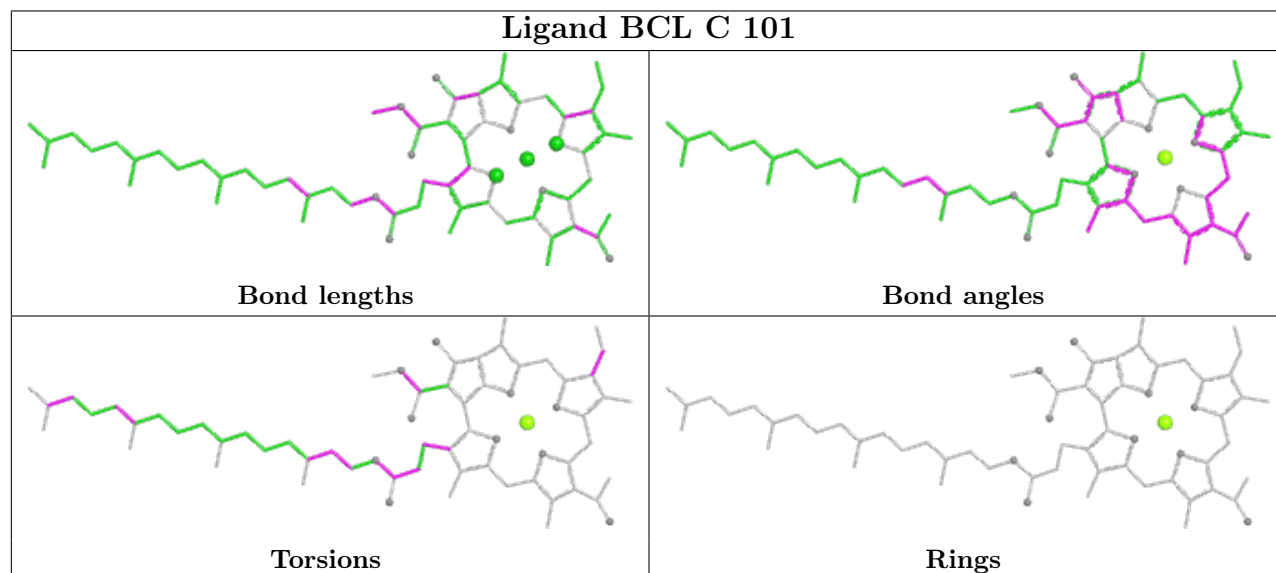
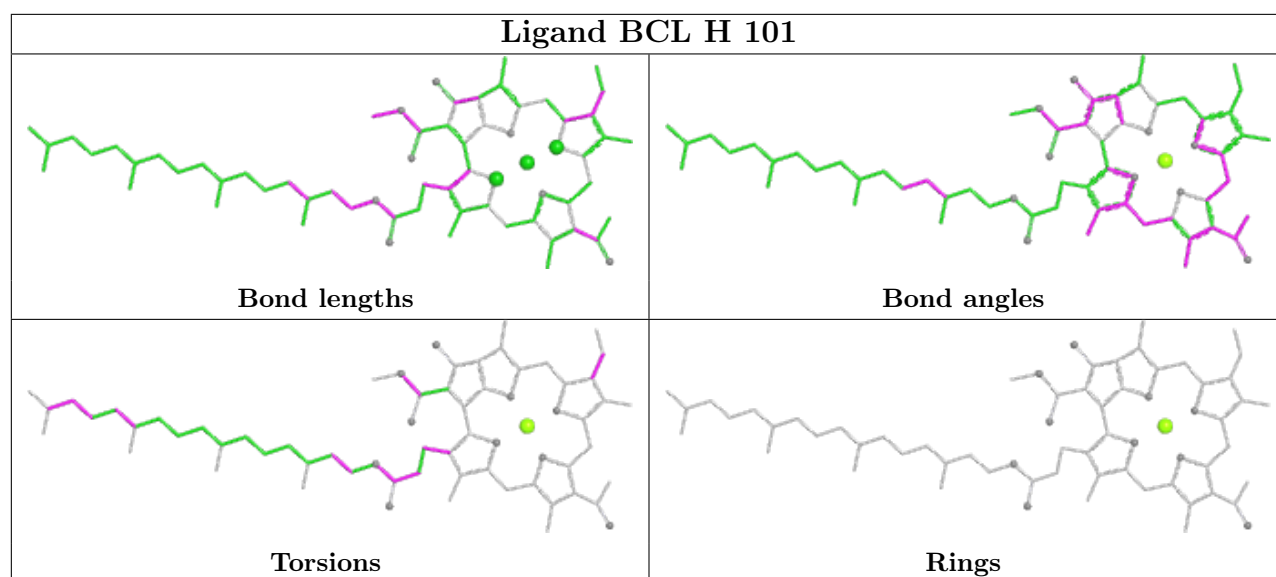
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

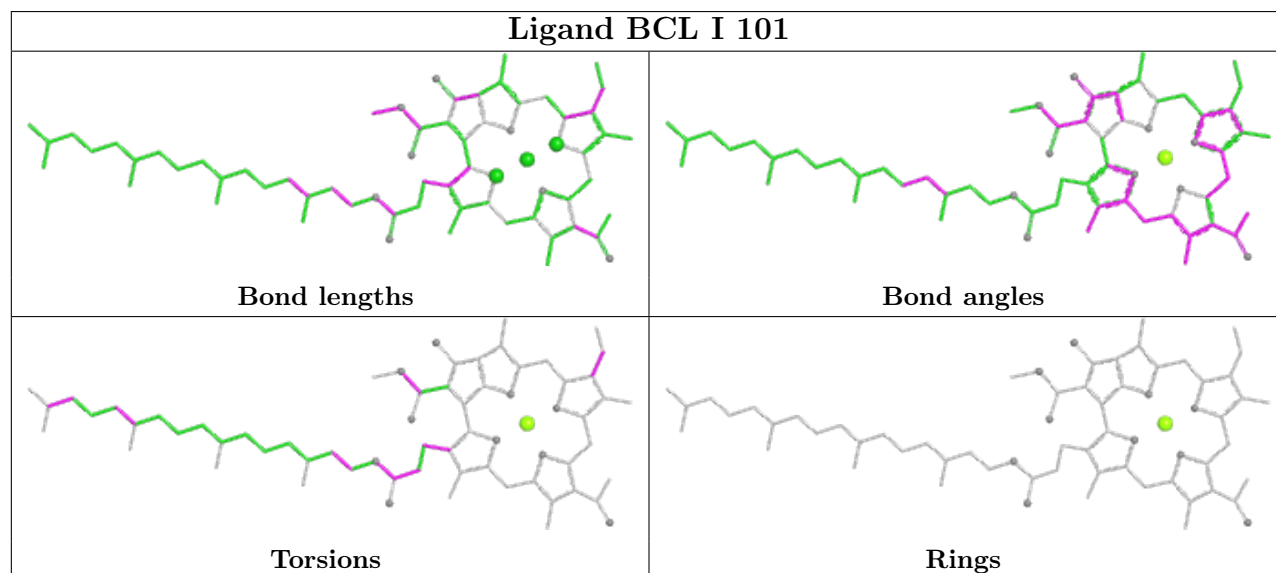
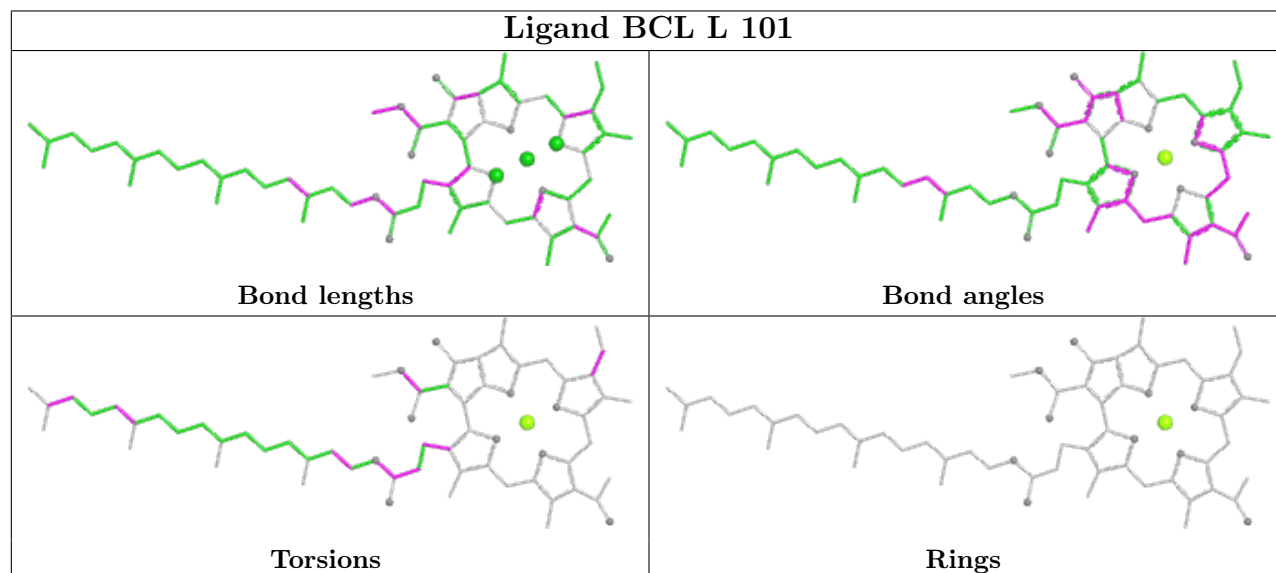
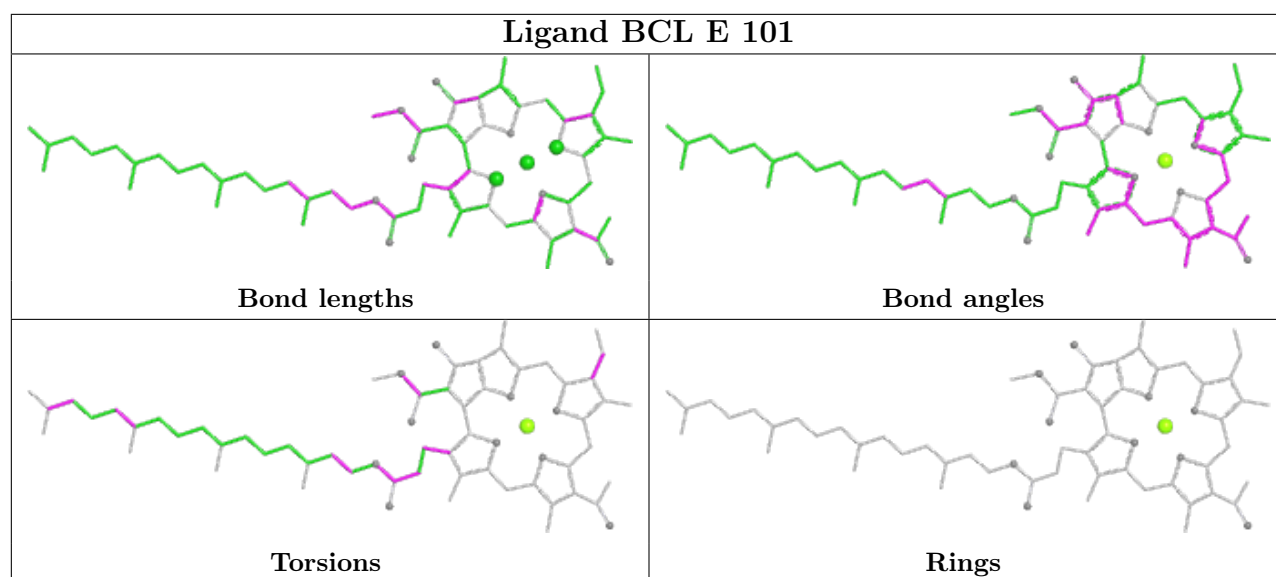


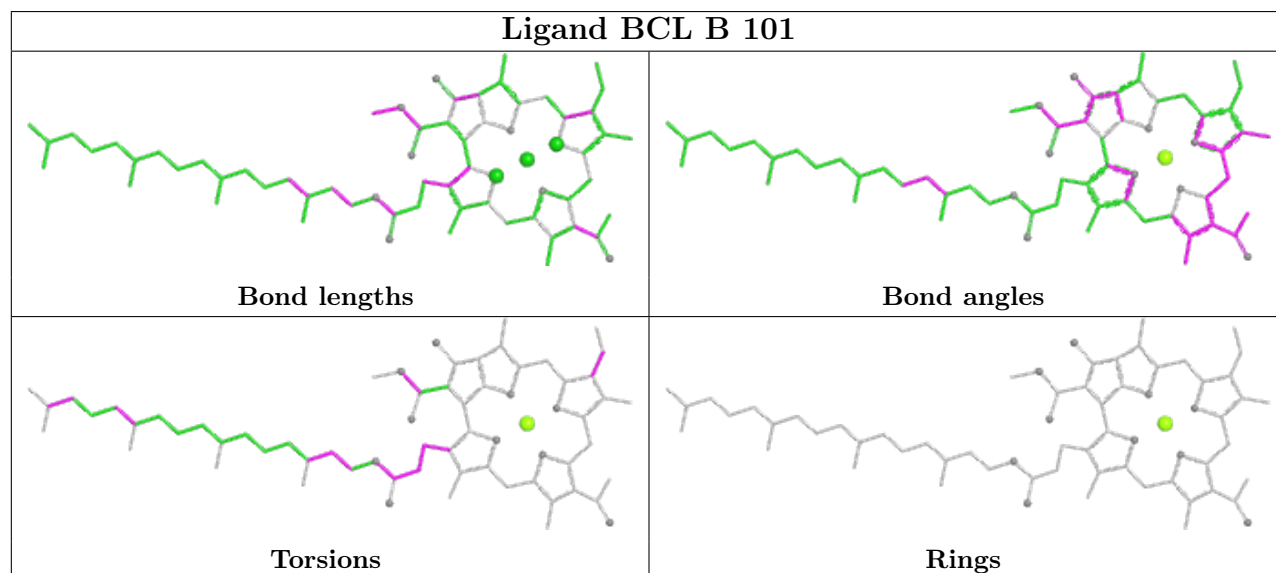
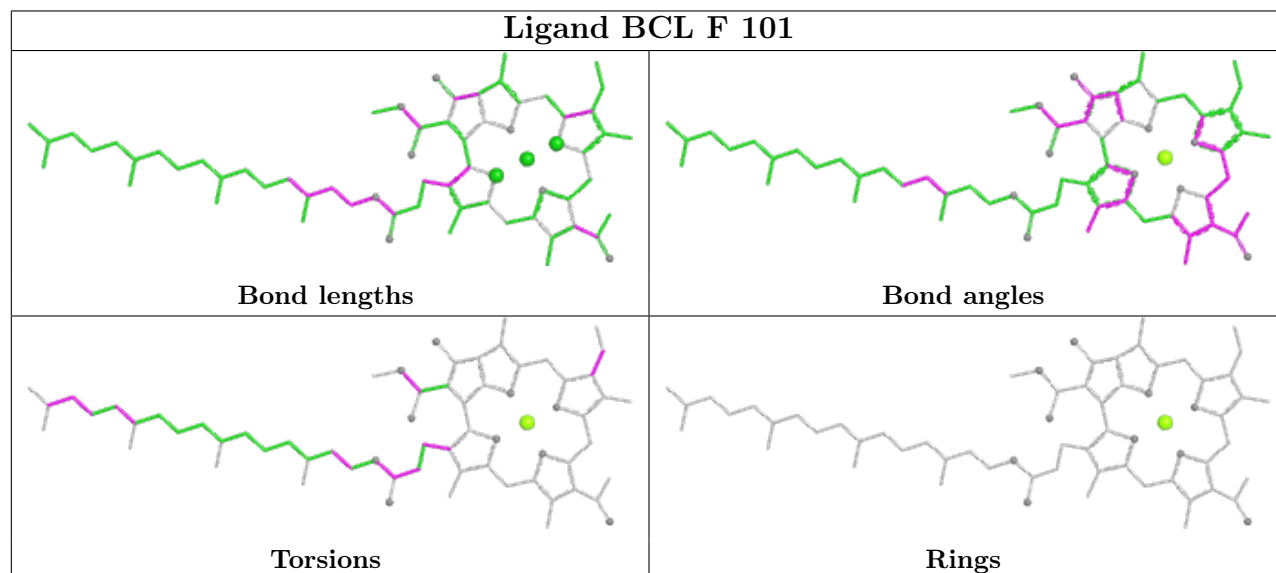
