



## Full wwPDB EM Validation Report ⓘ

Jul 22, 2024 – 12:56 PM EDT

PDB ID : 9BER  
EMDB ID : EMD-44482  
Title : Cryo-EM structure of the HIV-1 JR-FL IDL Env trimer in complex with PGT122 Fab  
Authors : Gorman, J.; Kwong, P.D.  
Deposited on : 2024-04-16  
Resolution : 4.10 Å (reported)  
Based on initial model : 5FUU

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

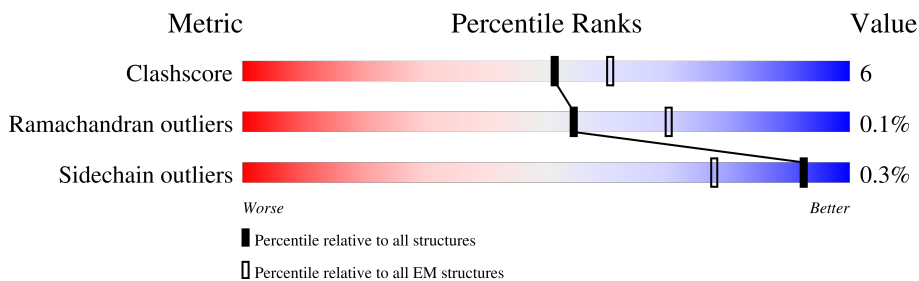
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	477	
1	F	477	
1	G	477	
2	B	153	
2	C	153	
2	I	153	
3	D	132	
3	H	132	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	J	132	 7% 90% 10%
4	E	105	 84% 16%
4	K	105	 87% 12%
4	L	105	 90% 10%
5	M	2	 50% 50%
5	N	2	 100%
5	P	2	 100%
5	Q	2	 50% 50%
5	S	2	 50% 50%
5	T	2	 100%
5	V	2	 100%
5	W	2	 50% 50%
5	Y	2	 50% 50%
5	Z	2	 100%
5	b	2	 50% 50%
5	c	2	 50% 50%
6	O	4	 75% 25%
6	U	4	 50% 50%
6	a	4	 75% 25%
7	R	6	 33% 50% 17%
7	X	6	 33% 67%
7	d	6	 50% 50%

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20350 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	445	3504	2207	612	658	27	0	0
1	A	445	3504	2207	612	658	27	0	0
1	F	445	3504	2207	612	658	27	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	113	CYS	ASP	conflict	UNP Q75760
G	168	LYS	GLU	conflict	UNP Q75760
G	197	ASN	ASP	conflict	UNP Q75760
G	236	THR	LYS	conflict	UNP Q75760
G	431A	GLY	-	insertion	UNP Q75760
G	431B	CYS	-	insertion	UNP Q75760
G	432	GLY	LYS	conflict	UNP Q75760
G	506	VAL	-	expression tag	UNP Q75760
G	507	GLY	-	expression tag	UNP Q75760
G	508	ARG	-	expression tag	UNP Q75760
G	509	ARG	-	expression tag	UNP Q75760
G	510	ARG	-	expression tag	UNP Q75760
G	511	ARG	-	expression tag	UNP Q75760
G	512	ARG	-	expression tag	UNP Q75760
G	513	ARG	-	expression tag	UNP Q75760
A	113	CYS	ASP	conflict	UNP Q75760
A	168	LYS	GLU	conflict	UNP Q75760
A	197	ASN	ASP	conflict	UNP Q75760
A	236	THR	LYS	conflict	UNP Q75760
A	431A	GLY	-	insertion	UNP Q75760
A	431B	CYS	-	insertion	UNP Q75760
A	432	GLY	LYS	conflict	UNP Q75760
A	506	VAL	-	expression tag	UNP Q75760
A	507	GLY	-	expression tag	UNP Q75760

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	ARG	-	expression tag	UNP Q75760
A	509	ARG	-	expression tag	UNP Q75760
A	510	ARG	-	expression tag	UNP Q75760
A	511	ARG	-	expression tag	UNP Q75760
A	512	ARG	-	expression tag	UNP Q75760
A	513	ARG	-	expression tag	UNP Q75760
F	113	CYS	ASP	conflict	UNP Q75760
F	168	LYS	GLU	conflict	UNP Q75760
F	197	ASN	ASP	conflict	UNP Q75760
F	236	THR	LYS	conflict	UNP Q75760
F	431A	GLY	-	insertion	UNP Q75760
F	431B	CYS	-	insertion	UNP Q75760
F	432	GLY	LYS	conflict	UNP Q75760
F	506	VAL	-	expression tag	UNP Q75760
F	507	GLY	-	expression tag	UNP Q75760
F	508	ARG	-	expression tag	UNP Q75760
F	509	ARG	-	expression tag	UNP Q75760
F	510	ARG	-	expression tag	UNP Q75760
F	511	ARG	-	expression tag	UNP Q75760
F	512	ARG	-	expression tag	UNP Q75760
F	513	ARG	-	expression tag	UNP Q75760

