



Full wwPDB EM Validation Report ⓘ

Jul 14, 2026 – 11:13 PM JST

PDB ID : 21NS / pdb_000021ns
EMDB ID : EMD-67849
Title : Cryo-EM structure of TLP-4b
Authors : Yan, N.; Li, Z.; Wang, T.
Deposited on : 2025-12-21
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

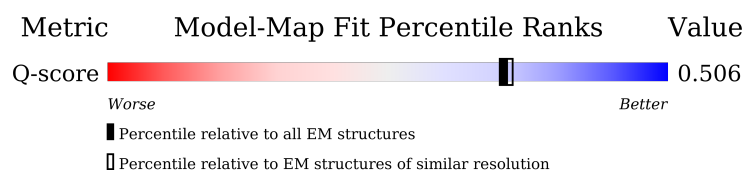
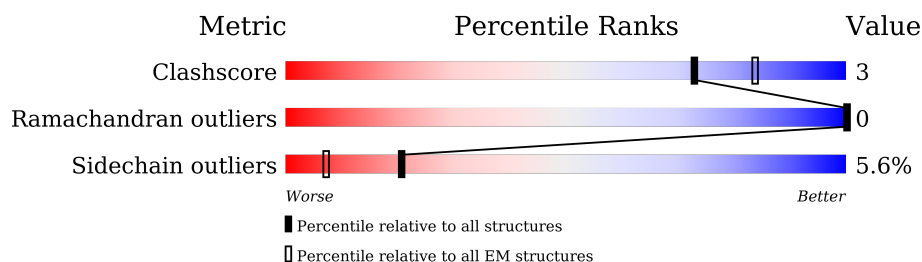
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	36	 94% . .
2	C	25	 72% 20% 8%
2	E	25	 72% 20% 8%
2	H	25	 68% 28% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	25	
2	N	25	
2	Q	25	
2	T	25	
2	W	25	
2	Z	25	
3	B	43	
3	F	43	
3	I	43	
3	L	43	
3	O	43	
3	R	43	
3	U	43	
3	X	43	
3	a	43	
4	D	19	
4	G	19	
4	J	19	
4	M	19	
4	P	19	
4	S	19	
4	V	19	
4	Y	19	
4	b	19	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8019 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 TLP-4b.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	36	Total	C	N	O	0	0
			279	153	63	63		

- Molecule 2 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-[alpha-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-5)-[beta-L-arabinofuranose-(1-2)]beta-L-arabinofuranose-(1-5)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-L-arabinofuranose-(1-4)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-D-galactofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	25	Total	C	N	O	0	0
			247	137	2	108		
2	E	25	Total	C	N	O	0	0
			247	137	2	108		
2	H	25	Total	C	N	O	0	0
			247	137	2	108		
2	K	25	Total	C	N	O	0	0
			247	137	2	108		
2	N	25	Total	C	N	O	0	0
			247	137	2	108		
2	Q	25	Total	C	N	O	0	0
			247	137	2	108		
2	T	25	Total	C	N	O	0	0
			247	137	2	108		
2	W	25	Total	C	N	O	0	0
			247	137	2	108		
2	Z	25	Total	C	N	O	0	0
			247	137	2	108		

- Molecule 3 is an oligosaccharide called alpha-L-arabinofuranose-(1-2)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-[alpha-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-5)-[beta-L-arabinofuranose-(1-2)]beta-L-arabinofuranose-(1-5)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-L-arabinofuranose-(1-4)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-D-galactofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose.

e-(1-3)]alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-3)-[alpha-D-galactofuranose-(1-2)]alpha-L-arabinofuranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-glucopyranose-(1-3)-[alpha-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-2)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-[beta-D-xylopyranose-(1-2)-[beta-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-3)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-3)-[beta-D-glucopyranose-(1-2)-alpha-D-galactofuranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[beta-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-4)]beta-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
3	B	43	Total	C	O	0	0
			419	231	188		
3	F	43	Total	C	O	0	0
			419	231	188		
3	I	43	Total	C	O	0	0
			419	231	188		
3	L	43	Total	C	O	0	0
			419	231	188		
3	O	43	Total	C	O	0	0
			419	231	188		
3	R	43	Total	C	O	0	0
			419	231	188		
3	U	43	Total	C	O	0	0
			419	231	188		
3	X	43	Total	C	O	0	0
			419	231	188		
3	a	43	Total	C	O	0	0
			419	231	188		

- Molecule 4 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]beta-D-glucopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-3)-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]alpha-L-arabinofuranose-(1-6)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-2)-beta-D-xylopyranose-(1-4)]alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose.

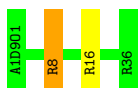
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	19	Total 194	C 108	N 3	O 83	0	0
4	G	19	Total 194	C 108	N 3	O 83	0	0
4	J	19	Total 194	C 108	N 3	O 83	0	0
4	M	19	Total 194	C 108	N 3	O 83	0	0
4	P	19	Total 194	C 108	N 3	O 83	0	0
4	S	19	Total 194	C 108	N 3	O 83	0	0
4	V	19	Total 194	C 108	N 3	O 83	0	0
4	Y	19	Total 194	C 108	N 3	O 83	0	0
4	b	19	Total 194	C 108	N 3	O 83	0	0

3 Residue-property plots

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: TLP-4b

Chain A:  94%



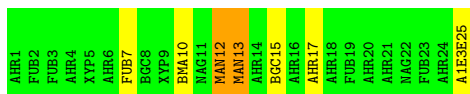
- Molecule 2: alpha-L-arabinofuranose-(1-3)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-[alpha-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-5)-[beta-L-arabinofuranose-(1-2)]beta-L-arabinofuranose-(1-5)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-L-arabinofuranose-(1-4)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-D-galactofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain C:  72% 20% 8%



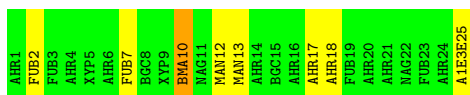
- Molecule 2: alpha-L-arabinofuranose-(1-3)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-[alpha-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-5)-[beta-L-arabinofuranose-(1-2)]beta-L-arabinofuranose-(1-5)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-L-arabinofuranose-(1-4)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-D-galactofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain E:  72% 20% 8%



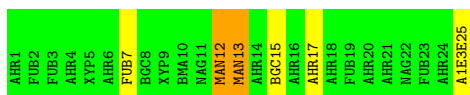
● Molecule 2: alpha-L-arabinofuranose-(1-3)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-[alpha-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-5)-[beta-L-arabinofuranose-(1-2)]beta-L-arabinofuranose-(1-5)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-L-arabinofuranose-(1-4)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-D-galactofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain H: 68% 28%



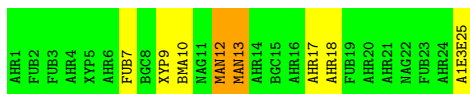
● Molecule 2: alpha-L-arabinofuranose-(1-3)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-[alpha-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-5)-[beta-L-arabinofuranose-(1-2)]beta-L-arabinofuranose-(1-5)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-L-arabinofuranose-(1-4)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-D-galactofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain K: 76% 16% 8%



● Molecule 2: alpha-L-arabinofuranose-(1-3)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-[alpha-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-5)-[beta-L-arabinofuranose-(1-2)]beta-L-arabinofuranose-(1-5)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-L-arabinofuranose-(1-4)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-D-galactofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain N: 68% 24% 8%



● Molecule 2: alpha-L-arabinofuranose-(1-3)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-[alpha-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-5)-[beta-L-arabinofuranose-(1-2)]beta-L-arabinofuranose-(1-5)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-L-arabinofuranose-(1-4)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-D-galactofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain Q: 68% 24% 8%



● Molecule 2: alpha-L-arabinofuranose-(1-3)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-[alpha-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-5)-[beta-L-arabinofuranose-(1-2)]beta-L-arabinofuranose-(1-5)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-L-arabinofuranose-(1-4)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-D-galactofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain T: 60% 40%



● Molecule 2: alpha-L-arabinofuranose-(1-3)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-[alpha-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-5)-[beta-L-arabinofuranose-(1-2)]beta-L-arabinofuranose-(1-5)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-L-arabinofuranose-(1-4)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-D-galactofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain W: 68% 24% 8%

AHR1
FUB2
FUB3
AHR4
XYP5
AHR6
FUB7
BGC8
XYP9
BMA10
NAG11
MAN12
MAN13
AHR14
BGC15
AHR16
AHR17
AHR18
FUB19
AHR20
AHR21
NAG22
FUB23
AHR24
A1E3E25

• Molecule 2: alpha-L-arabinofuranose-(1-3)-[beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-[alpha-L-arabinofuranose-(1-2)]beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-5)-[beta-L-arabinofuranose-(1-2)]beta-L-arabinofuranose-(1-5)-[alpha-L-arabinofuranose-(1-2)]alpha-L-arabinofuranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-L-arabinofuranose-(1-4)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(1-2)-[alpha-D-galactofuranose-(1-3)]beta-L-arabinofuranose-(1-3)-alpha-L-arabinofuranose

Chain Z:  68% 32%

AHR1
FUB2
FUB3
AHR4
XYP5
AHR6
FUB7
BGC8
XYP9
BMA10
NAG11
MAN12
MAN13
AHR14
BGC15
AHR16
AHR17
AHR18
FUB19
AHR20
AHR21
NAG22
FUB23
AHR24
A1E3E25

• Molecule 3: alpha-L-arabinofuranose-(1-2)-[beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-3)-[alpha-D-galactofuranose-(1-2)]alpha-L-arabinofuranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-glucopyranose-(1-3)-[alpha-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-2)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-[beta-D-xylopyranose-(1-2)-[beta-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-3)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-3)-[beta-D-glucopyranose-(1-2)-alpha-D-galactofuranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[beta-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-4)]beta-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-2)-beta-L-arabinofuranose

Chain B:  60% 35% 5%

FUB1
XYP2
MAN3
MAN4
XYP5
XYP6
XYP7
AHR8
XYP9
XYP10
XYP11
MAN12
AHR13
BGC14
FUB15
AHR16
A1E3E17
MAN18
BGC19
AHR20
AHR21
AHR22
BGC23
XYP24
MAN25
AHR26
FUB27
AHR28
XYP29
FUB30
MAN31
FUB32
A1E3E33
BGC34
XYP35
BGC36
BGC37
XYP38
XYP39
BMA40
AHR41
FUB42
BMA43

• Molecule 3: alpha-L-arabinofuranose-(1-2)-[beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-3)-[alpha-D-galactofuranose-(1-2)]alpha-L-arabinofuranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-glucopyranose-(1-3)-[alpha-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-2)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-[beta-D-xylopyranose-(1-2)-[beta-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-3)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-3)-[beta-D-glucopyranose-(1-2)-alpha-

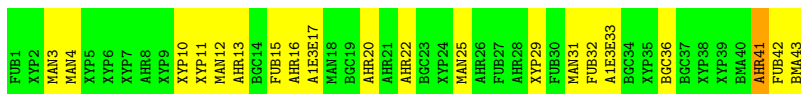
Chain F:  60% 35% 5%

Category	Green (%)	Yellow (%)	Red (%)
FUB1	60	35	5
XP2	60	35	5
MAN3	60	35	5
MAN4	60	35	5
XP5	60	35	5
XP6	60	35	5
XP7	60	35	5
XHR8	60	35	5
XP9	60	35	5
XP10	60	35	5
XP11	60	35	5
MAN12	60	35	5
XHR13	60	35	5
BGC14	60	35	5
FUB15	60	35	5
XHR16	60	35	5
A1E3E17	60	35	5
MAN18	60	35	5
BGC19	60	35	5
XHR20	60	35	5
XHR21	60	35	5
XHR22	60	35	5
BGC23	60	35	5
XP24	60	35	5
MAN25	60	35	5
BGC26	60	35	5
FUB27	60	35	5
XHR28	60	35	5
XP29	60	35	5
FUB30	60	35	5
MAN31	60	35	5
FUB32	60	35	5
A1E3E33	60	35	5
BGC34	60	35	5
XP35	60	35	5
BGC36	60	35	5
XP38	60	35	5
XP39	60	35	5
BMA40	60	35	5
XHR41	60	35	5
FUB42	60	35	5
BMA43	60	35	5

Chain I:  53% 44%

Category	Label	Percentage
1	FUB1	1.14%
2	XP2	1.14%
3	MAN3	1.14%
4	MAN4	1.14%
5	XP6	1.14%
6	XP7	1.14%
7	AHR8	1.14%
8	XP9	1.14%
9	XP10	1.14%
10	XP11	1.14%
11	MAN12	1.14%
12	AHR13	1.14%
13	BGC14	1.14%
14	FUB15	1.14%
15	AHR16	1.14%
16	ATE3E17	1.14%
17	MAN18	1.14%
18	BGC19	1.14%
19	AHR20	1.14%
20	AHR21	1.14%
21	AHR22	1.14%
22	BGC23	1.14%
23	XP24	1.14%
24	MAN25	1.14%
25	AHR26	1.14%
26	FUB27	1.14%
27	AHR28	1.14%
28	XP29	1.14%
29	FUB30	1.14%
30	MAN31	1.14%
31	FUB32	1.14%
32	ATE3E33	1.14%
33	BGC34	1.14%
34	XP35	1.14%
35	BGC36	1.14%
36	BGC37	1.14%
37	XP38	1.14%
38	XP39	1.14%
39	BMA40	1.14%
40	FUB41	1.14%
41	AHR42	1.14%
42	BMA43	1.14%

Chain L: 53% 44%



● Molecule 3: alpha-L-arabinofuranose-(1-2)-[beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-3)-[alpha-D-galactofuranose-(1-2)]alpha-L-arabinofuranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-glucopyranose-(1-3)-[alpha-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-2)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-[beta-D-xylopyranose-(1-2)-[beta-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-3)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-3)-[beta-D-glucopyranose-(1-2)-alpha-D-galactofuranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[beta-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-4)]beta-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-2)-beta-L-arabinofuranose

Chain O: 53% 44%



● Molecule 3: alpha-L-arabinofuranose-(1-2)-[beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-3)-[alpha-D-galactofuranose-(1-2)]alpha-L-arabinofuranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-glucopyranose-(1-3)-[alpha-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-2)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-[beta-D-xylopyranose-(1-2)-[beta-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-3)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-3)-[beta-D-glucopyranose-(1-2)-alpha-D-galactofuranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[beta-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-4)]beta-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-2)-beta-L-arabinofuranose

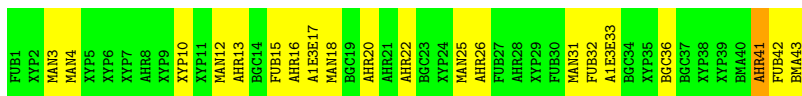
Chain R: 53% 44%



● Molecule 3: alpha-L-arabinofuranose-(1-2)-[beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-3)-[alpha-D-galactofuranose-(1-2)]alpha-L-arabinofuranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-glucopyra

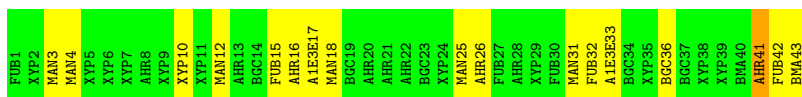
nose-(1-3)-[alpha-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-2)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-[beta-D-xylopyranose-(1-2)-[beta-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-3)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-3)-[beta-D-glucopyranose-(1-2)-alpha-D-galactofuranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[beta-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-4)]beta-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-2)-beta-L-arabinofuranose

Chain U:  53% 44%



• Molecule 3: alpha-L-arabinofuranose-(1-2)-[beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-3)-[alpha-D-galactofuranose-(1-2)]alpha-L-arabinofuranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-glucopyranose-(1-3)-[alpha-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-2)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-[beta-D-xylopyranose-(1-2)-[beta-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-3)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-3)-[beta-D-glucopyranose-(1-2)-alpha-D-galactofuranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[beta-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-4)]beta-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-2)-beta-L-arabinofuranose

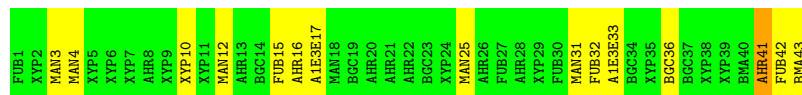
Chain X:  60% 37%



• Molecule 3: alpha-L-arabinofuranose-(1-2)-[beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-2)-[beta-L-arabinofuranose-(1-4)]beta-D-xylopyranose-(1-3)-[alpha-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-3)-[alpha-D-galactofuranose-(1-2)]alpha-L-arabinofuranose-(1-4)-[alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-6)]beta-D-glucopyranose-(1-3)-[alpha-L-arabinofuranose-(1-2)]alpha-D-mannopyranose-(1-2)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-[beta-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)-[beta-D-xylopyranose-(1-2)-[beta-L-arabinofuranose-(1-3)]alpha-L-arabinofuranose-(1-4)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-3)]beta-L-arabinofuranose-(1-2)]beta-D-xylopyranose-(1-3)-[beta-D-glucopyranose-(1-2)-alpha-D-galactofuranose-(1-6)]alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-beta-D-xylopyranose-(1-2)-[beta-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-4)]beta-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-2)-beta-L-arabinofuranose

ose-(1-4)]beta-D-mannopyranose-(1-3)]beta-D-xylopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-2)-beta-L-arabinofuranose

Chain a:  65% 33%



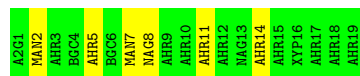
• Molecule 4: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]beta-D-glucopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-3)-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]alpha-L-arabinofuranose-(1-6)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-2)-beta-D-xylopyranose-(1-4)]alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain D:  68% 32%



• Molecule 4: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]beta-D-glucopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-3)-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]alpha-L-arabinofuranose-(1-6)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-2)-beta-D-xylopyranose-(1-4)]alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain G:  68% 32%



• Molecule 4: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]beta-D-glucopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-3)-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]alpha-L-arabinofuranose-(1-6)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-2)-beta-D-xylopyranose-(1-4)]alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain J:  68% 26% 5%



• Molecule 4: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]beta-D-glucopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-3)-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]alpha-L-arabinofuranose-(1-6)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-2)-beta-D-xylopyranose-(1-4)][alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain M:  58% 37% 5%



• Molecule 4: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]beta-D-glucopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-3)-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]alpha-L-arabinofuranose-(1-6)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-2)-beta-D-xylopyranose-(1-4)][alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain P:  58% 42%



• Molecule 4: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]beta-D-glucopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-3)-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]alpha-L-arabinofuranose-(1-6)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-2)-beta-D-xylopyranose-(1-4)][alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain S:  68% 32%



• Molecule 4: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]beta-D-glucopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-3)-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]alpha-L-arabinofuranose-(1-6)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-2)-beta-D-xylopyranose-(1-4)][alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain V:  47% 42% 11%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]beta-D-glucopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-3)-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]alpha-L-arabinofuranose-(1-6)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-2)-beta-D-xylopyranose-(1-4)]alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain Y: 47% 47% 5%



- Molecule 4: alpha-L-arabinofuranose-(1-3)-[alpha-L-arabinofuranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-[alpha-L-arabinofuranose-(1-3)]beta-D-glucopyranose-(1-2)-[alpha-L-arabinofuranose-(1-5)]alpha-L-arabinofuranose-(1-3)-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)]alpha-L-arabinofuranose-(1-6)-[alpha-L-arabinofuranose-(1-2)-alpha-L-arabinofuranose-(1-3)]alpha-D-mannopyranose-(1-3)-[alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-2)-beta-D-xylopyranose-(1-4)]alpha-L-arabinofuranose-(1-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain b: 53% 42% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-138.7°, rise=12.3 Å, axial sym=C1	Depositor
Number of segments used	44738	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.582	Depositor
Minimum map value	-1.063	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.253	Depositor
Map size (Å)	281.0624, 281.0624, 281.0624	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	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: FUB, BMA, MAN, NAG, BGC, A1D9O, AHR, XYP, A1E3E, A2G

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	A	0.32	0/189	0.31	0/234

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	279	0	198	2	0
2	C	247	0	67	2	0
2	E	247	0	67	2	0
2	H	247	0	67	2	0
2	K	247	0	67	2	0
2	N	247	0	67	1	0
2	Q	247	0	67	1	0
2	T	247	0	67	1	0
2	W	247	0	67	1	0
2	Z	247	0	67	0	0
3	B	419	0	125	2	0
3	F	419	0	125	2	0
3	I	419	0	125	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	419	0	125	4	0
3	O	419	0	125	3	0
3	R	419	0	125	3	0
3	U	419	0	125	2	0
3	X	419	0	125	1	0
3	a	419	0	125	1	0
4	D	194	0	67	0	0
4	G	194	0	67	0	0
4	J	194	0	67	1	0
4	M	194	0	67	1	0
4	P	194	0	67	0	0
4	S	194	0	67	0	0
4	V	194	0	67	2	0
4	Y	194	0	67	1	0
4	b	194	0	67	1	0
All	All	8019	0	2529	35	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 3.

All (35) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ARG:CG	1:A:8:ARG:O	2.58	0.51
3:I:20:HR:O5	3:I:22:HR:O3	2.28	0.51
3:O:41:HR:O4	3:O:42:FUB:O2	2.29	0.51
3:a:41:HR:O4	3:a:42:FUB:O2	2.30	0.49
3:F:20:HR:O5	3:F:22:HR:O3	2.29	0.49
3:O:20:HR:O5	3:O:22:HR:O3	2.29	0.49
3:U:41:HR:O4	3:U:42:FUB:O2	2.30	0.49
2:E:15:BGC:O6	3:L:13:HR:O5	2.31	0.49
3:B:20:HR:O5	3:B:22:HR:O3	2.30	0.49
3:R:20:HR:O5	3:R:22:HR:O3	2.31	0.48
3:X:41:HR:O4	3:X:42:FUB:O2	2.31	0.48
3:R:41:HR:O4	3:R:42:FUB:O2	2.31	0.47
3:L:20:HR:O5	3:L:22:HR:O3	2.32	0.47
2:N:12:MAN:H4	2:N:13:MAN:H2	1.72	0.46
2:T:22:NAG:O4	4:V:11:HR:O2	2.34	0.46
2:Q:12:MAN:H4	2:Q:13:MAN:H2	1.76	0.45
2:W:12:MAN:H4	2:W:13:MAN:H2	1.74	0.45
2:C:15:BGC:O6	3:I:13:HR:O5	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:20:AHR:O5	3:U:22:AHR:O3	2.34	0.45
2:C:12:MAN:H4	2:C:13:MAN:H2	1.75	0.44
3:B:41:AHR:O4	3:B:42:FUB:O2	2.35	0.44
3:I:41:AHR:O4	3:I:42:FUB:O2	2.35	0.44
4:b:6:BGC:H6C2	4:b:7:MAN:H2	1.99	0.44
3:L:41:AHR:O4	3:L:42:FUB:O2	2.36	0.43
2:E:12:MAN:H4	2:E:13:MAN:H2	1.73	0.43
4:J:6:BGC:H6C2	4:J:7:MAN:H2	2.00	0.43
4:Y:6:BGC:H6C2	4:Y:7:MAN:H2	2.00	0.42
3:L:22:AHR:O4	3:L:29:XYP:O4	2.37	0.42
2:K:15:BGC:O6	3:R:13:AHR:O5	2.35	0.42
3:F:41:AHR:O4	3:F:42:FUB:O2	2.38	0.42
4:V:6:BGC:H6C2	4:V:7:MAN:H2	2.01	0.42
2:H:10:BMA:O4	3:O:42:FUB:O3	2.38	0.41
2:K:12:MAN:H4	2:K:13:MAN:H2	1.75	0.41
4:M:6:BGC:H6C2	4:M:7:MAN:H2	2.02	0.41
1:A:16:ARG:HB2	2:H:2:FUB:O5	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	A	26/36 (72%)	26 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	A	18/18 (100%)	17 (94%)	1 (6%)	19	47

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	A1D9O	A	13	1	7,9,10	1.00	0	5,12,14	1.15	0
1	A1D9O	A	9	1	7,9,10	1.05	0	5,12,14	1.17	0
1	A1D9O	A	29	1	7,9,10	1.02	0	5,12,14	1.14	0
1	A1D9O	A	5	1	7,9,10	1.00	0	5,12,14	1.10	0
1	A1D9O	A	21	1	7,9,10	1.02	0	5,12,14	1.14	0
1	A1D9O	A	25	1	7,9,10	1.03	0	5,12,14	1.12	0
1	A1D9O	A	1	1	7,9,10	0.94	0	5,12,14	0.99	0
1	A1D9O	A	33	1	7,9,10	1.04	0	5,12,14	1.18	0
1	A1D9O	A	17	1	7,9,10	1.02	0	5,12,14	1.14	0

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
1	A1D9O	A	13	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	9	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	29	1	-	1/1/15/17	0/1/1/1
1	A1D9O	A	5	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	21	1	-	1/1/15/17	0/1/1/1
1	A1D9O	A	25	1	-	1/1/15/17	0/1/1/1
1	A1D9O	A	1	1	-	1/1/15/17	0/1/1/1
1	A1D9O	A	33	1	-	0/1/15/17	0/1/1/1
1	A1D9O	A	17	1	-	0/1/15/17	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	A1D9O	O-C-CA-CB
1	A	21	A1D9O	O-C-CA-CB
1	A	25	A1D9O	O-C-CA-CB
1	A	29	A1D9O	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