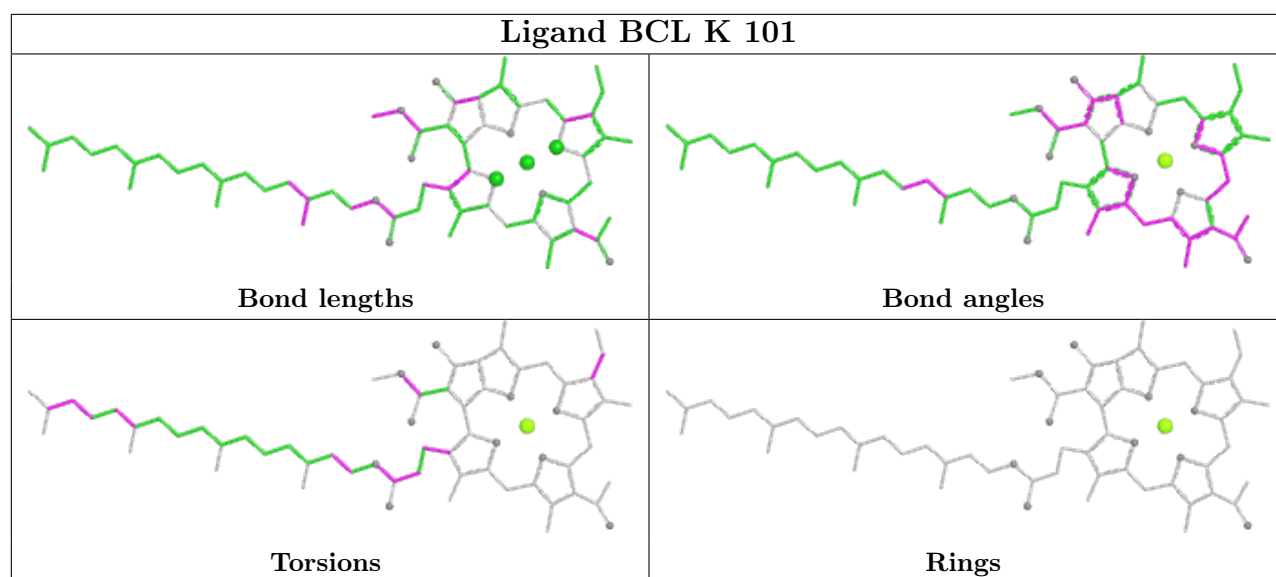
Ligand BCL D 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

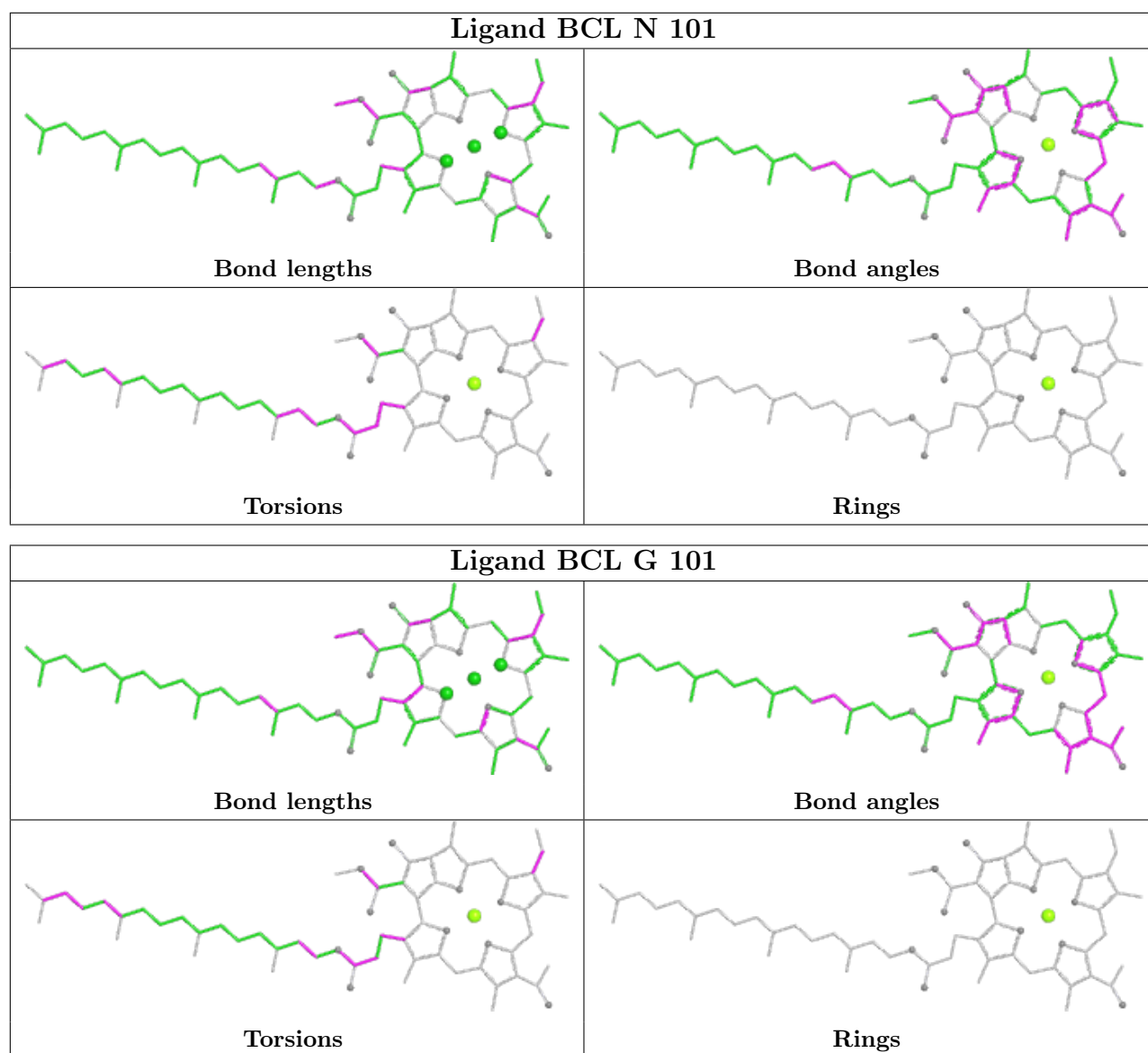
Ligand BCL J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL M 101	
	
Bond lengths	Bond angles
	
Torsions	Rings









## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 2% for