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms				AltConf	Trace	
2	B	125	Total	C	N	O	S	0	0
			994	631	168	189	6		
2	C	121	Total	C	N	O	S	0	0
			966	613	163	184	6		
2	I	124	Total	C	N	O	S	0	0
			985	626	166	187	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q6BC19
C	559	PRO	ILE	conflict	UNP Q6BC19
I	559	PRO	ILE	conflict	UNP Q6BC19

- Molecule 3 is a protein called PGT122 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		
3	D	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		
3	J	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		

- Molecule 4 is a protein called PGT122 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	105	Total	C	N	O	S	0	0
			805	504	139	160	2		
4	E	105	Total	C	N	O	S	0	0
			805	504	139	160	2		
4	K	105	Total	C	N	O	S	0	0
			805	504	139	160	2		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		

*Continued on next page...*

Continued from previous page...

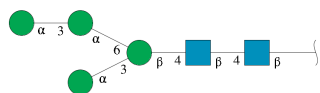
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	Z	2	Total 28	C 16	N 2	O 10	0	0
5	b	2	Total 28	C 16	N 2	O 10	0	0
5	c	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	O	4	Total 50	C 28	N 2	O 20	0	0
6	U	4	Total 50	C 28	N 2	O 20	0	0
6	a	4	Total 50	C 28	N 2	O 20	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	R	6	Total 72	C 40	N 2	O 30	0	0
7	X	6	Total 72	C 40	N 2	O 30	0	0
7	d	6	Total 72	C 40	N 2	O 30	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	G	1	14	8	1	5	0
8	G	1	14	8	1	5	0
8	G	1	14	8	1	5	0
8	G	1	14	8	1	5	0
8	G	1	14	8	1	5	0
8	G	1	14	8	1	5	0
8	G	1	14	8	1	5	0
8	G	1	14	8	1	5	0
8	G	1	14	8	1	5	0
8	G	1	14	8	1	5	0
8	G	1	14	8	1	5	0
8	G	1	14	8	1	5	0
8	B	1	14	8	1	5	0
8	B	1	14	8	1	5	0

*Continued on next page...*



*Continued from previous page...*

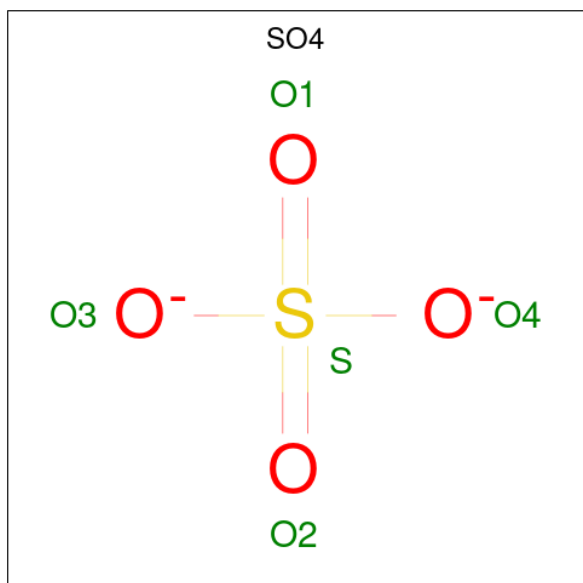
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	B	1	Total 14	C 8	N 1	O 5	0
8	A	1	Total 14	C 8	N 1	O 5	0
8	A	1	Total 14	C 8	N 1	O 5	0
8	A	1	Total 14	C 8	N 1	O 5	0
8	A	1	Total 14	C 8	N 1	O 5	0
8	A	1	Total 14	C 8	N 1	O 5	0
8	A	1	Total 14	C 8	N 1	O 5	0
8	A	1	Total 14	C 8	N 1	O 5	0
8	A	1	Total 14	C 8	N 1	O 5	0
8	A	1	Total 14	C 8	N 1	O 5	0
8	A	1	Total 14	C 8	N 1	O 5	0
8	A	1	Total 14	C 8	N 1	O 5	0
8	A	1	Total 14	C 8	N 1	O 5	0
8	A	1	Total 14	C 8	N 1	O 5	0
8	C	1	Total 14	C 8	N 1	O 5	0
8	C	1	Total 14	C 8	N 1	O 5	0
8	C	1	Total 14	C 8	N 1	O 5	0
8	C	1	Total 14	C 8	N 1	O 5	0
8	F	1	Total 14	C 8	N 1	O 5	0
8	F	1	Total 14	C 8	N 1	O 5	0
8	F	1	Total 14	C 8	N 1	O 5	0
8	F	1	Total 14	C 8	N 1	O 5	0

*Continued on next page...*

Continued from previous page...