783 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FUB	B	1	3	9,9,10	0.58	0	10,12,14	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	XYP	B	10	3	9,9,10	0.16	0	10,12,14	0.86	1 (10%)
3	XYP	B	11	3	9,9,10	0.18	0	10,12,14	0.70	0
3	MAN	B	12	3	11,11,12	0.23	0	15,15,17	0.83	1 (6%)
3	AHR	B	13	3	9,9,10	0.57	0	10,12,14	1.00	0
3	BGC	B	14	3	11,11,12	0.21	0	15,15,17	0.57	0
3	FUB	B	15	3	9,9,10	0.56	0	10,12,14	1.07	1 (10%)
3	AHR	B	16	3	9,9,10	0.58	0	10,12,14	1.03	1 (10%)
3	A1E3E	B	17	3	11,11,12	6.63	7 (63%)	14,15,17	1.72	2 (14%)
3	MAN	B	18	3	11,11,12	0.20	0	15,15,17	0.79	0
3	BGC	B	19	3	11,11,12	0.19	0	15,15,17	0.69	0
3	XYP	B	2	3	9,9,10	0.18	0	10,12,14	0.66	0
3	AHR	B	20	3	9,9,10	0.55	0	10,12,14	0.80	0
3	AHR	B	21	3	9,9,10	0.57	0	10,12,14	0.82	0
3	AHR	B	22	3	9,9,10	0.55	0	10,12,14	0.93	0
3	BGC	B	23	3	11,11,12	0.21	0	15,15,17	0.50	0
3	XYP	B	24	3	9,9,10	0.18	0	10,12,14	0.61	0
3	MAN	B	25	3	11,11,12	0.22	0	15,15,17	0.86	2 (13%)
3	AHR	B	26	3	9,9,10	0.57	0	10,12,14	0.98	0
3	FUB	B	27	3	9,9,10	0.55	0	10,12,14	0.98	0
3	AHR	B	28	3	9,9,10	0.59	0	10,12,14	0.92	0
3	XYP	B	29	3	9,9,10	0.18	0	10,12,14	0.62	0
3	MAN	B	3	3	11,11,12	0.29	0	15,15,17	0.98	2 (13%)
3	FUB	B	30	3	9,9,10	0.56	0	10,12,14	0.67	0
3	MAN	B	31	3	11,11,12	0.26	0	15,15,17	0.87	2 (13%)
3	FUB	B	32	3	9,9,10	0.56	0	10,12,14	1.06	1 (10%)
3	A1E3E	B	33	3	11,11,12	6.72	7 (63%)	14,15,17	1.46	1 (7%)
3	BGC	B	34	3	11,11,12	0.19	0	15,15,17	0.56	0
3	XYP	B	35	3	9,9,10	0.16	0	10,12,14	0.45	0
3	BGC	B	36	3	11,11,12	0.25	0	15,15,17	1.00	1 (6%)
3	BGC	B	37	3	11,11,12	0.18	0	15,15,17	0.51	0
3	XYP	B	38	3	9,9,10	0.17	0	10,12,14	0.66	0
3	XYP	B	39	3	9,9,10	0.18	0	10,12,14	0.64	0
3	MAN	B	4	3	11,11,12	0.22	0	15,15,17	0.86	1 (6%)
3	BMA	B	40	3	11,11,12	0.21	0	15,15,17	0.85	0
3	AHR	B	41	3	9,9,10	0.57	0	10,12,14	1.06	1 (10%)
3	FUB	B	42	3	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
3	BMA	B	43	3	11,11,12	0.24	0	15,15,17	1.13	2 (13%)
3	XYP	B	5	3	9,9,10	0.17	0	10,12,14	0.71	0
3	XYP	B	6	3	9,9,10	0.15	0	10,12,14	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	XYP	B	7	3	9,9,10	0.18	0	10,12,14	0.61	0
3	AHR	B	8	3	9,9,10	0.58	0	10,12,14	0.98	0
3	XYP	B	9	3	9,9,10	0.18	0	10,12,14	0.56	0
2	AHR	C	1	2	9,9,10	0.58	0	10,12,14	1.01	0
2	BMA	C	10	2	11,11,12	0.24	0	15,15,17	0.77	1 (6%)
2	NAG	C	11	2	14,14,15	0.28	0	17,19,21	0.70	0
2	MAN	C	12	2	11,11,12	0.24	0	15,15,17	0.91	2 (13%)
2	MAN	C	13	2	11,11,12	0.22	0	15,15,17	0.85	2 (13%)
2	AHR	C	14	2	9,9,10	0.59	0	10,12,14	0.89	0
2	BGC	C	15	2	11,11,12	0.21	0	15,15,17	0.60	0
2	AHR	C	16	2	9,9,10	0.58	0	10,12,14	0.94	0
2	AHR	C	17	2	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
2	AHR	C	18	2	9,9,10	0.58	0	10,12,14	0.98	1 (10%)
2	FUB	C	19	2	9,9,10	0.59	0	10,12,14	0.95	0
2	FUB	C	2	2	9,9,10	0.60	0	10,12,14	0.99	0
2	AHR	C	20	2	9,9,10	0.57	0	10,12,14	0.89	0
2	AHR	C	21	2	9,9,10	0.58	0	10,12,14	0.94	0
2	NAG	C	22	2	14,14,15	0.33	0	17,19,21	0.78	0
2	FUB	C	23	2	9,9,10	0.57	0	10,12,14	0.93	0
2	AHR	C	24	2	9,9,10	0.57	0	10,12,14	0.89	0
2	A1E3E	C	25	2	11,11,12	6.69	7 (63%)	14,15,17	1.62	3 (21%)
2	FUB	C	3	2	9,9,10	0.58	0	10,12,14	0.97	0
2	AHR	C	4	2	9,9,10	0.59	0	10,12,14	0.88	0
2	XYP	C	5	2	9,9,10	0.18	0	10,12,14	0.61	0
2	AHR	C	6	2	9,9,10	0.59	0	10,12,14	0.86	0
2	FUB	C	7	2	9,9,10	0.59	0	10,12,14	1.06	0
2	BGC	C	8	2	11,11,12	0.18	0	15,15,17	0.48	0
2	XYP	C	9	2	9,9,10	0.23	0	10,12,14	0.92	0
4	A2G	D	1	4,1	14,14,15	0.40	0	17,19,21	0.75	0
4	AHR	D	10	4	9,9,10	0.57	0	10,12,14	0.93	0
4	AHR	D	11	4	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
4	AHR	D	12	4	9,9,10	0.57	0	10,12,14	0.95	0
4	NAG	D	13	4	14,14,15	0.34	0	17,19,21	0.76	0
4	AHR	D	14	4	9,9,10	0.57	0	10,12,14	1.13	1 (10%)
4	AHR	D	15	4	9,9,10	0.57	0	10,12,14	0.92	0
4	XYP	D	16	4	9,9,10	0.19	0	10,12,14	0.58	0
4	AHR	D	17	4	9,9,10	0.59	0	10,12,14	0.79	0
4	AHR	D	18	4	9,9,10	0.58	0	10,12,14	0.96	0
4	AHR	D	19	4	9,9,10	0.59	0	10,12,14	0.87	0
4	MAN	D	2	4	11,11,12	0.22	0	15,15,17	0.84	2 (13%)
4	AHR	D	3	4	9,9,10	0.56	0	10,12,14	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BGC	D	4	4	11,11,12	0.20	0	15,15,17	0.54	0
4	AHR	D	5	4	9,9,10	0.55	0	10,12,14	1.09	1 (10%)
4	BGC	D	6	4	11,11,12	0.17	0	15,15,17	0.53	0
4	MAN	D	7	4	11,11,12	0.31	0	15,15,17	1.64	2 (13%)
4	NAG	D	8	4	14,14,15	0.38	0	17,19,21	0.93	1 (5%)
4	AHR	D	9	4	9,9,10	0.58	0	10,12,14	0.84	0
2	AHR	E	1	2	9,9,10	0.57	0	10,12,14	0.95	0
2	BMA	E	10	2	11,11,12	0.23	0	15,15,17	0.77	1 (6%)
2	NAG	E	11	2	14,14,15	0.27	0	17,19,21	0.62	0
2	MAN	E	12	2	11,11,12	0.24	0	15,15,17	0.90	2 (13%)
2	MAN	E	13	2	11,11,12	0.21	0	15,15,17	0.85	2 (13%)
2	AHR	E	14	2	9,9,10	0.58	0	10,12,14	0.92	0
2	BGC	E	15	2	11,11,12	0.21	0	15,15,17	0.59	0
2	AHR	E	16	2	9,9,10	0.58	0	10,12,14	0.95	0
2	AHR	E	17	2	9,9,10	0.57	0	10,12,14	1.01	1 (10%)
2	AHR	E	18	2	9,9,10	0.57	0	10,12,14	0.95	0
2	FUB	E	19	2	9,9,10	0.59	0	10,12,14	0.95	0
2	FUB	E	2	2	9,9,10	0.60	0	10,12,14	0.99	0
2	AHR	E	20	2	9,9,10	0.58	0	10,12,14	0.94	0
2	AHR	E	21	2	9,9,10	0.58	0	10,12,14	0.94	0
2	NAG	E	22	2	14,14,15	0.33	0	17,19,21	0.78	0
2	FUB	E	23	2	9,9,10	0.58	0	10,12,14	0.95	0
2	AHR	E	24	2	9,9,10	0.58	0	10,12,14	0.91	0
2	A1E3E	E	25	2	11,11,12	6.68	7 (63%)	14,15,17	1.63	2 (14%)
2	FUB	E	3	2	9,9,10	0.58	0	10,12,14	0.97	0
2	AHR	E	4	2	9,9,10	0.57	0	10,12,14	0.91	0
2	XYP	E	5	2	9,9,10	0.18	0	10,12,14	0.60	0
2	AHR	E	6	2	9,9,10	0.58	0	10,12,14	0.89	0
2	FUB	E	7	2	9,9,10	0.57	0	10,12,14	1.10	1 (10%)
2	BGC	E	8	2	11,11,12	0.18	0	15,15,17	0.47	0
2	XYP	E	9	2	9,9,10	0.22	0	10,12,14	0.87	0
3	FUB	F	1	3	9,9,10	0.58	0	10,12,14	1.07	0
3	XYP	F	10	3	9,9,10	0.17	0	10,12,14	0.86	1 (10%)
3	XYP	F	11	3	9,9,10	0.18	0	10,12,14	0.69	0
3	MAN	F	12	3	11,11,12	0.23	0	15,15,17	0.83	1 (6%)
3	AHR	F	13	3	9,9,10	0.58	0	10,12,14	0.98	0
3	BGC	F	14	3	11,11,12	0.19	0	15,15,17	0.56	0
3	FUB	F	15	3	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
3	AHR	F	16	3	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
3	A1E3E	F	17	3	11,11,12	6.64	7 (63%)	14,15,17	1.75	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	F	18	3	11,11,12	0.20	0	15,15,17	0.78	0
3	BGC	F	19	3	11,11,12	0.19	0	15,15,17	0.67	0
3	XYP	F	2	3	9,9,10	0.18	0	10,12,14	0.61	0
3	AHR	F	20	3	9,9,10	0.57	0	10,12,14	0.83	0
3	AHR	F	21	3	9,9,10	0.56	0	10,12,14	0.89	0
3	AHR	F	22	3	9,9,10	0.59	0	10,12,14	0.94	0
3	BGC	F	23	3	11,11,12	0.21	0	15,15,17	0.51	0
3	XYP	F	24	3	9,9,10	0.19	0	10,12,14	0.61	0
3	MAN	F	25	3	11,11,12	0.22	0	15,15,17	0.85	2 (13%)
3	AHR	F	26	3	9,9,10	0.57	0	10,12,14	0.95	0
3	FUB	F	27	3	9,9,10	0.56	0	10,12,14	0.97	0
3	AHR	F	28	3	9,9,10	0.59	0	10,12,14	0.92	0
3	XYP	F	29	3	9,9,10	0.16	0	10,12,14	0.61	0
3	MAN	F	3	3	11,11,12	0.28	0	15,15,17	0.98	2 (13%)
3	FUB	F	30	3	9,9,10	0.57	0	10,12,14	0.67	0
3	MAN	F	31	3	11,11,12	0.26	0	15,15,17	0.86	2 (13%)
3	FUB	F	32	3	9,9,10	0.56	0	10,12,14	1.04	1 (10%)
3	A1E3E	F	33	3	11,11,12	6.72	7 (63%)	14,15,17	1.44	1 (7%)
3	BGC	F	34	3	11,11,12	0.17	0	15,15,17	0.57	0
3	XYP	F	35	3	9,9,10	0.17	0	10,12,14	0.46	0
3	BGC	F	36	3	11,11,12	0.24	0	15,15,17	0.95	1 (6%)
3	BGC	F	37	3	11,11,12	0.19	0	15,15,17	0.51	0
3	XYP	F	38	3	9,9,10	0.18	0	10,12,14	0.67	0
3	XYP	F	39	3	9,9,10	0.17	0	10,12,14	0.65	0
3	MAN	F	4	3	11,11,12	0.23	0	15,15,17	0.88	1 (6%)
3	BMA	F	40	3	11,11,12	0.22	0	15,15,17	0.86	0
3	AHR	F	41	3	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
3	FUB	F	42	3	9,9,10	0.57	0	10,12,14	1.04	1 (10%)
3	BMA	F	43	3	11,11,12	0.25	0	15,15,17	1.11	2 (13%)
3	XYP	F	5	3	9,9,10	0.18	0	10,12,14	0.74	0
3	XYP	F	6	3	9,9,10	0.16	0	10,12,14	0.61	0
3	XYP	F	7	3	9,9,10	0.17	0	10,12,14	0.63	0
3	AHR	F	8	3	9,9,10	0.58	0	10,12,14	0.96	0
3	XYP	F	9	3	9,9,10	0.17	0	10,12,14	0.54	0
4	A2G	G	1	4,1	14,14,15	0.39	0	17,19,21	0.75	0
4	AHR	G	10	4	9,9,10	0.59	0	10,12,14	0.93	0
4	AHR	G	11	4	9,9,10	0.58	0	10,12,14	0.99	1 (10%)
4	AHR	G	12	4	9,9,10	0.58	0	10,12,14	0.95	0
4	NAG	G	13	4	14,14,15	0.31	0	17,19,21	0.71	0
4	AHR	G	14	4	9,9,10	0.55	0	10,12,14	1.13	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AHR	G	15	4	9,9,10	0.55	0	10,12,14	0.95	0
4	XYP	G	16	4	9,9,10	0.18	0	10,12,14	0.57	0
4	AHR	G	17	4	9,9,10	0.59	0	10,12,14	0.82	0
4	AHR	G	18	4	9,9,10	0.56	0	10,12,14	0.96	0
4	AHR	G	19	4	9,9,10	0.57	0	10,12,14	0.88	0
4	MAN	G	2	4	11,11,12	0.23	0	15,15,17	0.85	2 (13%)
4	AHR	G	3	4	9,9,10	0.57	0	10,12,14	0.99	0
4	BGC	G	4	4	11,11,12	0.19	0	15,15,17	0.54	0
4	AHR	G	5	4	9,9,10	0.54	0	10,12,14	1.10	1 (10%)
4	BGC	G	6	4	11,11,12	0.17	0	15,15,17	0.52	0
4	MAN	G	7	4	11,11,12	0.31	0	15,15,17	1.64	2 (13%)
4	NAG	G	8	4	14,14,15	0.38	0	17,19,21	0.94	1 (5%)
4	AHR	G	9	4	9,9,10	0.56	0	10,12,14	0.82	0
2	AHR	H	1	2	9,9,10	0.56	0	10,12,14	0.98	0
2	BMA	H	10	2	11,11,12	0.22	0	15,15,17	0.80	1 (6%)
2	NAG	H	11	2	14,14,15	0.30	0	17,19,21	0.66	0
2	MAN	H	12	2	11,11,12	0.24	0	15,15,17	0.91	2 (13%)
2	MAN	H	13	2	11,11,12	0.21	0	15,15,17	0.85	2 (13%)
2	AHR	H	14	2	9,9,10	0.59	0	10,12,14	0.88	0
2	BGC	H	15	2	11,11,12	0.21	0	15,15,17	0.61	0
2	AHR	H	16	2	9,9,10	0.56	0	10,12,14	0.93	0
2	AHR	H	17	2	9,9,10	0.55	0	10,12,14	1.03	1 (10%)
2	AHR	H	18	2	9,9,10	0.57	0	10,12,14	0.97	1 (10%)
2	FUB	H	19	2	9,9,10	0.60	0	10,12,14	0.95	0
2	FUB	H	2	2	9,9,10	0.59	0	10,12,14	0.96	0
2	AHR	H	20	2	9,9,10	0.58	0	10,12,14	0.89	0
2	AHR	H	21	2	9,9,10	0.59	0	10,12,14	0.96	0
2	NAG	H	22	2	14,14,15	0.32	0	17,19,21	0.73	0
2	FUB	H	23	2	9,9,10	0.57	0	10,12,14	0.95	0
2	AHR	H	24	2	9,9,10	0.59	0	10,12,14	0.83	0
2	A1E3E	H	25	2	11,11,12	6.68	7 (63%)	14,15,17	1.63	3 (21%)
2	FUB	H	3	2	9,9,10	0.58	0	10,12,14	0.95	0
2	AHR	H	4	2	9,9,10	0.57	0	10,12,14	0.92	0
2	XYP	H	5	2	9,9,10	0.17	0	10,12,14	0.61	0
2	AHR	H	6	2	9,9,10	0.59	0	10,12,14	0.92	0
2	FUB	H	7	2	9,9,10	0.59	0	10,12,14	1.12	1 (10%)
2	BGC	H	8	2	11,11,12	0.20	0	15,15,17	0.48	0
2	XYP	H	9	2	9,9,10	0.22	0	10,12,14	0.91	0
3	FUB	I	1	3	9,9,10	0.57	0	10,12,14	0.98	0
3	XYP	I	10	3	9,9,10	0.16	0	10,12,14	0.94	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	XYP	I	11	3	9,9,10	0.18	0	10,12,14	0.69	0
3	MAN	I	12	3	11,11,12	0.23	0	15,15,17	0.83	1 (6%)
3	AHR	I	13	3	9,9,10	0.57	0	10,12,14	1.00	0
3	BGC	I	14	3	11,11,12	0.21	0	15,15,17	0.57	0
3	FUB	I	15	3	9,9,10	0.58	0	10,12,14	1.07	1 (10%)
3	AHR	I	16	3	9,9,10	0.56	0	10,12,14	1.07	1 (10%)
3	A1E3E	I	17	3	11,11,12	6.65	7 (63%)	14,15,17	1.69	3 (21%)
3	MAN	I	18	3	11,11,12	0.21	0	15,15,17	0.79	1 (6%)
3	BGC	I	19	3	11,11,12	0.19	0	15,15,17	0.70	0
3	XYP	I	2	3	9,9,10	0.17	0	10,12,14	0.66	0
3	AHR	I	20	3	9,9,10	0.57	0	10,12,14	0.82	0
3	AHR	I	21	3	9,9,10	0.55	0	10,12,14	0.82	0
3	AHR	I	22	3	9,9,10	0.58	0	10,12,14	0.93	0
3	BGC	I	23	3	11,11,12	0.21	0	15,15,17	0.53	0
3	XYP	I	24	3	9,9,10	0.18	0	10,12,14	0.61	0
3	MAN	I	25	3	11,11,12	0.20	0	15,15,17	0.86	2 (13%)
3	AHR	I	26	3	9,9,10	0.58	0	10,12,14	1.00	1 (10%)
3	FUB	I	27	3	9,9,10	0.57	0	10,12,14	0.88	0
3	AHR	I	28	3	9,9,10	0.58	0	10,12,14	0.93	0
3	XYP	I	29	3	9,9,10	0.19	0	10,12,14	0.62	0
3	MAN	I	3	3	11,11,12	0.30	0	15,15,17	0.99	1 (6%)
3	FUB	I	30	3	9,9,10	0.57	0	10,12,14	0.67	0
3	MAN	I	31	3	11,11,12	0.28	0	15,15,17	0.87	2 (13%)
3	FUB	I	32	3	9,9,10	0.55	0	10,12,14	1.09	1 (10%)
3	A1E3E	I	33	3	11,11,12	6.73	7 (63%)	14,15,17	1.47	1 (7%)
3	BGC	I	34	3	11,11,12	0.21	0	15,15,17	0.61	0
3	XYP	I	35	3	9,9,10	0.16	0	10,12,14	0.42	0
3	BGC	I	36	3	11,11,12	0.26	0	15,15,17	1.05	1 (6%)
3	BGC	I	37	3	11,11,12	0.19	0	15,15,17	0.52	0
3	XYP	I	38	3	9,9,10	0.18	0	10,12,14	0.70	0
3	XYP	I	39	3	9,9,10	0.17	0	10,12,14	0.66	0
3	MAN	I	4	3	11,11,12	0.25	0	15,15,17	0.88	1 (6%)
3	BMA	I	40	3	11,11,12	0.21	0	15,15,17	0.85	0
3	AHR	I	41	3	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
3	FUB	I	42	3	9,9,10	0.58	0	10,12,14	1.03	0
3	BMA	I	43	3	11,11,12	0.27	0	15,15,17	1.16	2 (13%)
3	XYP	I	5	3	9,9,10	0.18	0	10,12,14	0.73	0
3	XYP	I	6	3	9,9,10	0.16	0	10,12,14	0.59	0
3	XYP	I	7	3	9,9,10	0.17	0	10,12,14	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AHR	I	8	3	9,9,10	0.58	0	10,12,14	0.96	0
3	XYP	I	9	3	9,9,10	0.17	0	10,12,14	0.59	0
4	A2G	J	1	4,1	14,14,15	0.40	0	17,19,21	0.77	0
4	AHR	J	10	4	9,9,10	0.56	0	10,12,14	0.89	0
4	AHR	J	11	4	9,9,10	0.58	0	10,12,14	0.99	0
4	AHR	J	12	4	9,9,10	0.58	0	10,12,14	0.96	0
4	NAG	J	13	4	14,14,15	0.32	0	17,19,21	0.76	0
4	AHR	J	14	4	9,9,10	0.55	0	10,12,14	1.13	1 (10%)
4	AHR	J	15	4	9,9,10	0.56	0	10,12,14	0.90	0
4	XYP	J	16	4	9,9,10	0.18	0	10,12,14	0.58	0
4	AHR	J	17	4	9,9,10	0.59	0	10,12,14	0.79	0
4	AHR	J	18	4	9,9,10	0.58	0	10,12,14	0.96	0
4	AHR	J	19	4	9,9,10	0.56	0	10,12,14	0.85	0
4	MAN	J	2	4	11,11,12	0.23	0	15,15,17	0.84	2 (13%)
4	AHR	J	3	4	9,9,10	0.57	0	10,12,14	1.00	0
4	BGC	J	4	4	11,11,12	0.19	0	15,15,17	0.54	0
4	AHR	J	5	4	9,9,10	0.52	0	10,12,14	1.10	1 (10%)
4	BGC	J	6	4	11,11,12	0.18	0	15,15,17	0.53	0
4	MAN	J	7	4	11,11,12	0.30	0	15,15,17	1.66	2 (13%)
4	NAG	J	8	4	14,14,15	0.39	0	17,19,21	1.00	1 (5%)
4	AHR	J	9	4	9,9,10	0.58	0	10,12,14	0.84	0
2	AHR	K	1	2	9,9,10	0.55	0	10,12,14	1.03	0
2	BMA	K	10	2	11,11,12	0.21	0	15,15,17	0.75	0
2	NAG	K	11	2	14,14,15	0.28	0	17,19,21	0.66	0
2	MAN	K	12	2	11,11,12	0.25	0	15,15,17	0.91	2 (13%)
2	MAN	K	13	2	11,11,12	0.20	0	15,15,17	0.85	2 (13%)
2	AHR	K	14	2	9,9,10	0.59	0	10,12,14	0.88	0
2	BGC	K	15	2	11,11,12	0.21	0	15,15,17	0.61	0
2	AHR	K	16	2	9,9,10	0.57	0	10,12,14	0.93	0
2	AHR	K	17	2	9,9,10	0.57	0	10,12,14	1.04	1 (10%)
2	AHR	K	18	2	9,9,10	0.56	0	10,12,14	0.95	0
2	FUB	K	19	2	9,9,10	0.57	0	10,12,14	0.96	0
2	FUB	K	2	2	9,9,10	0.60	0	10,12,14	0.96	0
2	AHR	K	20	2	9,9,10	0.58	0	10,12,14	0.89	0
2	AHR	K	21	2	9,9,10	0.57	0	10,12,14	0.92	0
2	NAG	K	22	2	14,14,15	0.32	0	17,19,21	0.79	0
2	FUB	K	23	2	9,9,10	0.56	0	10,12,14	0.93	0
2	AHR	K	24	2	9,9,10	0.56	0	10,12,14	0.89	0
2	A1E3E	K	25	2	11,11,12	6.68	7 (63%)	14,15,17	1.63	3 (21%)
2	FUB	K	3	2	9,9,10	0.57	0	10,12,14	1.00	0
2	AHR	K	4	2	9,9,10	0.58	0	10,12,14	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	XYP	K	5	2	9,9,10	0.18	0	10,12,14	0.62	0
2	AHR	K	6	2	9,9,10	0.57	0	10,12,14	0.87	0
2	FUB	K	7	2	9,9,10	0.56	0	10,12,14	1.09	1 (10%)
2	BGC	K	8	2	11,11,12	0.19	0	15,15,17	0.49	0
2	XYP	K	9	2	9,9,10	0.22	0	10,12,14	0.89	0
3	FUB	L	1	3	9,9,10	0.58	0	10,12,14	0.95	0
3	XYP	L	10	3	9,9,10	0.17	0	10,12,14	0.93	1 (10%)
3	XYP	L	11	3	9,9,10	0.17	0	10,12,14	0.72	1 (10%)
3	MAN	L	12	3	11,11,12	0.22	0	15,15,17	0.83	1 (6%)
3	AHR	L	13	3	9,9,10	0.58	0	10,12,14	0.99	0
3	BGC	L	14	3	11,11,12	0.20	0	15,15,17	0.57	0
3	FUB	L	15	3	9,9,10	0.57	0	10,12,14	1.07	1 (10%)
3	AHR	L	16	3	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
3	A1E3E	L	17	3	11,11,12	6.65	7 (63%)	14,15,17	1.65	3 (21%)
3	MAN	L	18	3	11,11,12	0.21	0	15,15,17	0.78	0
3	BGC	L	19	3	11,11,12	0.20	0	15,15,17	0.73	0
3	XYP	L	2	3	9,9,10	0.17	0	10,12,14	0.64	0
3	AHR	L	20	3	9,9,10	0.57	0	10,12,14	0.81	0
3	AHR	L	21	3	9,9,10	0.55	0	10,12,14	0.79	0
3	AHR	L	22	3	9,9,10	0.57	0	10,12,14	0.92	0
3	BGC	L	23	3	11,11,12	0.20	0	15,15,17	0.51	0
3	XYP	L	24	3	9,9,10	0.17	0	10,12,14	0.61	0
3	MAN	L	25	3	11,11,12	0.22	0	15,15,17	0.85	2 (13%)
3	AHR	L	26	3	9,9,10	0.57	0	10,12,14	0.95	0
3	FUB	L	27	3	9,9,10	0.57	0	10,12,14	0.97	0
3	AHR	L	28	3	9,9,10	0.58	0	10,12,14	0.91	0
3	XYP	L	29	3	9,9,10	0.18	0	10,12,14	0.62	0
3	MAN	L	3	3	11,11,12	0.30	0	15,15,17	0.97	1 (6%)
3	FUB	L	30	3	9,9,10	0.56	0	10,12,14	0.69	0
3	MAN	L	31	3	11,11,12	0.27	0	15,15,17	0.86	2 (13%)
3	FUB	L	32	3	9,9,10	0.55	0	10,12,14	1.08	1 (10%)
3	A1E3E	L	33	3	11,11,12	6.74	7 (63%)	14,15,17	1.41	1 (7%)
3	BGC	L	34	3	11,11,12	0.20	0	15,15,17	0.60	0
3	XYP	L	35	3	9,9,10	0.16	0	10,12,14	0.41	0
3	BGC	L	36	3	11,11,12	0.25	0	15,15,17	1.03	1 (6%)
3	BGC	L	37	3	11,11,12	0.19	0	15,15,17	0.52	0
3	XYP	L	38	3	9,9,10	0.18	0	10,12,14	0.69	0
3	XYP	L	39	3	9,9,10	0.17	0	10,12,14	0.65	0
3	MAN	L	4	3	11,11,12	0.24	0	15,15,17	0.88	1 (6%)
3	BMA	L	40	3	11,11,12	0.21	0	15,15,17	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AHR	L	41	3	9,9,10	0.60	0	10,12,14	1.06	1 (10%)
3	FUB	L	42	3	9,9,10	0.58	0	10,12,14	1.02	0
3	BMA	L	43	3	11,11,12	0.25	0	15,15,17	1.15	2 (13%)
3	XYP	L	5	3	9,9,10	0.18	0	10,12,14	0.70	0
3	XYP	L	6	3	9,9,10	0.16	0	10,12,14	0.58	0
3	XYP	L	7	3	9,9,10	0.17	0	10,12,14	0.60	0
3	AHR	L	8	3	9,9,10	0.58	0	10,12,14	0.97	0
3	XYP	L	9	3	9,9,10	0.17	0	10,12,14	0.53	0
4	A2G	M	1	4,1	14,14,15	0.38	0	17,19,21	0.78	0
4	AHR	M	10	4	9,9,10	0.56	0	10,12,14	0.92	0
4	AHR	M	11	4	9,9,10	0.58	0	10,12,14	1.02	1 (10%)
4	AHR	M	12	4	9,9,10	0.57	0	10,12,14	0.96	0
4	NAG	M	13	4	14,14,15	0.33	0	17,19,21	0.82	1 (5%)
4	AHR	M	14	4	9,9,10	0.56	0	10,12,14	1.11	1 (10%)
4	AHR	M	15	4	9,9,10	0.57	0	10,12,14	0.92	0
4	XYP	M	16	4	9,9,10	0.18	0	10,12,14	0.58	0
4	AHR	M	17	4	9,9,10	0.58	0	10,12,14	0.82	0
4	AHR	M	18	4	9,9,10	0.56	0	10,12,14	0.95	0
4	AHR	M	19	4	9,9,10	0.56	0	10,12,14	0.87	0
4	MAN	M	2	4	11,11,12	0.23	0	15,15,17	0.85	2 (13%)
4	AHR	M	3	4	9,9,10	0.56	0	10,12,14	1.00	0
4	BGC	M	4	4	11,11,12	0.19	0	15,15,17	0.55	0
4	AHR	M	5	4	9,9,10	0.54	0	10,12,14	1.11	1 (10%)
4	BGC	M	6	4	11,11,12	0.18	0	15,15,17	0.52	0
4	MAN	M	7	4	11,11,12	0.31	0	15,15,17	1.63	2 (13%)
4	NAG	M	8	4	14,14,15	0.38	0	17,19,21	0.95	1 (5%)
4	AHR	M	9	4	9,9,10	0.58	0	10,12,14	0.83	0
2	AHR	N	1	2	9,9,10	0.57	0	10,12,14	1.01	0
2	BMA	N	10	2	11,11,12	0.24	0	15,15,17	0.84	1 (6%)
2	NAG	N	11	2	14,14,15	0.29	0	17,19,21	0.74	0
2	MAN	N	12	2	11,11,12	0.25	0	15,15,17	0.92	2 (13%)
2	MAN	N	13	2	11,11,12	0.21	0	15,15,17	0.86	2 (13%)
2	AHR	N	14	2	9,9,10	0.59	0	10,12,14	0.89	0
2	BGC	N	15	2	11,11,12	0.20	0	15,15,17	0.61	0
2	AHR	N	16	2	9,9,10	0.57	0	10,12,14	0.92	0
2	AHR	N	17	2	9,9,10	0.58	0	10,12,14	1.03	1 (10%)
2	AHR	N	18	2	9,9,10	0.58	0	10,12,14	1.02	1 (10%)
2	FUB	N	19	2	9,9,10	0.57	0	10,12,14	0.93	0
2	FUB	N	2	2	9,9,10	0.60	0	10,12,14	0.97	0
2	AHR	N	20	2	9,9,10	0.58	0	10,12,14	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AHR	N	21	2	9,9,10	0.58	0	10,12,14	0.92	0
2	NAG	N	22	2	14,14,15	0.30	0	17,19,21	0.65	0
2	FUB	N	23	2	9,9,10	0.58	0	10,12,14	0.92	0
2	AHR	N	24	2	9,9,10	0.59	0	10,12,14	0.84	0
2	A1E3E	N	25	2	11,11,12	6.69	7 (63%)	14,15,17	1.65	3 (21%)
2	FUB	N	3	2	9,9,10	0.58	0	10,12,14	0.95	0
2	AHR	N	4	2	9,9,10	0.58	0	10,12,14	0.94	0
2	XYP	N	5	2	9,9,10	0.17	0	10,12,14	0.60	0
2	AHR	N	6	2	9,9,10	0.59	0	10,12,14	0.95	0
2	FUB	N	7	2	9,9,10	0.58	0	10,12,14	1.11	1 (10%)
2	BGC	N	8	2	11,11,12	0.20	0	15,15,17	0.48	0
2	XYP	N	9	2	9,9,10	0.24	0	10,12,14	0.97	1 (10%)
3	FUB	O	1	3	9,9,10	0.57	0	10,12,14	0.99	0
3	XYP	O	10	3	9,9,10	0.17	0	10,12,14	0.94	1 (10%)
3	XYP	O	11	3	9,9,10	0.17	0	10,12,14	0.70	0
3	MAN	O	12	3	11,11,12	0.23	0	15,15,17	0.82	1 (6%)
3	AHR	O	13	3	9,9,10	0.58	0	10,12,14	1.00	0
3	BGC	O	14	3	11,11,12	0.21	0	15,15,17	0.58	0
3	FUB	O	15	3	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
3	AHR	O	16	3	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
3	A1E3E	O	17	3	11,11,12	6.67	7 (63%)	14,15,17	1.72	2 (14%)
3	MAN	O	18	3	11,11,12	0.20	0	15,15,17	0.78	1 (6%)
3	BGC	O	19	3	11,11,12	0.20	0	15,15,17	0.72	0
3	XYP	O	2	3	9,9,10	0.18	0	10,12,14	0.66	0
3	AHR	O	20	3	9,9,10	0.58	0	10,12,14	0.80	0
3	AHR	O	21	3	9,9,10	0.56	0	10,12,14	0.81	0
3	AHR	O	22	3	9,9,10	0.57	0	10,12,14	0.91	0
3	BGC	O	23	3	11,11,12	0.22	0	15,15,17	0.54	0
3	XYP	O	24	3	9,9,10	0.18	0	10,12,14	0.62	0
3	MAN	O	25	3	11,11,12	0.23	0	15,15,17	0.85	2 (13%)
3	AHR	O	26	3	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
3	FUB	O	27	3	9,9,10	0.55	0	10,12,14	0.94	0
3	AHR	O	28	3	9,9,10	0.58	0	10,12,14	0.96	0
3	XYP	O	29	3	9,9,10	0.17	0	10,12,14	0.64	0
3	MAN	O	3	3	11,11,12	0.31	0	15,15,17	1.00	2 (13%)
3	FUB	O	30	3	9,9,10	0.58	0	10,12,14	0.68	0
3	MAN	O	31	3	11,11,12	0.28	0	15,15,17	0.88	2 (13%)
3	FUB	O	32	3	9,9,10	0.57	0	10,12,14	1.03	1 (10%)
3	A1E3E	O	33	3	11,11,12	6.72	7 (63%)	14,15,17	1.52	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	O	34	3	11,11,12	0.21	0	15,15,17	0.60	0
3	XYP	O	35	3	9,9,10	0.16	0	10,12,14	0.41	0
3	BGC	O	36	3	11,11,12	0.28	0	15,15,17	1.07	1 (6%)
3	BGC	O	37	3	11,11,12	0.19	0	15,15,17	0.50	0
3	XYP	O	38	3	9,9,10	0.19	0	10,12,14	0.71	1 (10%)
3	XYP	O	39	3	9,9,10	0.17	0	10,12,14	0.67	0
3	MAN	O	4	3	11,11,12	0.25	0	15,15,17	0.88	1 (6%)
3	BMA	O	40	3	11,11,12	0.22	0	15,15,17	0.88	0
3	AHR	O	41	3	9,9,10	0.59	0	10,12,14	1.06	1 (10%)
3	FUB	O	42	3	9,9,10	0.58	0	10,12,14	1.01	0
3	BMA	O	43	3	11,11,12	0.26	0	15,15,17	1.20	2 (13%)
3	XYP	O	5	3	9,9,10	0.17	0	10,12,14	0.74	0
3	XYP	O	6	3	9,9,10	0.15	0	10,12,14	0.58	0
3	XYP	O	7	3	9,9,10	0.17	0	10,12,14	0.60	0
3	AHR	O	8	3	9,9,10	0.58	0	10,12,14	0.98	0
3	XYP	O	9	3	9,9,10	0.17	0	10,12,14	0.58	0
4	A2G	P	1	4,1	14,14,15	0.39	0	17,19,21	0.77	0
4	AHR	P	10	4	9,9,10	0.56	0	10,12,14	0.96	1 (10%)
4	AHR	P	11	4	9,9,10	0.58	0	10,12,14	1.01	1 (10%)
4	AHR	P	12	4	9,9,10	0.57	0	10,12,14	0.98	0
4	NAG	P	13	4	14,14,15	0.34	0	17,19,21	0.80	0
4	AHR	P	14	4	9,9,10	0.57	0	10,12,14	1.13	1 (10%)
4	AHR	P	15	4	9,9,10	0.55	0	10,12,14	0.89	0
4	XYP	P	16	4	9,9,10	0.18	0	10,12,14	0.61	0
4	AHR	P	17	4	9,9,10	0.59	0	10,12,14	0.78	0
4	AHR	P	18	4	9,9,10	0.55	0	10,12,14	0.97	1 (10%)
4	AHR	P	19	4	9,9,10	0.57	0	10,12,14	0.87	0
4	MAN	P	2	4	11,11,12	0.22	0	15,15,17	0.85	2 (13%)
4	AHR	P	3	4	9,9,10	0.57	0	10,12,14	1.01	0
4	BGC	P	4	4	11,11,12	0.20	0	15,15,17	0.52	0
4	AHR	P	5	4	9,9,10	0.54	0	10,12,14	1.10	1 (10%)
4	BGC	P	6	4	11,11,12	0.18	0	15,15,17	0.52	0
4	MAN	P	7	4	11,11,12	0.29	0	15,15,17	1.63	2 (13%)
4	NAG	P	8	4	14,14,15	0.38	0	17,19,21	0.97	1 (5%)
4	AHR	P	9	4	9,9,10	0.57	0	10,12,14	0.83	0
2	AHR	Q	1	2	9,9,10	0.57	0	10,12,14	0.96	0
2	BMA	Q	10	2	11,11,12	0.23	0	15,15,17	0.79	1 (6%)
2	NAG	Q	11	2	14,14,15	0.29	0	17,19,21	0.67	0
2	MAN	Q	12	2	11,11,12	0.25	0	15,15,17	0.92	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	Q	13	2	11,11,12	0.19	0	15,15,17	0.86	2 (13%)
2	AHR	Q	14	2	9,9,10	0.58	0	10,12,14	0.88	0
2	BGC	Q	15	2	11,11,12	0.21	0	15,15,17	0.60	0
2	AHR	Q	16	2	9,9,10	0.58	0	10,12,14	0.92	0
2	AHR	Q	17	2	9,9,10	0.56	0	10,12,14	1.03	1 (10%)
2	AHR	Q	18	2	9,9,10	0.59	0	10,12,14	0.97	1 (10%)
2	FUB	Q	19	2	9,9,10	0.58	0	10,12,14	0.95	0
2	FUB	Q	2	2	9,9,10	0.59	0	10,12,14	0.98	0
2	AHR	Q	20	2	9,9,10	0.57	0	10,12,14	0.89	0
2	AHR	Q	21	2	9,9,10	0.57	0	10,12,14	0.97	0
2	NAG	Q	22	2	14,14,15	0.30	0	17,19,21	0.65	0
2	FUB	Q	23	2	9,9,10	0.59	0	10,12,14	0.96	0
2	AHR	Q	24	2	9,9,10	0.57	0	10,12,14	0.84	0
2	A1E3E	Q	25	2	11,11,12	6.69	7 (63%)	14,15,17	1.61	3 (21%)
2	FUB	Q	3	2	9,9,10	0.58	0	10,12,14	0.95	0
2	AHR	Q	4	2	9,9,10	0.57	0	10,12,14	0.96	0
2	XYP	Q	5	2	9,9,10	0.17	0	10,12,14	0.59	0
2	AHR	Q	6	2	9,9,10	0.58	0	10,12,14	0.99	0
2	FUB	Q	7	2	9,9,10	0.59	0	10,12,14	1.13	1 (10%)
2	BGC	Q	8	2	11,11,12	0.20	0	15,15,17	0.50	0
2	XYP	Q	9	2	9,9,10	0.24	0	10,12,14	0.95	1 (10%)
3	FUB	R	1	3	9,9,10	0.56	0	10,12,14	1.01	0
3	XYP	R	10	3	9,9,10	0.18	0	10,12,14	0.94	1 (10%)
3	XYP	R	11	3	9,9,10	0.17	0	10,12,14	0.69	0
3	MAN	R	12	3	11,11,12	0.23	0	15,15,17	0.82	1 (6%)
3	AHR	R	13	3	9,9,10	0.56	0	10,12,14	0.99	0
3	BGC	R	14	3	11,11,12	0.21	0	15,15,17	0.57	0
3	FUB	R	15	3	9,9,10	0.56	0	10,12,14	1.08	1 (10%)
3	AHR	R	16	3	9,9,10	0.59	0	10,12,14	1.03	1 (10%)
3	A1E3E	R	17	3	11,11,12	6.67	7 (63%)	14,15,17	1.70	3 (21%)
3	MAN	R	18	3	11,11,12	0.20	0	15,15,17	0.78	0
3	BGC	R	19	3	11,11,12	0.19	0	15,15,17	0.70	0
3	XYP	R	2	3	9,9,10	0.19	0	10,12,14	0.65	0
3	AHR	R	20	3	9,9,10	0.59	0	10,12,14	0.80	0
3	AHR	R	21	3	9,9,10	0.56	0	10,12,14	0.82	0
3	AHR	R	22	3	9,9,10	0.56	0	10,12,14	0.93	0
3	BGC	R	23	3	11,11,12	0.22	0	15,15,17	0.52	0
3	XYP	R	24	3	9,9,10	0.17	0	10,12,14	0.62	0
3	MAN	R	25	3	11,11,12	0.21	0	15,15,17	0.86	2 (13%)
3	AHR	R	26	3	9,9,10	0.58	0	10,12,14	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUB	R	27	3	9,9,10	0.56	0	10,12,14	0.96	0
3	AHR	R	28	3	9,9,10	0.59	0	10,12,14	0.94	0
3	XYP	R	29	3	9,9,10	0.18	0	10,12,14	0.63	0
3	MAN	R	3	3	11,11,12	0.31	0	15,15,17	1.01	2 (13%)
3	FUB	R	30	3	9,9,10	0.56	0	10,12,14	0.68	0
3	MAN	R	31	3	11,11,12	0.28	0	15,15,17	0.87	2 (13%)
3	FUB	R	32	3	9,9,10	0.55	0	10,12,14	1.08	1 (10%)
3	A1E3E	R	33	3	11,11,12	6.74	7 (63%)	14,15,17	1.43	1 (7%)
3	BGC	R	34	3	11,11,12	0.21	0	15,15,17	0.61	0
3	XYP	R	35	3	9,9,10	0.17	0	10,12,14	0.42	0
3	BGC	R	36	3	11,11,12	0.25	0	15,15,17	1.05	1 (6%)
3	BGC	R	37	3	11,11,12	0.19	0	15,15,17	0.53	0
3	XYP	R	38	3	9,9,10	0.18	0	10,12,14	0.71	1 (10%)
3	XYP	R	39	3	9,9,10	0.17	0	10,12,14	0.67	0
3	MAN	R	4	3	11,11,12	0.24	0	15,15,17	0.90	1 (6%)
3	BMA	R	40	3	11,11,12	0.22	0	15,15,17	0.94	1 (6%)
3	AHR	R	41	3	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
3	FUB	R	42	3	9,9,10	0.58	0	10,12,14	1.02	0
3	BMA	R	43	3	11,11,12	0.27	0	15,15,17	1.27	2 (13%)
3	XYP	R	5	3	9,9,10	0.18	0	10,12,14	0.74	0
3	XYP	R	6	3	9,9,10	0.16	0	10,12,14	0.57	0
3	XYP	R	7	3	9,9,10	0.17	0	10,12,14	0.60	0
3	AHR	R	8	3	9,9,10	0.58	0	10,12,14	0.96	0
3	XYP	R	9	3	9,9,10	0.18	0	10,12,14	0.60	0
4	A2G	S	1	4,1	14,14,15	0.39	0	17,19,21	0.77	0
4	AHR	S	10	4	9,9,10	0.56	0	10,12,14	0.94	0
4	AHR	S	11	4	9,9,10	0.57	0	10,12,14	1.04	1 (10%)
4	AHR	S	12	4	9,9,10	0.59	0	10,12,14	0.95	0
4	NAG	S	13	4	14,14,15	0.32	0	17,19,21	0.78	0
4	AHR	S	14	4	9,9,10	0.57	0	10,12,14	1.12	1 (10%)
4	AHR	S	15	4	9,9,10	0.57	0	10,12,14	0.91	0
4	XYP	S	16	4	9,9,10	0.19	0	10,12,14	0.60	0
4	AHR	S	17	4	9,9,10	0.59	0	10,12,14	0.79	0
4	AHR	S	18	4	9,9,10	0.58	0	10,12,14	0.97	1 (10%)
4	AHR	S	19	4	9,9,10	0.58	0	10,12,14	0.83	0
4	MAN	S	2	4	11,11,12	0.23	0	15,15,17	0.83	2 (13%)
4	AHR	S	3	4	9,9,10	0.57	0	10,12,14	0.99	0
4	BGC	S	4	4	11,11,12	0.19	0	15,15,17	0.54	0
4	AHR	S	5	4	9,9,10	0.54	0	10,12,14	1.11	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BGC	S	6	4	11,11,12	0.17	0	15,15,17	0.52	0
4	MAN	S	7	4	11,11,12	0.30	0	15,15,17	1.64	2 (13%)
4	NAG	S	8	4	14,14,15	0.38	0	17,19,21	0.94	0
4	AHR	S	9	4	9,9,10	0.58	0	10,12,14	0.83	0
2	AHR	T	1	2	9,9,10	0.57	0	10,12,14	0.97	0
2	BMA	T	10	2	11,11,12	0.25	0	15,15,17	0.83	1 (6%)
2	NAG	T	11	2	14,14,15	0.29	0	17,19,21	0.66	0
2	MAN	T	12	2	11,11,12	0.23	0	15,15,17	0.90	2 (13%)
2	MAN	T	13	2	11,11,12	0.20	0	15,15,17	0.86	2 (13%)
2	AHR	T	14	2	9,9,10	0.59	0	10,12,14	0.93	0
2	BGC	T	15	2	11,11,12	0.21	0	15,15,17	0.60	0
2	AHR	T	16	2	9,9,10	0.57	0	10,12,14	0.92	0
2	AHR	T	17	2	9,9,10	0.57	0	10,12,14	1.04	1 (10%)
2	AHR	T	18	2	9,9,10	0.58	0	10,12,14	1.04	1 (10%)
2	FUB	T	19	2	9,9,10	0.58	0	10,12,14	0.94	0
2	FUB	T	2	2	9,9,10	0.60	0	10,12,14	0.99	0
2	AHR	T	20	2	9,9,10	0.58	0	10,12,14	0.93	0
2	AHR	T	21	2	9,9,10	0.58	0	10,12,14	0.98	1 (10%)
2	NAG	T	22	2	14,14,15	0.29	0	17,19,21	0.62	0
2	FUB	T	23	2	9,9,10	0.57	0	10,12,14	0.94	0
2	AHR	T	24	2	9,9,10	0.59	0	10,12,14	0.83	0
2	A1E3E	T	25	2	11,11,12	6.70	7 (63%)	14,15,17	1.60	2 (14%)
2	FUB	T	3	2	9,9,10	0.57	0	10,12,14	0.96	0
2	AHR	T	4	2	9,9,10	0.58	0	10,12,14	0.95	0
2	XYP	T	5	2	9,9,10	0.17	0	10,12,14	0.61	0
2	AHR	T	6	2	9,9,10	0.57	0	10,12,14	0.99	0
2	FUB	T	7	2	9,9,10	0.57	0	10,12,14	1.12	1 (10%)
2	BGC	T	8	2	11,11,12	0.19	0	15,15,17	0.51	0
2	XYP	T	9	2	9,9,10	0.24	0	10,12,14	0.94	1 (10%)
3	FUB	U	1	3	9,9,10	0.57	0	10,12,14	1.01	0
3	XYP	U	10	3	9,9,10	0.17	0	10,12,14	0.93	1 (10%)
3	XYP	U	11	3	9,9,10	0.17	0	10,12,14	0.69	0
3	MAN	U	12	3	11,11,12	0.23	0	15,15,17	0.82	1 (6%)
3	AHR	U	13	3	9,9,10	0.58	0	10,12,14	1.01	1 (10%)
3	BGC	U	14	3	11,11,12	0.20	0	15,15,17	0.57	0
3	FUB	U	15	3	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
3	AHR	U	16	3	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
3	A1E3E	U	17	3	11,11,12	6.66	7 (63%)	14,15,17	1.72	3 (21%)
3	MAN	U	18	3	11,11,12	0.20	0	15,15,17	0.79	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	U	19	3	11,11,12	0.19	0	15,15,17	0.70	0
3	XYP	U	2	3	9,9,10	0.16	0	10,12,14	0.64	0
3	AHR	U	20	3	9,9,10	0.59	0	10,12,14	0.80	0
3	AHR	U	21	3	9,9,10	0.56	0	10,12,14	0.82	0
3	AHR	U	22	3	9,9,10	0.57	0	10,12,14	0.88	0
3	BGC	U	23	3	11,11,12	0.21	0	15,15,17	0.54	0
3	XYP	U	24	3	9,9,10	0.18	0	10,12,14	0.61	0
3	MAN	U	25	3	11,11,12	0.21	0	15,15,17	0.86	2 (13%)
3	AHR	U	26	3	9,9,10	0.56	0	10,12,14	1.00	1 (10%)
3	FUB	U	27	3	9,9,10	0.57	0	10,12,14	0.91	0
3	AHR	U	28	3	9,9,10	0.59	0	10,12,14	0.93	0
3	XYP	U	29	3	9,9,10	0.17	0	10,12,14	0.64	0
3	MAN	U	3	3	11,11,12	0.32	0	15,15,17	1.01	2 (13%)
3	FUB	U	30	3	9,9,10	0.57	0	10,12,14	0.70	0
3	MAN	U	31	3	11,11,12	0.29	0	15,15,17	0.86	2 (13%)
3	FUB	U	32	3	9,9,10	0.55	0	10,12,14	1.08	1 (10%)
3	A1E3E	U	33	3	11,11,12	6.74	7 (63%)	14,15,17	1.51	1 (7%)
3	BGC	U	34	3	11,11,12	0.21	0	15,15,17	0.59	0
3	XYP	U	35	3	9,9,10	0.15	0	10,12,14	0.46	0
3	BGC	U	36	3	11,11,12	0.25	0	15,15,17	1.00	1 (6%)
3	BGC	U	37	3	11,11,12	0.20	0	15,15,17	0.50	0
3	XYP	U	38	3	9,9,10	0.18	0	10,12,14	0.68	0
3	XYP	U	39	3	9,9,10	0.17	0	10,12,14	0.66	0
3	MAN	U	4	3	11,11,12	0.25	0	15,15,17	0.89	1 (6%)
3	BMA	U	40	3	11,11,12	0.22	0	15,15,17	0.89	0
3	AHR	U	41	3	9,9,10	0.58	0	10,12,14	1.06	1 (10%)
3	FUB	U	42	3	9,9,10	0.58	0	10,12,14	1.02	0
3	BMA	U	43	3	11,11,12	0.25	0	15,15,17	1.12	2 (13%)
3	XYP	U	5	3	9,9,10	0.17	0	10,12,14	0.74	0
3	XYP	U	6	3	9,9,10	0.16	0	10,12,14	0.60	0
3	XYP	U	7	3	9,9,10	0.17	0	10,12,14	0.60	0
3	AHR	U	8	3	9,9,10	0.58	0	10,12,14	0.96	0
3	XYP	U	9	3	9,9,10	0.18	0	10,12,14	0.58	0
4	A2G	V	1	4,1	14,14,15	0.40	0	17,19,21	0.78	0
4	AHR	V	10	4	9,9,10	0.57	0	10,12,14	0.99	1 (10%)
4	AHR	V	11	4	9,9,10	0.58	0	10,12,14	1.02	1 (10%)
4	AHR	V	12	4	9,9,10	0.58	0	10,12,14	0.96	0
4	NAG	V	13	4	14,14,15	0.32	0	17,19,21	0.83	1 (5%)
4	AHR	V	14	4	9,9,10	0.57	0	10,12,14	1.11	1 (10%)
4	AHR	V	15	4	9,9,10	0.58	0	10,12,14	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	XYP	V	16	4	9,9,10	0.18	0	10,12,14	0.58	0
4	AHR	V	17	4	9,9,10	0.59	0	10,12,14	0.79	0
4	AHR	V	18	4	9,9,10	0.57	0	10,12,14	0.98	1 (10%)
4	AHR	V	19	4	9,9,10	0.58	0	10,12,14	0.83	0
4	MAN	V	2	4	11,11,12	0.24	0	15,15,17	0.84	2 (13%)
4	AHR	V	3	4	9,9,10	0.56	0	10,12,14	1.01	0
4	BGC	V	4	4	11,11,12	0.19	0	15,15,17	0.54	0
4	AHR	V	5	4	9,9,10	0.55	0	10,12,14	1.10	1 (10%)
4	BGC	V	6	4	11,11,12	0.18	0	15,15,17	0.52	0
4	MAN	V	7	4	11,11,12	0.30	0	15,15,17	1.62	2 (13%)
4	NAG	V	8	4	14,14,15	0.38	0	17,19,21	1.01	1 (5%)
4	AHR	V	9	4	9,9,10	0.56	0	10,12,14	0.87	0
2	AHR	W	1	2	9,9,10	0.58	0	10,12,14	0.98	0
2	BMA	W	10	2	11,11,12	0.23	0	15,15,17	0.83	1 (6%)
2	NAG	W	11	2	14,14,15	0.28	0	17,19,21	0.71	0
2	MAN	W	12	2	11,11,12	0.25	0	15,15,17	0.91	2 (13%)
2	MAN	W	13	2	11,11,12	0.19	0	15,15,17	0.87	2 (13%)
2	AHR	W	14	2	9,9,10	0.58	0	10,12,14	0.95	0
2	BGC	W	15	2	11,11,12	0.22	0	15,15,17	0.61	0
2	AHR	W	16	2	9,9,10	0.59	0	10,12,14	0.91	0
2	AHR	W	17	2	9,9,10	0.56	0	10,12,14	1.04	1 (10%)
2	AHR	W	18	2	9,9,10	0.58	0	10,12,14	1.01	1 (10%)
2	FUB	W	19	2	9,9,10	0.59	0	10,12,14	0.90	0
2	FUB	W	2	2	9,9,10	0.59	0	10,12,14	0.99	0
2	AHR	W	20	2	9,9,10	0.57	0	10,12,14	0.92	0
2	AHR	W	21	2	9,9,10	0.58	0	10,12,14	1.00	1 (10%)
2	NAG	W	22	2	14,14,15	0.31	0	17,19,21	0.67	0
2	FUB	W	23	2	9,9,10	0.57	0	10,12,14	0.92	0
2	AHR	W	24	2	9,9,10	0.58	0	10,12,14	0.82	0
2	A1E3E	W	25	2	11,11,12	6.69	7 (63%)	14,15,17	1.66	3 (21%)
2	FUB	W	3	2	9,9,10	0.56	0	10,12,14	0.94	0
2	AHR	W	4	2	9,9,10	0.57	0	10,12,14	0.94	0
2	XYP	W	5	2	9,9,10	0.16	0	10,12,14	0.59	0
2	AHR	W	6	2	9,9,10	0.58	0	10,12,14	1.01	0
2	FUB	W	7	2	9,9,10	0.58	0	10,12,14	1.12	1 (10%)
2	BGC	W	8	2	11,11,12	0.20	0	15,15,17	0.49	0
2	XYP	W	9	2	9,9,10	0.22	0	10,12,14	0.90	0
3	FUB	X	1	3	9,9,10	0.58	0	10,12,14	1.01	0
3	XYP	X	10	3	9,9,10	0.18	0	10,12,14	0.93	1 (10%)
3	XYP	X	11	3	9,9,10	0.17	0	10,12,14	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	X	12	3	11,11,12	0.23	0	15,15,17	0.82	1 (6%)
3	AHR	X	13	3	9,9,10	0.57	0	10,12,14	1.00	0
3	BGC	X	14	3	11,11,12	0.20	0	15,15,17	0.57	0
3	FUB	X	15	3	9,9,10	0.58	0	10,12,14	1.05	1 (10%)
3	AHR	X	16	3	9,9,10	0.58	0	10,12,14	1.03	1 (10%)
3	A1E3E	X	17	3	11,11,12	6.65	7 (63%)	14,15,17	1.72	3 (21%)
3	MAN	X	18	3	11,11,12	0.20	0	15,15,17	0.78	1 (6%)
3	BGC	X	19	3	11,11,12	0.20	0	15,15,17	0.72	0
3	XYP	X	2	3	9,9,10	0.18	0	10,12,14	0.64	0
3	AHR	X	20	3	9,9,10	0.57	0	10,12,14	0.82	0
3	AHR	X	21	3	9,9,10	0.56	0	10,12,14	0.79	0
3	AHR	X	22	3	9,9,10	0.56	0	10,12,14	0.91	0
3	BGC	X	23	3	11,11,12	0.21	0	15,15,17	0.54	0
3	XYP	X	24	3	9,9,10	0.17	0	10,12,14	0.61	0
3	MAN	X	25	3	11,11,12	0.23	0	15,15,17	0.86	2 (13%)
3	AHR	X	26	3	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
3	FUB	X	27	3	9,9,10	0.55	0	10,12,14	0.94	0
3	AHR	X	28	3	9,9,10	0.59	0	10,12,14	0.96	0
3	XYP	X	29	3	9,9,10	0.17	0	10,12,14	0.64	0
3	MAN	X	3	3	11,11,12	0.30	0	15,15,17	1.00	2 (13%)
3	FUB	X	30	3	9,9,10	0.57	0	10,12,14	0.68	0
3	MAN	X	31	3	11,11,12	0.28	0	15,15,17	0.87	2 (13%)
3	FUB	X	32	3	9,9,10	0.55	0	10,12,14	1.05	1 (10%)
3	A1E3E	X	33	3	11,11,12	6.74	7 (63%)	14,15,17	1.51	1 (7%)
3	BGC	X	34	3	11,11,12	0.21	0	15,15,17	0.61	0
3	XYP	X	35	3	9,9,10	0.16	0	10,12,14	0.42	0
3	BGC	X	36	3	11,11,12	0.25	0	15,15,17	1.04	1 (6%)
3	BGC	X	37	3	11,11,12	0.21	0	15,15,17	0.50	0
3	XYP	X	38	3	9,9,10	0.19	0	10,12,14	0.71	0
3	XYP	X	39	3	9,9,10	0.16	0	10,12,14	0.66	0
3	MAN	X	4	3	11,11,12	0.25	0	15,15,17	0.88	1 (6%)
3	BMA	X	40	3	11,11,12	0.22	0	15,15,17	0.86	0
3	AHR	X	41	3	9,9,10	0.56	0	10,12,14	1.04	1 (10%)
3	FUB	X	42	3	9,9,10	0.59	0	10,12,14	1.01	0
3	BMA	X	43	3	11,11,12	0.27	0	15,15,17	1.23	2 (13%)
3	XYP	X	5	3	9,9,10	0.18	0	10,12,14	0.73	0
3	XYP	X	6	3	9,9,10	0.17	0	10,12,14	0.59	0
3	XYP	X	7	3	9,9,10	0.18	0	10,12,14	0.59	0
3	AHR	X	8	3	9,9,10	0.57	0	10,12,14	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	XYP	X	9	3	9,9,10	0.16	0	10,12,14	0.57	0
4	A2G	Y	1	4,1	14,14,15	0.40	0	17,19,21	0.78	0
4	AHR	Y	10	4	9,9,10	0.57	0	10,12,14	0.96	1 (10%)
4	AHR	Y	11	4	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
4	AHR	Y	12	4	9,9,10	0.57	0	10,12,14	0.96	0
4	NAG	Y	13	4	14,14,15	0.34	0	17,19,21	0.85	1 (5%)
4	AHR	Y	14	4	9,9,10	0.56	0	10,12,14	1.13	1 (10%)
4	AHR	Y	15	4	9,9,10	0.57	0	10,12,14	0.89	0
4	XYP	Y	16	4	9,9,10	0.17	0	10,12,14	0.59	0
4	AHR	Y	17	4	9,9,10	0.58	0	10,12,14	0.79	0
4	AHR	Y	18	4	9,9,10	0.56	0	10,12,14	0.97	1 (10%)
4	AHR	Y	19	4	9,9,10	0.59	0	10,12,14	0.87	0
4	MAN	Y	2	4	11,11,12	0.23	0	15,15,17	0.85	2 (13%)
4	AHR	Y	3	4	9,9,10	0.57	0	10,12,14	1.02	0
4	BGC	Y	4	4	11,11,12	0.20	0	15,15,17	0.54	0
4	AHR	Y	5	4	9,9,10	0.54	0	10,12,14	1.11	1 (10%)
4	BGC	Y	6	4	11,11,12	0.16	0	15,15,17	0.52	0
4	MAN	Y	7	4	11,11,12	0.29	0	15,15,17	1.64	2 (13%)
4	NAG	Y	8	4	14,14,15	0.39	0	17,19,21	1.03	1 (5%)
4	AHR	Y	9	4	9,9,10	0.59	0	10,12,14	0.83	0
2	AHR	Z	1	2	9,9,10	0.57	0	10,12,14	0.98	0
2	BMA	Z	10	2	11,11,12	0.24	0	15,15,17	0.82	1 (6%)
2	NAG	Z	11	2	14,14,15	0.29	0	17,19,21	0.63	0
2	MAN	Z	12	2	11,11,12	0.24	0	15,15,17	0.89	2 (13%)
2	MAN	Z	13	2	11,11,12	0.21	0	15,15,17	0.86	2 (13%)
2	AHR	Z	14	2	9,9,10	0.58	0	10,12,14	0.94	0
2	BGC	Z	15	2	11,11,12	0.21	0	15,15,17	0.58	0
2	AHR	Z	16	2	9,9,10	0.57	0	10,12,14	0.92	0
2	AHR	Z	17	2	9,9,10	0.55	0	10,12,14	1.03	1 (10%)
2	AHR	Z	18	2	9,9,10	0.57	0	10,12,14	1.02	1 (10%)
2	FUB	Z	19	2	9,9,10	0.60	0	10,12,14	0.93	0
2	FUB	Z	2	2	9,9,10	0.58	0	10,12,14	0.99	0
2	AHR	Z	20	2	9,9,10	0.57	0	10,12,14	0.94	0
2	AHR	Z	21	2	9,9,10	0.57	0	10,12,14	1.00	1 (10%)
2	NAG	Z	22	2	14,14,15	0.30	0	17,19,21	0.64	0
2	FUB	Z	23	2	9,9,10	0.58	0	10,12,14	0.94	0
2	AHR	Z	24	2	9,9,10	0.58	0	10,12,14	0.84	0
2	A1E3E	Z	25	2	11,11,12	6.69	7 (63%)	14,15,17	1.61	2 (14%)
2	FUB	Z	3	2	9,9,10	0.59	0	10,12,14	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AHR	Z	4	2	9,9,10	0.58	0	10,12,14	0.95	0
2	XYP	Z	5	2	9,9,10	0.17	0	10,12,14	0.60	0
2	AHR	Z	6	2	9,9,10	0.57	0	10,12,14	0.97	0
2	FUB	Z	7	2	9,9,10	0.59	0	10,12,14	1.13	1 (10%)
2	BGC	Z	8	2	11,11,12	0.20	0	15,15,17	0.52	0
2	XYP	Z	9	2	9,9,10	0.25	0	10,12,14	0.92	0
3	FUB	a	1	3	9,9,10	0.58	0	10,12,14	1.00	0
3	XYP	a	10	3	9,9,10	0.19	0	10,12,14	0.92	1 (10%)
3	XYP	a	11	3	9,9,10	0.17	0	10,12,14	0.70	0
3	MAN	a	12	3	11,11,12	0.23	0	15,15,17	0.83	1 (6%)
3	AHR	a	13	3	9,9,10	0.57	0	10,12,14	0.99	0
3	BGC	a	14	3	11,11,12	0.20	0	15,15,17	0.56	0
3	FUB	a	15	3	9,9,10	0.59	0	10,12,14	1.04	1 (10%)
3	AHR	a	16	3	9,9,10	0.58	0	10,12,14	1.00	1 (10%)
3	A1E3E	a	17	3	11,11,12	6.67	7 (63%)	14,15,17	1.72	3 (21%)
3	MAN	a	18	3	11,11,12	0.21	0	15,15,17	0.78	0
3	BGC	a	19	3	11,11,12	0.20	0	15,15,17	0.70	0
3	XYP	a	2	3	9,9,10	0.18	0	10,12,14	0.64	0
3	AHR	a	20	3	9,9,10	0.56	0	10,12,14	0.82	0
3	AHR	a	21	3	9,9,10	0.57	0	10,12,14	0.80	0
3	AHR	a	22	3	9,9,10	0.57	0	10,12,14	0.90	0
3	BGC	a	23	3	11,11,12	0.21	0	15,15,17	0.54	0
3	XYP	a	24	3	9,9,10	0.17	0	10,12,14	0.61	0
3	MAN	a	25	3	11,11,12	0.22	0	15,15,17	0.85	2 (13%)
3	AHR	a	26	3	9,9,10	0.58	0	10,12,14	1.00	0
3	FUB	a	27	3	9,9,10	0.57	0	10,12,14	0.90	0
3	AHR	a	28	3	9,9,10	0.59	0	10,12,14	0.90	0
3	XYP	a	29	3	9,9,10	0.17	0	10,12,14	0.62	0
3	MAN	a	3	3	11,11,12	0.33	0	15,15,17	1.01	2 (13%)
3	FUB	a	30	3	9,9,10	0.58	0	10,12,14	0.70	0
3	MAN	a	31	3	11,11,12	0.26	0	15,15,17	0.85	2 (13%)
3	FUB	a	32	3	9,9,10	0.55	0	10,12,14	1.08	1 (10%)
3	A1E3E	a	33	3	11,11,12	6.72	7 (63%)	14,15,17	1.51	1 (7%)
3	BGC	a	34	3	11,11,12	0.22	0	15,15,17	0.60	0
3	XYP	a	35	3	9,9,10	0.17	0	10,12,14	0.44	0
3	BGC	a	36	3	11,11,12	0.26	0	15,15,17	1.00	1 (6%)
3	BGC	a	37	3	11,11,12	0.19	0	15,15,17	0.49	0
3	XYP	a	38	3	9,9,10	0.17	0	10,12,14	0.69	0
3	XYP	a	39	3	9,9,10	0.16	0	10,12,14	0.66	0
3	MAN	a	4	3	11,11,12	0.24	0	15,15,17	0.89	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	a	40	3	11,11,12	0.22	0	15,15,17	0.91	0
3	AHR	a	41	3	9,9,10	0.57	0	10,12,14	1.04	1 (10%)
3	FUB	a	42	3	9,9,10	0.57	0	10,12,14	1.02	0
3	BMA	a	43	3	11,11,12	0.26	0	15,15,17	1.19	2 (13%)
3	XYP	a	5	3	9,9,10	0.16	0	10,12,14	0.73	0
3	XYP	a	6	3	9,9,10	0.17	0	10,12,14	0.58	0
3	XYP	a	7	3	9,9,10	0.17	0	10,12,14	0.60	0
3	AHR	a	8	3	9,9,10	0.57	0	10,12,14	0.98	0
3	XYP	a	9	3	9,9,10	0.17	0	10,12,14	0.57	0
4	A2G	b	1	4,1	14,14,15	0.40	0	17,19,21	0.73	0
4	AHR	b	10	4	9,9,10	0.56	0	10,12,14	0.97	1 (10%)
4	AHR	b	11	4	9,9,10	0.59	0	10,12,14	1.02	1 (10%)
4	AHR	b	12	4	9,9,10	0.58	0	10,12,14	0.97	0
4	NAG	b	13	4	14,14,15	0.33	0	17,19,21	0.83	0
4	AHR	b	14	4	9,9,10	0.55	0	10,12,14	1.13	1 (10%)
4	AHR	b	15	4	9,9,10	0.57	0	10,12,14	0.91	0
4	XYP	b	16	4	9,9,10	0.18	0	10,12,14	0.59	0
4	AHR	b	17	4	9,9,10	0.57	0	10,12,14	0.80	0
4	AHR	b	18	4	9,9,10	0.56	0	10,12,14	0.99	1 (10%)
4	AHR	b	19	4	9,9,10	0.58	0	10,12,14	0.85	0
4	MAN	b	2	4	11,11,12	0.24	0	15,15,17	0.84	2 (13%)
4	AHR	b	3	4	9,9,10	0.56	0	10,12,14	1.02	0
4	BGC	b	4	4	11,11,12	0.19	0	15,15,17	0.55	0
4	AHR	b	5	4	9,9,10	0.56	0	10,12,14	1.11	1 (10%)
4	BGC	b	6	4	11,11,12	0.19	0	15,15,17	0.52	0
4	MAN	b	7	4	11,11,12	0.30	0	15,15,17	1.62	2 (13%)
4	NAG	b	8	4	14,14,15	0.38	0	17,19,21	1.02	1 (5%)
4	AHR	b	9	4	9,9,10	0.58	0	10,12,14	0.90	0