the well-defined parts and 2% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *csmanewer31.str*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	207
Number of shifts mapped to atoms	207
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	44	$-1.07 \pm 0.21$	Should be applied
$^{13}\text{C}_\beta$	34	$0.85 \pm 0.52$	None needed (imprecise)
$^{13}\text{C}'$	43	$-0.61 \pm 0.37$	None needed (imprecise)
$^{15}\text{N}$	44	$2.02 \pm 0.32$	Should be applied

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 2%, i.e. 201 atoms were assigned a chemical shift out of a possible 9198. 4 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	131/4130 (3%)	0/1652 (0%)	87/1652 (5%)	44/826 (5%)
Sidechain	70/4312 (2%)	0/2520 (0%)	70/1582 (4%)	0/210 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/756 (0%)	0/406 (0%)	0/322 (0%)	0/28 (0%)
Overall	201/9198 (2%)	0/4578 (0%)	157/3556 (4%)	44/1064 (4%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 201 atoms were assigned a chemical shift out of a possible 9198. 4 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	131/4130 (3%)	0/1652 (0%)	87/1652 (5%)	44/826 (5%)
Sidechain	70/4312 (2%)	0/2520 (0%)	70/1582 (4%)	0/210 (0%)
Aromatic	0/756 (0%)	0/406 (0%)	0/322 (0%)	0/28 (0%)
Overall	201/9198 (2%)	0/4578 (0%)	157/3556 (4%)	44/1064 (4%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