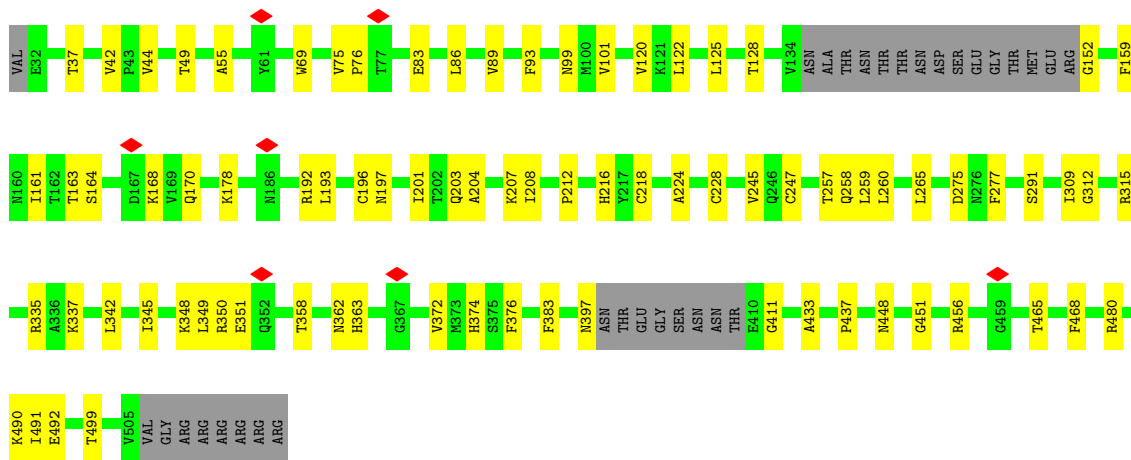
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	F	1	Total 14	C 8	N 1	O 5	0
8	F	1	Total 14	C 8	N 1	O 5	0
8	F	1	Total 14	C 8	N 1	O 5	0
8	F	1	Total 14	C 8	N 1	O 5	0
8	F	1	Total 14	C 8	N 1	O 5	0
8	F	1	Total 14	C 8	N 1	O 5	0
8	F	1	Total 14	C 8	N 1	O 5	0
8	I	1	Total 14	C 8	N 1	O 5	0
8	I	1	Total 14	C 8	N 1	O 5	0
8	I	1	Total 14	C 8	N 1	O 5	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

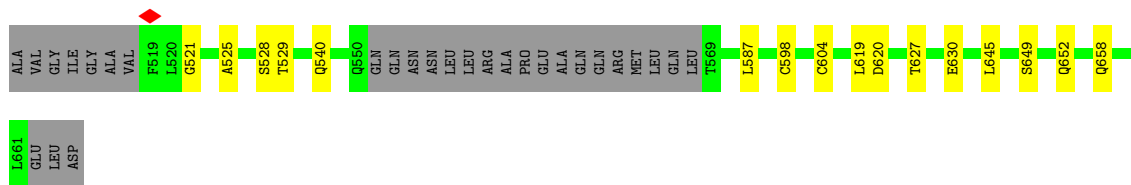


Mol	Chain	Residues	Atoms			AltConf
			Total	O	S	
9	A	1	Total 5	O 4	S 1	0

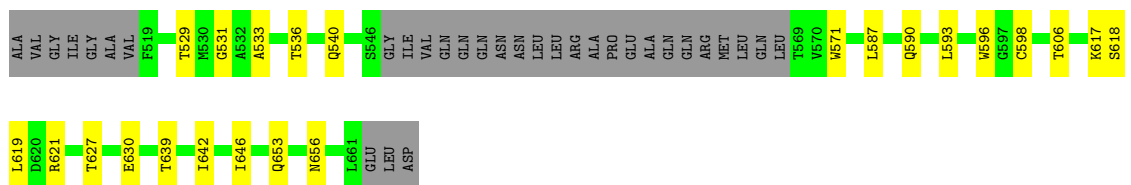




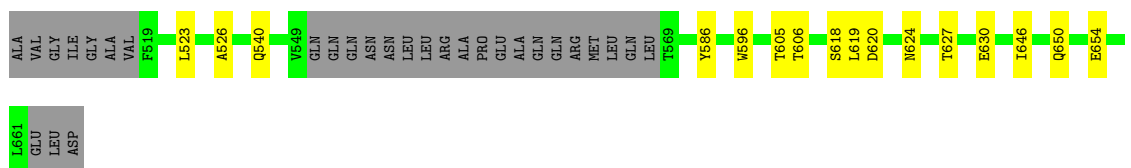
• Molecule 2: Envelope glycoprotein gp41



• Molecule 2: Envelope glycoprotein gp41

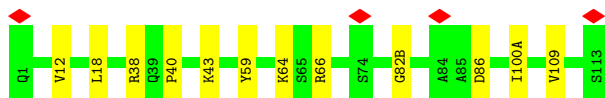


• Molecule 2: Envelope glycoprotein gp41

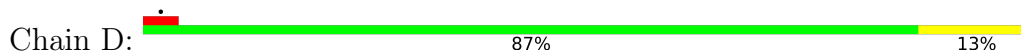


• Molecule 3: PGT122 heavy chain

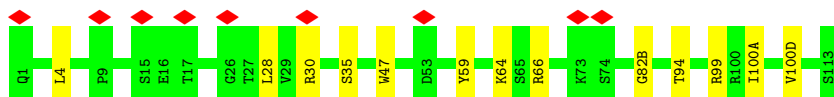
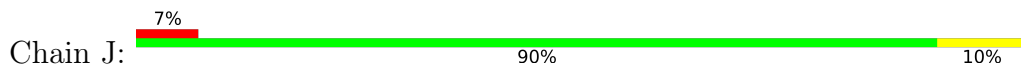