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
3	FUB	B	1	3	-	0/2/15/18	0/1/1/1
3	XYP	B	10	3	-	-	0/1/1/1
3	XYP	B	11	3	-	-	0/1/1/1
3	MAN	B	12	3	-	0/2/19/22	0/1/1/1
3	AHR	B	13	3	-	0/2/15/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	B	14	3	-	0/2/19/22	0/1/1/1
3	FUB	B	15	3	-	0/2/15/18	0/1/1/1
3	AHR	B	16	3	-	0/2/15/18	0/1/1/1
3	A1E3E	B	17	3	-	4/6/19/22	0/1/1/1
3	MAN	B	18	3	-	0/2/19/22	0/1/1/1
3	BGC	B	19	3	-	0/2/19/22	0/1/1/1
3	XYP	B	2	3	-	-	0/1/1/1
3	AHR	B	20	3	-	0/2/15/18	0/1/1/1
3	AHR	B	21	3	-	0/2/15/18	0/1/1/1
3	AHR	B	22	3	-	0/2/15/18	0/1/1/1
3	BGC	B	23	3	-	1/2/19/22	0/1/1/1
3	XYP	B	24	3	-	-	0/1/1/1
3	MAN	B	25	3	-	0/2/19/22	0/1/1/1
3	AHR	B	26	3	-	0/2/15/18	0/1/1/1
3	FUB	B	27	3	-	0/2/15/18	0/1/1/1
3	AHR	B	28	3	-	0/2/15/18	0/1/1/1
3	XYP	B	29	3	-	-	0/1/1/1
3	MAN	B	3	3	-	0/2/19/22	0/1/1/1
3	FUB	B	30	3	-	0/2/15/18	0/1/1/1
3	MAN	B	31	3	-	0/2/19/22	0/1/1/1
3	FUB	B	32	3	-	0/2/15/18	0/1/1/1
3	A1E3E	B	33	3	-	0/6/19/22	0/1/1/1
3	BGC	B	34	3	-	0/2/19/22	0/1/1/1
3	XYP	B	35	3	-	-	0/1/1/1
3	BGC	B	36	3	-	0/2/19/22	0/1/1/1
3	BGC	B	37	3	-	0/2/19/22	0/1/1/1
3	XYP	B	38	3	-	-	0/1/1/1
3	XYP	B	39	3	-	-	0/1/1/1
3	MAN	B	4	3	-	0/2/19/22	0/1/1/1
3	BMA	B	40	3	-	0/2/19/22	0/1/1/1
3	AHR	B	41	3	-	0/2/15/18	0/1/1/1
3	FUB	B	42	3	-	0/2/15/18	0/1/1/1
3	BMA	B	43	3	-	0/2/19/22	0/1/1/1
3	XYP	B	5	3	-	-	0/1/1/1
3	XYP	B	6	3	-	-	0/1/1/1
3	XYP	B	7	3	-	-	0/1/1/1
3	AHR	B	8	3	-	0/2/15/18	0/1/1/1
3	XYP	B	9	3	-	-	0/1/1/1
2	AHR	C	1	2	-	0/2/15/18	0/1/1/1
2	BMA	C	10	2	-	0/2/19/22	0/1/1/1
2	NAG	C	11	2	-	2/6/23/26	0/1/1/1
2	MAN	C	12	2	-	1/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	C	13	2	-	0/2/19/22	0/1/1/1
2	AHR	C	14	2	-	0/2/15/18	0/1/1/1
2	BGC	C	15	2	-	0/2/19/22	0/1/1/1
2	AHR	C	16	2	-	0/2/15/18	0/1/1/1
2	AHR	C	17	2	-	0/2/15/18	0/1/1/1
2	AHR	C	18	2	-	0/2/15/18	0/1/1/1
2	FUB	C	19	2	-	0/2/15/18	0/1/1/1
2	FUB	C	2	2	-	0/2/15/18	0/1/1/1
2	AHR	C	20	2	-	0/2/15/18	0/1/1/1
2	AHR	C	21	2	-	0/2/15/18	0/1/1/1
2	NAG	C	22	2	-	4/6/23/26	0/1/1/1
2	FUB	C	23	2	-	0/2/15/18	0/1/1/1
2	AHR	C	24	2	-	0/2/15/18	0/1/1/1
2	A1E3E	C	25	2	-	4/6/19/22	0/1/1/1
2	FUB	C	3	2	-	0/2/15/18	0/1/1/1
2	AHR	C	4	2	-	0/2/15/18	0/1/1/1
2	XYP	C	5	2	-	-	0/1/1/1
2	AHR	C	6	2	-	0/2/15/18	0/1/1/1
2	FUB	C	7	2	-	0/2/15/18	0/1/1/1
2	BGC	C	8	2	-	0/2/19/22	0/1/1/1
2	XYP	C	9	2	-	-	0/1/1/1
4	A2G	D	1	4,1	-	0/6/23/26	0/1/1/1
4	AHR	D	10	4	-	0/2/15/18	0/1/1/1
4	AHR	D	11	4	-	0/2/15/18	0/1/1/1
4	AHR	D	12	4	-	0/2/15/18	0/1/1/1
4	NAG	D	13	4	-	2/6/23/26	0/1/1/1
4	AHR	D	14	4	-	0/2/15/18	0/1/1/1
4	AHR	D	15	4	-	0/2/15/18	0/1/1/1
4	XYP	D	16	4	-	-	0/1/1/1
4	AHR	D	17	4	-	0/2/15/18	0/1/1/1
4	AHR	D	18	4	-	0/2/15/18	0/1/1/1
4	AHR	D	19	4	-	0/2/15/18	0/1/1/1
4	MAN	D	2	4	-	0/2/19/22	0/1/1/1
4	AHR	D	3	4	-	0/2/15/18	0/1/1/1
4	BGC	D	4	4	-	0/2/19/22	0/1/1/1
4	AHR	D	5	4	-	0/2/15/18	0/1/1/1
4	BGC	D	6	4	-	0/2/19/22	0/1/1/1
4	MAN	D	7	4	-	0/2/19/22	0/1/1/1
4	NAG	D	8	4	-	0/6/23/26	0/1/1/1
4	AHR	D	9	4	-	0/2/15/18	0/1/1/1
2	AHR	E	1	2	-	0/2/15/18	0/1/1/1
2	BMA	E	10	2	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	11	2	-	2/6/23/26	0/1/1/1
2	MAN	E	12	2	-	1/2/19/22	0/1/1/1
2	MAN	E	13	2	-	0/2/19/22	0/1/1/1
2	AHR	E	14	2	-	0/2/15/18	0/1/1/1
2	BGC	E	15	2	-	0/2/19/22	0/1/1/1
2	AHR	E	16	2	-	0/2/15/18	0/1/1/1
2	AHR	E	17	2	-	0/2/15/18	0/1/1/1
2	AHR	E	18	2	-	0/2/15/18	0/1/1/1
2	FUB	E	19	2	-	0/2/15/18	0/1/1/1
2	FUB	E	2	2	-	0/2/15/18	0/1/1/1
2	AHR	E	20	2	-	0/2/15/18	0/1/1/1
2	AHR	E	21	2	-	0/2/15/18	0/1/1/1
2	NAG	E	22	2	-	4/6/23/26	0/1/1/1
2	FUB	E	23	2	-	0/2/15/18	0/1/1/1
2	AHR	E	24	2	-	0/2/15/18	0/1/1/1
2	A1E3E	E	25	2	-	6/6/19/22	0/1/1/1
2	FUB	E	3	2	-	0/2/15/18	0/1/1/1
2	AHR	E	4	2	-	0/2/15/18	0/1/1/1
2	XYP	E	5	2	-	-	0/1/1/1
2	AHR	E	6	2	-	0/2/15/18	0/1/1/1
2	FUB	E	7	2	-	0/2/15/18	0/1/1/1
2	BGC	E	8	2	-	0/2/19/22	0/1/1/1
2	XYP	E	9	2	-	-	0/1/1/1
3	FUB	F	1	3	-	0/2/15/18	0/1/1/1
3	XYP	F	10	3	-	-	0/1/1/1
3	XYP	F	11	3	-	-	0/1/1/1
3	MAN	F	12	3	-	0/2/19/22	0/1/1/1
3	AHR	F	13	3	-	0/2/15/18	0/1/1/1
3	BGC	F	14	3	-	0/2/19/22	0/1/1/1
3	FUB	F	15	3	-	0/2/15/18	0/1/1/1
3	AHR	F	16	3	-	0/2/15/18	0/1/1/1
3	A1E3E	F	17	3	-	4/6/19/22	0/1/1/1
3	MAN	F	18	3	-	0/2/19/22	0/1/1/1
3	BGC	F	19	3	-	0/2/19/22	0/1/1/1
3	XYP	F	2	3	-	-	0/1/1/1
3	AHR	F	20	3	-	0/2/15/18	0/1/1/1
3	AHR	F	21	3	-	0/2/15/18	0/1/1/1
3	AHR	F	22	3	-	0/2/15/18	0/1/1/1
3	BGC	F	23	3	-	1/2/19/22	0/1/1/1
3	XYP	F	24	3	-	-	0/1/1/1
3	MAN	F	25	3	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHR	F	26	3	-	0/2/15/18	0/1/1/1
3	FUB	F	27	3	-	0/2/15/18	0/1/1/1
3	AHR	F	28	3	-	0/2/15/18	0/1/1/1
3	XYP	F	29	3	-	-	0/1/1/1
3	MAN	F	3	3	-	0/2/19/22	0/1/1/1
3	FUB	F	30	3	-	0/2/15/18	0/1/1/1
3	MAN	F	31	3	-	0/2/19/22	0/1/1/1
3	FUB	F	32	3	-	0/2/15/18	0/1/1/1
3	A1E3E	F	33	3	-	2/6/19/22	0/1/1/1
3	BGC	F	34	3	-	0/2/19/22	0/1/1/1
3	XYP	F	35	3	-	-	0/1/1/1
3	BGC	F	36	3	-	0/2/19/22	0/1/1/1
3	BGC	F	37	3	-	0/2/19/22	0/1/1/1
3	XYP	F	38	3	-	-	0/1/1/1
3	XYP	F	39	3	-	-	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	BMA	F	40	3	-	0/2/19/22	0/1/1/1
3	AHR	F	41	3	-	0/2/15/18	0/1/1/1
3	FUB	F	42	3	-	0/2/15/18	0/1/1/1
3	BMA	F	43	3	-	0/2/19/22	0/1/1/1
3	XYP	F	5	3	-	-	0/1/1/1
3	XYP	F	6	3	-	-	0/1/1/1
3	XYP	F	7	3	-	-	0/1/1/1
3	AHR	F	8	3	-	0/2/15/18	0/1/1/1
3	XYP	F	9	3	-	-	0/1/1/1
4	A2G	G	1	4,1	-	0/6/23/26	0/1/1/1
4	AHR	G	10	4	-	0/2/15/18	0/1/1/1
4	AHR	G	11	4	-	0/2/15/18	0/1/1/1
4	AHR	G	12	4	-	0/2/15/18	0/1/1/1
4	NAG	G	13	4	-	2/6/23/26	0/1/1/1
4	AHR	G	14	4	-	0/2/15/18	0/1/1/1
4	AHR	G	15	4	-	0/2/15/18	0/1/1/1
4	XYP	G	16	4	-	-	0/1/1/1
4	AHR	G	17	4	-	0/2/15/18	0/1/1/1
4	AHR	G	18	4	-	0/2/15/18	0/1/1/1
4	AHR	G	19	4	-	0/2/15/18	0/1/1/1
4	MAN	G	2	4	-	0/2/19/22	0/1/1/1
4	AHR	G	3	4	-	0/2/15/18	0/1/1/1
4	BGC	G	4	4	-	0/2/19/22	0/1/1/1
4	AHR	G	5	4	-	0/2/15/18	0/1/1/1
4	BGC	G	6	4	-	0/2/19/22	0/1/1/1
4	MAN	G	7	4	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	8	4	-	0/6/23/26	0/1/1/1
4	AHR	G	9	4	-	0/2/15/18	0/1/1/1
2	AHR	H	1	2	-	0/2/15/18	0/1/1/1
2	BMA	H	10	2	-	0/2/19/22	0/1/1/1
2	NAG	H	11	2	-	2/6/23/26	0/1/1/1
2	MAN	H	12	2	-	1/2/19/22	0/1/1/1
2	MAN	H	13	2	-	0/2/19/22	0/1/1/1
2	AHR	H	14	2	-	0/2/15/18	0/1/1/1
2	BGC	H	15	2	-	0/2/19/22	0/1/1/1
2	AHR	H	16	2	-	0/2/15/18	0/1/1/1
2	AHR	H	17	2	-	0/2/15/18	0/1/1/1
2	AHR	H	18	2	-	0/2/15/18	0/1/1/1
2	FUB	H	19	2	-	0/2/15/18	0/1/1/1
2	FUB	H	2	2	-	0/2/15/18	0/1/1/1
2	AHR	H	20	2	-	0/2/15/18	0/1/1/1
2	AHR	H	21	2	-	0/2/15/18	0/1/1/1
2	NAG	H	22	2	-	4/6/23/26	0/1/1/1
2	FUB	H	23	2	-	0/2/15/18	0/1/1/1
2	AHR	H	24	2	-	0/2/15/18	0/1/1/1
2	A1E3E	H	25	2	-	4/6/19/22	0/1/1/1
2	FUB	H	3	2	-	0/2/15/18	0/1/1/1
2	AHR	H	4	2	-	0/2/15/18	0/1/1/1
2	XYP	H	5	2	-	-	0/1/1/1
2	AHR	H	6	2	-	0/2/15/18	0/1/1/1
2	FUB	H	7	2	-	0/2/15/18	0/1/1/1
2	BGC	H	8	2	-	0/2/19/22	0/1/1/1
2	XYP	H	9	2	-	-	0/1/1/1
3	FUB	I	1	3	-	0/2/15/18	0/1/1/1
3	XYP	I	10	3	-	-	0/1/1/1
3	XYP	I	11	3	-	-	0/1/1/1
3	MAN	I	12	3	-	0/2/19/22	0/1/1/1
3	AHR	I	13	3	-	0/2/15/18	0/1/1/1
3	BGC	I	14	3	-	0/2/19/22	0/1/1/1
3	FUB	I	15	3	-	0/2/15/18	0/1/1/1
3	AHR	I	16	3	-	0/2/15/18	0/1/1/1
3	A1E3E	I	17	3	-	4/6/19/22	0/1/1/1
3	MAN	I	18	3	-	0/2/19/22	0/1/1/1
3	BGC	I	19	3	-	0/2/19/22	0/1/1/1
3	XYP	I	2	3	-	-	0/1/1/1
3	AHR	I	20	3	-	0/2/15/18	0/1/1/1
3	AHR	I	21	3	-	0/2/15/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHR	I	22	3	-	0/2/15/18	0/1/1/1
3	BGC	I	23	3	-	1/2/19/22	0/1/1/1
3	XYP	I	24	3	-	-	0/1/1/1
3	MAN	I	25	3	-	0/2/19/22	0/1/1/1
3	AHR	I	26	3	-	0/2/15/18	0/1/1/1
3	FUB	I	27	3	-	0/2/15/18	0/1/1/1
3	AHR	I	28	3	-	0/2/15/18	0/1/1/1
3	XYP	I	29	3	-	-	0/1/1/1
3	MAN	I	3	3	-	0/2/19/22	0/1/1/1
3	FUB	I	30	3	-	0/2/15/18	0/1/1/1
3	MAN	I	31	3	-	0/2/19/22	0/1/1/1
3	FUB	I	32	3	-	0/2/15/18	0/1/1/1
3	A1E3E	I	33	3	-	2/6/19/22	0/1/1/1
3	BGC	I	34	3	-	0/2/19/22	0/1/1/1
3	XYP	I	35	3	-	-	0/1/1/1
3	BGC	I	36	3	-	0/2/19/22	0/1/1/1
3	BGC	I	37	3	-	0/2/19/22	0/1/1/1
3	XYP	I	38	3	-	-	0/1/1/1
3	XYP	I	39	3	-	-	0/1/1/1
3	MAN	I	4	3	-	0/2/19/22	0/1/1/1
3	BMA	I	40	3	-	0/2/19/22	0/1/1/1
3	AHR	I	41	3	-	0/2/15/18	0/1/1/1
3	FUB	I	42	3	-	0/2/15/18	0/1/1/1
3	BMA	I	43	3	-	0/2/19/22	0/1/1/1
3	XYP	I	5	3	-	-	0/1/1/1
3	XYP	I	6	3	-	-	0/1/1/1
3	XYP	I	7	3	-	-	0/1/1/1
3	AHR	I	8	3	-	0/2/15/18	0/1/1/1
3	XYP	I	9	3	-	-	0/1/1/1
4	A2G	J	1	4,1	-	0/6/23/26	0/1/1/1
4	AHR	J	10	4	-	0/2/15/18	0/1/1/1
4	AHR	J	11	4	-	0/2/15/18	0/1/1/1
4	AHR	J	12	4	-	0/2/15/18	0/1/1/1
4	NAG	J	13	4	-	2/6/23/26	0/1/1/1
4	AHR	J	14	4	-	0/2/15/18	0/1/1/1
4	AHR	J	15	4	-	0/2/15/18	0/1/1/1
4	XYP	J	16	4	-	-	0/1/1/1
4	AHR	J	17	4	-	0/2/15/18	0/1/1/1
4	AHR	J	18	4	-	0/2/15/18	0/1/1/1
4	AHR	J	19	4	-	0/2/15/18	0/1/1/1
4	MAN	J	2	4	-	0/2/19/22	0/1/1/1
4	AHR	J	3	4	-	0/2/15/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	J	4	4	-	0/2/19/22	0/1/1/1
4	AHR	J	5	4	-	0/2/15/18	0/1/1/1
4	BGC	J	6	4	-	0/2/19/22	0/1/1/1
4	MAN	J	7	4	-	0/2/19/22	0/1/1/1
4	NAG	J	8	4	-	0/6/23/26	0/1/1/1
4	AHR	J	9	4	-	0/2/15/18	0/1/1/1
2	AHR	K	1	2	-	0/2/15/18	0/1/1/1
2	BMA	K	10	2	-	0/2/19/22	0/1/1/1
2	NAG	K	11	2	-	2/6/23/26	0/1/1/1
2	MAN	K	12	2	-	1/2/19/22	0/1/1/1
2	MAN	K	13	2	-	0/2/19/22	0/1/1/1
2	AHR	K	14	2	-	0/2/15/18	0/1/1/1
2	BGC	K	15	2	-	0/2/19/22	0/1/1/1
2	AHR	K	16	2	-	0/2/15/18	0/1/1/1
2	AHR	K	17	2	-	0/2/15/18	0/1/1/1
2	AHR	K	18	2	-	0/2/15/18	0/1/1/1
2	FUB	K	19	2	-	0/2/15/18	0/1/1/1
2	FUB	K	2	2	-	0/2/15/18	0/1/1/1
2	AHR	K	20	2	-	0/2/15/18	0/1/1/1
2	AHR	K	21	2	-	0/2/15/18	0/1/1/1
2	NAG	K	22	2	-	4/6/23/26	0/1/1/1
2	FUB	K	23	2	-	0/2/15/18	0/1/1/1
2	AHR	K	24	2	-	0/2/15/18	0/1/1/1
2	A1E3E	K	25	2	-	5/6/19/22	0/1/1/1
2	FUB	K	3	2	-	0/2/15/18	0/1/1/1
2	AHR	K	4	2	-	0/2/15/18	0/1/1/1
2	XYP	K	5	2	-	-	0/1/1/1
2	AHR	K	6	2	-	0/2/15/18	0/1/1/1
2	FUB	K	7	2	-	0/2/15/18	0/1/1/1
2	BGC	K	8	2	-	0/2/19/22	0/1/1/1
2	XYP	K	9	2	-	-	0/1/1/1
3	FUB	L	1	3	-	0/2/15/18	0/1/1/1
3	XYP	L	10	3	-	-	0/1/1/1
3	XYP	L	11	3	-	-	0/1/1/1
3	MAN	L	12	3	-	0/2/19/22	0/1/1/1
3	AHR	L	13	3	-	0/2/15/18	0/1/1/1
3	BGC	L	14	3	-	0/2/19/22	0/1/1/1
3	FUB	L	15	3	-	0/2/15/18	0/1/1/1
3	AHR	L	16	3	-	0/2/15/18	0/1/1/1
3	A1E3E	L	17	3	-	4/6/19/22	0/1/1/1
3	MAN	L	18	3	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	L	19	3	-	0/2/19/22	0/1/1/1
3	XYP	L	2	3	-	-	0/1/1/1
3	AHR	L	20	3	-	0/2/15/18	0/1/1/1
3	AHR	L	21	3	-	0/2/15/18	0/1/1/1
3	AHR	L	22	3	-	0/2/15/18	0/1/1/1
3	BGC	L	23	3	-	1/2/19/22	0/1/1/1
3	XYP	L	24	3	-	-	0/1/1/1
3	MAN	L	25	3	-	0/2/19/22	0/1/1/1
3	AHR	L	26	3	-	0/2/15/18	0/1/1/1
3	FUB	L	27	3	-	0/2/15/18	0/1/1/1
3	AHR	L	28	3	-	0/2/15/18	0/1/1/1
3	XYP	L	29	3	-	-	0/1/1/1
3	MAN	L	3	3	-	0/2/19/22	0/1/1/1
3	FUB	L	30	3	-	0/2/15/18	0/1/1/1
3	MAN	L	31	3	-	0/2/19/22	0/1/1/1
3	FUB	L	32	3	-	0/2/15/18	0/1/1/1
3	A1E3E	L	33	3	-	2/6/19/22	0/1/1/1
3	BGC	L	34	3	-	0/2/19/22	0/1/1/1
3	XYP	L	35	3	-	-	0/1/1/1
3	BGC	L	36	3	-	0/2/19/22	0/1/1/1
3	BGC	L	37	3	-	0/2/19/22	0/1/1/1
3	XYP	L	38	3	-	-	0/1/1/1
3	XYP	L	39	3	-	-	0/1/1/1
3	MAN	L	4	3	-	0/2/19/22	0/1/1/1
3	BMA	L	40	3	-	0/2/19/22	0/1/1/1
3	AHR	L	41	3	-	0/2/15/18	0/1/1/1
3	FUB	L	42	3	-	0/2/15/18	0/1/1/1
3	BMA	L	43	3	-	0/2/19/22	0/1/1/1
3	XYP	L	5	3	-	-	0/1/1/1
3	XYP	L	6	3	-	-	0/1/1/1
3	XYP	L	7	3	-	-	0/1/1/1
3	AHR	L	8	3	-	0/2/15/18	0/1/1/1
3	XYP	L	9	3	-	-	0/1/1/1
4	A2G	M	1	4,1	-	0/6/23/26	0/1/1/1
4	AHR	M	10	4	-	0/2/15/18	0/1/1/1
4	AHR	M	11	4	-	0/2/15/18	0/1/1/1
4	AHR	M	12	4	-	0/2/15/18	0/1/1/1
4	NAG	M	13	4	-	2/6/23/26	0/1/1/1
4	AHR	M	14	4	-	0/2/15/18	0/1/1/1
4	AHR	M	15	4	-	0/2/15/18	0/1/1/1
4	XYP	M	16	4	-	-	0/1/1/1
4	AHR	M	17	4	-	0/2/15/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AHR	M	18	4	-	0/2/15/18	0/1/1/1
4	AHR	M	19	4	-	0/2/15/18	0/1/1/1
4	MAN	M	2	4	-	0/2/19/22	0/1/1/1
4	AHR	M	3	4	-	0/2/15/18	0/1/1/1
4	BGC	M	4	4	-	0/2/19/22	0/1/1/1
4	AHR	M	5	4	-	0/2/15/18	0/1/1/1
4	BGC	M	6	4	-	0/2/19/22	0/1/1/1
4	MAN	M	7	4	-	0/2/19/22	0/1/1/1
4	NAG	M	8	4	-	2/6/23/26	0/1/1/1
4	AHR	M	9	4	-	0/2/15/18	0/1/1/1
2	AHR	N	1	2	-	0/2/15/18	0/1/1/1
2	BMA	N	10	2	-	0/2/19/22	0/1/1/1
2	NAG	N	11	2	-	2/6/23/26	0/1/1/1
2	MAN	N	12	2	-	1/2/19/22	0/1/1/1
2	MAN	N	13	2	-	0/2/19/22	0/1/1/1
2	AHR	N	14	2	-	0/2/15/18	0/1/1/1
2	BGC	N	15	2	-	0/2/19/22	0/1/1/1
2	AHR	N	16	2	-	0/2/15/18	0/1/1/1
2	AHR	N	17	2	-	0/2/15/18	0/1/1/1
2	AHR	N	18	2	-	0/2/15/18	0/1/1/1
2	FUB	N	19	2	-	0/2/15/18	0/1/1/1
2	FUB	N	2	2	-	0/2/15/18	0/1/1/1
2	AHR	N	20	2	-	0/2/15/18	0/1/1/1
2	AHR	N	21	2	-	0/2/15/18	0/1/1/1
2	NAG	N	22	2	-	4/6/23/26	0/1/1/1
2	FUB	N	23	2	-	0/2/15/18	0/1/1/1
2	AHR	N	24	2	-	0/2/15/18	0/1/1/1
2	A1E3E	N	25	2	-	6/6/19/22	0/1/1/1
2	FUB	N	3	2	-	0/2/15/18	0/1/1/1
2	AHR	N	4	2	-	0/2/15/18	0/1/1/1
2	XYP	N	5	2	-	-	0/1/1/1
2	AHR	N	6	2	-	0/2/15/18	0/1/1/1
2	FUB	N	7	2	-	0/2/15/18	0/1/1/1
2	BGC	N	8	2	-	0/2/19/22	0/1/1/1
2	XYP	N	9	2	-	-	0/1/1/1
3	FUB	O	1	3	-	0/2/15/18	0/1/1/1
3	XYP	O	10	3	-	-	0/1/1/1
3	XYP	O	11	3	-	-	0/1/1/1
3	MAN	O	12	3	-	0/2/19/22	0/1/1/1
3	AHR	O	13	3	-	0/2/15/18	0/1/1/1
3	BGC	O	14	3	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUB	O	15	3	-	0/2/15/18	0/1/1/1
3	AHR	O	16	3	-	0/2/15/18	0/1/1/1
3	A1E3E	O	17	3	-	4/6/19/22	0/1/1/1
3	MAN	O	18	3	-	0/2/19/22	0/1/1/1
3	BGC	O	19	3	-	0/2/19/22	0/1/1/1
3	XYP	O	2	3	-	-	0/1/1/1
3	AHR	O	20	3	-	0/2/15/18	0/1/1/1
3	AHR	O	21	3	-	0/2/15/18	0/1/1/1
3	AHR	O	22	3	-	0/2/15/18	0/1/1/1
3	BGC	O	23	3	-	1/2/19/22	0/1/1/1
3	XYP	O	24	3	-	-	0/1/1/1
3	MAN	O	25	3	-	0/2/19/22	0/1/1/1
3	AHR	O	26	3	-	0/2/15/18	0/1/1/1
3	FUB	O	27	3	-	0/2/15/18	0/1/1/1
3	AHR	O	28	3	-	0/2/15/18	0/1/1/1
3	XYP	O	29	3	-	-	0/1/1/1
3	MAN	O	3	3	-	0/2/19/22	0/1/1/1
3	FUB	O	30	3	-	0/2/15/18	0/1/1/1
3	MAN	O	31	3	-	0/2/19/22	0/1/1/1
3	FUB	O	32	3	-	0/2/15/18	0/1/1/1
3	A1E3E	O	33	3	-	2/6/19/22	0/1/1/1
3	BGC	O	34	3	-	0/2/19/22	0/1/1/1
3	XYP	O	35	3	-	-	0/1/1/1
3	BGC	O	36	3	-	0/2/19/22	0/1/1/1
3	BGC	O	37	3	-	0/2/19/22	0/1/1/1
3	XYP	O	38	3	-	-	0/1/1/1
3	XYP	O	39	3	-	-	0/1/1/1
3	MAN	O	4	3	-	0/2/19/22	0/1/1/1
3	BMA	O	40	3	-	0/2/19/22	0/1/1/1
3	AHR	O	41	3	-	0/2/15/18	0/1/1/1
3	FUB	O	42	3	-	0/2/15/18	0/1/1/1
3	BMA	O	43	3	-	0/2/19/22	0/1/1/1
3	XYP	O	5	3	-	-	0/1/1/1
3	XYP	O	6	3	-	-	0/1/1/1
3	XYP	O	7	3	-	-	0/1/1/1
3	AHR	O	8	3	-	0/2/15/18	0/1/1/1
3	XYP	O	9	3	-	-	0/1/1/1
4	A2G	P	1	4,1	-	0/6/23/26	0/1/1/1
4	AHR	P	10	4	-	0/2/15/18	0/1/1/1
4	AHR	P	11	4	-	0/2/15/18	0/1/1/1
4	AHR	P	12	4	-	0/2/15/18	0/1/1/1
4	NAG	P	13	4	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AHR	P	14	4	-	0/2/15/18	0/1/1/1
4	AHR	P	15	4	-	0/2/15/18	0/1/1/1
4	XYP	P	16	4	-	-	0/1/1/1
4	AHR	P	17	4	-	0/2/15/18	0/1/1/1
4	AHR	P	18	4	-	0/2/15/18	0/1/1/1
4	AHR	P	19	4	-	0/2/15/18	0/1/1/1
4	MAN	P	2	4	-	0/2/19/22	0/1/1/1
4	AHR	P	3	4	-	0/2/15/18	0/1/1/1
4	BGC	P	4	4	-	0/2/19/22	0/1/1/1
4	AHR	P	5	4	-	0/2/15/18	0/1/1/1
4	BGC	P	6	4	-	0/2/19/22	0/1/1/1
4	MAN	P	7	4	-	0/2/19/22	0/1/1/1
4	NAG	P	8	4	-	0/6/23/26	0/1/1/1
4	AHR	P	9	4	-	0/2/15/18	0/1/1/1
2	AHR	Q	1	2	-	0/2/15/18	0/1/1/1
2	BMA	Q	10	2	-	0/2/19/22	0/1/1/1
2	NAG	Q	11	2	-	2/6/23/26	0/1/1/1
2	MAN	Q	12	2	-	1/2/19/22	0/1/1/1
2	MAN	Q	13	2	-	0/2/19/22	0/1/1/1
2	AHR	Q	14	2	-	0/2/15/18	0/1/1/1
2	BGC	Q	15	2	-	0/2/19/22	0/1/1/1
2	AHR	Q	16	2	-	0/2/15/18	0/1/1/1
2	AHR	Q	17	2	-	0/2/15/18	0/1/1/1
2	AHR	Q	18	2	-	0/2/15/18	0/1/1/1
2	FUB	Q	19	2	-	0/2/15/18	0/1/1/1
2	FUB	Q	2	2	-	0/2/15/18	0/1/1/1
2	AHR	Q	20	2	-	0/2/15/18	0/1/1/1
2	AHR	Q	21	2	-	0/2/15/18	0/1/1/1
2	NAG	Q	22	2	-	4/6/23/26	0/1/1/1
2	FUB	Q	23	2	-	0/2/15/18	0/1/1/1
2	AHR	Q	24	2	-	0/2/15/18	0/1/1/1
2	A1E3E	Q	25	2	-	6/6/19/22	0/1/1/1
2	FUB	Q	3	2	-	0/2/15/18	0/1/1/1
2	AHR	Q	4	2	-	0/2/15/18	0/1/1/1
2	XYP	Q	5	2	-	-	0/1/1/1
2	AHR	Q	6	2	-	0/2/15/18	0/1/1/1
2	FUB	Q	7	2	-	0/2/15/18	0/1/1/1
2	BGC	Q	8	2	-	0/2/19/22	0/1/1/1
2	XYP	Q	9	2	-	-	0/1/1/1
3	FUB	R	1	3	-	0/2/15/18	0/1/1/1
3	XYP	R	10	3	-	-	0/1/1/1
3	XYP	R	11	3	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	R	12	3	-	0/2/19/22	0/1/1/1
3	AHR	R	13	3	-	0/2/15/18	0/1/1/1
3	BGC	R	14	3	-	0/2/19/22	0/1/1/1
3	FUB	R	15	3	-	0/2/15/18	0/1/1/1
3	AHR	R	16	3	-	0/2/15/18	0/1/1/1
3	A1E3E	R	17	3	-	4/6/19/22	0/1/1/1
3	MAN	R	18	3	-	0/2/19/22	0/1/1/1
3	BGC	R	19	3	-	0/2/19/22	0/1/1/1
3	XYP	R	2	3	-	-	0/1/1/1
3	AHR	R	20	3	-	0/2/15/18	0/1/1/1
3	AHR	R	21	3	-	0/2/15/18	0/1/1/1
3	AHR	R	22	3	-	0/2/15/18	0/1/1/1
3	BGC	R	23	3	-	1/2/19/22	0/1/1/1
3	XYP	R	24	3	-	-	0/1/1/1
3	MAN	R	25	3	-	0/2/19/22	0/1/1/1
3	AHR	R	26	3	-	0/2/15/18	0/1/1/1
3	FUB	R	27	3	-	0/2/15/18	0/1/1/1
3	AHR	R	28	3	-	0/2/15/18	0/1/1/1
3	XYP	R	29	3	-	-	0/1/1/1
3	MAN	R	3	3	-	0/2/19/22	0/1/1/1
3	FUB	R	30	3	-	0/2/15/18	0/1/1/1
3	MAN	R	31	3	-	0/2/19/22	0/1/1/1
3	FUB	R	32	3	-	0/2/15/18	0/1/1/1
3	A1E3E	R	33	3	-	2/6/19/22	0/1/1/1
3	BGC	R	34	3	-	0/2/19/22	0/1/1/1
3	XYP	R	35	3	-	-	0/1/1/1
3	BGC	R	36	3	-	0/2/19/22	0/1/1/1
3	BGC	R	37	3	-	0/2/19/22	0/1/1/1
3	XYP	R	38	3	-	-	0/1/1/1
3	XYP	R	39	3	-	-	0/1/1/1
3	MAN	R	4	3	-	0/2/19/22	0/1/1/1
3	BMA	R	40	3	-	0/2/19/22	0/1/1/1
3	AHR	R	41	3	-	0/2/15/18	0/1/1/1
3	FUB	R	42	3	-	0/2/15/18	0/1/1/1
3	BMA	R	43	3	-	0/2/19/22	0/1/1/1
3	XYP	R	5	3	-	-	0/1/1/1
3	XYP	R	6	3	-	-	0/1/1/1
3	XYP	R	7	3	-	-	0/1/1/1
3	AHR	R	8	3	-	0/2/15/18	0/1/1/1
3	XYP	R	9	3	-	-	0/1/1/1
4	A2G	S	1	4,1	-	0/6/23/26	0/1/1/1
4	AHR	S	10	4	-	0/2/15/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AHR	S	11	4	-	0/2/15/18	0/1/1/1
4	AHR	S	12	4	-	0/2/15/18	0/1/1/1
4	NAG	S	13	4	-	2/6/23/26	0/1/1/1
4	AHR	S	14	4	-	0/2/15/18	0/1/1/1
4	AHR	S	15	4	-	0/2/15/18	0/1/1/1
4	XYP	S	16	4	-	-	0/1/1/1
4	AHR	S	17	4	-	0/2/15/18	0/1/1/1
4	AHR	S	18	4	-	0/2/15/18	0/1/1/1
4	AHR	S	19	4	-	0/2/15/18	0/1/1/1
4	MAN	S	2	4	-	0/2/19/22	0/1/1/1
4	AHR	S	3	4	-	0/2/15/18	0/1/1/1
4	BGC	S	4	4	-	0/2/19/22	0/1/1/1
4	AHR	S	5	4	-	0/2/15/18	0/1/1/1
4	BGC	S	6	4	-	0/2/19/22	0/1/1/1
4	MAN	S	7	4	-	0/2/19/22	0/1/1/1
4	NAG	S	8	4	-	0/6/23/26	0/1/1/1
4	AHR	S	9	4	-	0/2/15/18	0/1/1/1
2	AHR	T	1	2	-	0/2/15/18	0/1/1/1
2	BMA	T	10	2	-	0/2/19/22	0/1/1/1
2	NAG	T	11	2	-	2/6/23/26	0/1/1/1
2	MAN	T	12	2	-	1/2/19/22	0/1/1/1
2	MAN	T	13	2	-	0/2/19/22	0/1/1/1
2	AHR	T	14	2	-	0/2/15/18	0/1/1/1
2	BGC	T	15	2	-	0/2/19/22	0/1/1/1
2	AHR	T	16	2	-	0/2/15/18	0/1/1/1
2	AHR	T	17	2	-	0/2/15/18	0/1/1/1
2	AHR	T	18	2	-	0/2/15/18	0/1/1/1
2	FUB	T	19	2	-	0/2/15/18	0/1/1/1
2	FUB	T	2	2	-	0/2/15/18	0/1/1/1
2	AHR	T	20	2	-	0/2/15/18	0/1/1/1
2	AHR	T	21	2	-	0/2/15/18	0/1/1/1
2	NAG	T	22	2	-	4/6/23/26	0/1/1/1
2	FUB	T	23	2	-	0/2/15/18	0/1/1/1
2	AHR	T	24	2	-	0/2/15/18	0/1/1/1
2	A1E3E	T	25	2	-	3/6/19/22	0/1/1/1
2	FUB	T	3	2	-	0/2/15/18	0/1/1/1
2	AHR	T	4	2	-	0/2/15/18	0/1/1/1
2	XYP	T	5	2	-	-	0/1/1/1
2	AHR	T	6	2	-	0/2/15/18	0/1/1/1
2	FUB	T	7	2	-	0/2/15/18	0/1/1/1
2	BGC	T	8	2	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XYP	T	9	2	-	-	0/1/1/1
3	FUB	U	1	3	-	0/2/15/18	0/1/1/1
3	XYP	U	10	3	-	-	0/1/1/1
3	XYP	U	11	3	-	-	0/1/1/1
3	MAN	U	12	3	-	0/2/19/22	0/1/1/1
3	AHR	U	13	3	-	0/2/15/18	0/1/1/1
3	BGC	U	14	3	-	0/2/19/22	0/1/1/1
3	FUB	U	15	3	-	0/2/15/18	0/1/1/1
3	AHR	U	16	3	-	0/2/15/18	0/1/1/1
3	A1E3E	U	17	3	-	4/6/19/22	0/1/1/1
3	MAN	U	18	3	-	0/2/19/22	0/1/1/1
3	BGC	U	19	3	-	0/2/19/22	0/1/1/1
3	XYP	U	2	3	-	-	0/1/1/1
3	AHR	U	20	3	-	0/2/15/18	0/1/1/1
3	AHR	U	21	3	-	0/2/15/18	0/1/1/1
3	AHR	U	22	3	-	0/2/15/18	0/1/1/1
3	BGC	U	23	3	-	1/2/19/22	0/1/1/1
3	XYP	U	24	3	-	-	0/1/1/1
3	MAN	U	25	3	-	0/2/19/22	0/1/1/1
3	AHR	U	26	3	-	0/2/15/18	0/1/1/1
3	FUB	U	27	3	-	0/2/15/18	0/1/1/1
3	AHR	U	28	3	-	0/2/15/18	0/1/1/1
3	XYP	U	29	3	-	-	0/1/1/1
3	MAN	U	3	3	-	0/2/19/22	0/1/1/1
3	FUB	U	30	3	-	0/2/15/18	0/1/1/1
3	MAN	U	31	3	-	0/2/19/22	0/1/1/1
3	FUB	U	32	3	-	0/2/15/18	0/1/1/1
3	A1E3E	U	33	3	-	2/6/19/22	0/1/1/1
3	BGC	U	34	3	-	0/2/19/22	0/1/1/1
3	XYP	U	35	3	-	-	0/1/1/1
3	BGC	U	36	3	-	0/2/19/22	0/1/1/1
3	BGC	U	37	3	-	0/2/19/22	0/1/1/1
3	XYP	U	38	3	-	-	0/1/1/1
3	XYP	U	39	3	-	-	0/1/1/1
3	MAN	U	4	3	-	0/2/19/22	0/1/1/1
3	BMA	U	40	3	-	0/2/19/22	0/1/1/1
3	AHR	U	41	3	-	0/2/15/18	0/1/1/1
3	FUB	U	42	3	-	0/2/15/18	0/1/1/1
3	BMA	U	43	3	-	0/2/19/22	0/1/1/1
3	XYP	U	5	3	-	-	0/1/1/1
3	XYP	U	6	3	-	-	0/1/1/1
3	XYP	U	7	3	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHR	U	8	3	-	0/2/15/18	0/1/1/1
3	XYP	U	9	3	-	-	0/1/1/1
4	A2G	V	1	4,1	-	0/6/23/26	0/1/1/1
4	AHR	V	10	4	-	0/2/15/18	0/1/1/1
4	AHR	V	11	4	-	0/2/15/18	0/1/1/1
4	AHR	V	12	4	-	0/2/15/18	0/1/1/1
4	NAG	V	13	4	-	2/6/23/26	0/1/1/1
4	AHR	V	14	4	-	0/2/15/18	0/1/1/1
4	AHR	V	15	4	-	0/2/15/18	0/1/1/1
4	XYP	V	16	4	-	-	0/1/1/1
4	AHR	V	17	4	-	0/2/15/18	0/1/1/1
4	AHR	V	18	4	-	0/2/15/18	0/1/1/1
4	AHR	V	19	4	-	0/2/15/18	0/1/1/1
4	MAN	V	2	4	-	0/2/19/22	0/1/1/1
4	AHR	V	3	4	-	0/2/15/18	0/1/1/1
4	BGC	V	4	4	-	0/2/19/22	0/1/1/1
4	AHR	V	5	4	-	0/2/15/18	0/1/1/1
4	BGC	V	6	4	-	0/2/19/22	0/1/1/1
4	MAN	V	7	4	-	0/2/19/22	0/1/1/1
4	NAG	V	8	4	-	0/6/23/26	0/1/1/1
4	AHR	V	9	4	-	0/2/15/18	0/1/1/1
2	AHR	W	1	2	-	0/2/15/18	0/1/1/1
2	BMA	W	10	2	-	0/2/19/22	0/1/1/1
2	NAG	W	11	2	-	2/6/23/26	0/1/1/1
2	MAN	W	12	2	-	1/2/19/22	0/1/1/1
2	MAN	W	13	2	-	0/2/19/22	0/1/1/1
2	AHR	W	14	2	-	0/2/15/18	0/1/1/1
2	BGC	W	15	2	-	0/2/19/22	0/1/1/1
2	AHR	W	16	2	-	0/2/15/18	0/1/1/1
2	AHR	W	17	2	-	0/2/15/18	0/1/1/1
2	AHR	W	18	2	-	0/2/15/18	0/1/1/1
2	FUB	W	19	2	-	0/2/15/18	0/1/1/1
2	FUB	W	2	2	-	0/2/15/18	0/1/1/1
2	AHR	W	20	2	-	0/2/15/18	0/1/1/1
2	AHR	W	21	2	-	0/2/15/18	0/1/1/1
2	NAG	W	22	2	-	4/6/23/26	0/1/1/1
2	FUB	W	23	2	-	0/2/15/18	0/1/1/1
2	AHR	W	24	2	-	0/2/15/18	0/1/1/1
2	A1E3E	W	25	2	-	6/6/19/22	0/1/1/1
2	FUB	W	3	2	-	0/2/15/18	0/1/1/1
2	AHR	W	4	2	-	0/2/15/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XYP	W	5	2	-	-	0/1/1/1
2	AHR	W	6	2	-	0/2/15/18	0/1/1/1
2	FUB	W	7	2	-	0/2/15/18	0/1/1/1
2	BGC	W	8	2	-	0/2/19/22	0/1/1/1
2	XYP	W	9	2	-	-	0/1/1/1
3	FUB	X	1	3	-	0/2/15/18	0/1/1/1
3	XYP	X	10	3	-	-	0/1/1/1
3	XYP	X	11	3	-	-	0/1/1/1
3	MAN	X	12	3	-	0/2/19/22	0/1/1/1
3	AHR	X	13	3	-	0/2/15/18	0/1/1/1
3	BGC	X	14	3	-	0/2/19/22	0/1/1/1
3	FUB	X	15	3	-	0/2/15/18	0/1/1/1
3	AHR	X	16	3	-	0/2/15/18	0/1/1/1
3	A1E3E	X	17	3	-	4/6/19/22	0/1/1/1
3	MAN	X	18	3	-	0/2/19/22	0/1/1/1
3	BGC	X	19	3	-	0/2/19/22	0/1/1/1
3	XYP	X	2	3	-	-	0/1/1/1
3	AHR	X	20	3	-	0/2/15/18	0/1/1/1
3	AHR	X	21	3	-	0/2/15/18	0/1/1/1
3	AHR	X	22	3	-	0/2/15/18	0/1/1/1
3	BGC	X	23	3	-	1/2/19/22	0/1/1/1
3	XYP	X	24	3	-	-	0/1/1/1
3	MAN	X	25	3	-	0/2/19/22	0/1/1/1
3	AHR	X	26	3	-	0/2/15/18	0/1/1/1
3	FUB	X	27	3	-	0/2/15/18	0/1/1/1
3	AHR	X	28	3	-	0/2/15/18	0/1/1/1
3	XYP	X	29	3	-	-	0/1/1/1
3	MAN	X	3	3	-	0/2/19/22	0/1/1/1
3	FUB	X	30	3	-	0/2/15/18	0/1/1/1
3	MAN	X	31	3	-	0/2/19/22	0/1/1/1
3	FUB	X	32	3	-	0/2/15/18	0/1/1/1
3	A1E3E	X	33	3	-	2/6/19/22	0/1/1/1
3	BGC	X	34	3	-	0/2/19/22	0/1/1/1
3	XYP	X	35	3	-	-	0/1/1/1
3	BGC	X	36	3	-	0/2/19/22	0/1/1/1
3	BGC	X	37	3	-	0/2/19/22	0/1/1/1
3	XYP	X	38	3	-	-	0/1/1/1
3	XYP	X	39	3	-	-	0/1/1/1
3	MAN	X	4	3	-	0/2/19/22	0/1/1/1
3	BMA	X	40	3	-	0/2/19/22	0/1/1/1
3	AHR	X	41	3	-	0/2/15/18	0/1/1/1
3	FUB	X	42	3	-	0/2/15/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	X	43	3	-	0/2/19/22	0/1/1/1
3	XYP	X	5	3	-	-	0/1/1/1
3	XYP	X	6	3	-	-	0/1/1/1
3	XYP	X	7	3	-	-	0/1/1/1
3	AHR	X	8	3	-	0/2/15/18	0/1/1/1
3	XYP	X	9	3	-	-	0/1/1/1
4	A2G	Y	1	4,1	-	0/6/23/26	0/1/1/1
4	AHR	Y	10	4	-	0/2/15/18	0/1/1/1
4	AHR	Y	11	4	-	0/2/15/18	0/1/1/1
4	AHR	Y	12	4	-	0/2/15/18	0/1/1/1
4	NAG	Y	13	4	-	2/6/23/26	0/1/1/1
4	AHR	Y	14	4	-	0/2/15/18	0/1/1/1
4	AHR	Y	15	4	-	0/2/15/18	0/1/1/1
4	XYP	Y	16	4	-	-	0/1/1/1
4	AHR	Y	17	4	-	0/2/15/18	0/1/1/1
4	AHR	Y	18	4	-	0/2/15/18	0/1/1/1
4	AHR	Y	19	4	-	0/2/15/18	0/1/1/1
4	MAN	Y	2	4	-	0/2/19/22	0/1/1/1
4	AHR	Y	3	4	-	0/2/15/18	0/1/1/1
4	BGC	Y	4	4	-	0/2/19/22	0/1/1/1
4	AHR	Y	5	4	-	0/2/15/18	0/1/1/1
4	BGC	Y	6	4	-	0/2/19/22	0/1/1/1
4	MAN	Y	7	4	-	0/2/19/22	0/1/1/1
4	NAG	Y	8	4	-	0/6/23/26	0/1/1/1
4	AHR	Y	9	4	-	0/2/15/18	0/1/1/1
2	AHR	Z	1	2	-	0/2/15/18	0/1/1/1
2	BMA	Z	10	2	-	0/2/19/22	0/1/1/1
2	NAG	Z	11	2	-	2/6/23/26	0/1/1/1
2	MAN	Z	12	2	-	1/2/19/22	0/1/1/1
2	MAN	Z	13	2	-	0/2/19/22	0/1/1/1
2	AHR	Z	14	2	-	0/2/15/18	0/1/1/1
2	BGC	Z	15	2	-	0/2/19/22	0/1/1/1
2	AHR	Z	16	2	-	0/2/15/18	0/1/1/1
2	AHR	Z	17	2	-	0/2/15/18	0/1/1/1
2	AHR	Z	18	2	-	0/2/15/18	0/1/1/1
2	FUB	Z	19	2	-	0/2/15/18	0/1/1/1
2	FUB	Z	2	2	-	0/2/15/18	0/1/1/1
2	AHR	Z	20	2	-	0/2/15/18	0/1/1/1
2	AHR	Z	21	2	-	0/2/15/18	0/1/1/1
2	NAG	Z	22	2	-	4/6/23/26	0/1/1/1
2	FUB	Z	23	2	-	0/2/15/18	0/1/1/1
2	AHR	Z	24	2	-	0/2/15/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1E3E	Z	25	2	-	6/6/19/22	0/1/1/1
2	FUB	Z	3	2	-	0/2/15/18	0/1/1/1
2	AHR	Z	4	2	-	0/2/15/18	0/1/1/1
2	XYP	Z	5	2	-	-	0/1/1/1
2	AHR	Z	6	2	-	0/2/15/18	0/1/1/1
2	FUB	Z	7	2	-	0/2/15/18	0/1/1/1
2	BGC	Z	8	2	-	0/2/19/22	0/1/1/1
2	XYP	Z	9	2	-	-	0/1/1/1
3	FUB	a	1	3	-	0/2/15/18	0/1/1/1
3	XYP	a	10	3	-	-	0/1/1/1
3	XYP	a	11	3	-	-	0/1/1/1
3	MAN	a	12	3	-	0/2/19/22	0/1/1/1
3	AHR	a	13	3	-	0/2/15/18	0/1/1/1
3	BGC	a	14	3	-	0/2/19/22	0/1/1/1
3	FUB	a	15	3	-	0/2/15/18	0/1/1/1
3	AHR	a	16	3	-	0/2/15/18	0/1/1/1
3	A1E3E	a	17	3	-	4/6/19/22	0/1/1/1
3	MAN	a	18	3	-	0/2/19/22	0/1/1/1
3	BGC	a	19	3	-	0/2/19/22	0/1/1/1
3	XYP	a	2	3	-	-	0/1/1/1
3	AHR	a	20	3	-	0/2/15/18	0/1/1/1
3	AHR	a	21	3	-	0/2/15/18	0/1/1/1
3	AHR	a	22	3	-	0/2/15/18	0/1/1/1
3	BGC	a	23	3	-	1/2/19/22	0/1/1/1
3	XYP	a	24	3	-	-	0/1/1/1
3	MAN	a	25	3	-	0/2/19/22	0/1/1/1
3	AHR	a	26	3	-	0/2/15/18	0/1/1/1
3	FUB	a	27	3	-	0/2/15/18	0/1/1/1
3	AHR	a	28	3	-	0/2/15/18	0/1/1/1
3	XYP	a	29	3	-	-	0/1/1/1
3	MAN	a	3	3	-	0/2/19/22	0/1/1/1
3	FUB	a	30	3	-	0/2/15/18	0/1/1/1
3	MAN	a	31	3	-	0/2/19/22	0/1/1/1
3	FUB	a	32	3	-	0/2/15/18	0/1/1/1
3	A1E3E	a	33	3	-	2/6/19/22	0/1/1/1
3	BGC	a	34	3	-	0/2/19/22	0/1/1/1
3	XYP	a	35	3	-	-	0/1/1/1
3	BGC	a	36	3	-	0/2/19/22	0/1/1/1
3	BGC	a	37	3	-	0/2/19/22	0/1/1/1
3	XYP	a	38	3	-	-	0/1/1/1
3	XYP	a	39	3	-	-	0/1/1/1
3	MAN	a	4	3	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	a	40	3	-	0/2/19/22	0/1/1/1
3	AHR	a	41	3	-	0/2/15/18	0/1/1/1
3	FUB	a	42	3	-	0/2/15/18	0/1/1/1
3	BMA	a	43	3	-	0/2/19/22	0/1/1/1
3	XYP	a	5	3	-	-	0/1/1/1
3	XYP	a	6	3	-	-	0/1/1/1
3	XYP	a	7	3	-	-	0/1/1/1
3	AHR	a	8	3	-	0/2/15/18	0/1/1/1
3	XYP	a	9	3	-	-	0/1/1/1
4	A2G	b	1	4,1	-	0/6/23/26	0/1/1/1
4	AHR	b	10	4	-	0/2/15/18	0/1/1/1
4	AHR	b	11	4	-	0/2/15/18	0/1/1/1
4	AHR	b	12	4	-	0/2/15/18	0/1/1/1
4	NAG	b	13	4	-	2/6/23/26	0/1/1/1
4	AHR	b	14	4	-	0/2/15/18	0/1/1/1
4	AHR	b	15	4	-	0/2/15/18	0/1/1/1
4	XYP	b	16	4	-	-	0/1/1/1
4	AHR	b	17	4	-	0/2/15/18	0/1/1/1
4	AHR	b	18	4	-	0/2/15/18	0/1/1/1
4	AHR	b	19	4	-	0/2/15/18	0/1/1/1
4	MAN	b	2	4	-	0/2/19/22	0/1/1/1
4	AHR	b	3	4	-	0/2/15/18	0/1/1/1
4	BGC	b	4	4	-	0/2/19/22	0/1/1/1
4	AHR	b	5	4	-	0/2/15/18	0/1/1/1
4	BGC	b	6	4	-	0/2/19/22	0/1/1/1
4	MAN	b	7	4	-	0/2/19/22	0/1/1/1
4	NAG	b	8	4	-	0/6/23/26	0/1/1/1
4	AHR	b	9	4	-	0/2/15/18	0/1/1/1