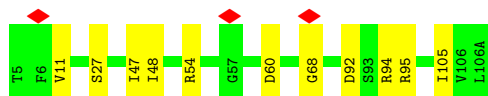
• Molecule 3: PGT122 heavy chain



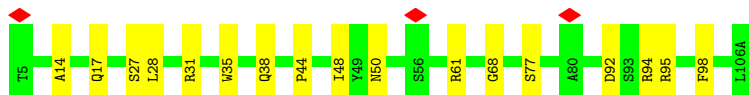
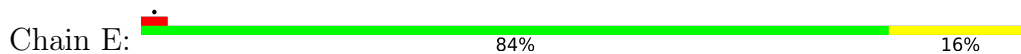
• Molecule 3: PGT122 heavy chain



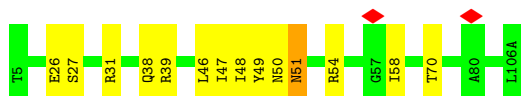
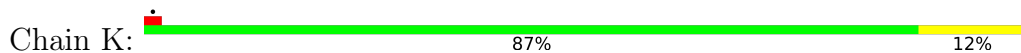
• Molecule 4: PGT122 light chain



• Molecule 4: PGT122 light chain



• Molecule 4: PGT122 light chain



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  50% 50%

MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  50% 50%

MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%

MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%

MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 50% 50%



- Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 75% 25%



- Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 50% 50%



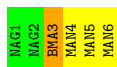
- Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  75% 25%



- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  33% 50% 17%



- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  33% 67%



- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  50% 50%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	31576	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	70.73	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.430	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.12	Depositor
Map size ( $\text{\AA}$ )	343.456, 343.456, 343.456	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0733, 1.0733, 1.0733	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: BMA, MAN, SO4, NAG

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	0.30	0/3578	0.59	0/4859
1	F	0.26	0/3577	0.54	1/4856 (0.0%)
1	G	0.26	0/3578	0.53	0/4859
2	B	0.25	0/1012	0.55	1/1372 (0.1%)
2	C	0.24	0/984	0.53	0/1334
2	I	0.24	0/1003	0.53	0/1360
3	D	0.24	0/1076	0.52	0/1465
3	H	0.24	0/1076	0.50	0/1465
3	J	0.25	0/1075	0.53	0/1462
4	E	0.25	0/826	0.52	0/1130
4	K	0.25	0/826	0.53	0/1130
4	L	0.25	0/826	0.53	0/1130
All	All	0.26	0/19437	0.54	2/26422 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	645	LEU	CA-CB-CG	6.78	130.88	115.30
1	F	259	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	100(D)	VAL	Peptide

## 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	3504	0	3435	61	0
1	F	3504	0	3435	47	0
1	G	3504	0	3435	41	0
2	B	994	0	973	12	0
2	C	966	0	941	15	0
2	I	985	0	966	10	0
3	D	1047	0	1026	19	0
3	H	1047	0	1026	7	0
3	J	1047	0	1025	6	0
4	E	805	0	761	18	0
4	K	805	0	761	8	0
4	L	805	0	761	6	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	P	28	0	25	0	0
5	Q	28	0	25	0	0
5	S	28	0	25	0	0
5	T	28	0	25	0	0
5	V	28	0	25	0	0
5	W	28	0	25	1	0
5	Y	28	0	25	0	0
5	Z	28	0	25	0	0
5	b	28	0	25	0	0
5	c	28	0	25	0	0
6	O	50	0	43	0	0
6	U	50	0	43	1	0
6	a	50	0	43	0	0
7	R	72	0	61	1	0
7	X	72	0	61	0	0
7	d	72	0	61	0	0
8	A	168	0	156	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	42	0	39	0	0
8	C	56	0	52	0	0
8	F	154	0	143	0	0
8	G	168	0	156	1	0
8	I	42	0	39	0	0
9	A	5	0	0	0	0
All	All	20350	0	19742	230	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (230) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:100:ARG:NH1	4:E:50:ASN:OD1	1.90	1.04
3:D:39:GLN:NE2	4:E:38:GLN:HE22	1.78	0.81
3:D:39:GLN:CD	4:E:38:GLN:HE22	1.84	0.80
1:G:304:ARG:HG2	1:G:440:ARG:HH21	1.50	0.76
4:E:28:LEU:H	4:E:31:ARG:HH12	1.35	0.75
1:F:376:PHE:HB3	1:F:383:PHE:HB2	1.70	0.74
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.75	0.69
2:C:587:LEU:HA	2:C:590:GLN:HB3	1.77	0.67
2:C:606:THR:HG21	2:C:646:ILE:HG23	1.75	0.67
1:A:297:THR:HG21	1:A:444:ARG:HH21	1.59	0.65
1:G:204:ALA:HB3	1:G:437:PRO:HD3	1.78	0.65
2:I:606:THR:HG21	2:I:646:ILE:HG23	1.78	0.64
1:A:101:VAL:HG21	1:A:480:ARG:HG3	1.80	0.63
4:L:47:ILE:HG22	4:L:48:ILE:HG13	1.81	0.60
1:G:101:VAL:HG21	1:G:480:ARG:HG3	1.84	0.60
4:K:26:GLU:HA	4:K:70:THR:HG22	1.83	0.60
3:D:39:GLN:OE1	4:E:38:GLN:NE2	2.34	0.60
1:G:55:ALA:HB3	1:G:216:HIS:HB2	1.83	0.59
1:A:358:THR:HG23	1:A:465:THR:H	1.68	0.59
1:G:342:LEU:HA	1:G:345:ILE:HD12	1.85	0.59
3:D:39:GLN:HE22	4:E:38:GLN:NE2	2.00	0.58
4:E:35:TRP:HB2	4:E:48:ILE:HB	1.85	0.58
1:F:49:THR:OG1	1:F:99:ASN:ND2	2.36	0.58
3:D:44:GLN:HB2	4:E:98:PHE:HB2	1.83	0.58
1:A:203:GLN:HA	1:A:435:TYR:HB3	1.84	0.58
1:F:122:LEU:HD23	1:F:203:GLN:HB2	1.84	0.58
1:G:43:PRO:HG3	2:B:540:GLN:HE22	1.69	0.58