All (189) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	25	A1E3E	C2-C3	-18.59	1.23	1.53
3	R	33	A1E3E	C2-C3	-18.58	1.23	1.53
2	T	25	A1E3E	C2-C3	-18.57	1.23	1.53
3	U	33	A1E3E	C2-C3	-18.57	1.23	1.53
2	C	25	A1E3E	C2-C3	-18.57	1.23	1.53
2	N	25	A1E3E	C2-C3	-18.56	1.23	1.53
3	X	33	A1E3E	C2-C3	-18.56	1.23	1.53
2	W	25	A1E3E	C2-C3	-18.56	1.23	1.53
3	L	33	A1E3E	C2-C3	-18.55	1.23	1.53
3	I	33	A1E3E	C2-C3	-18.55	1.23	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	25	A1E3E	C2-C3	-18.54	1.23	1.53
2	E	25	A1E3E	C2-C3	-18.54	1.23	1.53
3	O	33	A1E3E	C2-C3	-18.53	1.23	1.53
3	B	33	A1E3E	C2-C3	-18.53	1.23	1.53
2	Z	25	A1E3E	C2-C3	-18.52	1.23	1.53
3	a	33	A1E3E	C2-C3	-18.51	1.23	1.53
2	K	25	A1E3E	C2-C3	-18.51	1.23	1.53
3	F	33	A1E3E	C2-C3	-18.49	1.23	1.53
3	R	17	A1E3E	C2-C3	-18.38	1.24	1.53
3	U	17	A1E3E	C2-C3	-18.37	1.24	1.53
3	a	17	A1E3E	C2-C3	-18.35	1.24	1.53
3	L	17	A1E3E	C2-C3	-18.34	1.24	1.53
3	O	17	A1E3E	C2-C3	-18.33	1.24	1.53
3	I	17	A1E3E	C2-C3	-18.32	1.24	1.53
3	X	17	A1E3E	C2-C3	-18.29	1.24	1.53
3	F	17	A1E3E	C2-C3	-18.22	1.24	1.53
3	B	17	A1E3E	C2-C3	-18.21	1.24	1.53
3	a	33	A1E3E	O4-C4	-7.29	1.27	1.43
3	O	17	A1E3E	O4-C4	-7.26	1.27	1.43
3	O	33	A1E3E	O4-C4	-7.25	1.27	1.43
3	L	33	A1E3E	O4-C4	-7.24	1.27	1.43
3	U	33	A1E3E	O4-C4	-7.23	1.27	1.43
3	X	33	A1E3E	O4-C4	-7.23	1.27	1.43
3	B	17	A1E3E	O4-C4	-7.23	1.27	1.43
3	F	33	A1E3E	O4-C4	-7.22	1.27	1.43
3	B	33	A1E3E	O4-C4	-7.22	1.27	1.43
3	I	33	A1E3E	O4-C4	-7.22	1.27	1.43
3	F	17	A1E3E	O4-C4	-7.21	1.27	1.43
3	I	17	A1E3E	O4-C4	-7.20	1.27	1.43
3	a	17	A1E3E	O4-C4	-7.19	1.27	1.43
3	X	17	A1E3E	O4-C4	-7.18	1.27	1.43
3	R	17	A1E3E	O4-C4	-7.16	1.27	1.43
3	R	33	A1E3E	O4-C4	-7.15	1.27	1.43
3	U	17	A1E3E	O4-C4	-7.15	1.27	1.43
3	L	17	A1E3E	O4-C4	-7.13	1.27	1.43
2	Z	25	A1E3E	O4-C4	-7.05	1.28	1.43
2	K	25	A1E3E	O4-C4	-7.04	1.28	1.43
2	H	25	A1E3E	O4-C4	-7.03	1.28	1.43
2	N	25	A1E3E	O4-C4	-7.02	1.28	1.43
2	W	25	A1E3E	O4-C4	-7.01	1.28	1.43
2	C	25	A1E3E	O4-C4	-7.01	1.28	1.43
2	Q	25	A1E3E	O4-C4	-7.00	1.28	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	25	A1E3E	O4-C4	-6.99	1.28	1.43
2	T	25	A1E3E	O4-C4	-6.99	1.28	1.43
2	T	25	A1E3E	C3-C4	6.67	1.67	1.52
2	Z	25	A1E3E	C3-C4	6.67	1.67	1.52
2	K	25	A1E3E	C3-C4	6.67	1.67	1.52
2	C	25	A1E3E	C3-C4	6.67	1.67	1.52
2	N	25	A1E3E	C3-C4	6.66	1.67	1.52
2	H	25	A1E3E	C3-C4	6.64	1.67	1.52
2	E	25	A1E3E	C3-C4	6.64	1.67	1.52
2	W	25	A1E3E	C3-C4	6.64	1.67	1.52
2	Q	25	A1E3E	C3-C4	6.62	1.67	1.52
3	a	17	A1E3E	C3-C4	6.58	1.67	1.52
3	L	17	A1E3E	C3-C4	6.57	1.67	1.52
3	U	17	A1E3E	C3-C4	6.56	1.67	1.52
3	X	17	A1E3E	C3-C4	6.55	1.67	1.52
3	R	17	A1E3E	C3-C4	6.54	1.67	1.52
3	F	17	A1E3E	C3-C4	6.54	1.67	1.52
3	I	17	A1E3E	C3-C4	6.52	1.67	1.52
3	O	17	A1E3E	C3-C4	6.52	1.67	1.52
3	B	17	A1E3E	C3-C4	6.47	1.67	1.52
3	B	33	A1E3E	C3-C4	6.18	1.66	1.52
3	F	33	A1E3E	C3-C4	6.16	1.66	1.52
3	L	33	A1E3E	C3-C4	6.14	1.66	1.52
3	O	33	A1E3E	C3-C4	6.14	1.66	1.52
3	R	33	A1E3E	C3-C4	6.11	1.66	1.52
3	U	33	A1E3E	C3-C4	6.11	1.66	1.52
3	X	33	A1E3E	C3-C4	6.10	1.66	1.52
3	a	33	A1E3E	C3-C4	6.10	1.66	1.52
3	I	33	A1E3E	C3-C4	6.08	1.66	1.52
3	X	33	A1E3E	C1-C2	5.14	1.60	1.51
3	R	33	A1E3E	C1-C2	5.12	1.60	1.51
3	I	33	A1E3E	C1-C2	5.10	1.60	1.51
3	L	33	A1E3E	C1-C2	5.10	1.60	1.51
3	U	33	A1E3E	C1-C2	5.09	1.60	1.51
3	F	33	A1E3E	C1-C2	5.06	1.60	1.51
3	a	33	A1E3E	C1-C2	5.05	1.60	1.51
3	O	33	A1E3E	C1-C2	5.04	1.60	1.51
3	B	33	A1E3E	C1-C2	5.03	1.60	1.51
3	B	17	A1E3E	C1-C2	4.71	1.59	1.51
3	F	17	A1E3E	C1-C2	4.64	1.59	1.51
3	O	17	A1E3E	C1-C2	4.63	1.59	1.51
3	a	17	A1E3E	C1-C2	4.60	1.59	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	17	A1E3E	C1-C2	4.58	1.59	1.51
3	I	17	A1E3E	C1-C2	4.57	1.59	1.51
3	U	17	A1E3E	C1-C2	4.57	1.59	1.51
3	R	17	A1E3E	C1-C2	4.56	1.59	1.51
3	L	17	A1E3E	C1-C2	4.56	1.59	1.51
2	Z	25	A1E3E	C1-C2	4.43	1.59	1.51
2	T	25	A1E3E	C1-C2	4.42	1.59	1.51
2	E	25	A1E3E	C1-C2	4.38	1.59	1.51
2	H	25	A1E3E	C1-C2	4.36	1.59	1.51
2	W	25	A1E3E	C1-C2	4.36	1.59	1.51
2	N	25	A1E3E	C1-C2	4.36	1.59	1.51
2	C	25	A1E3E	C1-C2	4.35	1.59	1.51
2	Q	25	A1E3E	C1-C2	4.34	1.59	1.51
2	K	25	A1E3E	C1-C2	4.33	1.59	1.51
3	R	33	A1E3E	O4-C1	4.12	1.52	1.43
3	I	33	A1E3E	O4-C1	4.09	1.52	1.43
3	U	33	A1E3E	O4-C1	4.08	1.52	1.43
3	L	33	A1E3E	O4-C1	4.08	1.52	1.43
3	X	33	A1E3E	O4-C1	4.08	1.52	1.43
3	a	33	A1E3E	O4-C1	4.05	1.52	1.43
3	F	33	A1E3E	O4-C1	4.04	1.52	1.43
3	B	33	A1E3E	O4-C1	4.02	1.52	1.43
3	O	33	A1E3E	O4-C1	4.01	1.52	1.43
3	I	33	A1E3E	O2-C2	3.91	1.51	1.43
3	X	33	A1E3E	O2-C2	3.89	1.51	1.43
3	R	33	A1E3E	O2-C2	3.87	1.51	1.43
3	L	33	A1E3E	O2-C2	3.86	1.51	1.43
3	U	33	A1E3E	O2-C2	3.82	1.51	1.43
3	F	33	A1E3E	O2-C2	3.81	1.51	1.43
2	W	25	A1E3E	O4-C1	3.81	1.52	1.43
2	N	25	A1E3E	O4-C1	3.80	1.52	1.43
2	Z	25	A1E3E	O4-C1	3.80	1.52	1.43
3	a	33	A1E3E	O2-C2	3.80	1.51	1.43
3	B	17	A1E3E	O2-C2	3.80	1.51	1.43
3	X	17	A1E3E	O2-C2	3.79	1.51	1.43
3	B	33	A1E3E	O2-C2	3.79	1.51	1.43
3	O	33	A1E3E	O2-C2	3.79	1.51	1.43
2	E	25	A1E3E	O4-C1	3.78	1.52	1.43
3	O	17	A1E3E	O2-C2	3.78	1.51	1.43
3	B	17	A1E3E	O4-C1	3.78	1.52	1.43
3	F	17	A1E3E	O4-C1	3.78	1.52	1.43
3	X	17	A1E3E	O4-C1	3.77	1.52	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	17	A1E3E	O2-C2	3.77	1.51	1.43
3	a	17	A1E3E	O2-C2	3.77	1.51	1.43
3	a	17	A1E3E	O4-C1	3.77	1.52	1.43
3	L	17	A1E3E	O2-C2	3.77	1.51	1.43
2	T	25	A1E3E	O4-C1	3.77	1.52	1.43
3	U	17	A1E3E	O2-C2	3.77	1.51	1.43
2	C	25	A1E3E	O4-C1	3.76	1.52	1.43
3	F	17	A1E3E	O2-C2	3.76	1.51	1.43
3	U	17	A1E3E	O4-C1	3.76	1.52	1.43
3	R	17	A1E3E	O4-C1	3.75	1.52	1.43
3	L	17	A1E3E	O4-C1	3.74	1.52	1.43
3	O	17	A1E3E	O4-C1	3.74	1.52	1.43
3	I	17	A1E3E	O2-C2	3.74	1.51	1.43
2	Q	25	A1E3E	O4-C1	3.74	1.52	1.43
2	K	25	A1E3E	O4-C1	3.74	1.52	1.43
3	I	17	A1E3E	O4-C1	3.72	1.52	1.43
2	H	25	A1E3E	O2-C2	3.71	1.51	1.43
2	Q	25	A1E3E	O2-C2	3.70	1.51	1.43
2	H	25	A1E3E	O4-C1	3.70	1.52	1.43
2	E	25	A1E3E	O2-C2	3.70	1.51	1.43
2	T	25	A1E3E	O2-C2	3.69	1.51	1.43
2	K	25	A1E3E	O2-C2	3.68	1.51	1.43
2	Z	25	A1E3E	O2-C2	3.68	1.51	1.43
2	N	25	A1E3E	O2-C2	3.67	1.51	1.43
2	C	25	A1E3E	O2-C2	3.67	1.51	1.43
2	W	25	A1E3E	O2-C2	3.64	1.51	1.43
2	C	25	A1E3E	O3-C3	2.17	1.48	1.43
3	X	17	A1E3E	O3-C3	2.15	1.48	1.43
3	R	17	A1E3E	O3-C3	2.15	1.48	1.43
3	L	17	A1E3E	O3-C3	2.14	1.48	1.43
2	Z	25	A1E3E	O3-C3	2.14	1.48	1.43
2	W	25	A1E3E	O3-C3	2.13	1.48	1.43
2	K	25	A1E3E	O3-C3	2.13	1.48	1.43
2	T	25	A1E3E	O3-C3	2.13	1.48	1.43
2	H	25	A1E3E	O3-C3	2.12	1.48	1.43
2	Q	25	A1E3E	O3-C3	2.12	1.48	1.43
3	F	17	A1E3E	O3-C3	2.12	1.48	1.43
3	X	33	A1E3E	O3-C3	2.11	1.47	1.43
3	a	33	A1E3E	O3-C3	2.11	1.47	1.43
2	E	25	A1E3E	O3-C3	2.11	1.47	1.43
3	O	17	A1E3E	O3-C3	2.11	1.47	1.43
3	B	17	A1E3E	O3-C3	2.11	1.47	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	17	A1E3E	O3-C3	2.10	1.47	1.43
3	I	17	A1E3E	O3-C3	2.10	1.47	1.43
2	N	25	A1E3E	O3-C3	2.10	1.47	1.43
3	a	17	A1E3E	O3-C3	2.10	1.47	1.43
3	U	33	A1E3E	O3-C3	2.09	1.47	1.43
3	F	33	A1E3E	O3-C3	2.09	1.47	1.43
3	B	33	A1E3E	O3-C3	2.08	1.47	1.43
3	I	33	A1E3E	O3-C3	2.08	1.47	1.43
3	O	33	A1E3E	O3-C3	2.08	1.47	1.43
3	L	33	A1E3E	O3-C3	2.04	1.47	1.43
3	R	33	A1E3E	O3-C3	2.04	1.47	1.43