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:VAL:HG13	1:F:315:ARG:HB2	1.86	0.58
1:A:258:GLN:HG3	1:A:470:PRO:O	2.03	0.58
1:A:289:LYS:HG2	1:A:290:GLU:HG3	1.86	0.57
1:A:475:MET:HA	1:A:475:MET:CE	2.34	0.57
2:I:620:ASP:O	2:I:624:ASN:ND2	2.37	0.57
1:A:165:ILE:HG12	1:F:128:THR:HG23	1.87	0.57
4:K:38:GLN:NE2	4:K:39:ARG:O	2.33	0.57
4:E:92:ASP:HB3	4:E:95:ARG:HB2	1.86	0.57
2:C:653:GLN:O	2:C:656:ASN:ND2	2.37	0.57
3:H:12:VAL:HG21	3:H:18:LEU:HD13	1.87	0.57
1:G:41:GLY:O	2:B:540:GLN:NE2	2.35	0.56
3:D:39:GLN:NE2	4:E:38:GLN:NE2	2.51	0.56
1:G:34:LEU:HD21	2:B:619:LEU:HD21	1.87	0.56
1:A:475:MET:HA	1:A:475:MET:HE1	1.86	0.56
4:K:27:SER:HA	4:K:31:ARG:HH12	1.69	0.56
2:B:528:SER:OG	2:B:529:THR:N	2.39	0.56
1:A:302:ASN:HB3	1:A:322:ILE:HA	1.87	0.56
1:F:204:ALA:HB3	1:F:437:PRO:HD3	1.88	0.55
1:G:122:LEU:HD23	1:G:203:GLN:HB2	1.88	0.55
1:F:37:THR:HG22	2:I:605:THR:HA	1.87	0.55
1:G:502:LYS:NZ	1:G:503:ARG:O	2.40	0.55
1:A:269:GLU:HA	1:A:289:LYS:HD2	1.89	0.55
1:G:192:ARG:HH21	1:G:196:CYS:HB2	1.72	0.54
1:A:474:ASP:C	1:A:476:ARG:N	2.61	0.54
1:A:38:VAL:HG12	1:A:496:VAL:HG12	1.90	0.54
1:A:474:ASP:C	1:A:476:ARG:H	2.11	0.54
3:J:35:SER:HB2	3:J:47:TRP:HE1	1.73	0.54
3:J:66:ARG:NH1	3:J:82(B):GLY:O	2.41	0.54
3:D:39:GLN:HE22	4:E:38:GLN:CD	2.10	0.54
3:D:39:GLN:HE22	4:E:38:GLN:HE22	1.51	0.53
3:D:29:VAL:HA	3:D:34:TRP:HZ2	1.74	0.53
1:F:309:ILE:O	1:F:312:GLY:N	2.42	0.53
1:G:360:VAL:HG23	1:G:394:THR:HA	1.91	0.53
2:B:649:SER:HA	2:B:652:GLN:HB2	1.90	0.53
1:A:67:ASN:OD1	1:A:209:SER:OG	2.22	0.53
4:L:92:ASP:HB3	4:L:95:ARG:HB2	1.90	0.53
1:F:350:ARG:NH1	1:F:397:ASN:OD1	2.42	0.52
6:U:1:NAG:H61	5:W:1:NAG:H81	1.90	0.52
2:B:627:THR:HG23	2:B:630:GLU:H	1.75	0.52
2:C:529:THR:HG22	2:C:531:GLY:H	1.74	0.52
2:I:596:TRP:HB3	2:I:646:ILE:HG22	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:HIS:NE2	1:A:482:GLU:OE2	2.39	0.51
1:G:499:THR:HG23	1:G:501:ALA:H	1.74	0.51
3:D:62:SER:O	3:D:66:ARG:NH1	2.43	0.51
1:G:376:PHE:HB3	1:G:383:PHE:HB2	1.92	0.51
4:K:54:ARG:HB3	4:K:58:ILE:HD11	1.93	0.51
1:F:86:LEU:HB3	1:F:89:VAL:HG11	1.93	0.50
1:F:342:LEU:HD23	1:F:345:ILE:HD12	1.92	0.50
3:D:35:SER:HB3	3:D:47:TRP:HE1	1.76	0.50
1:A:334:SER:HA	1:A:413:THR:HG22	1.94	0.50
3:H:38:ARG:HH12	3:H:109:VAL:HB	1.76	0.50
1:A:389:GLN:NE2	1:A:415:THR:O	2.40	0.50