All (370) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	7	MAN	O2-C2-C3	5.22	120.60	110.14
4	S	7	MAN	O2-C2-C3	5.20	120.55	110.14
4	G	7	MAN	O2-C2-C3	5.17	120.49	110.14
4	Y	7	MAN	O2-C2-C3	5.15	120.46	110.14
4	D	7	MAN	O2-C2-C3	5.14	120.43	110.14
4	M	7	MAN	O2-C2-C3	5.13	120.42	110.14
4	P	7	MAN	O2-C2-C3	5.10	120.36	110.14
4	b	7	MAN	O2-C2-C3	5.06	120.28	110.14
4	V	7	MAN	O2-C2-C3	5.04	120.24	110.14
3	U	17	A1E3E	C5-C4-C3	-4.55	109.78	115.86
3	F	17	A1E3E	C5-C4-C3	-4.51	109.83	115.86
3	R	17	A1E3E	C5-C4-C3	-4.48	109.87	115.86
3	U	33	A1E3E	C5-C4-C3	-4.45	109.90	115.86
3	X	17	A1E3E	C5-C4-C3	-4.45	109.90	115.86
3	a	17	A1E3E	C5-C4-C3	-4.42	109.94	115.86
3	X	33	A1E3E	C5-C4-C3	-4.41	109.97	115.86
3	O	33	A1E3E	C5-C4-C3	-4.34	110.05	115.86
3	a	33	A1E3E	C5-C4-C3	-4.32	110.08	115.86
3	I	17	A1E3E	C5-C4-C3	-4.31	110.09	115.86
3	O	17	A1E3E	C5-C4-C3	-4.29	110.12	115.86
3	B	17	A1E3E	C5-C4-C3	-4.27	110.15	115.86
3	R	33	A1E3E	C5-C4-C3	-4.26	110.17	115.86
3	I	33	A1E3E	C5-C4-C3	-4.26	110.17	115.86
3	B	33	A1E3E	C5-C4-C3	-4.22	110.22	115.86
3	L	17	A1E3E	C5-C4-C3	-4.20	110.25	115.86
2	E	25	A1E3E	C5-C4-C3	-4.13	110.34	115.86
2	N	25	A1E3E	C5-C4-C3	-4.12	110.35	115.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	33	A1E3E	C5-C4-C3	-4.10	110.37	115.86
2	W	25	A1E3E	C5-C4-C3	-4.09	110.39	115.86
2	Z	25	A1E3E	C5-C4-C3	-4.06	110.43	115.86
3	L	33	A1E3E	C5-C4-C3	-4.04	110.46	115.86
2	Q	25	A1E3E	C5-C4-C3	-3.97	110.55	115.86
2	C	25	A1E3E	C5-C4-C3	-3.97	110.55	115.86
2	H	25	A1E3E	C5-C4-C3	-3.96	110.56	115.86
2	T	25	A1E3E	C5-C4-C3	-3.91	110.63	115.86
2	K	25	A1E3E	C5-C4-C3	-3.88	110.67	115.86
3	O	36	BGC	O2-C2-C3	3.54	117.23	110.14
3	I	36	BGC	O2-C2-C3	3.49	117.13	110.14
3	R	36	BGC	O2-C2-C3	3.44	117.03	110.14
3	X	36	BGC	O2-C2-C3	3.43	117.00	110.14
3	L	36	BGC	O2-C2-C3	3.37	116.89	110.14
3	a	36	BGC	O2-C2-C3	3.25	116.65	110.14
3	U	36	BGC	O2-C2-C3	3.25	116.65	110.14
3	B	36	BGC	O2-C2-C3	3.24	116.64	110.14
3	B	17	A1E3E	C1-C2-C3	3.18	106.48	101.63
3	O	17	A1E3E	C1-C2-C3	3.14	106.42	101.63
3	F	36	BGC	O2-C2-C3	3.00	116.15	110.14
3	F	17	A1E3E	C1-C2-C3	2.98	106.17	101.63
3	R	43	BMA	C1-C2-C3	2.96	113.31	109.67
3	X	43	BMA	C1-C2-C3	2.89	113.22	109.67
4	Y	5	AHR	C1-C2-C3	2.84	105.95	101.63
4	b	5	AHR	C1-C2-C3	2.81	105.91	101.63
4	S	5	AHR	C1-C2-C3	2.80	105.89	101.63
4	V	5	AHR	C1-C2-C3	2.78	105.86	101.63
4	M	5	AHR	C1-C2-C3	2.78	105.86	101.63
3	I	10	XYP	C1-C2-C3	2.76	113.06	109.67
3	O	10	XYP	C1-C2-C3	2.76	113.05	109.67
4	J	5	AHR	C1-C2-C3	2.75	105.82	101.63
3	R	10	XYP	C1-C2-C3	2.75	113.04	109.67
3	L	10	XYP	C1-C2-C3	2.74	113.03	109.67
3	U	10	XYP	C1-C2-C3	2.74	113.03	109.67
3	R	43	BMA	C1-O5-C5	2.74	115.90	112.19
3	X	17	A1E3E	C1-C2-C3	2.74	105.80	101.63
3	X	10	XYP	C1-C2-C3	2.73	113.03	109.67
4	P	5	AHR	C1-C2-C3	2.73	105.79	101.63
4	D	14	AHR	C1-C2-C3	2.73	105.79	101.63
4	b	14	AHR	C1-C2-C3	2.72	105.77	101.63
3	a	17	A1E3E	C1-C2-C3	2.70	105.75	101.63
3	a	10	XYP	C1-C2-C3	2.70	112.98	109.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	43	BMA	C1-C2-C3	2.69	112.97	109.67
4	P	14	AHR	C1-C2-C3	2.68	105.72	101.63
4	G	14	AHR	C1-C2-C3	2.68	105.72	101.63
4	J	14	AHR	C1-C2-C3	2.67	105.70	101.63
4	D	5	AHR	C1-C2-C3	2.67	105.70	101.63
4	Y	14	AHR	C1-C2-C3	2.67	105.69	101.63
3	O	43	BMA	C1-O5-C5	2.67	115.81	112.19
3	a	43	BMA	C1-C2-C3	2.65	112.93	109.67
3	O	43	BMA	C1-C2-C3	2.65	112.92	109.67
4	G	5	AHR	C1-C2-C3	2.63	105.63	101.63
4	V	14	AHR	C1-C2-C3	2.60	105.58	101.63
4	S	14	AHR	C1-C2-C3	2.59	105.58	101.63
3	B	43	BMA	C1-C2-C3	2.59	112.85	109.67
3	L	43	BMA	C1-C2-C3	2.58	112.83	109.67
3	I	17	A1E3E	C1-C2-C3	2.58	105.55	101.63
3	F	43	BMA	C1-C2-C3	2.56	112.81	109.67
4	M	14	AHR	C1-C2-C3	2.55	105.51	101.63
3	F	10	XYP	C1-C2-C3	2.55	112.80	109.67
3	B	10	XYP	C1-C2-C3	2.54	112.79	109.67
3	R	3	MAN	C1-C2-C3	2.53	112.78	109.67
3	X	43	BMA	C1-O5-C5	2.53	115.62	112.19
3	U	43	BMA	C1-C2-C3	2.52	112.77	109.67
3	a	3	MAN	C1-C2-C3	2.51	112.75	109.67
3	I	3	MAN	C1-C2-C3	2.50	112.74	109.67
3	U	17	A1E3E	C1-C2-C3	2.50	105.44	101.63
4	J	7	MAN	C1-C2-C3	2.50	112.73	109.67
3	a	43	BMA	C1-O5-C5	2.49	115.57	112.19
3	F	3	MAN	C1-C2-C3	2.49	112.73	109.67
3	U	3	MAN	C1-C2-C3	2.49	112.73	109.67
3	X	3	MAN	C1-C2-C3	2.47	112.70	109.67
3	R	17	A1E3E	C1-C2-C3	2.47	105.39	101.63
3	L	17	A1E3E	C1-C2-C3	2.46	105.38	101.63
3	O	3	MAN	C1-C2-C3	2.46	112.69	109.67
3	L	3	MAN	C1-C2-C3	2.46	112.69	109.67
3	L	43	BMA	C1-O5-C5	2.45	115.52	112.19
4	Y	7	MAN	C1-C2-C3	2.45	112.68	109.67
3	I	43	BMA	C1-O5-C5	2.45	115.51	112.19
4	V	7	MAN	C1-C2-C3	2.44	112.67	109.67
4	G	7	MAN	C1-C2-C3	2.44	112.66	109.67
4	D	7	MAN	C1-C2-C3	2.43	112.66	109.67
4	P	7	MAN	C1-C2-C3	2.43	112.66	109.67
3	B	3	MAN	C1-C2-C3	2.43	112.65	109.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	b	7	MAN	C1-C2-C3	2.42	112.64	109.67
4	S	7	MAN	C1-C2-C3	2.40	112.61	109.67
4	M	7	MAN	C1-C2-C3	2.39	112.60	109.67
3	R	15	FUB	C1-C2-C3	2.37	105.25	101.63
3	I	16	AHR	C1-C2-C3	2.36	105.23	101.63
3	I	4	MAN	C1-C2-C3	2.35	112.55	109.67
3	a	32	FUB	C1-C2-C3	2.35	105.20	101.63
3	U	43	BMA	C1-O5-C5	2.34	115.37	112.19
2	T	18	AHR	C1-C2-C3	2.34	105.19	101.63
2	W	7	FUB	C1-C2-C3	2.33	105.18	101.63
3	O	31	MAN	C1-C2-C3	2.32	112.52	109.67
3	R	4	MAN	C1-C2-C3	2.32	112.52	109.67
3	I	32	FUB	C1-C2-C3	2.32	105.16	101.63
3	I	15	FUB	C1-C2-C3	2.32	105.16	101.63
2	E	25	A1E3E	O4-C4-C3	2.32	107.73	103.59
3	I	31	MAN	C1-C2-C3	2.31	112.51	109.67
3	F	43	BMA	C1-O5-C5	2.31	115.33	112.19
3	R	31	MAN	C1-C2-C3	2.31	112.51	109.67
3	U	4	MAN	C1-C2-C3	2.31	112.51	109.67
3	O	4	MAN	C1-C2-C3	2.31	112.51	109.67
2	Q	12	MAN	C1-O5-C5	2.31	115.32	112.19
3	F	4	MAN	C1-C2-C3	2.30	112.50	109.67
3	R	17	A1E3E	O4-C4-C3	2.30	107.70	103.59
3	U	32	FUB	C1-C2-C3	2.29	105.12	101.63
3	B	4	MAN	C1-C2-C3	2.29	112.48	109.67
3	O	41	AHR	C1-C2-C3	2.29	105.12	101.63
3	O	16	AHR	C1-C2-C3	2.29	105.11	101.63
3	X	4	MAN	C1-C2-C3	2.29	112.48	109.67
3	R	32	FUB	C1-C2-C3	2.29	105.11	101.63
3	L	4	MAN	C1-C2-C3	2.28	112.47	109.67
3	B	15	FUB	C1-C2-C3	2.28	105.10	101.63
3	a	4	MAN	C1-C2-C3	2.28	112.47	109.67
2	T	7	FUB	C1-C2-C3	2.28	105.10	101.63
3	U	31	MAN	C1-C2-C3	2.28	112.46	109.67
3	B	31	MAN	C1-C2-C3	2.27	112.46	109.67
3	F	15	FUB	C1-C2-C3	2.27	105.09	101.63
3	L	15	FUB	C1-C2-C3	2.27	105.09	101.63
2	N	18	AHR	C1-C2-C3	2.27	105.09	101.63
4	Y	8	NAG	C1-O5-C5	2.27	115.26	112.19
2	Z	25	A1E3E	O4-C4-C3	2.26	107.64	103.59
3	L	32	FUB	C1-C2-C3	2.26	105.07	101.63
3	X	31	MAN	C1-C2-C3	2.25	112.43	109.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	41	AHR	C1-C2-C3	2.25	105.06	101.63
3	L	31	MAN	C1-C2-C3	2.25	112.43	109.67
4	S	11	AHR	C1-C2-C3	2.25	105.06	101.63
2	W	12	MAN	C1-O5-C5	2.25	115.24	112.19
2	Z	7	FUB	C1-C2-C3	2.25	105.06	101.63
2	N	12	MAN	C1-O5-C5	2.25	115.24	112.19
2	W	18	AHR	C1-C2-C3	2.24	105.05	101.63
3	L	16	AHR	C1-C2-C3	2.24	105.05	101.63
3	F	41	AHR	C1-C2-C3	2.24	105.05	101.63
2	N	7	FUB	C1-C2-C3	2.24	105.04	101.63
2	H	7	FUB	C1-C2-C3	2.24	105.04	101.63
2	C	12	MAN	C1-C2-C3	2.24	112.42	109.67
2	C	12	MAN	C1-O5-C5	2.24	115.22	112.19
2	Z	18	AHR	C1-C2-C3	2.24	105.04	101.63
2	H	12	MAN	C1-O5-C5	2.24	115.22	112.19
3	U	41	AHR	C1-C2-C3	2.24	105.03	101.63
3	B	43	BMA	C1-O5-C5	2.23	115.22	112.19
2	H	12	MAN	C1-C2-C3	2.23	112.41	109.67
2	Q	25	A1E3E	O4-C4-C3	2.23	107.58	103.59
3	O	15	FUB	C1-C2-C3	2.23	105.03	101.63
2	Q	7	FUB	C1-C2-C3	2.23	105.02	101.63
2	Q	12	MAN	C1-C2-C3	2.23	112.40	109.67
4	b	8	NAG	C1-O5-C5	2.22	115.21	112.19
3	a	31	MAN	C1-C2-C3	2.22	112.40	109.67
3	I	12	MAN	C1-C2-C3	2.22	112.40	109.67
3	U	15	FUB	C1-C2-C3	2.22	105.01	101.63
3	L	17	A1E3E	O4-C4-C3	2.22	107.56	103.59
2	N	12	MAN	C1-C2-C3	2.22	112.39	109.67
3	U	12	MAN	C1-C2-C3	2.22	112.39	109.67
3	X	41	AHR	C1-C2-C3	2.22	105.00	101.63
2	K	12	MAN	C1-C2-C3	2.22	112.39	109.67
3	F	31	MAN	C1-C2-C3	2.21	112.39	109.67
3	a	12	MAN	C1-C2-C3	2.21	112.39	109.67
3	B	41	AHR	C1-C2-C3	2.21	105.00	101.63
3	L	41	AHR	C1-C2-C3	2.21	105.00	101.63
2	T	25	A1E3E	O4-C4-C3	2.21	107.55	103.59
3	F	16	AHR	C1-C2-C3	2.21	105.00	101.63
2	W	12	MAN	C1-C2-C3	2.21	112.39	109.67
3	B	32	FUB	C1-C2-C3	2.21	105.00	101.63
3	a	25	MAN	C1-C2-C3	2.21	112.38	109.67
3	X	16	AHR	C1-C2-C3	2.21	105.00	101.63
2	T	12	MAN	C1-O5-C5	2.21	115.19	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	7	FUB	C1-C2-C3	2.21	104.99	101.63
3	X	12	MAN	C1-C2-C3	2.21	112.38	109.67
2	E	12	MAN	C1-O5-C5	2.21	115.18	112.19
3	B	16	AHR	C1-C2-C3	2.21	104.99	101.63
3	L	12	MAN	C1-C2-C3	2.21	112.38	109.67
2	K	12	MAN	C1-O5-C5	2.21	115.18	112.19
3	B	12	MAN	C1-C2-C3	2.21	112.38	109.67
3	R	12	MAN	C1-C2-C3	2.20	112.38	109.67
2	E	12	MAN	C1-C2-C3	2.20	112.37	109.67
3	F	12	MAN	C1-C2-C3	2.20	112.37	109.67
4	Y	11	AHR	C1-C2-C3	2.20	104.98	101.63
3	U	17	A1E3E	O4-C4-C3	2.20	107.52	103.59
3	X	15	FUB	C1-C2-C3	2.19	104.97	101.63
3	I	41	AHR	C1-C2-C3	2.19	104.97	101.63
2	Z	13	MAN	C1-C2-C3	2.19	112.35	109.67
2	W	13	MAN	C1-C2-C3	2.19	112.35	109.67
3	U	16	AHR	C1-C2-C3	2.18	104.96	101.63
3	I	25	MAN	C1-C2-C3	2.18	112.35	109.67
3	O	12	MAN	C1-C2-C3	2.18	112.35	109.67
2	Z	12	MAN	C1-O5-C5	2.18	115.15	112.19
3	U	25	MAN	C1-C2-C3	2.18	112.35	109.67
2	T	12	MAN	C1-C2-C3	2.18	112.34	109.67
2	K	17	AHR	C1-C2-C3	2.18	104.94	101.63
3	X	32	FUB	C1-C2-C3	2.17	104.94	101.63
2	Q	13	MAN	C1-C2-C3	2.17	112.34	109.67
4	J	8	NAG	C1-O5-C5	2.17	115.13	112.19
2	C	25	A1E3E	O4-C1-C2	-2.17	101.80	105.99
2	Q	17	AHR	C1-C2-C3	2.17	104.93	101.63
2	W	25	A1E3E	O4-C1-C2	-2.16	101.80	105.99
2	C	17	AHR	C1-C2-C3	2.16	104.92	101.63
2	W	17	AHR	C1-C2-C3	2.16	104.92	101.63
2	T	10	BMA	O5-C5-C6	2.16	110.59	107.20
3	X	25	MAN	C1-C2-C3	2.16	112.32	109.67
4	V	11	AHR	C1-C2-C3	2.16	104.92	101.63
2	N	25	A1E3E	O4-C4-C3	2.16	107.45	103.59
3	a	41	AHR	C1-C2-C3	2.16	104.91	101.63
3	R	25	MAN	C1-C2-C3	2.15	112.31	109.67
4	M	11	AHR	C1-C2-C3	2.15	104.91	101.63
3	O	31	MAN	C1-O5-C5	2.15	115.11	112.19
2	Z	12	MAN	C1-C2-C3	2.15	112.31	109.67
2	K	25	A1E3E	O4-C1-C2	-2.15	101.83	105.99
2	N	13	MAN	C1-C2-C3	2.15	112.31	109.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	16	AHR	C1-C2-C3	2.15	104.90	101.63
2	T	13	MAN	C1-C2-C3	2.14	112.30	109.67
3	O	25	MAN	C1-C2-C3	2.14	112.30	109.67
2	H	17	AHR	C1-C2-C3	2.14	104.89	101.63
3	F	32	FUB	C1-C2-C3	2.14	104.89	101.63
2	Z	10	BMA	O5-C5-C6	2.14	110.56	107.20
3	X	31	MAN	C1-O5-C5	2.14	115.09	112.19
3	F	25	MAN	C1-C2-C3	2.14	112.29	109.67
2	N	10	BMA	O5-C5-C6	2.14	110.55	107.20
2	H	13	MAN	C1-C2-C3	2.13	112.29	109.67
4	V	2	MAN	C1-O5-C5	2.13	115.08	112.19
3	F	42	FUB	C1-C2-C3	2.13	104.88	101.63
3	I	17	A1E3E	O4-C4-C3	2.13	107.41	103.59
4	M	2	MAN	C1-C2-C3	2.13	112.29	109.67
2	H	25	A1E3E	O4-C4-C3	2.13	107.39	103.59
2	K	13	MAN	C1-C2-C3	2.12	112.28	109.67
3	a	15	FUB	C1-C2-C3	2.12	104.86	101.63
4	Y	2	MAN	C1-O5-C5	2.12	115.06	112.19
2	H	25	A1E3E	O4-C1-C2	-2.12	101.89	105.99
2	T	17	AHR	C1-C2-C3	2.12	104.86	101.63
4	M	8	NAG	C1-O5-C5	2.12	115.06	112.19
2	W	10	BMA	O5-C5-C6	2.12	110.52	107.20
3	F	31	MAN	C1-O5-C5	2.11	115.06	112.19
2	Z	21	AHR	C1-C2-C3	2.11	104.84	101.63
3	B	31	MAN	C1-O5-C5	2.11	115.05	112.19
4	b	2	MAN	C1-C2-C3	2.11	112.26	109.67
4	P	2	MAN	C1-C2-C3	2.11	112.26	109.67
2	N	25	A1E3E	O4-C1-C2	-2.11	101.91	105.99
4	P	2	MAN	C1-O5-C5	2.11	115.05	112.19
4	M	2	MAN	C1-O5-C5	2.10	115.04	112.19
3	L	25	MAN	C1-C2-C3	2.10	112.25	109.67
3	R	31	MAN	C1-O5-C5	2.10	115.04	112.19
2	K	13	MAN	C1-O5-C5	2.10	115.04	112.19
2	K	7	FUB	C1-C2-C3	2.10	104.83	101.63
3	B	42	FUB	C1-C2-C3	2.10	104.83	101.63
4	G	2	MAN	C1-O5-C5	2.10	115.03	112.19
2	N	17	AHR	C1-C2-C3	2.10	104.83	101.63
4	D	11	AHR	C1-C2-C3	2.10	104.83	101.63
4	b	11	AHR	C1-C2-C3	2.10	104.82	101.63
3	O	32	FUB	C1-C2-C3	2.10	104.82	101.63
3	L	31	MAN	C1-O5-C5	2.09	115.03	112.19
4	V	8	NAG	C1-O5-C5	2.09	115.03	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	10	AHR	C1-C2-C3	2.09	104.82	101.63
2	C	25	A1E3E	O4-C4-C3	2.09	107.33	103.59
3	B	25	MAN	C1-C2-C3	2.09	112.24	109.67
2	E	17	AHR	C1-C2-C3	2.09	104.81	101.63
4	J	2	MAN	C1-C2-C3	2.09	112.23	109.67
4	J	2	MAN	C1-O5-C5	2.09	115.02	112.19
3	X	17	A1E3E	O4-C4-C3	2.08	107.32	103.59
2	Z	17	AHR	C1-C2-C3	2.08	104.80	101.63
4	D	2	MAN	C1-C2-C3	2.08	112.22	109.67
2	W	13	MAN	C1-O5-C5	2.08	115.01	112.19
4	Y	13	NAG	C1-O5-C5	2.08	115.01	112.19
4	D	2	MAN	C1-O5-C5	2.08	115.01	112.19
2	C	13	MAN	C1-C2-C3	2.08	112.22	109.67
4	b	2	MAN	C1-O5-C5	2.08	115.01	112.19
3	I	31	MAN	C1-O5-C5	2.08	115.00	112.19
4	Y	2	MAN	C1-C2-C3	2.08	112.22	109.67
2	W	25	A1E3E	O4-C4-C3	2.08	107.30	103.59
2	H	10	BMA	O5-C5-C6	2.08	110.46	107.20
2	E	13	MAN	C1-O5-C5	2.07	115.00	112.19
2	Q	13	MAN	C1-O5-C5	2.07	115.00	112.19
3	a	3	MAN	C1-O5-C5	2.07	115.00	112.19
3	L	25	MAN	C1-O5-C5	2.07	114.99	112.19
3	X	25	MAN	C1-O5-C5	2.06	114.99	112.19
3	I	25	MAN	C1-O5-C5	2.06	114.99	112.19
4	S	2	MAN	C1-C2-C3	2.06	112.20	109.67
4	G	8	NAG	C1-O5-C5	2.06	114.99	112.19
4	G	2	MAN	C1-C2-C3	2.06	112.20	109.67
2	C	13	MAN	C1-O5-C5	2.06	114.99	112.19
4	S	2	MAN	C1-O5-C5	2.06	114.99	112.19
2	N	13	MAN	C1-O5-C5	2.06	114.98	112.19
2	E	13	MAN	C1-C2-C3	2.06	112.20	109.67
3	a	31	MAN	C1-O5-C5	2.06	114.98	112.19
3	B	25	MAN	C1-O5-C5	2.06	114.98	112.19
2	W	21	AHR	C1-C2-C3	2.05	104.76	101.63
2	Z	13	MAN	C1-O5-C5	2.05	114.97	112.19
4	P	11	AHR	C1-C2-C3	2.05	104.75	101.63
3	a	17	A1E3E	O4-C4-C3	2.05	107.25	103.59
2	H	13	MAN	C1-O5-C5	2.05	114.96	112.19
2	C	10	BMA	O5-C5-C6	2.04	110.41	107.20
4	V	18	AHR	C1-C2-C3	2.04	104.74	101.63
4	D	8	NAG	C1-O5-C5	2.04	114.96	112.19
2	T	13	MAN	C1-O5-C5	2.04	114.95	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	25	MAN	C1-O5-C5	2.04	114.95	112.19
2	H	18	AHR	C1-C2-C3	2.04	104.73	101.63
3	O	25	MAN	C1-O5-C5	2.04	114.95	112.19
3	U	31	MAN	C1-O5-C5	2.04	114.95	112.19
2	E	10	BMA	O5-C5-C6	2.04	110.39	107.20
4	V	2	MAN	C1-C2-C3	2.03	112.17	109.67
3	U	25	MAN	C1-O5-C5	2.03	114.95	112.19
3	a	16	AHR	C1-C2-C3	2.03	104.73	101.63
2	C	18	AHR	C1-C2-C3	2.03	104.72	101.63
4	G	11	AHR	C1-C2-C3	2.03	104.72	101.63
3	U	13	AHR	C1-C2-C3	2.03	104.72	101.63
4	b	18	AHR	C1-C2-C3	2.03	104.72	101.63
2	K	25	A1E3E	O4-C4-C3	2.03	107.22	103.59
4	P	18	AHR	C1-C2-C3	2.03	104.72	101.63
3	R	25	MAN	C1-O5-C5	2.03	114.94	112.19
4	Y	10	AHR	C1-C2-C3	2.03	104.72	101.63
2	T	21	AHR	C1-C2-C3	2.02	104.71	101.63
3	U	26	AHR	C1-C2-C3	2.02	104.71	101.63
2	Q	18	AHR	C1-C2-C3	2.02	104.71	101.63
3	O	38	XYP	C1-C2-C3	2.02	112.15	109.67
2	Q	25	A1E3E	O4-C1-C2	-2.02	102.08	105.99
4	M	13	NAG	C1-O5-C5	2.02	114.93	112.19
2	T	9	XYP	O2-C2-C1	2.02	113.28	109.15
4	P	8	NAG	C1-O5-C5	2.02	114.92	112.19
2	Q	9	XYP	O2-C2-C1	2.02	113.28	109.15
3	I	26	AHR	C1-C2-C3	2.02	104.70	101.63
3	B	3	MAN	C1-O5-C5	2.02	114.92	112.19
3	O	3	MAN	C1-O5-C5	2.02	114.92	112.19
3	R	38	XYP	C1-C2-C3	2.02	112.14	109.67
3	O	18	MAN	C1-O5-C5	2.01	114.92	112.19
3	a	25	MAN	C1-O5-C5	2.01	114.92	112.19
4	b	10	AHR	C1-C2-C3	2.01	104.70	101.63
3	F	3	MAN	C1-O5-C5	2.01	114.92	112.19
3	O	26	AHR	C1-C2-C3	2.01	104.69	101.63
4	Y	18	AHR	C1-C2-C3	2.01	104.69	101.63
3	U	3	MAN	C1-O5-C5	2.01	114.91	112.19
3	R	40	BMA	C1-O5-C5	2.01	114.91	112.19
4	P	10	AHR	C1-C2-C3	2.01	104.69	101.63
3	X	3	MAN	C1-O5-C5	2.01	114.91	112.19
3	R	3	MAN	C1-O5-C5	2.01	114.91	112.19
4	V	13	NAG	C1-O5-C5	2.01	114.91	112.19
3	X	26	AHR	C1-C2-C3	2.01	104.68	101.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	18	MAN	C1-O5-C5	2.00	114.91	112.19
3	X	18	MAN	C1-O5-C5	2.00	114.91	112.19
3	L	11	XYP	C1-C2-C3	2.00	112.13	109.67
4	S	18	AHR	C1-C2-C3	2.00	104.68	101.63
2	Q	10	BMA	O5-C5-C6	2.00	110.34	107.20
3	U	18	MAN	C1-O5-C5	2.00	114.90	112.19
2	N	9	XYP	O2-C2-C1	2.00	113.25	109.15

There are no chirality outliers.

All (190) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	11	NAG	C8-C7-N2-C2
2	C	11	NAG	O7-C7-N2-C2
2	C	22	NAG	C3-C2-N2-C7
2	C	22	NAG	C8-C7-N2-C2
2	C	22	NAG	O7-C7-N2-C2
2	C	25	A1E3E	C3-C4-C5-C6
2	C	25	A1E3E	C3-C4-C5-O5
2	C	25	A1E3E	O4-C4-C5-C6
2	C	25	A1E3E	O4-C4-C5-O5
2	E	11	NAG	C8-C7-N2-C2
2	E	11	NAG	O7-C7-N2-C2
2	E	22	NAG	C3-C2-N2-C7
2	E	22	NAG	C8-C7-N2-C2
2	E	22	NAG	O7-C7-N2-C2
2	E	25	A1E3E	C3-C4-C5-C6
2	E	25	A1E3E	C3-C4-C5-O5
2	E	25	A1E3E	O4-C4-C5-C6
2	E	25	A1E3E	C4-C5-C6-O6
2	E	25	A1E3E	O5-C5-C6-O6
2	H	11	NAG	C8-C7-N2-C2
2	H	11	NAG	O7-C7-N2-C2
2	H	22	NAG	C8-C7-N2-C2
2	H	22	NAG	O7-C7-N2-C2
2	K	11	NAG	C8-C7-N2-C2
2	K	11	NAG	O7-C7-N2-C2
2	K	22	NAG	C8-C7-N2-C2
2	K	22	NAG	O7-C7-N2-C2
2	K	25	A1E3E	O4-C4-C5-C6
2	K	25	A1E3E	C4-C5-C6-O6
2	K	25	A1E3E	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	N	11	NAG	C8-C7-N2-C2
2	N	11	NAG	O7-C7-N2-C2
2	N	22	NAG	C8-C7-N2-C2
2	N	22	NAG	O7-C7-N2-C2
2	N	25	A1E3E	C3-C4-C5-C6
2	N	25	A1E3E	C3-C4-C5-O5
2	N	25	A1E3E	O4-C4-C5-C6
2	N	25	A1E3E	O4-C4-C5-O5
2	N	25	A1E3E	O5-C5-C6-O6
2	Q	11	NAG	C8-C7-N2-C2
2	Q	11	NAG	O7-C7-N2-C2
2	Q	22	NAG	C8-C7-N2-C2
2	Q	22	NAG	O7-C7-N2-C2
2	Q	25	A1E3E	C3-C4-C5-C6
2	Q	25	A1E3E	C3-C4-C5-O5
2	Q	25	A1E3E	O4-C4-C5-C6
2	Q	25	A1E3E	O5-C5-C6-O6
2	T	11	NAG	C8-C7-N2-C2
2	T	11	NAG	O7-C7-N2-C2
2	T	22	NAG	C8-C7-N2-C2
2	T	22	NAG	O7-C7-N2-C2
2	T	25	A1E3E	C4-C5-C6-O6
2	T	25	A1E3E	O5-C5-C6-O6
2	W	11	NAG	C8-C7-N2-C2
2	W	11	NAG	O7-C7-N2-C2
2	W	22	NAG	C8-C7-N2-C2
2	W	22	NAG	O7-C7-N2-C2
2	W	25	A1E3E	C3-C4-C5-C6
2	W	25	A1E3E	C3-C4-C5-O5
2	W	25	A1E3E	O4-C4-C5-C6
2	W	25	A1E3E	C4-C5-C6-O6
2	W	25	A1E3E	O5-C5-C6-O6
2	Z	11	NAG	C8-C7-N2-C2
2	Z	11	NAG	O7-C7-N2-C2
2	Z	22	NAG	C8-C7-N2-C2
2	Z	22	NAG	O7-C7-N2-C2
2	Z	25	A1E3E	O4-C4-C5-C6
2	Z	25	A1E3E	O5-C5-C6-O6
3	B	17	A1E3E	C3-C4-C5-C6
3	B	17	A1E3E	C3-C4-C5-O5
3	B	17	A1E3E	O4-C4-C5-C6
3	F	17	A1E3E	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	F	17	A1E3E	C3-C4-C5-O5
3	F	17	A1E3E	O4-C4-C5-C6
3	F	33	A1E3E	O5-C5-C6-O6
3	I	17	A1E3E	C3-C4-C5-C6
3	I	17	A1E3E	C3-C4-C5-O5
3	I	17	A1E3E	O4-C4-C5-C6
3	I	17	A1E3E	O4-C4-C5-O5
3	I	33	A1E3E	C4-C5-C6-O6
3	L	17	A1E3E	C3-C4-C5-C6
3	L	17	A1E3E	C3-C4-C5-O5
3	L	17	A1E3E	O4-C4-C5-C6
3	L	17	A1E3E	O4-C4-C5-O5
3	L	33	A1E3E	C4-C5-C6-O6
3	O	17	A1E3E	C3-C4-C5-C6
3	O	17	A1E3E	C3-C4-C5-O5
3	O	17	A1E3E	O4-C4-C5-C6
3	R	17	A1E3E	O4-C4-C5-C6
3	R	33	A1E3E	C4-C5-C6-O6
3	U	17	A1E3E	O4-C4-C5-C6
3	U	33	A1E3E	O4-C4-C5-C6
3	X	17	A1E3E	O4-C4-C5-C6
3	a	17	A1E3E	C3-C4-C5-C6
3	a	17	A1E3E	C3-C4-C5-O5
3	a	17	A1E3E	O4-C4-C5-C6
3	a	33	A1E3E	C4-C5-C6-O6
2	H	22	NAG	C1-C2-N2-C7
3	I	33	A1E3E	O5-C5-C6-O6
3	L	33	A1E3E	O5-C5-C6-O6
3	R	33	A1E3E	O5-C5-C6-O6
3	a	33	A1E3E	O5-C5-C6-O6
2	N	25	A1E3E	C4-C5-C6-O6
2	Q	25	A1E3E	C4-C5-C6-O6
2	Z	25	A1E3E	C4-C5-C6-O6
3	F	33	A1E3E	C4-C5-C6-O6
4	Y	13	NAG	C8-C7-N2-C2
4	D	13	NAG	C8-C7-N2-C2
4	G	13	NAG	C8-C7-N2-C2
4	J	13	NAG	C8-C7-N2-C2
4	P	13	NAG	C8-C7-N2-C2
4	S	13	NAG	C8-C7-N2-C2
4	V	13	NAG	C8-C7-N2-C2
2	K	22	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	13	NAG	O7-C7-N2-C2
4	G	13	NAG	O7-C7-N2-C2
4	J	13	NAG	O7-C7-N2-C2
4	M	13	NAG	C8-C7-N2-C2
4	M	13	NAG	O7-C7-N2-C2
4	P	13	NAG	O7-C7-N2-C2
4	S	13	NAG	O7-C7-N2-C2
4	V	13	NAG	O7-C7-N2-C2
4	Y	13	NAG	O7-C7-N2-C2
2	Q	22	NAG	C1-C2-N2-C7
2	W	22	NAG	C1-C2-N2-C7
2	H	25	A1E3E	O5-C5-C6-O6
4	b	13	NAG	C8-C7-N2-C2
2	Z	22	NAG	C1-C2-N2-C7
2	C	22	NAG	C1-C2-N2-C7
2	N	22	NAG	C1-C2-N2-C7
2	E	25	A1E3E	O4-C4-C5-O5
2	H	25	A1E3E	O4-C4-C5-O5
2	K	25	A1E3E	O4-C4-C5-O5
2	Q	25	A1E3E	O4-C4-C5-O5
2	T	25	A1E3E	O4-C4-C5-O5
2	W	25	A1E3E	O4-C4-C5-O5
2	Z	25	A1E3E	O4-C4-C5-O5
3	B	17	A1E3E	O4-C4-C5-O5
3	F	17	A1E3E	O4-C4-C5-O5
3	O	17	A1E3E	O4-C4-C5-O5
3	O	33	A1E3E	O4-C4-C5-O5
3	R	17	A1E3E	O4-C4-C5-O5
3	U	17	A1E3E	O4-C4-C5-O5
3	X	17	A1E3E	O4-C4-C5-O5
3	a	17	A1E3E	O4-C4-C5-O5
3	R	17	A1E3E	C3-C4-C5-O5
4	b	13	NAG	O7-C7-N2-C2
2	E	22	NAG	C1-C2-N2-C7
3	I	23	BGC	O5-C5-C6-O6
3	B	23	BGC	O5-C5-C6-O6
3	L	23	BGC	O5-C5-C6-O6
3	R	23	BGC	O5-C5-C6-O6
3	U	23	BGC	O5-C5-C6-O6
3	X	23	BGC	O5-C5-C6-O6
3	a	23	BGC	O5-C5-C6-O6
3	F	23	BGC	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	O	23	BGC	O5-C5-C6-O6
2	Z	25	A1E3E	C3-C4-C5-C6
3	R	17	A1E3E	C3-C4-C5-C6
2	H	25	A1E3E	O4-C4-C5-C6
2	N	12	MAN	O5-C5-C6-O6
2	Q	12	MAN	O5-C5-C6-O6
2	C	12	MAN	O5-C5-C6-O6
2	E	12	MAN	O5-C5-C6-O6
2	H	12	MAN	O5-C5-C6-O6
2	K	12	MAN	O5-C5-C6-O6
2	T	12	MAN	O5-C5-C6-O6
2	W	12	MAN	O5-C5-C6-O6
2	Z	12	MAN	O5-C5-C6-O6
2	H	22	NAG	C3-C2-N2-C7
2	K	22	NAG	C3-C2-N2-C7
3	U	33	A1E3E	O4-C4-C5-O5
2	Z	25	A1E3E	C3-C4-C5-O5
3	X	33	A1E3E	O5-C5-C6-O6
2	T	22	NAG	C1-C2-N2-C7
3	X	17	A1E3E	C3-C4-C5-C6
2	H	25	A1E3E	C4-C5-C6-O6
3	X	33	A1E3E	C4-C5-C6-O6
3	U	17	A1E3E	C3-C4-C5-C6
3	X	17	A1E3E	C3-C4-C5-O5
3	U	17	A1E3E	O5-C5-C6-O6
4	M	8	NAG	C8-C7-N2-C2
2	N	22	NAG	C3-C2-N2-C7
2	Q	22	NAG	C3-C2-N2-C7
2	T	22	NAG	C3-C2-N2-C7
2	W	22	NAG	C3-C2-N2-C7
2	Z	22	NAG	C3-C2-N2-C7
2	K	25	A1E3E	C3-C4-C5-C6
3	O	33	A1E3E	O4-C4-C5-C6
4	M	8	NAG	O7-C7-N2-C2

There are no ring outliers.

65 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	20	AHR	1	0
2	C	15	BGC	1	0
3	R	42	FUB	1	0

Continued on next page...

Continued from previous page...