2:C:617:LYS:HE2	2:C:621:ARG:HB3	1.92	0.49
1:A:43:PRO:HA	1:A:491:ILE:HD11	1.92	0.49
1:F:101:VAL:HG11	1:F:480:ARG:HE	1.77	0.49
1:F:55:ALA:HB3	1:F:216:HIS:HB2	1.95	0.49
1:F:218:CYS:HA	1:F:247:CYS:HB2	1.94	0.49
2:I:650:GLN:NE2	2:I:654:GLU:OE2	2.44	0.49
1:A:68:VAL:HG11	1:A:112:TRP:CD1	2.47	0.49
2:C:627:THR:HG23	2:C:630:GLU:H	1.78	0.49
1:F:349:LEU:HD21	1:F:468:PHE:HE1	1.78	0.49
1:A:302:ASN:HD22	1:A:322:ILE:HG22	1.78	0.49
1:A:298:ARG:HG3	1:A:329:ALA:HB2	1.94	0.49
1:F:201:ILE:HA	1:F:433:ALA:HB3	1.94	0.49
4:E:14:ALA:HB3	4:E:17:GLN:HE22	1.77	0.49
4:E:28:LEU:HD12	4:E:94:ARG:HH21	1.78	0.48
4:E:61:ARG:NH1	4:E:77:SER:O	2.46	0.48
1:G:38:VAL:HG12	1:G:496:VAL:HG12	1.94	0.48
1:F:122:LEU:HD13	1:F:125:LEU:HD12	1.95	0.48
2:I:526:ALA:O	2:I:627:THR:OG1	2.31	0.48
1:F:192:ARG:NH2	1:F:197:ASN:OD1	2.39	0.48
1:A:179:LEU:HD11	1:A:419:ARG:HD3	1.95	0.48
3:D:34:TRP:HZ3	3:D:94:THR:HG22	1.79	0.48
1:G:205:CYS:HB3	1:G:208:ILE:HD13	1.95	0.48
1:F:159:PHE:HE1	1:F:161:ILE:HD12	1.79	0.48
4:K:46:LEU:HD11	4:K:49:TYR:HB3	1.96	0.48
1:A:83:GLU:HB3	1:A:245:VAL:HG23	1.95	0.47
1:A:229:ASN:O	1:A:231:LYS:NZ	2.47	0.47
1:A:266:ALA:HB3	1:A:289:LYS:HA	1.95	0.47
1:F:258:GLN:NE2	1:F:372:VAL:O	2.47	0.47
1:G:296:CYS:HB3	1:G:331:CYS:HA	1.94	0.47
1:A:309:ILE:HB	1:A:315:ARG:HG3	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:47:ILE:HG22	4:K:48:ILE:HG13	1.97	0.47
1:G:218:CYS:HA	1:G:247:CYS:HB2	1.96	0.47
1:F:83:GLU:HG2	1:F:245:VAL:HG23	1.96	0.47
1:F:152:GLY:O	1:F:178:LYS:NZ	2.39	0.47
2:I:618:SER:OG	2:I:619:LEU:N	2.47	0.47
3:D:40:PRO:HG2	3:D:43:LYS:HB2	1.97	0.47
1:A:360:VAL:HG13	1:A:467:ILE:HG22	1.97	0.47
1:A:363:HIS:HB3	1:A:388:THR:HG23	1.97	0.47
3:H:38:ARG:NH2	3:H:86:ASP:O	2.44	0.47
1:A:195:SER:O	1:A:199:SER:OG	2.33	0.47
1:A:300:ASN:O	1:A:302:ASN:ND2	2.47	0.47
3:D:60:ASN:HB3	3:D:63:LEU:HB2	1.96	0.47
1:G:359:ILE:HG22	1:G:465:THR:HG21	1.96	0.47
2:B:587:LEU:HD21	2:I:586:TYR:CE2	2.50	0.47
2:C:596:TRP:CD1	2:C:646:ILE:HG22	2.50	0.47
3:J:28:LEU:HG	3:J:30:ARG:H	1.78	0.47
4:K:51:ASN:O	4:K:51:ASN:ND2	2.48	0.47
2:C:533:ALA:HA	2:C:536:THR:HG22	1.96	0.46
1:A:391:PHE:CD2	1:A:470:PRO:HG2	2.50	0.46
1:F:358:THR:HG23	1:F:465:THR:H	1.80	0.46
1:A:455:THR:O	1:A:469:ARG:N	2.47	0.46
1:A:185:ASP:OD1	1:A:186:ASN:N	2.45	0.46
1:A:58:ALA:HB2	1:A:76:PRO:HB3	1.98	0.45
1:A:475:MET:O	1:A:475:MET:SD	2.74	0.45