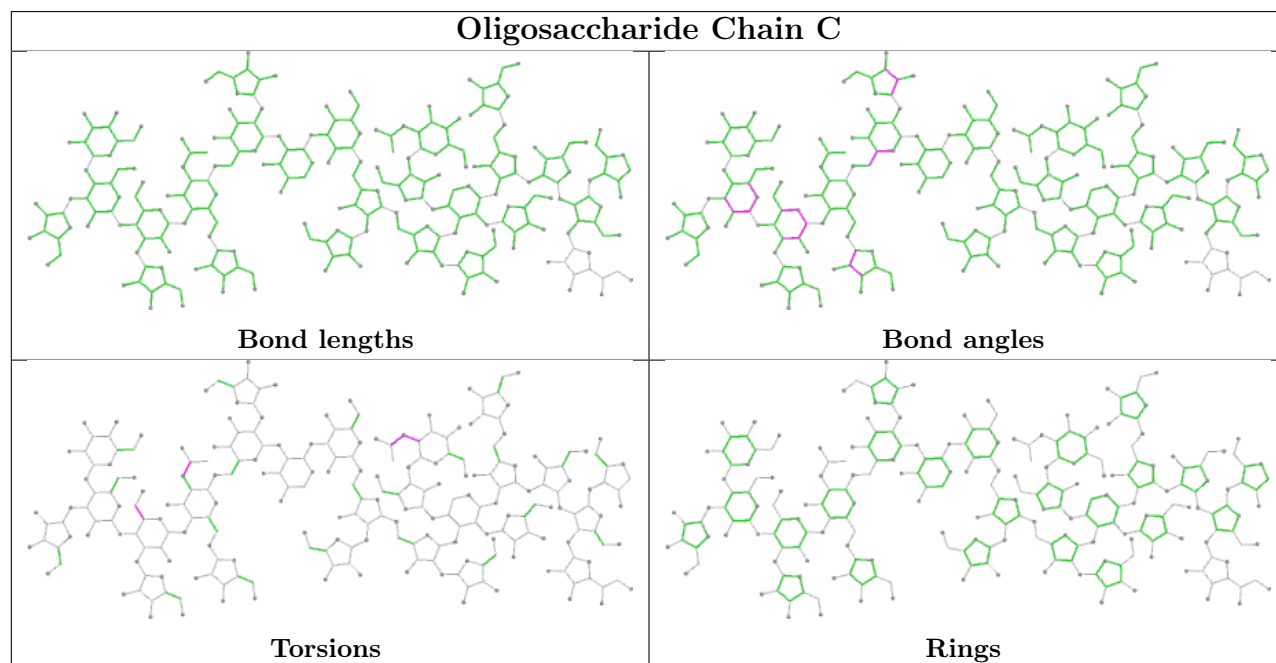
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	41	AHR	1	0
2	K	13	MAN	1	0
2	W	12	MAN	1	0
3	O	41	AHR	1	0
3	I	20	AHR	1	0
2	H	10	BMA	1	0
2	K	12	MAN	1	0
3	L	13	AHR	1	0
2	H	2	FUB	1	0
4	Y	6	BGC	1	0
3	B	20	AHR	1	0
4	J	7	MAN	1	0
3	B	42	FUB	1	0
2	T	22	NAG	1	0
3	O	42	FUB	2	0
4	b	6	BGC	1	0
3	B	22	AHR	1	0
3	F	20	AHR	1	0
3	L	22	AHR	2	0
3	U	41	AHR	1	0
4	M	7	MAN	1	0
2	W	13	MAN	1	0
3	I	41	AHR	1	0
3	I	13	AHR	1	0
2	E	12	MAN	1	0
2	N	12	MAN	1	0
2	K	15	BGC	1	0
3	F	42	FUB	1	0
2	E	13	MAN	1	0
4	V	11	AHR	1	0
3	U	20	AHR	1	0
3	L	41	AHR	1	0
3	X	41	AHR	1	0
3	F	22	AHR	1	0
3	U	22	AHR	1	0
3	L	42	FUB	1	0
2	E	15	BGC	1	0
4	V	6	BGC	1	0
3	I	42	FUB	1	0
2	Q	13	MAN	1	0
3	R	13	AHR	1	0
2	C	13	MAN	1	0

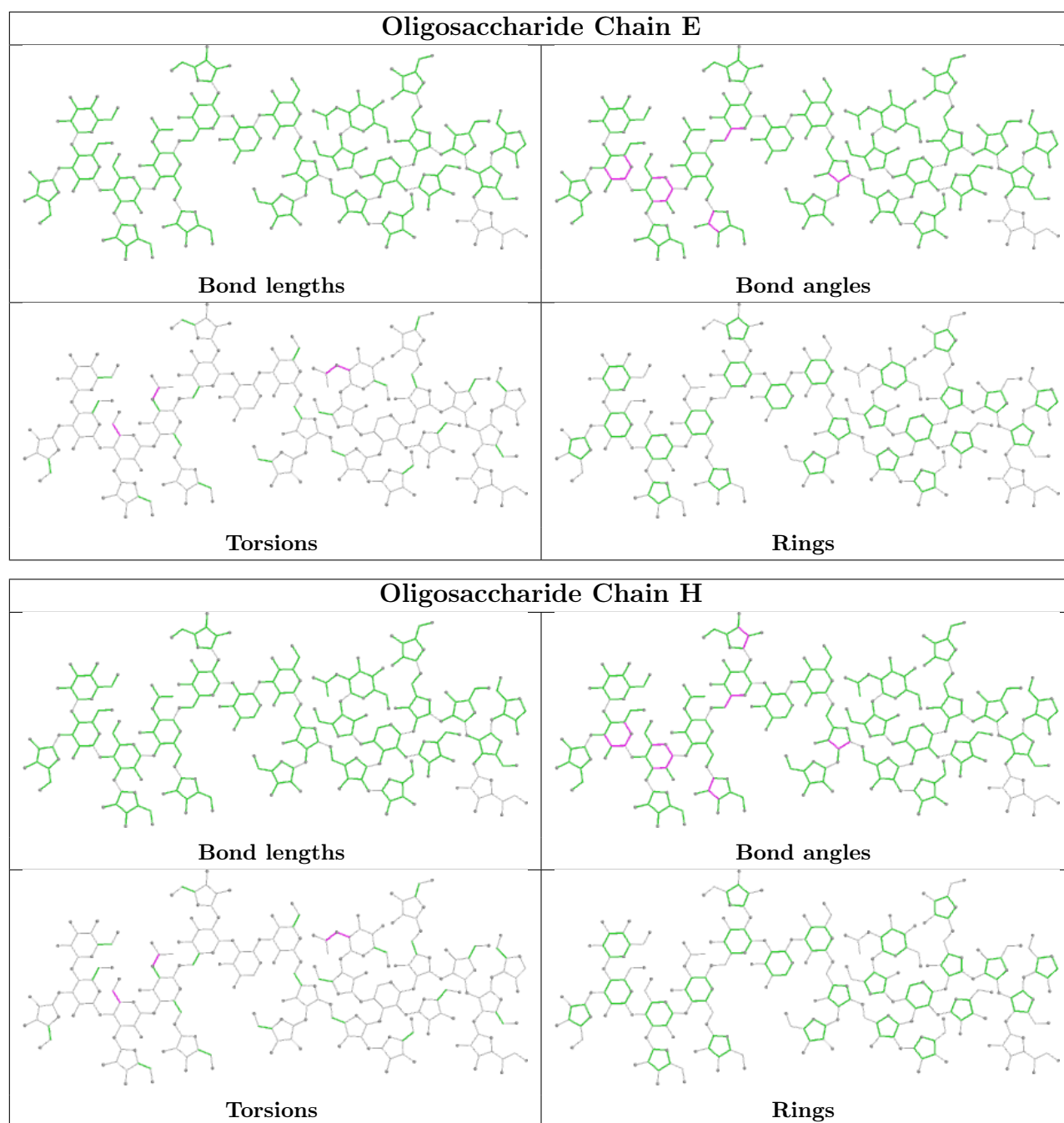
Continued on next page...

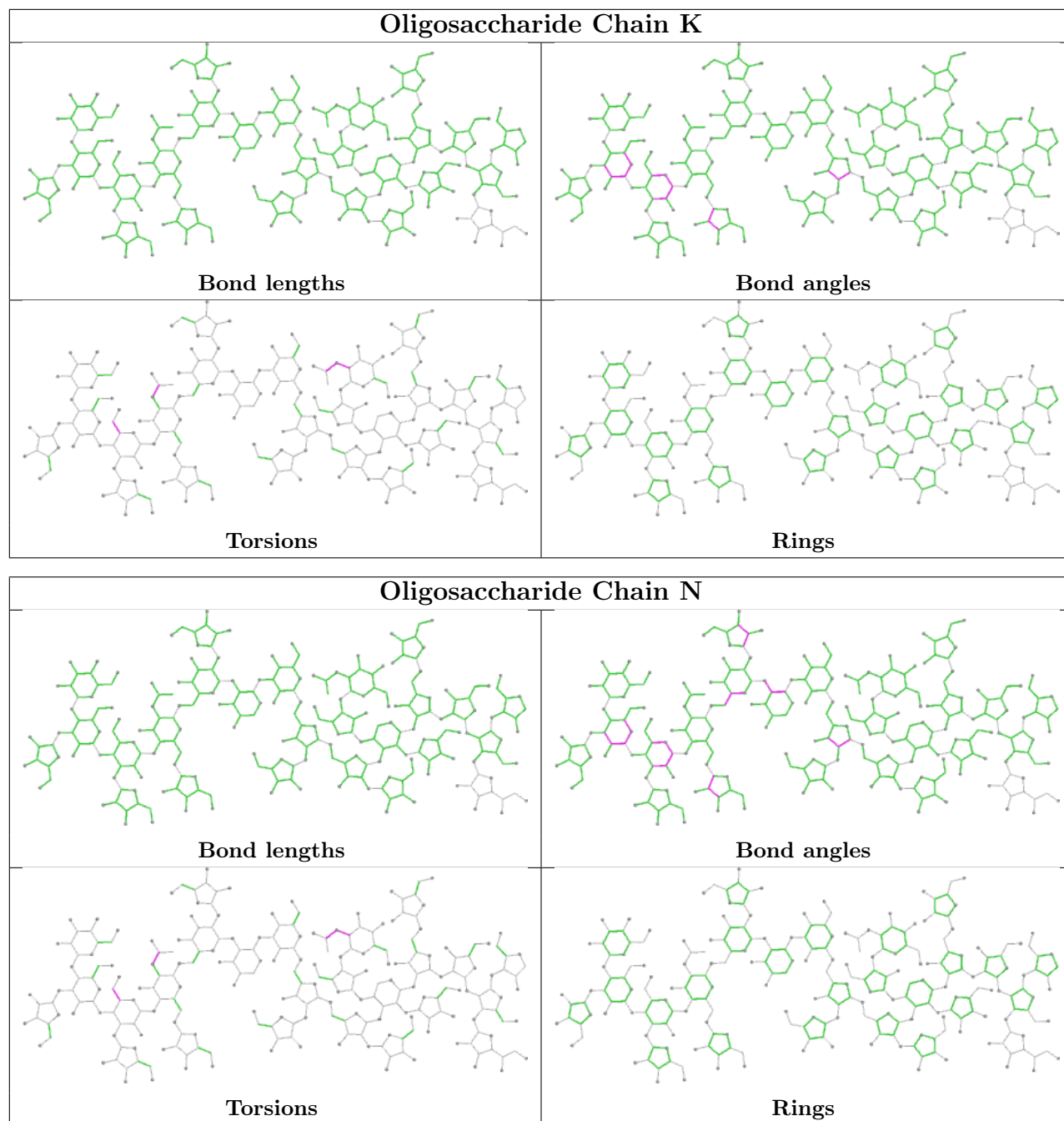
Continued from previous page...

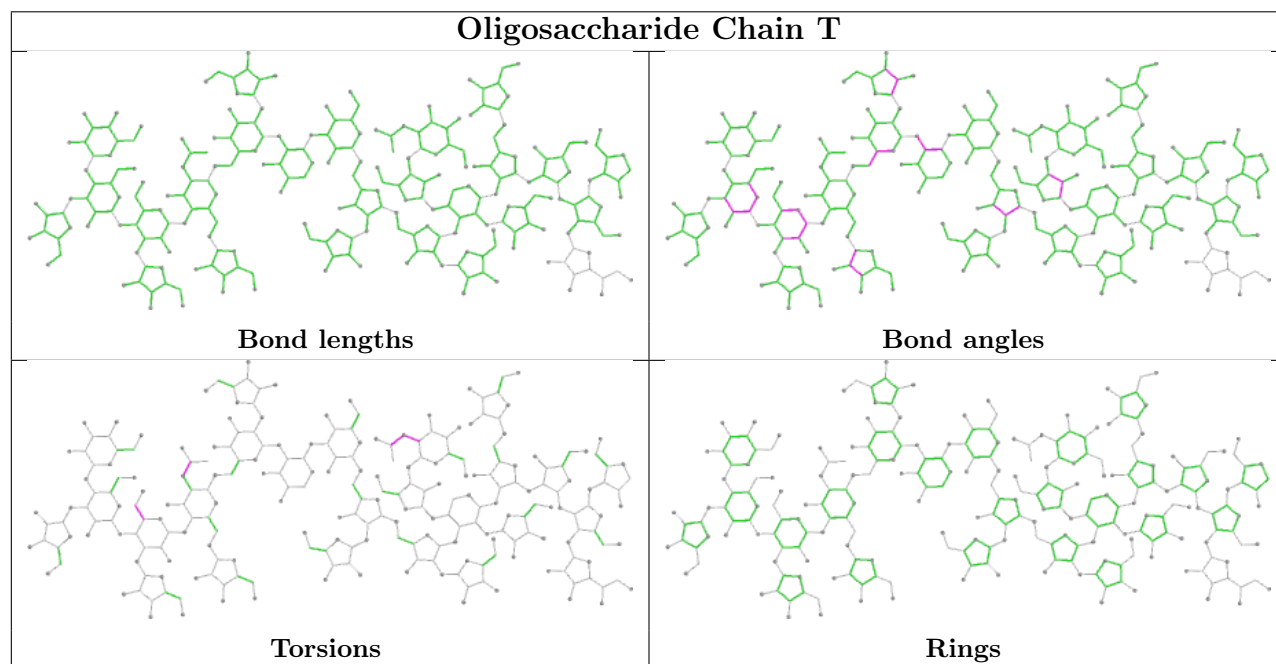
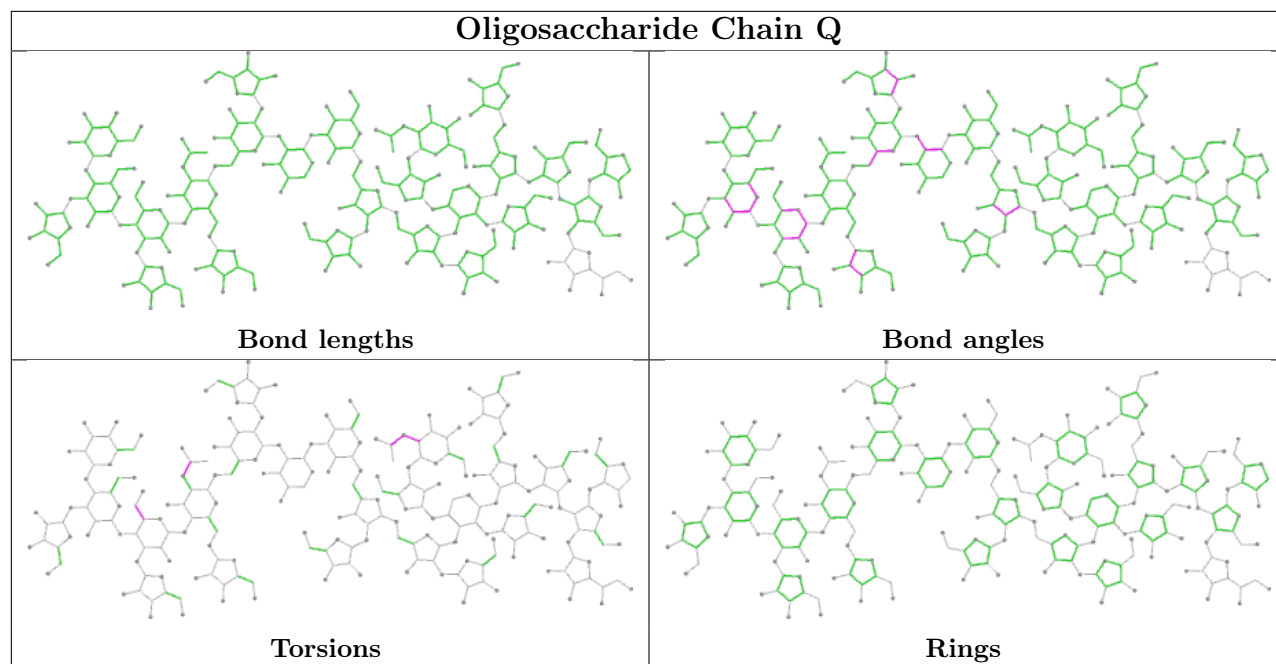
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	12	MAN	1	0
3	O	22	AHR	1	0
3	U	42	FUB	1	0
3	I	22	AHR	1	0
3	B	41	AHR	1	0
4	V	7	MAN	1	0
3	L	29	XYP	1	0
2	C	12	MAN	1	0
4	b	7	MAN	1	0
4	J	6	BGC	1	0
3	a	41	AHR	1	0
4	M	6	BGC	1	0
3	R	20	AHR	1	0
3	L	20	AHR	1	0
3	a	42	FUB	1	0
3	R	22	AHR	1	0
3	X	42	FUB	1	0
2	N	13	MAN	1	0
4	Y	7	MAN	1	0
3	R	41	AHR	1	0

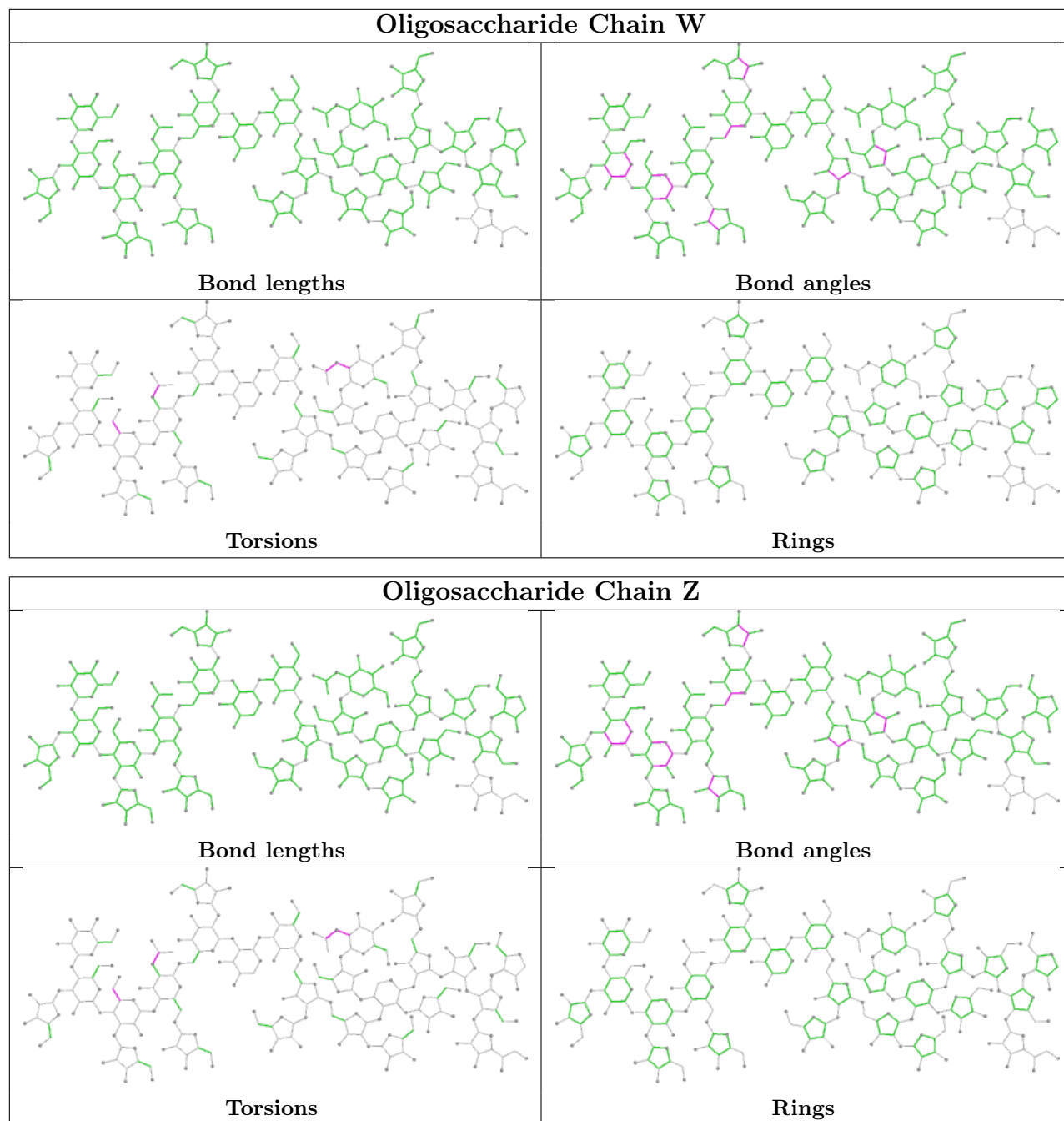
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