1:G:84:VAL:HG21	2:B:521:GLY:HA3	1.98	0.45
1:A:122:LEU:HD22	1:A:317:PHE:HE1	1.81	0.45
1:F:265:LEU:HD21	1:F:291:SER:HB3	1.98	0.45
1:F:362:ASN:OD1	1:F:363:HIS:N	2.49	0.45
4:E:38:GLN:HB2	4:E:44:PRO:HB3	1.99	0.45
1:G:164:SER:HB3	1:G:312:GLY:HA2	1.98	0.45
1:A:474:ASP:O	1:A:476:ARG:N	2.50	0.45
1:F:101:VAL:HG21	1:F:480:ARG:HG3	1.98	0.45
1:F:207:LYS:HG3	1:F:208:ILE:HD12	1.97	0.45
1:F:277:PHE:O	1:F:456:ARG:NH2	2.50	0.45
4:E:61:ARG:HD2	4:E:77:SER:HB2	1.98	0.45
1:A:201:ILE:HG13	1:A:433:ALA:HB3	1.99	0.44
1:F:69:TRP:CZ3	1:F:212:PRO:HA	2.52	0.44
4:L:11:VAL:O	4:L:105:ILE:N	2.45	0.44
1:G:275:ASP:N	1:G:275:ASP:OD1	2.48	0.44
2:C:639:THR:HA	2:C:642:ILE:HB	1.99	0.44
1:F:257:THR:O	1:F:374:HIS:ND1	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:CYS:HA	1:A:157:CYS:HA	1.98	0.44
1:A:296:CYS:HB3	1:A:331:CYS:HA	1.99	0.44
1:G:298:ARG:HB2	1:G:383:PHE:HZ	1.83	0.44
1:F:260:LEU:HD12	1:F:451:GLY:HA3	2.00	0.43
1:A:272:ILE:HG13	1:A:286:VAL:HG23	2.00	0.43
4:L:27:SER:OG	4:L:68:GLY:N	2.51	0.43
1:A:376:PHE:HB3	1:A:383:PHE:HB2	1.99	0.43
1:F:168:LYS:HB3	1:F:170:GLN:HE22	1.83	0.43
1:G:363:HIS:HB3	1:G:388:THR:HG23	2.00	0.43
1:F:224:ALA:HB2	1:F:491:ILE:HD11	2.01	0.43
1:A:50:THR:OG1	1:A:51:THR:N	2.51	0.43
1:A:251:ILE:HG13	1:A:482:GLU:HG2	2.00	0.43
2:B:658:GLN:NE2	1:F:499:THR:HG21	2.34	0.43
1:A:348:LYS:HA	1:A:348:LYS:HD3	1.78	0.43
1:A:54:CYS:HB3	1:A:74:CYS:HB3	1.93	0.43
3:H:66:ARG:NH1	3:H:82(B):GLY:O	2.52	0.43
3:D:4:LEU:HD11	3:D:94:THR:HG23	2.01	0.43
4:E:27:SER:OG	4:E:68:GLY:N	2.52	0.43
1:G:260:LEU:HD12	1:G:451:GLY:HA3	2.01	0.43
2:B:525:ALA:HB1	2:B:528:SER:HB3	2.00	0.43
1:A:499:THR:HA	2:C:619:LEU:HD11	2.01	0.43
2:I:627:THR:HG23	2:I:630:GLU:H	1.84	0.43
1:G:390:LEU:HD11	1:G:416:LEU:HD11	2.00	0.42
2:B:620:ASP:OD1	2:B:620:ASP:N	2.52	0.42
2:I:523:LEU:HA	2:I:540:GLN:HE21	1.84	0.42
2:C:593:LEU:HD22	2:C:598:CYS:HB2	2.01	0.42
3:H:59:TYR:HB2	3:H:64:LYS:HD3	2.01	0.42
1:G:163:THR:OG1	1:G:170:GLN:OE1	2.34	0.42
1:G:434:MET:HB2	1:G:434:MET:HE3	1.90	0.42
1:A:307:ILE:HD12	1:A:317:PHE:HD2	1.84	0.42
3:D:63:LEU:HD23	3:D:66:ARG:HH11	1.84	0.42
1:G:43:PRO:HA	1:G:491:ILE:HD11	2.00	0.42
1:G:188:ASN:OD1	1:G:189:THR:N	2.51	0.42
1:G:396:ASN:OD1	1:G:397:ASN:N	2.52	0.42
1:G:492:GLU:HA	1:G:493:PRO:HD3	1.90	0.42
3:D:1:GLN:HE22	3:D:3:HIS:HB2	1.84	0.42