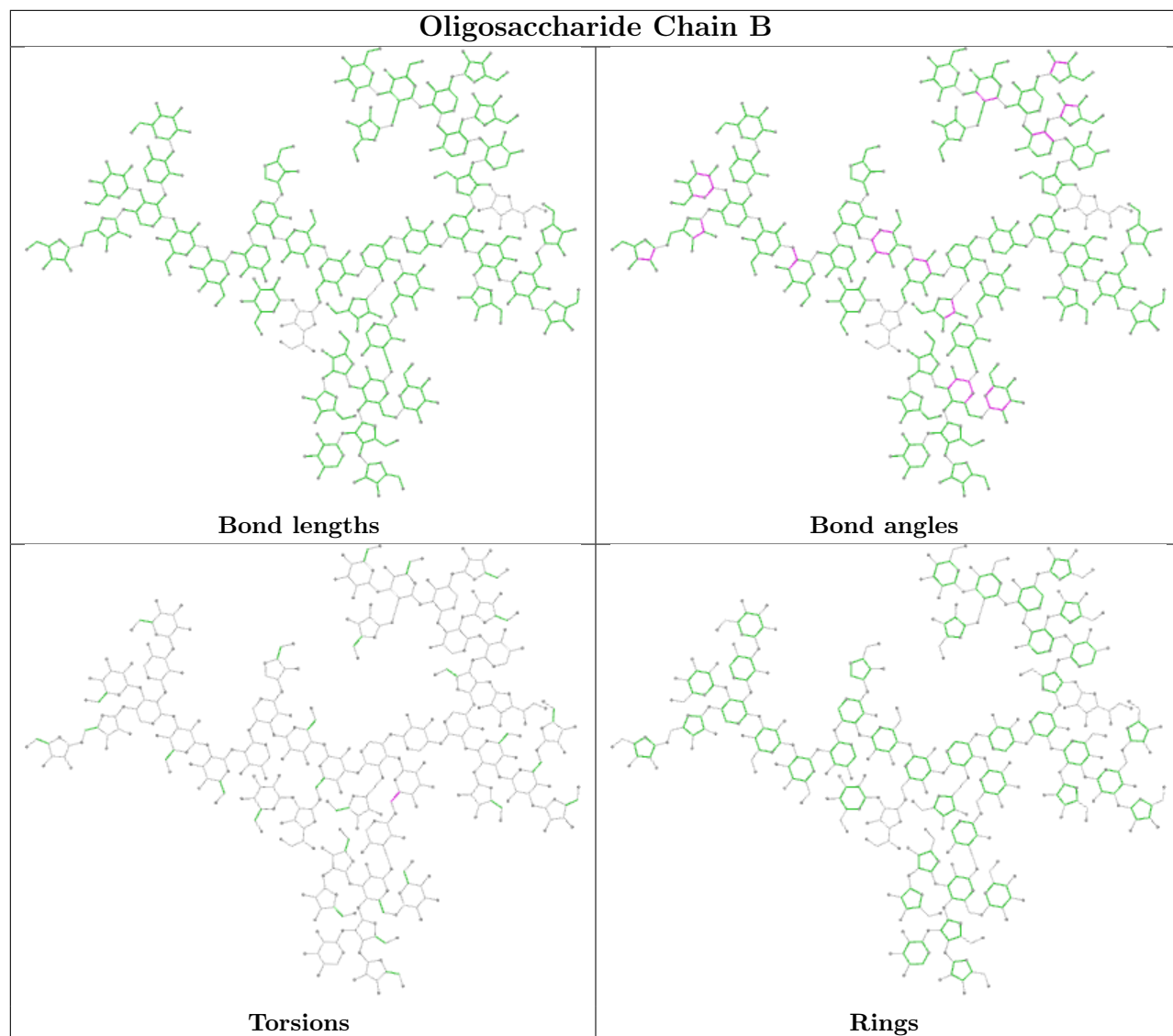


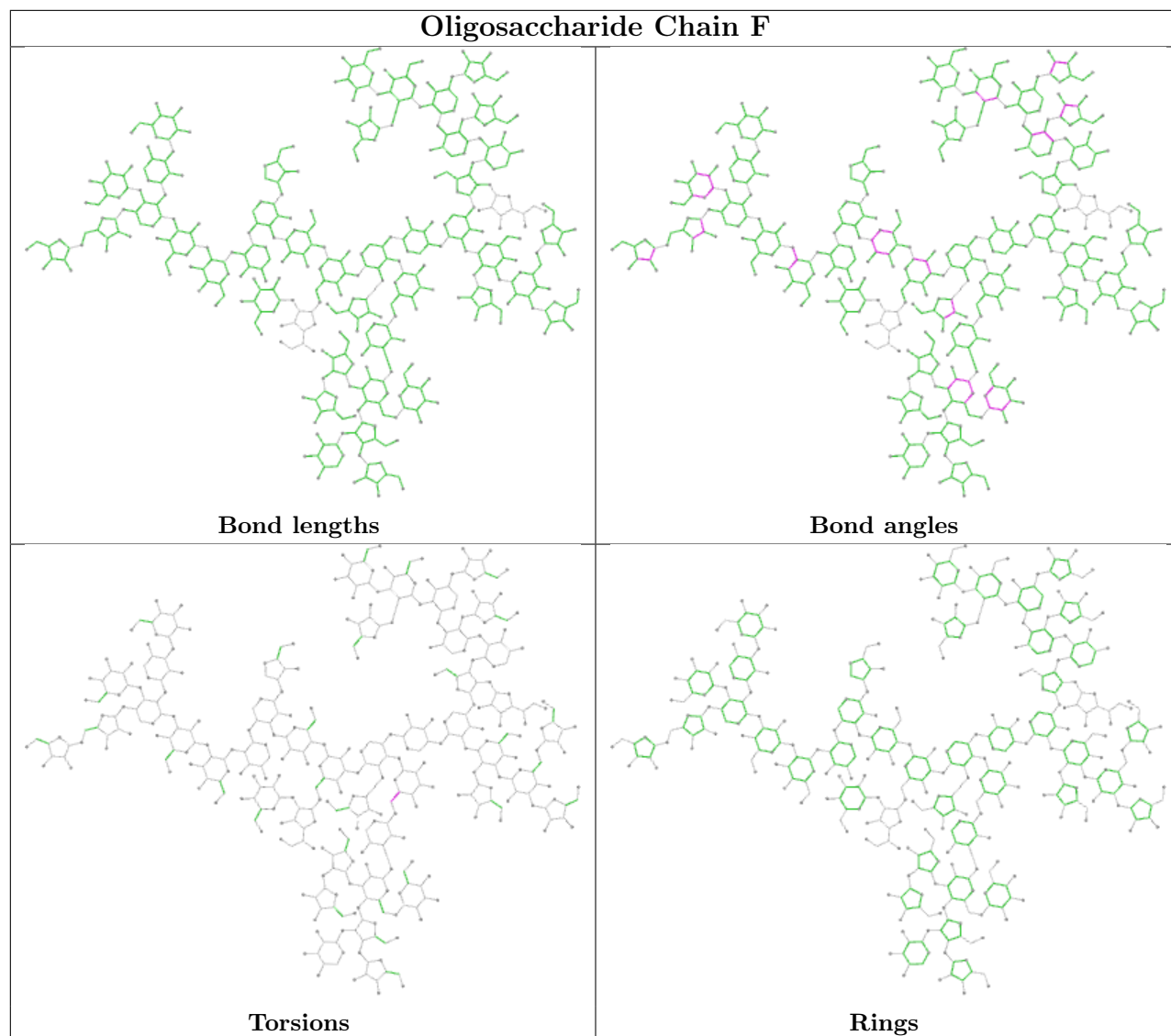


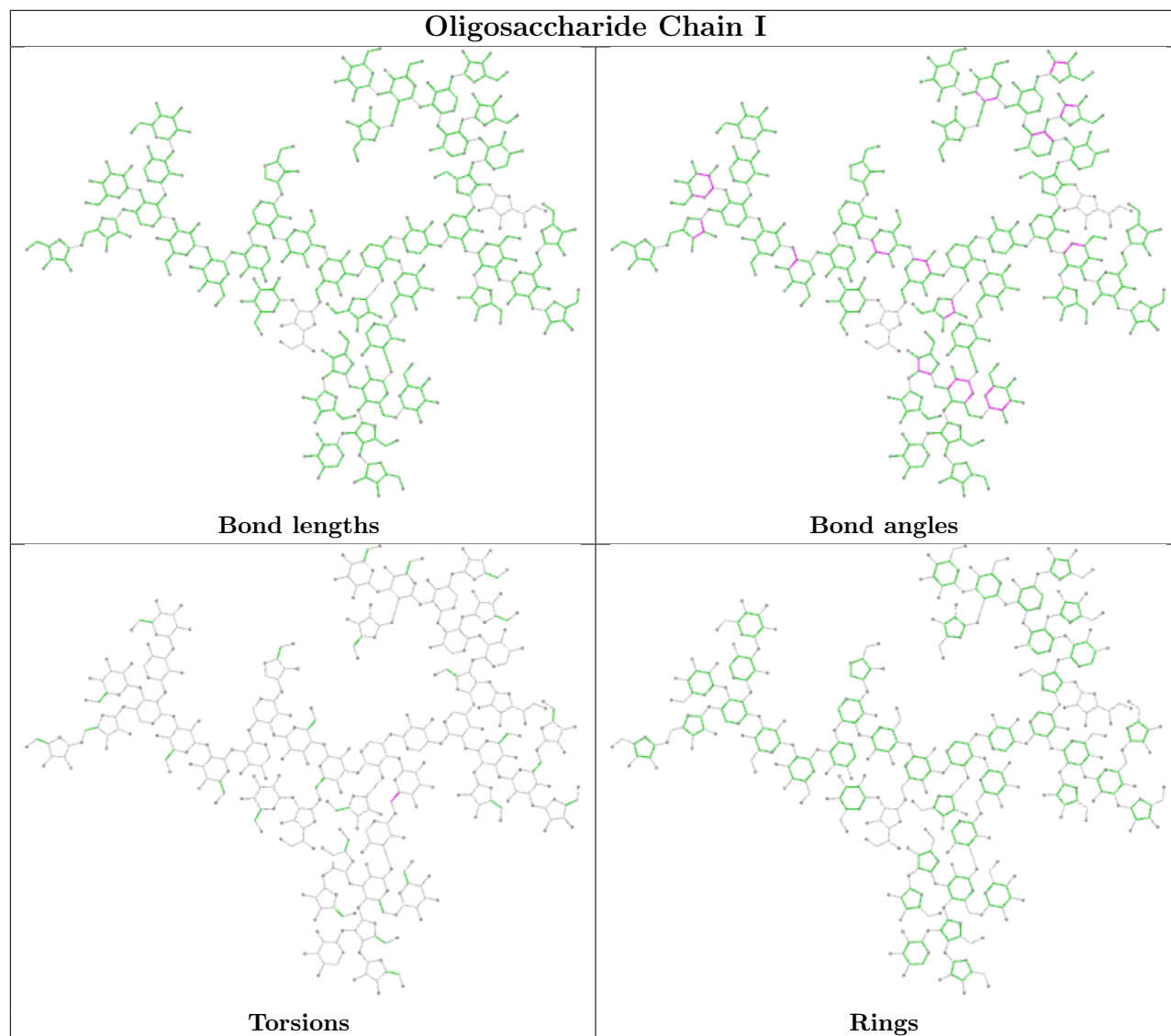


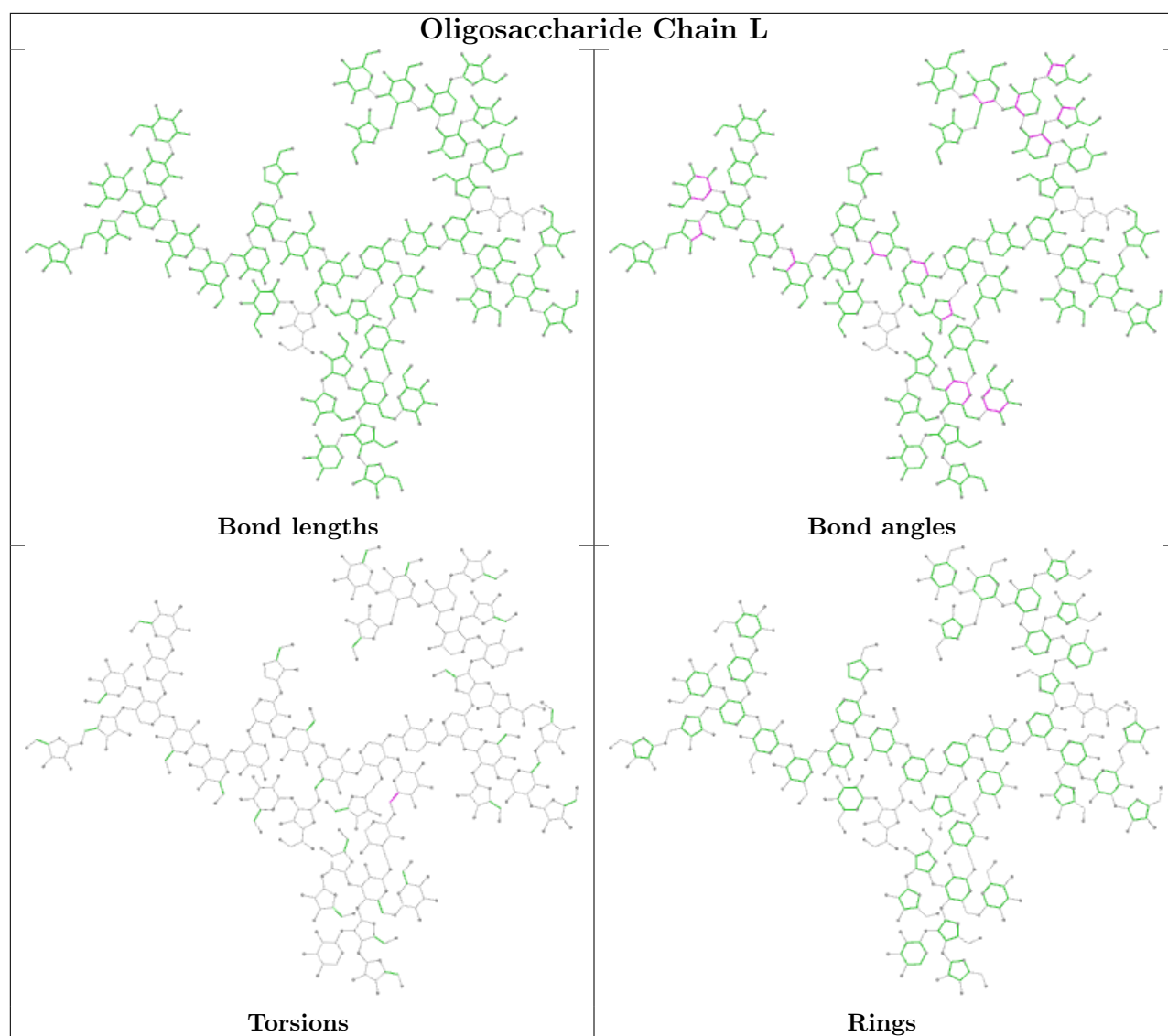


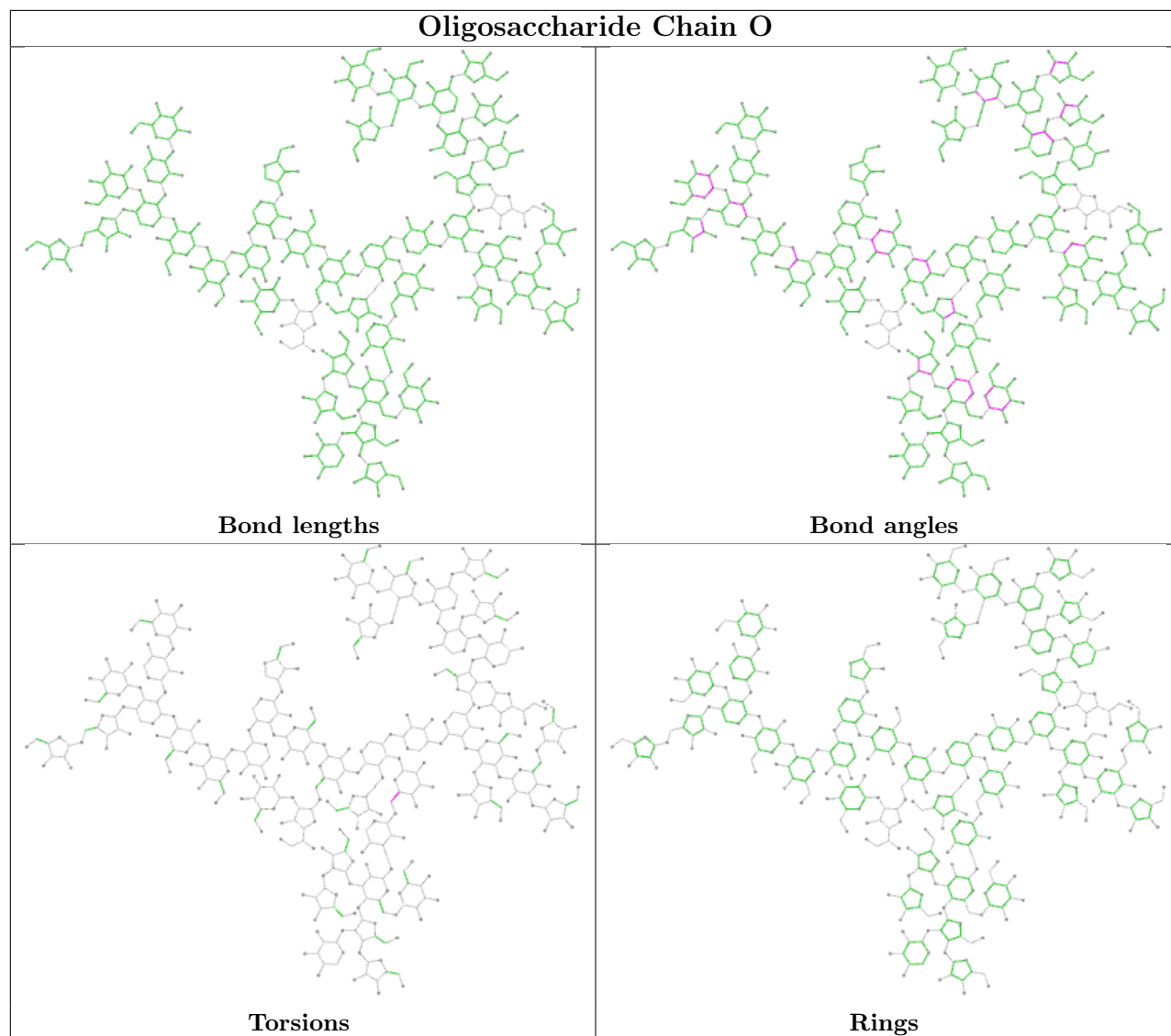


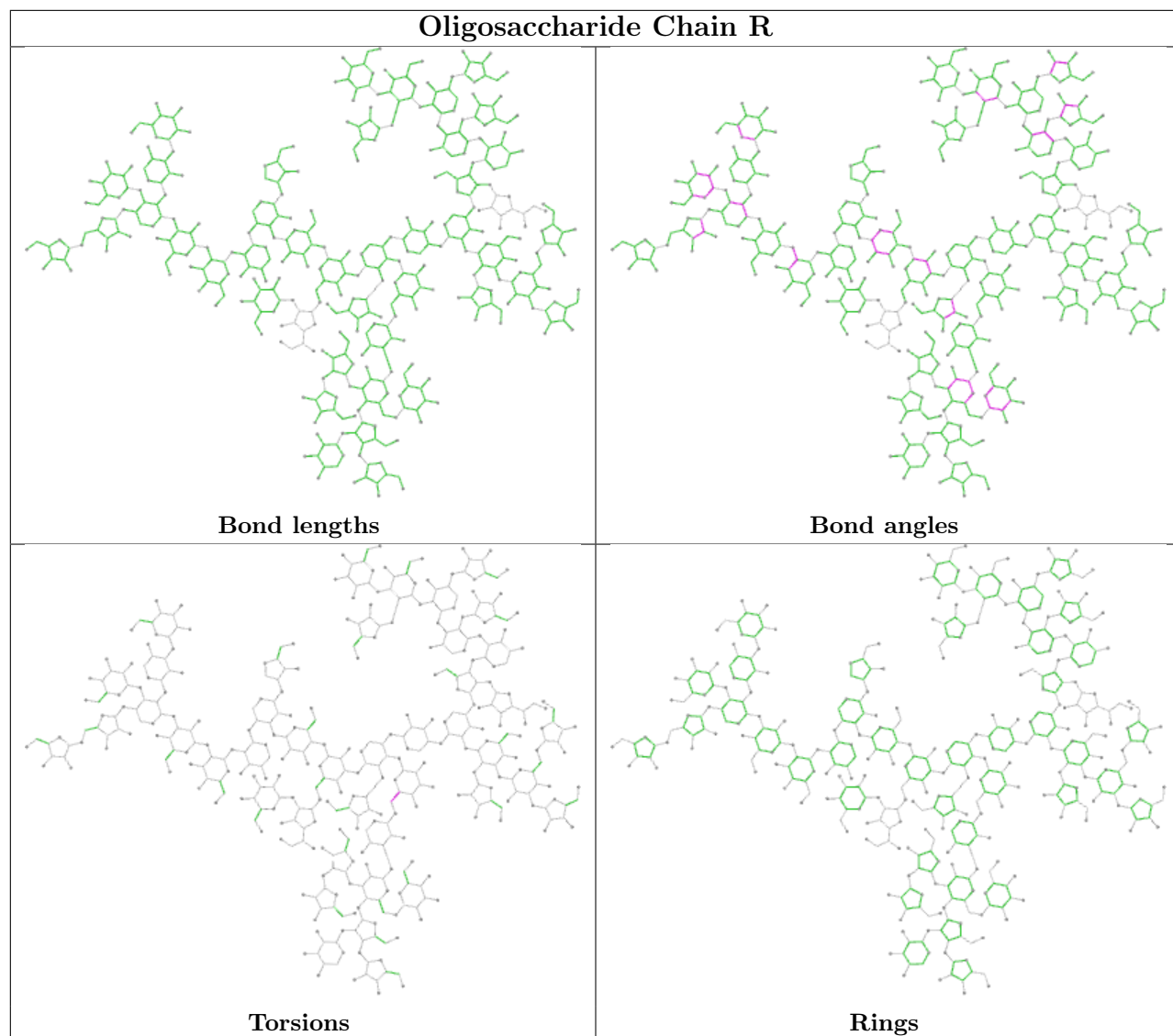


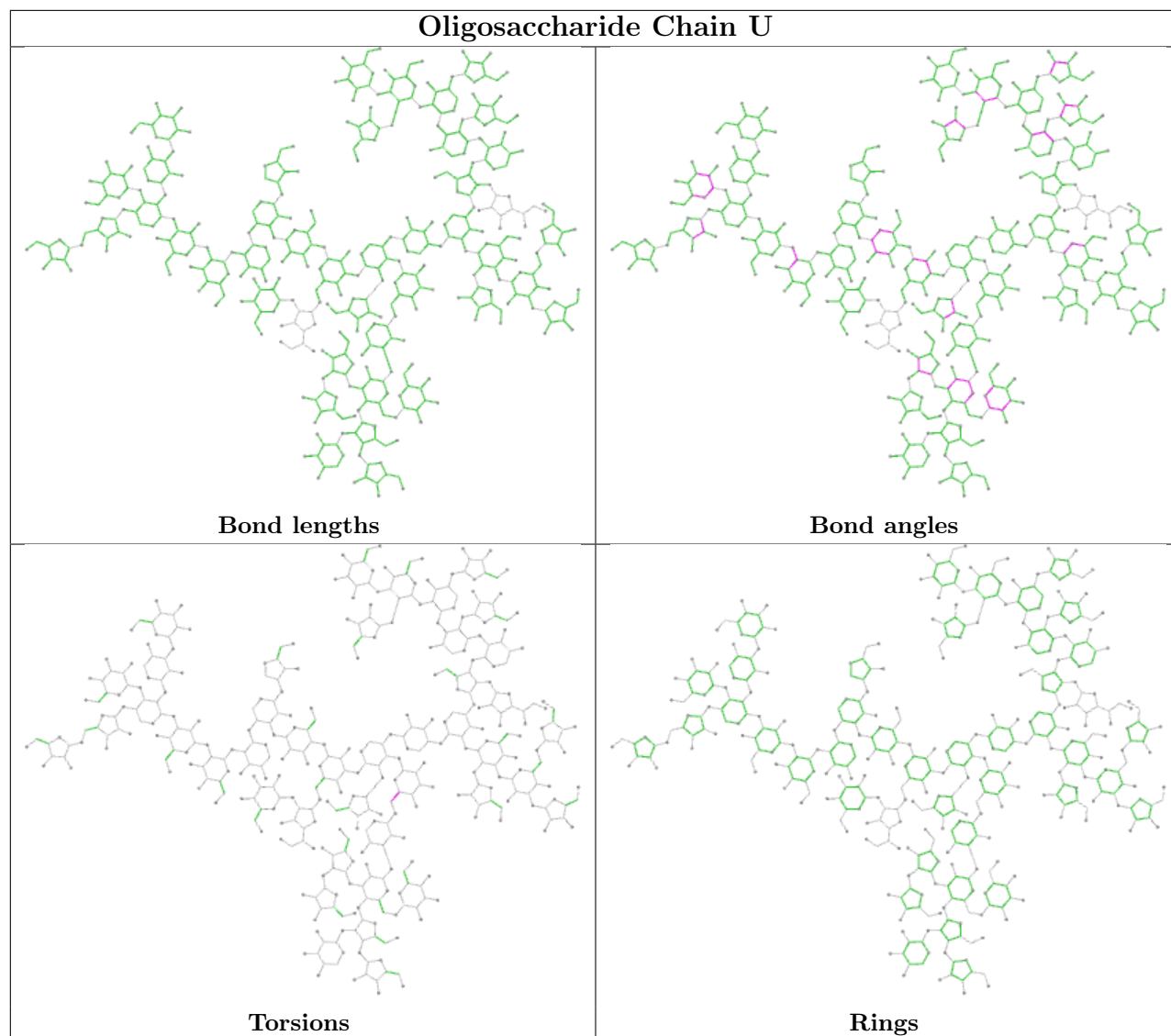


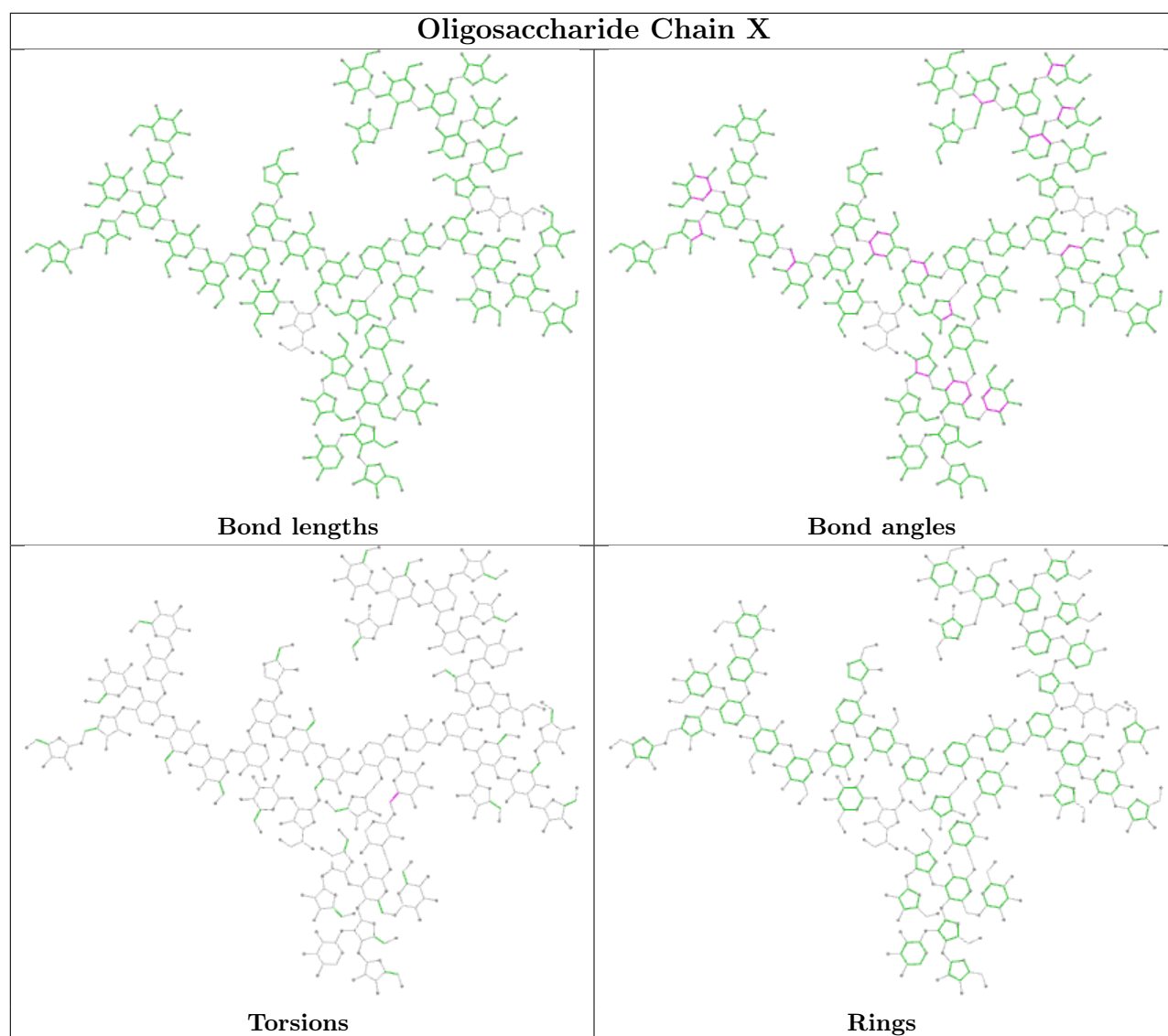


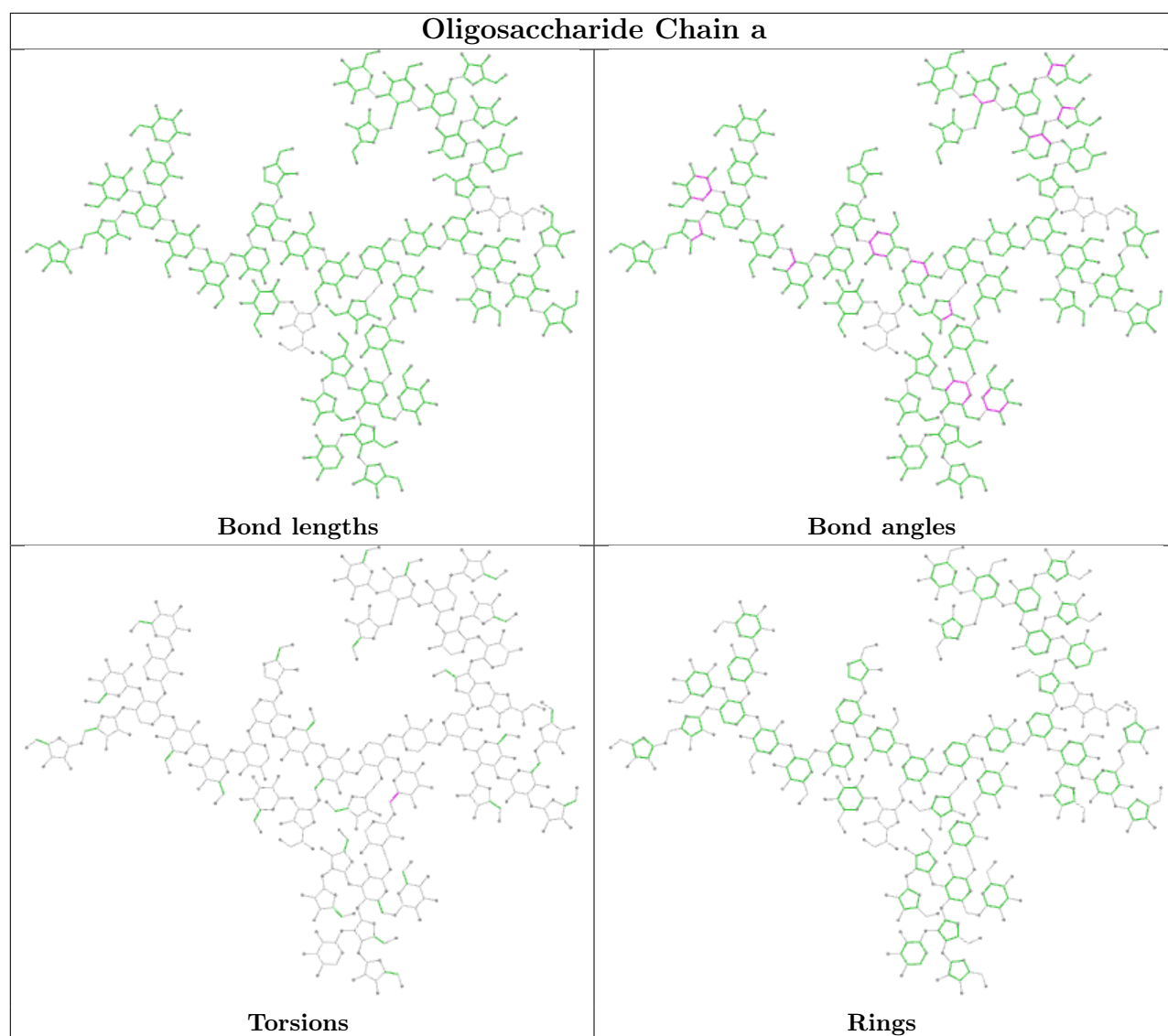


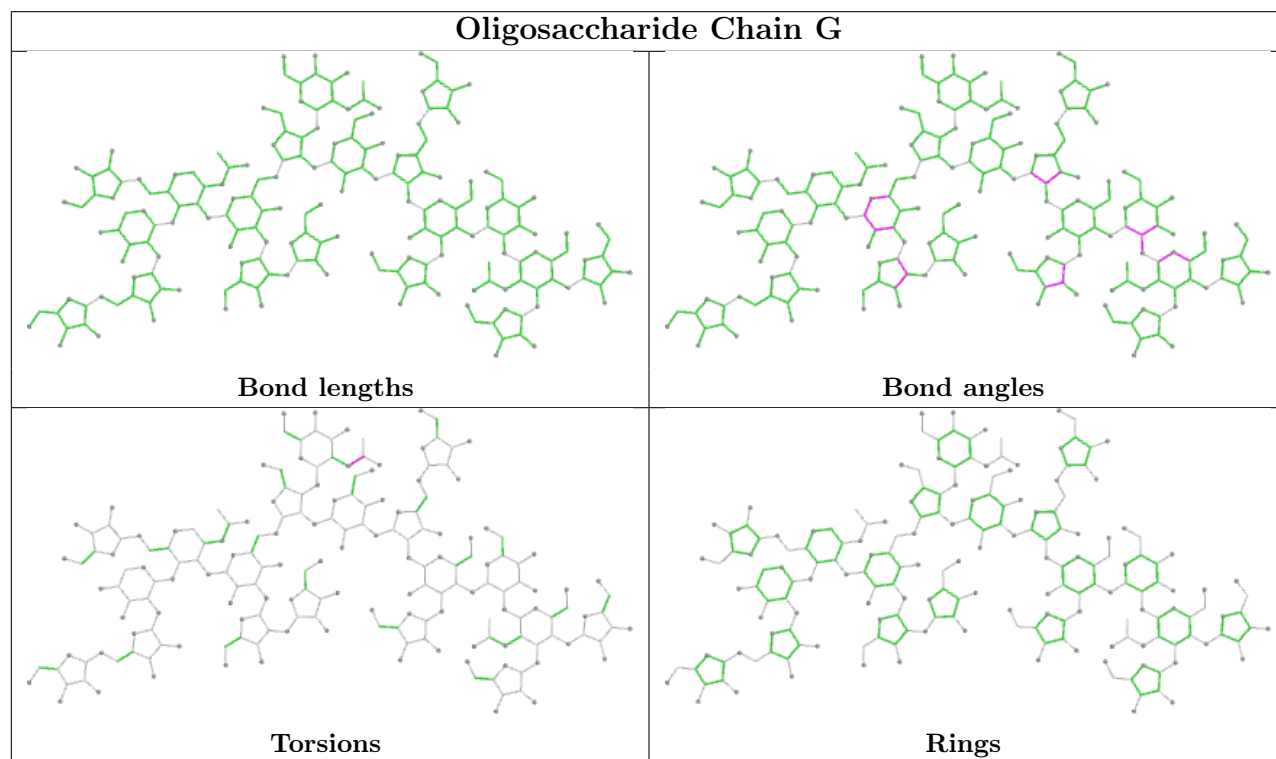
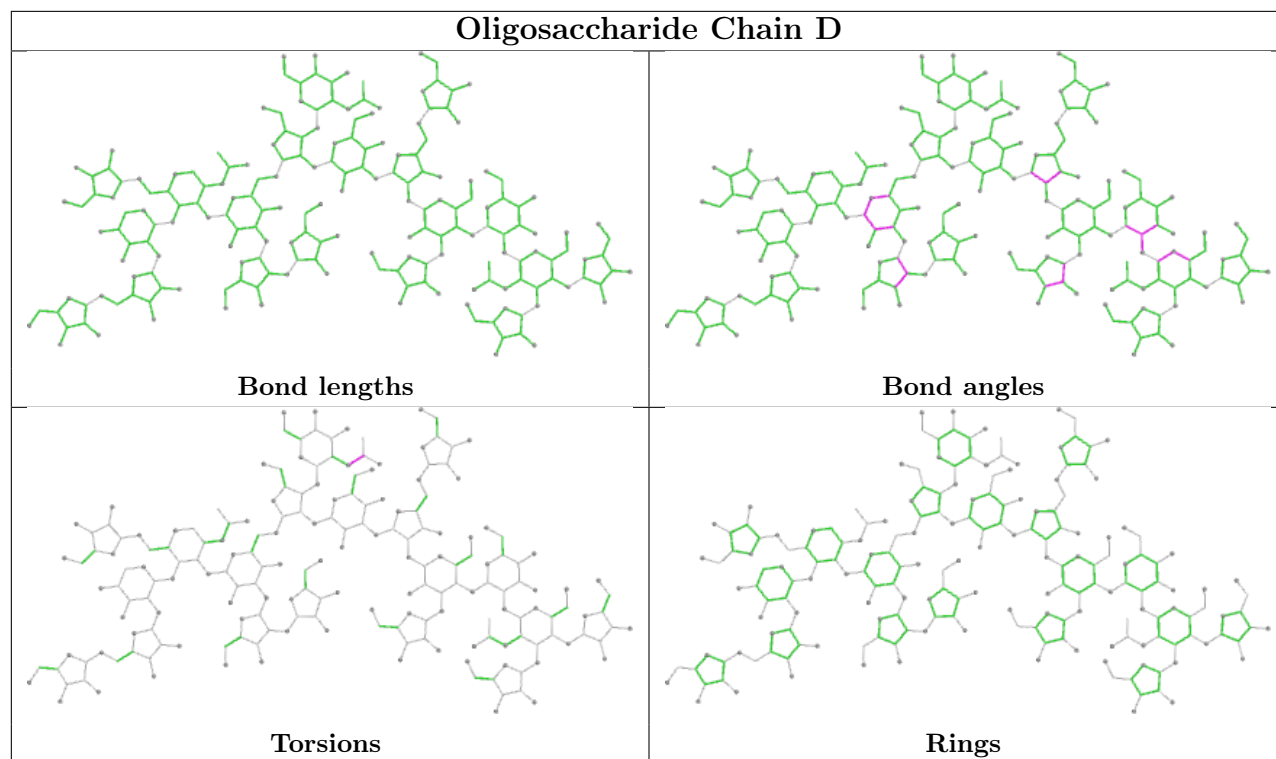


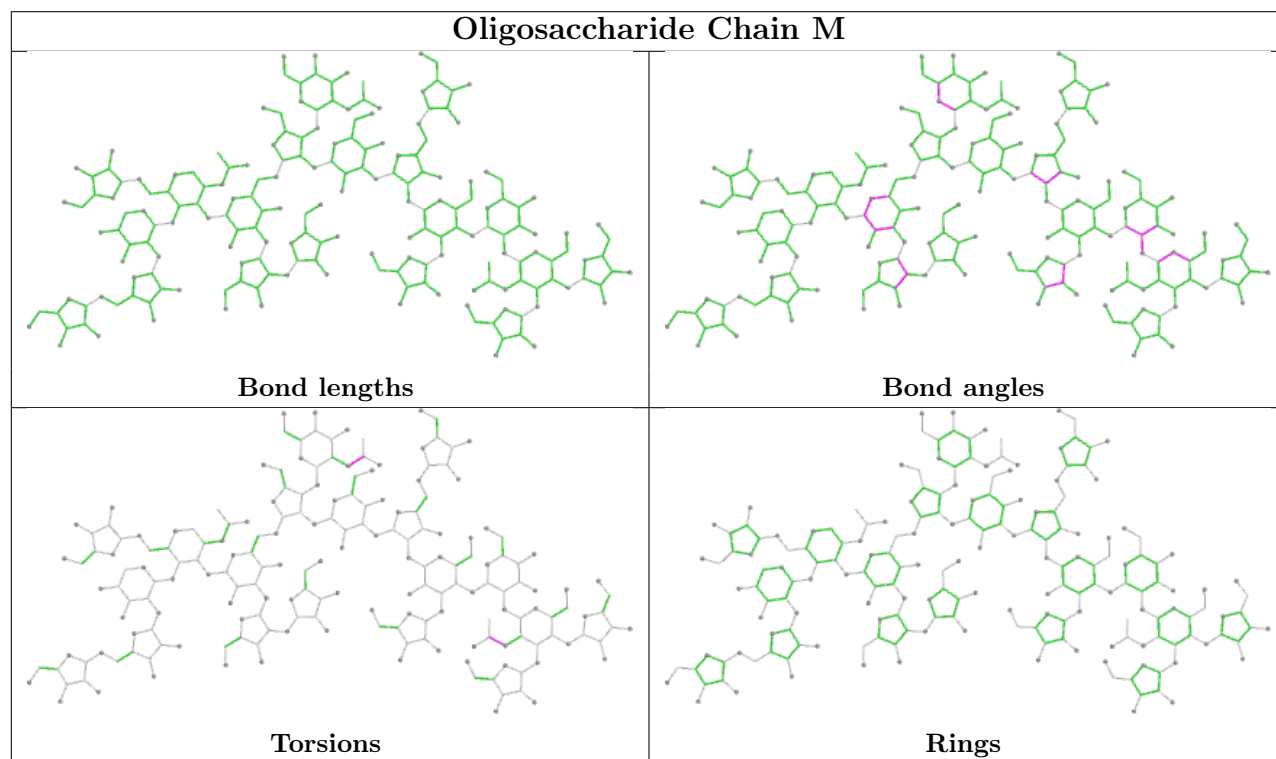
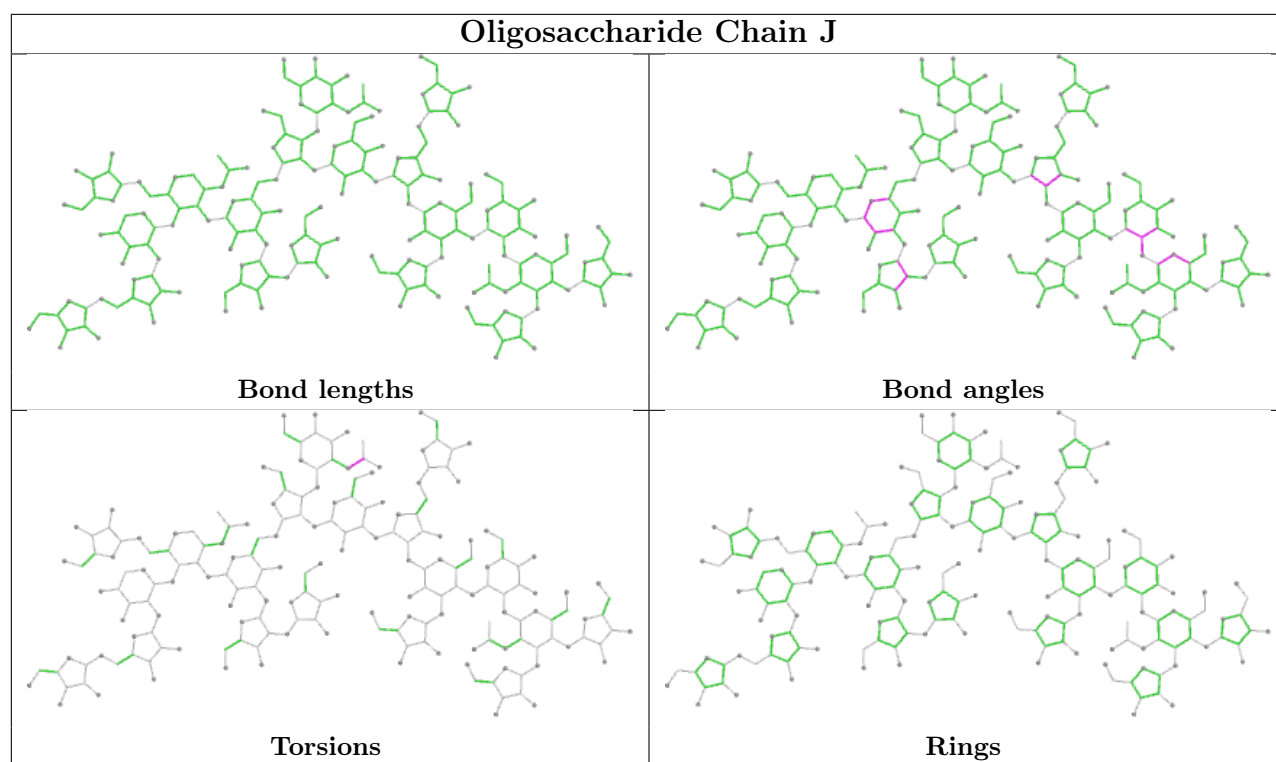


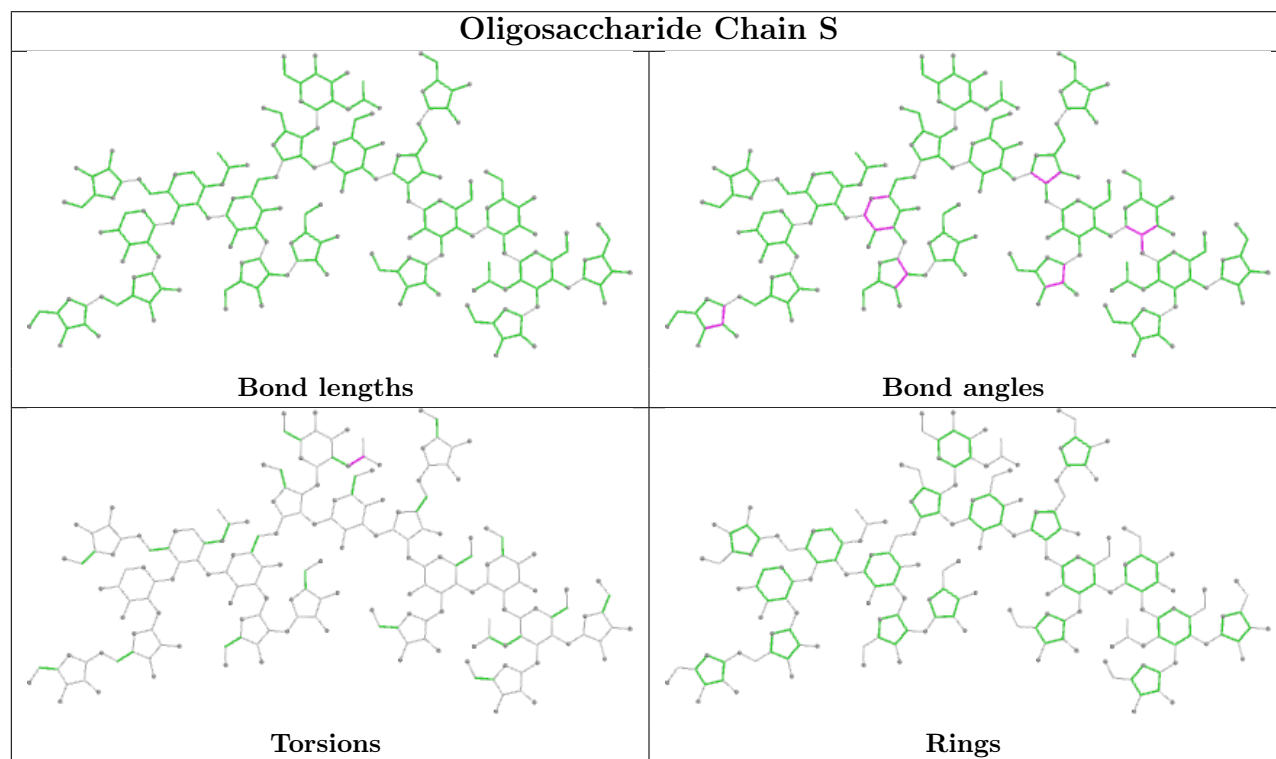
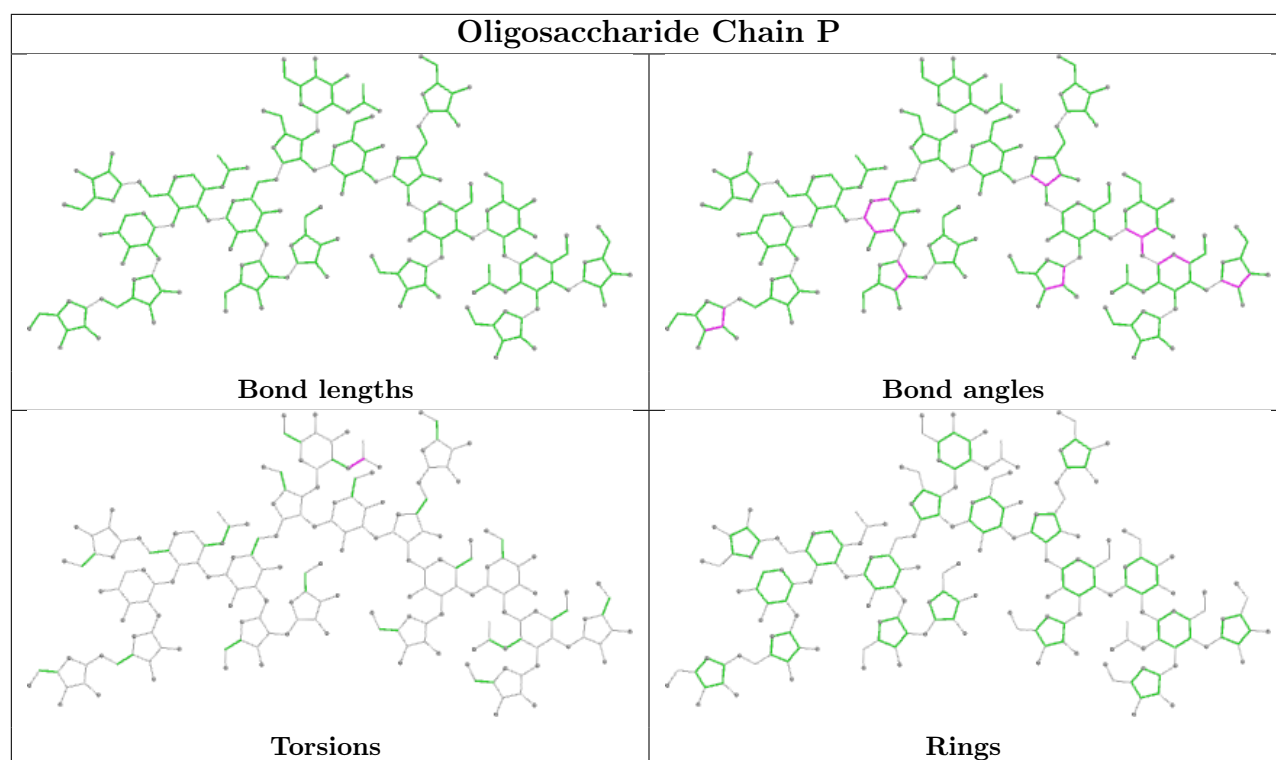


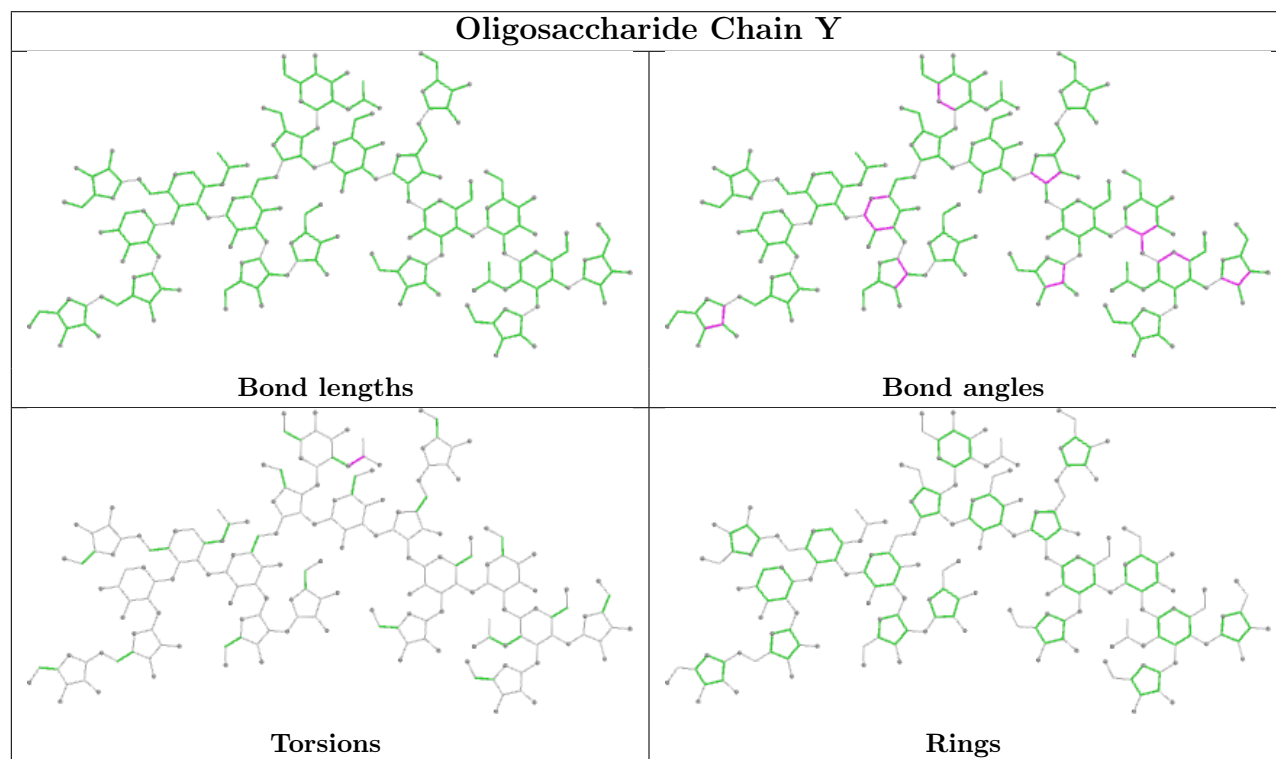
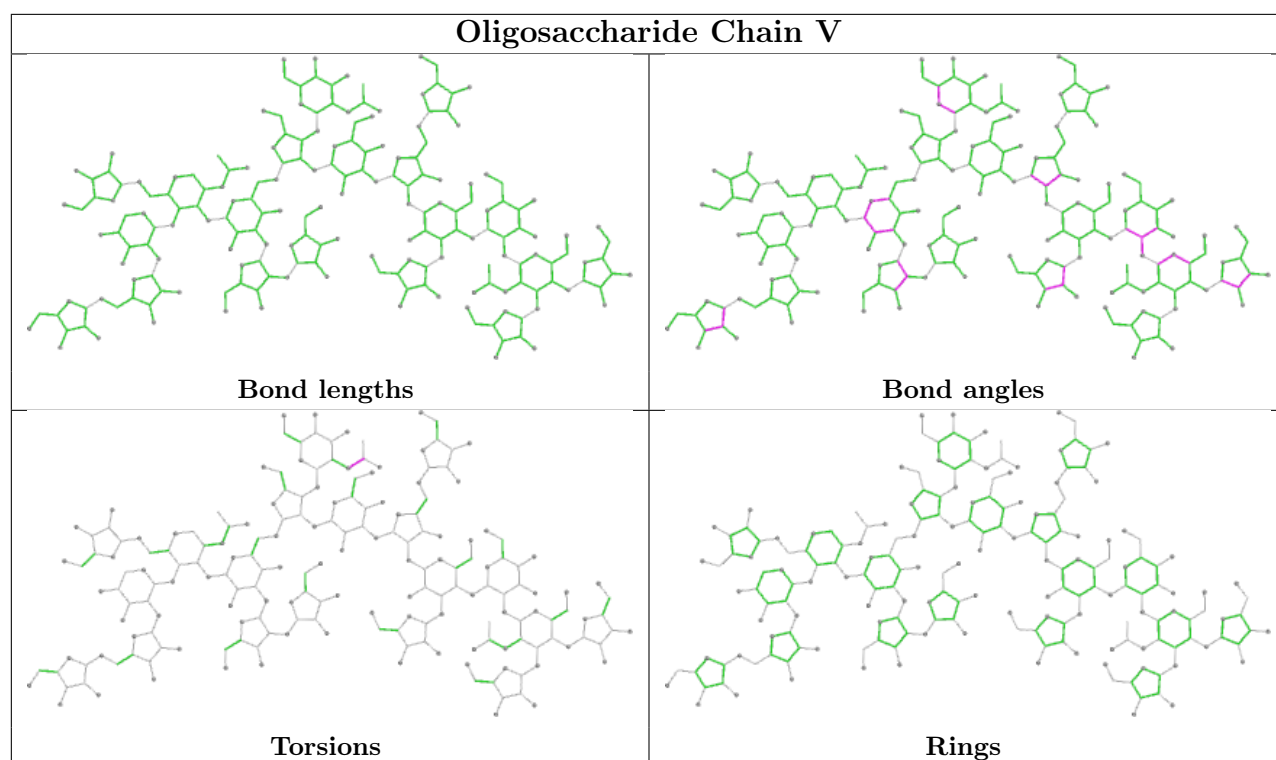


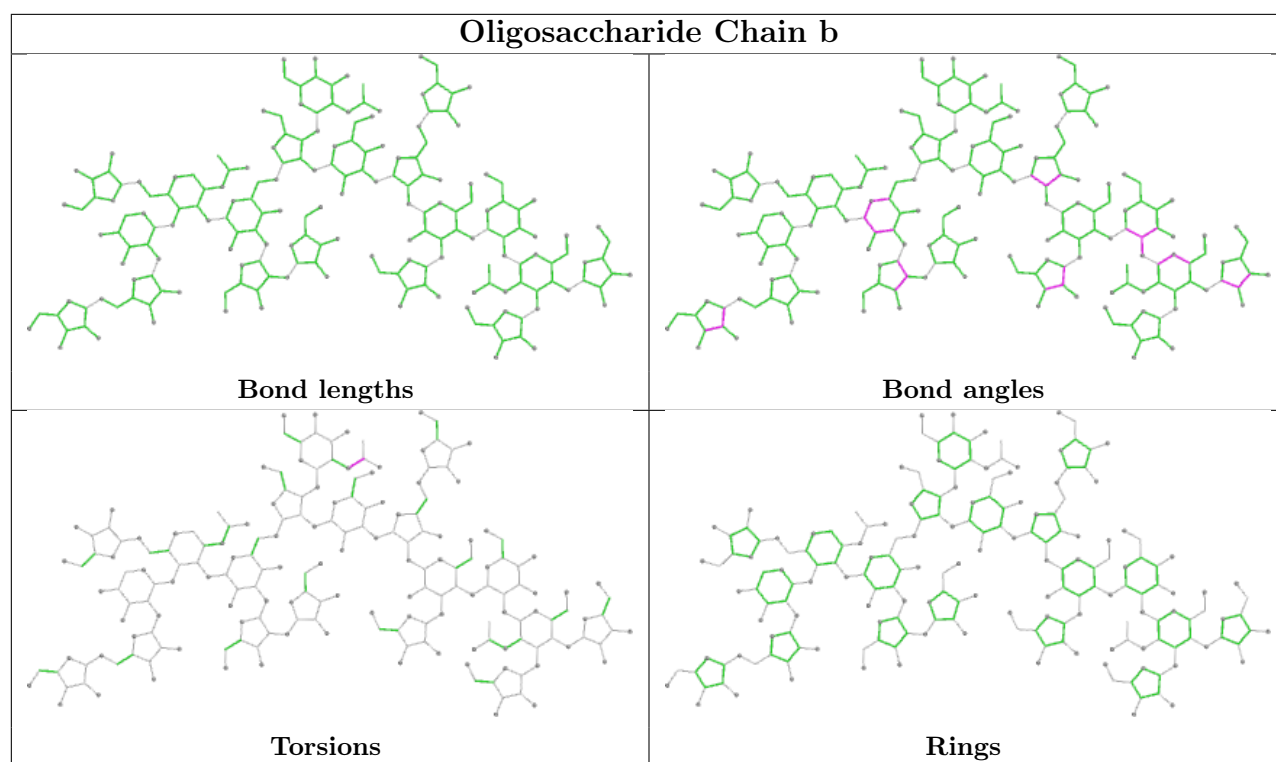












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

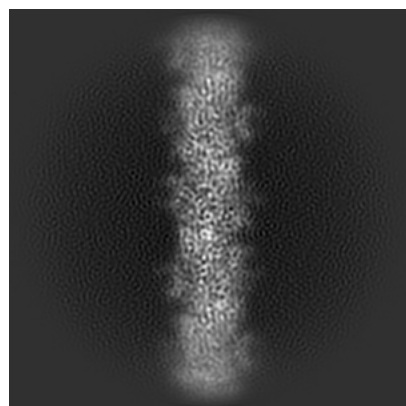
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67849. These allow visual inspection of the internal detail of the map and identification of artifacts.

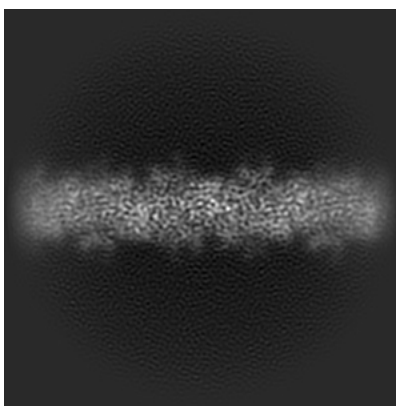
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

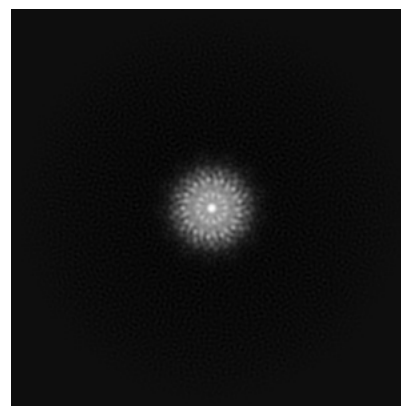
6.1.1 Primary map



X

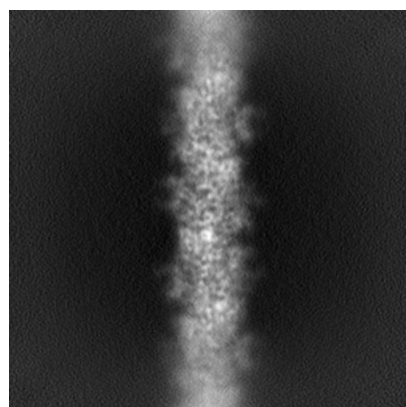


Y

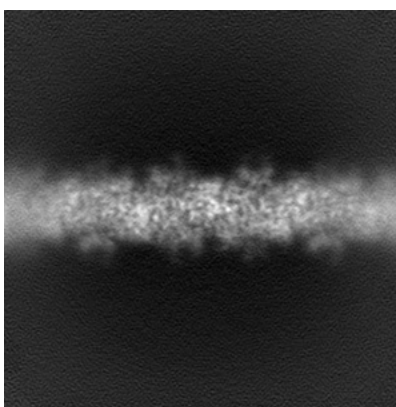


Z

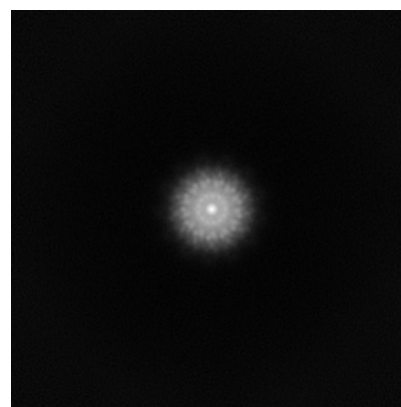
6.1.2 Raw map



X



Y

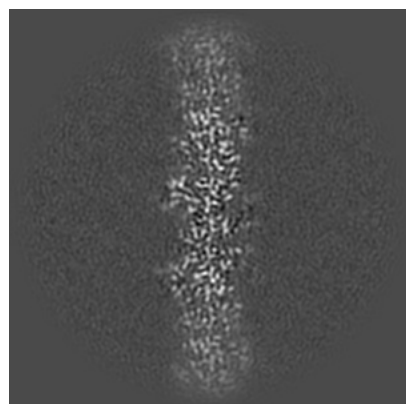


Z

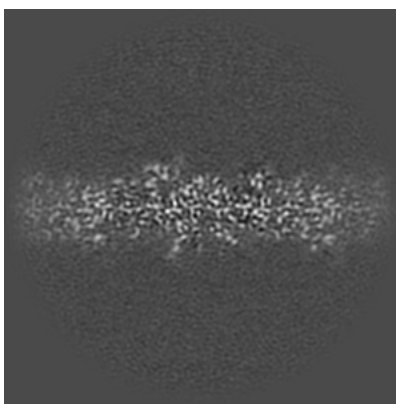
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

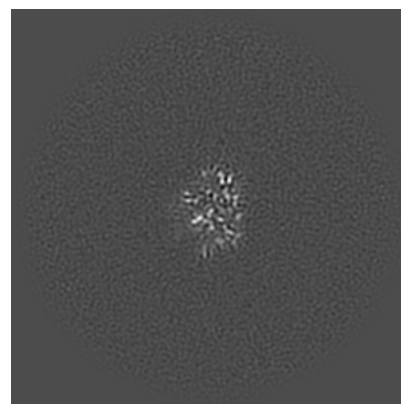
6.2.1 Primary map



X Index: 128

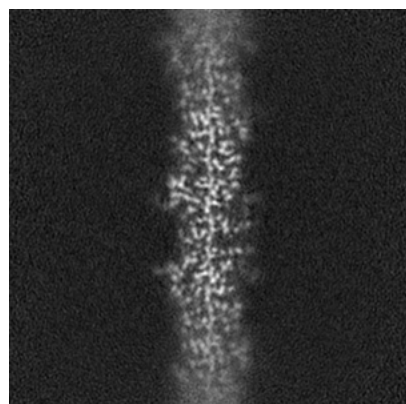


Y Index: 128

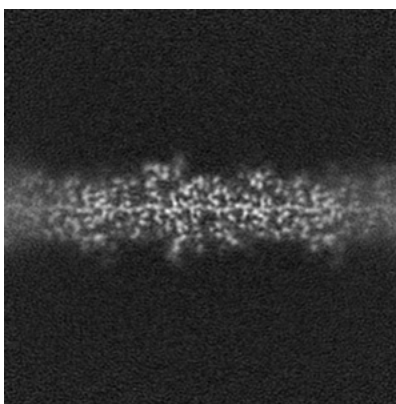


Z Index: 128

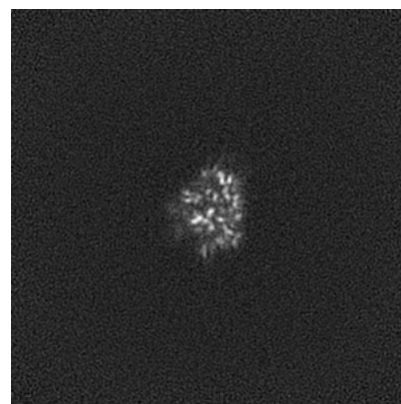
6.2.2 Raw map



X Index: 128



Y Index: 128

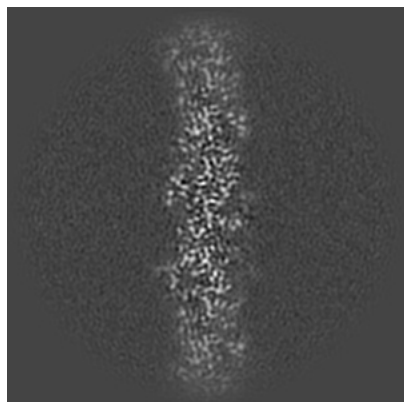


Z Index: 128

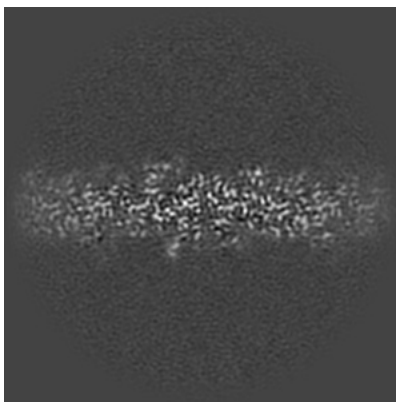
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

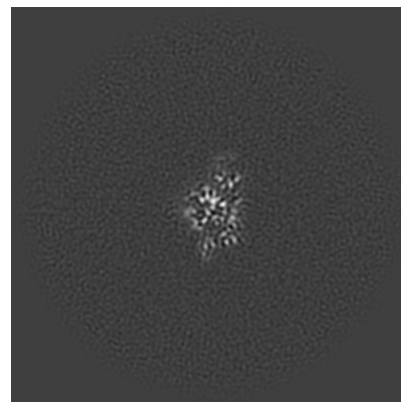
6.3.1 Primary map



X Index: 129

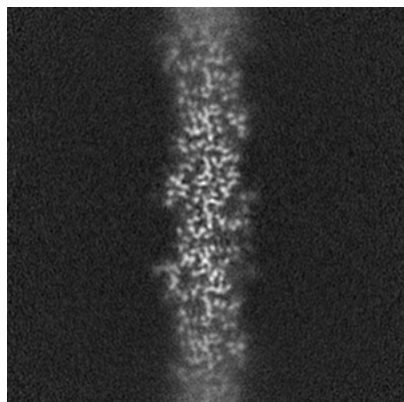


Y Index: 129

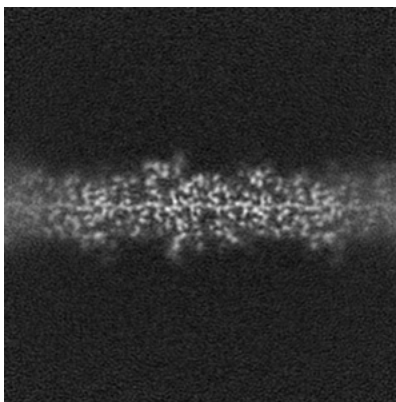


Z Index: 131

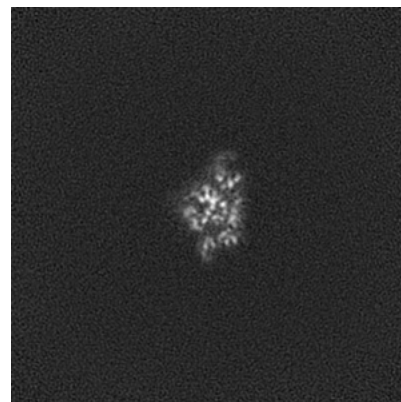
6.3.2 Raw map



X Index: 129



Y Index: 128

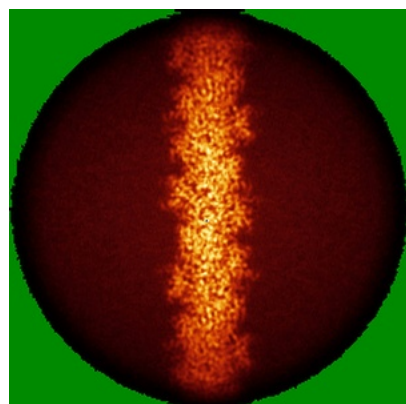


Z Index: 131

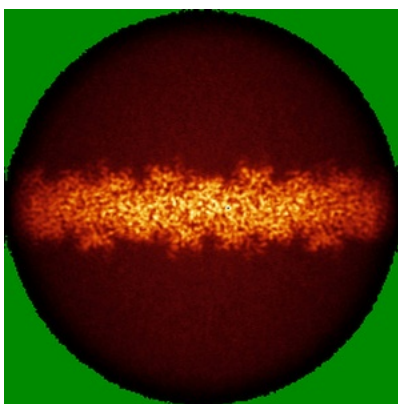
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

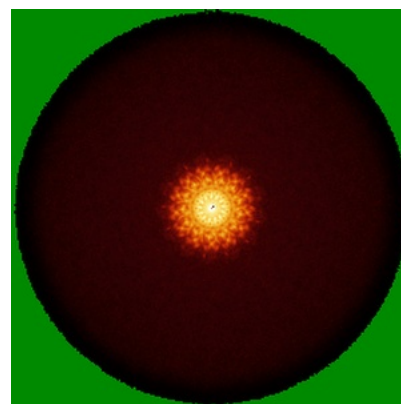
6.4.1 Primary map



X

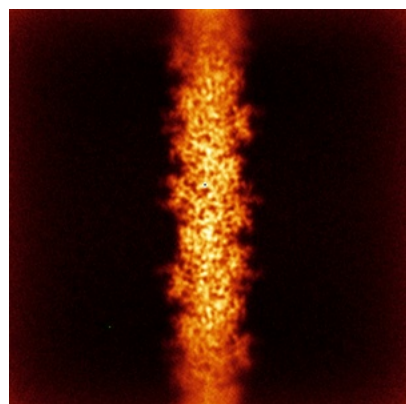


Y

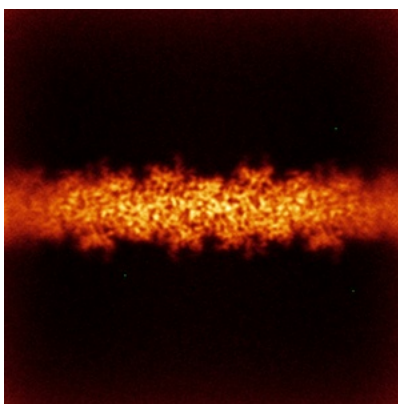


Z

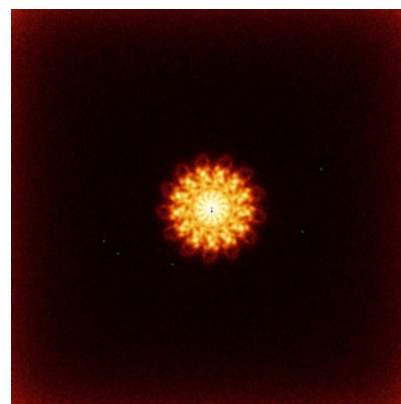
6.4.2 Raw map



X



Y

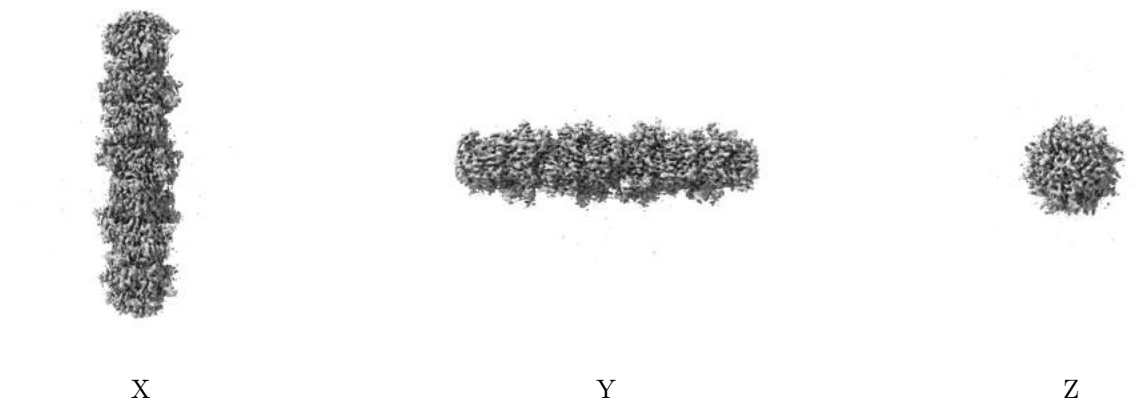


Z

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.

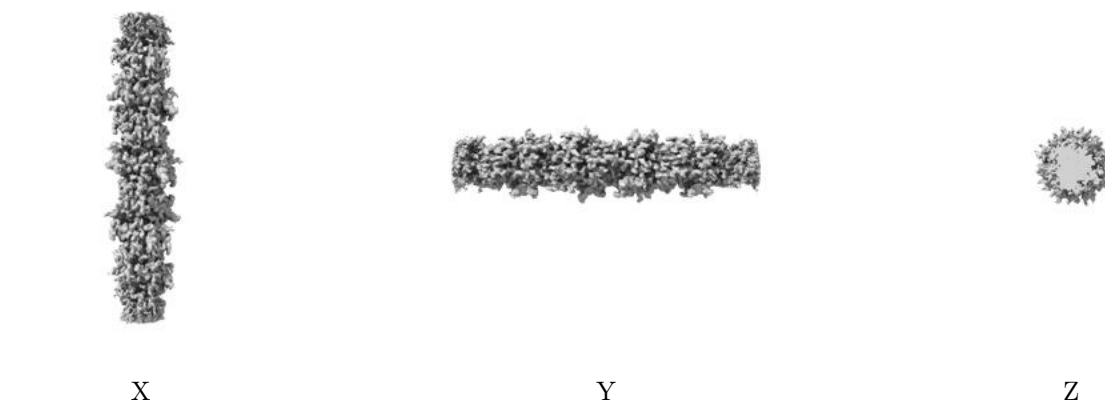
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.253. 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



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.

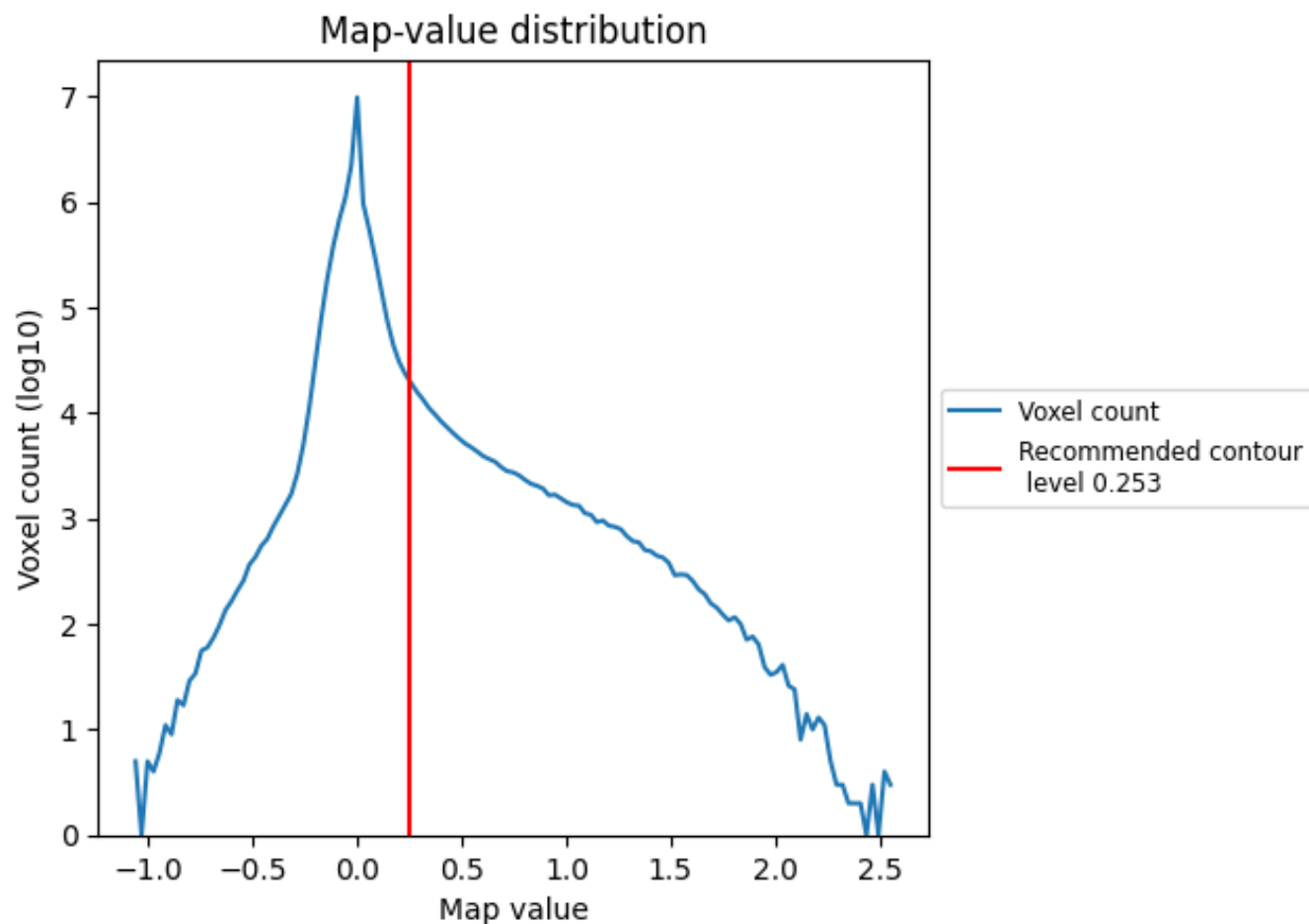
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

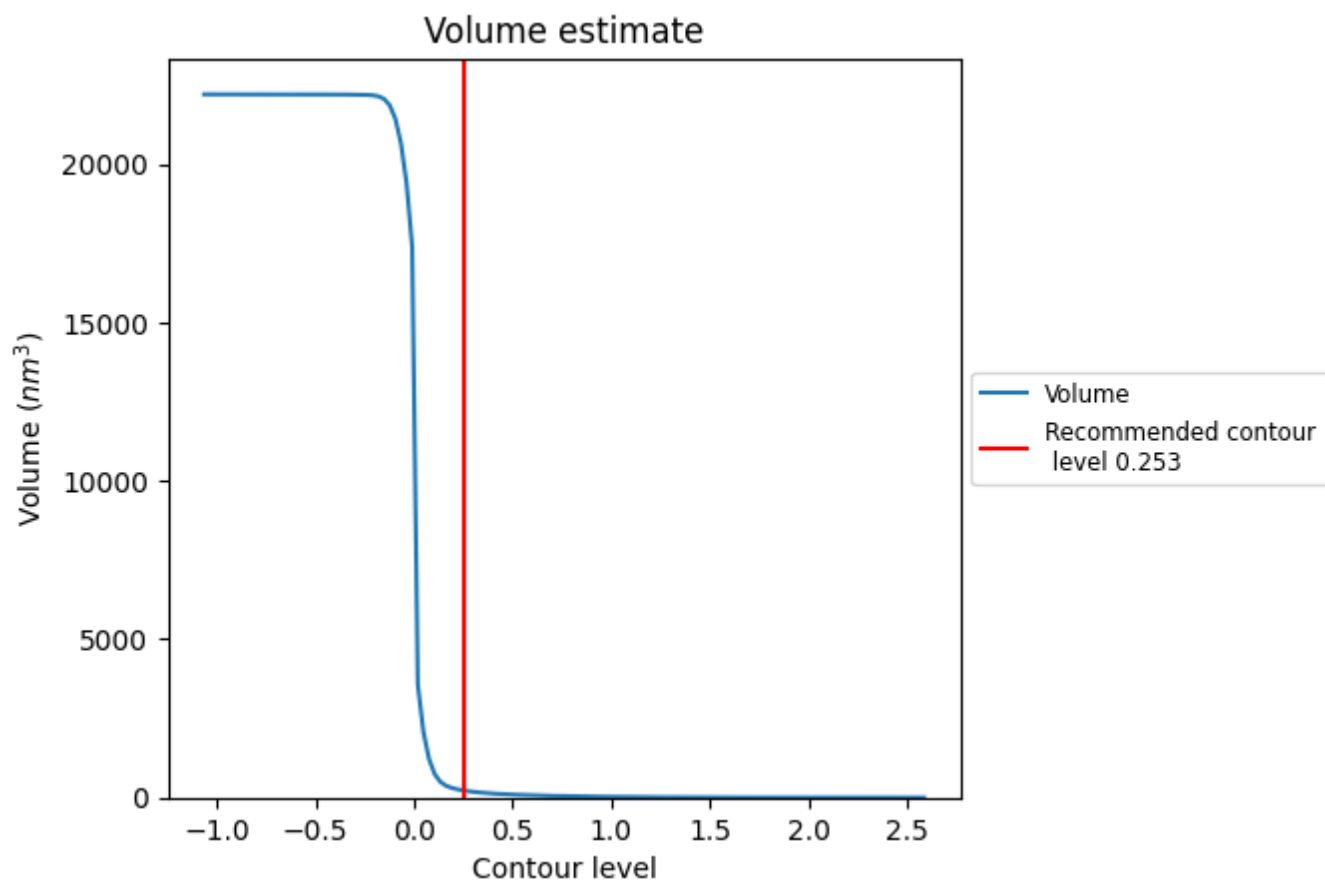
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

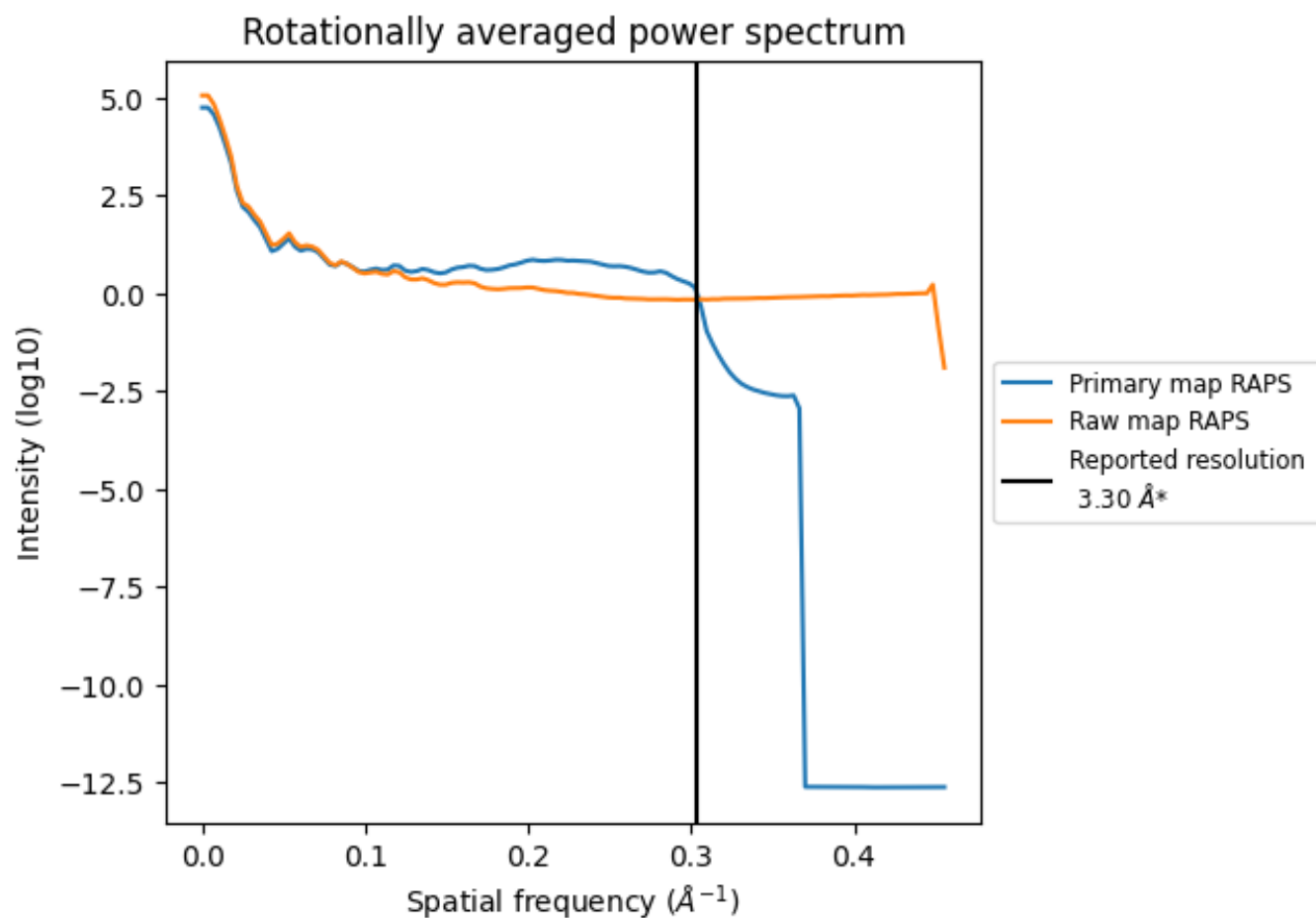
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 222 nm^3 ; this corresponds to an approximate mass of 201 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 ⓘ

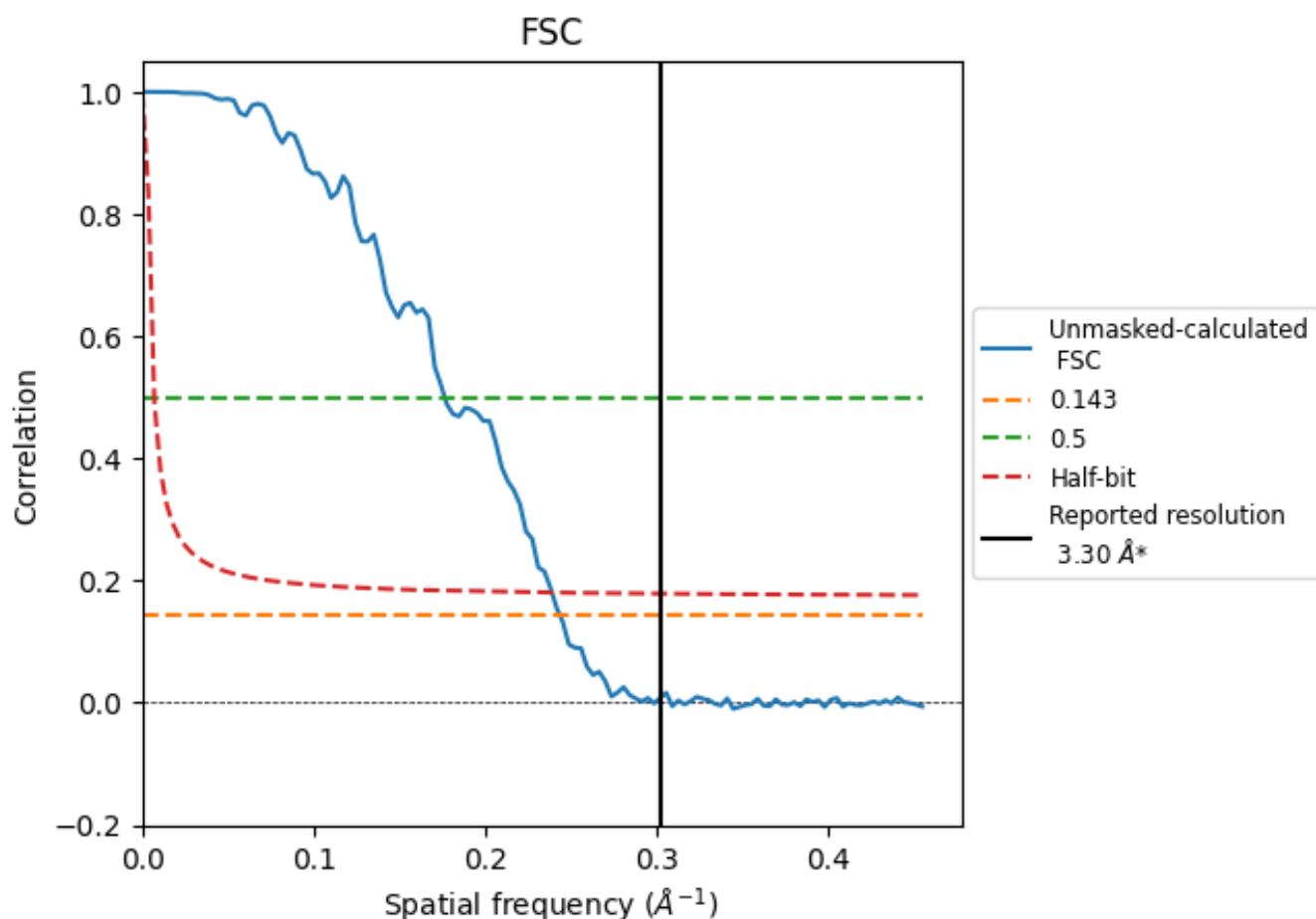


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

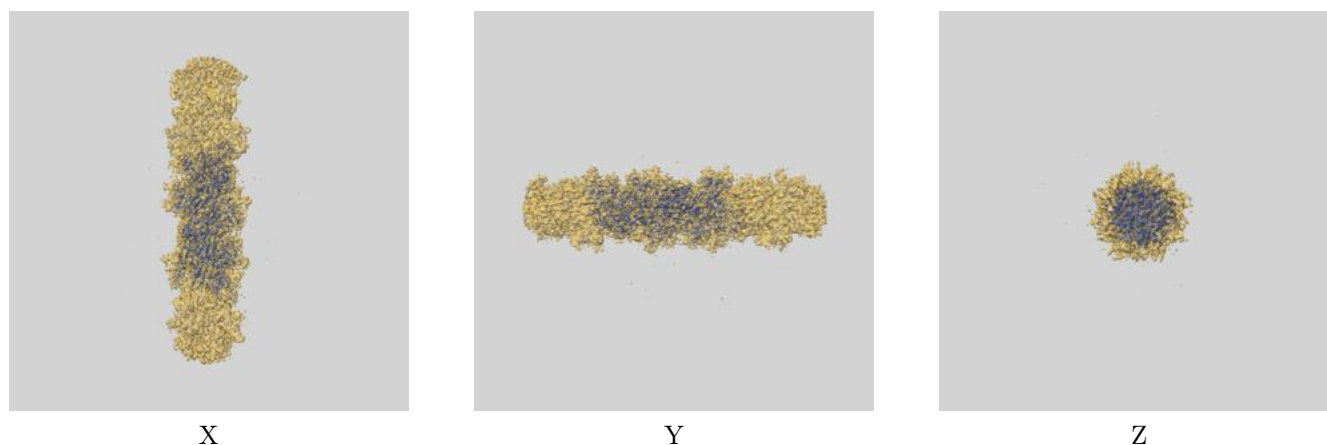
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.10	5.66	4.18

*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 4.10 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

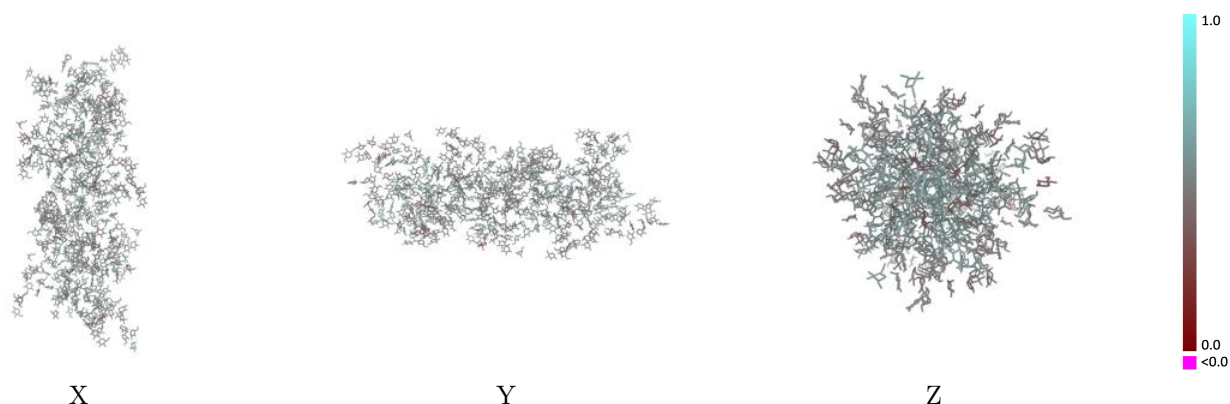
This section contains information regarding the fit between EMDB map EMD-67849 and PDB model 21NS. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



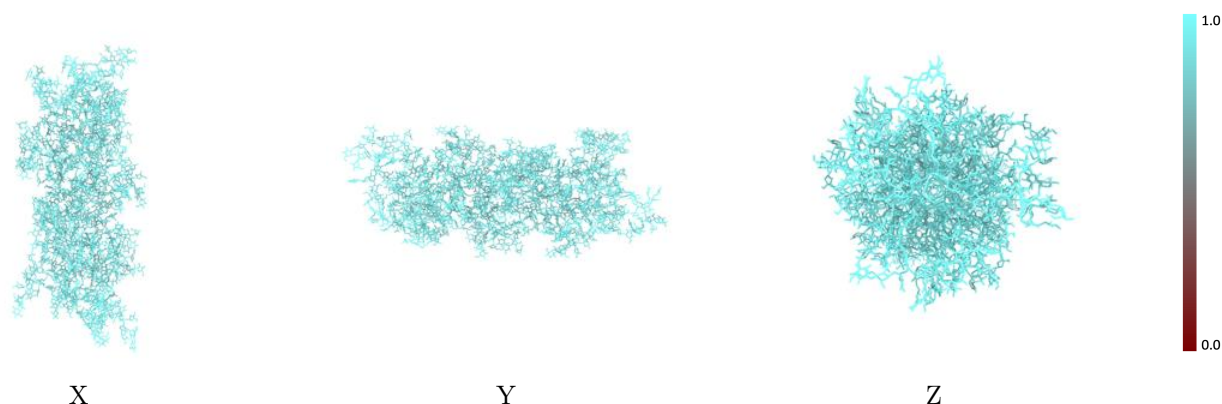
The images above show the 3D surface view of the map at the recommended contour level 0.253 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



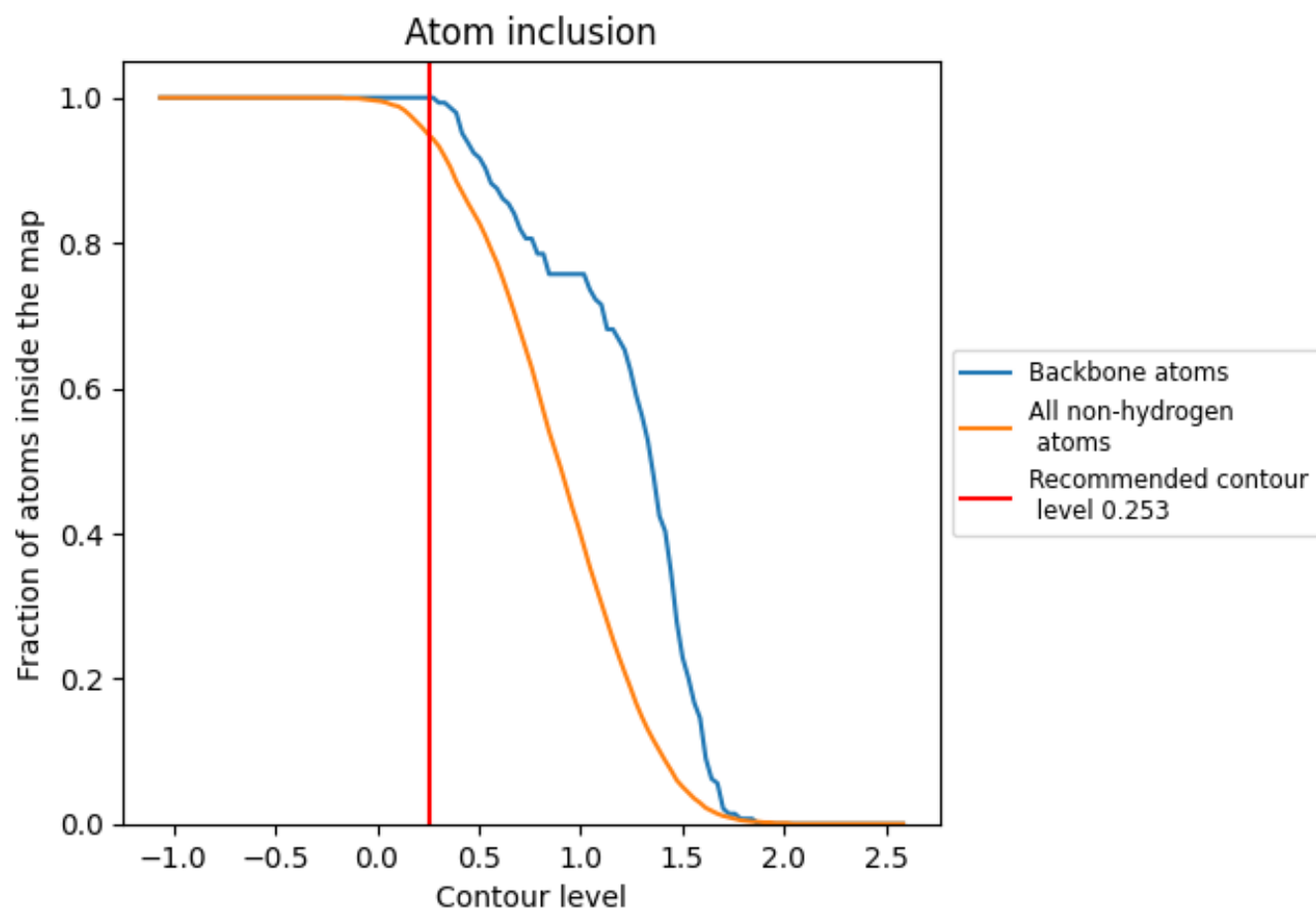
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.253).

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 95% 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 (0.253) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.5060
A	 1.0000	 0.5670
B	 0.9430	 0.4880
C	 0.9600	 0.5170
D	 0.9590	 0.5300
E	 0.9600	 0.5170
F	 0.9450	 0.4790
G	 0.9590	 0.5240
H	 0.9600	 0.5140
I	 0.9330	 0.4850
J	 0.9640	 0.5350
K	 0.9640	 0.5170
L	 0.9360	 0.4840
M	 0.9640	 0.5290
N	 0.9560	 0.5180
O	 0.9260	 0.4880
P	 0.9640	 0.5300
Q	 0.9640	 0.5140
R	 0.9330	 0.4870
S	 0.9540	 0.5310
T	 0.9640	 0.5110
U	 0.9240	 0.4820
V	 0.9690	 0.5310
W	 0.9640	 0.5160
X	 0.9280	 0.4850
Y	 0.9690	 0.5390
Z	 0.9510	 0.5120
a	 0.9260	 0.4890
b	 0.9640	 0.5300