1:G:334:SER:HA	1:G:413:THR:HG22	2.01	0.42
1:A:57:ASP:OD1	1:A:57:ASP:N	2.53	0.42
4:L:54:ARG:NH1	4:L:60:ASP:OD1	2.43	0.42
1:G:275:ASP:HB2	8:G:603:NAG:H82	2.00	0.42
1:A:223:PHE:CE2	1:A:490:LYS:HB3	2.54	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:618:SER:OG	2:C:619:LEU:N	2.53	0.42
1:G:322:ILE:O	4:L:94:ARG:NH1	2.53	0.41
1:F:163:THR:OG1	1:F:164:SER:N	2.52	0.41
3:H:100(A):ILE:O	7:R:3:BMA:O2	2.38	0.41
1:G:322:ILE:HG21	1:G:326:ILE:HG22	2.01	0.41
1:F:193:LEU:HB2	1:F:196:CYS:SG	2.61	0.41
1:F:42:VAL:HG12	1:F:44:VAL:HG23	2.03	0.41
1:G:232:THR:HA	1:G:271:VAL:HG11	2.01	0.41
1:A:114:GLN:OE1	2:C:571:TRP:NE1	2.48	0.41
1:A:346:VAL:O	1:A:350:ARG:HG2	2.21	0.41
1:G:122:LEU:HD22	1:G:317:PHE:CE1	2.56	0.41
1:A:275:ASP:OD1	1:A:276:ASN:N	2.53	0.41
1:A:165:ILE:HD12	1:A:165:ILE:H	1.86	0.41
1:F:275:ASP:OD1	1:F:275:ASP:N	2.49	0.41
1:F:291:SER:HB2	1:F:448:ASN:HB3	2.03	0.41
3:D:43:LYS:HB3	3:D:43:LYS:HE3	1.87	0.41
3:J:4:LEU:HD11	3:J:94:THR:HG23	2.01	0.41
2:B:598:CYS:N	2:B:604:CYS:SG	2.94	0.41
1:A:167:ASP:C	1:A:167:ASP:OD1	2.58	0.41
1:A:259:LEU:HD23	1:A:449:ILE:HD12	2.03	0.41
1:A:270:VAL:HG11	1:A:345:ILE:HD13	2.02	0.41
2:C:593:LEU:HD23	2:C:593:LEU:HA	1.92	0.41
1:G:105:GLN:HG2	1:G:479:TRP:HZ3	1.86	0.41
1:F:69:TRP:HZ3	1:F:212:PRO:HA	1.86	0.41
1:F:168:LYS:HA	1:F:168:LYS:HD3	1.85	0.41
1:F:337:LYS:HE2	1:F:337:LYS:HB3	1.93	0.41
1:F:490:LYS:NZ	1:F:492:GLU:OE2	2.54	0.41
3:H:40:PRO:HB2	3:H:43:LYS:HB2	2.03	0.41
1:G:463:ASN:OD1	1:G:463:ASN:N	2.54	0.41
1:F:335:ARG:HD2	1:F:411:GLY:O	2.21	0.41
1:F:348:LYS:HA	1:F:351:GLU:HG2	2.03	0.41
1:A:43:PRO:HG3	2:C:540:GLN:HE22	1.86	0.40
1:A:97:LYS:HD2	1:A:97:LYS:HA	1.83	0.40
1:F:93:PHE:CE2	1:F:228:CYS:HB2	2.56	0.40
3:J:59:TYR:HB2	3:J:64:LYS:HD3	2.03	0.40
1:G:184:ILE:HG13	1:G:184:ILE:O	2.21	0.40
1:F:75:VAL:HA	1:F:76:PRO:HD3	1.93	0.40
4:K:47:ILE:HD13	4:K:47:ILE:HA	1.96	0.40
3:J:99:ARG:HE	3:J:100(A):ILE:HD11	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	439/477 (92%)	398 (91%)	39 (9%)	2 (0%)	29	67
1	F	437/477 (92%)	401 (92%)	36 (8%)	0	100	100
1	G	439/477 (92%)	409 (93%)	30 (7%)	0	100	100
2	B	121/153 (79%)	109 (90%)	12 (10%)	0	100	100
2	C	117/153 (76%)	101 (86%)	16 (14%)	0	100	100
2	I	120/153 (78%)	108 (90%)	12 (10%)	0	100	100
3	D	130/132 (98%)	126 (97%)	4 (3%)	0	100	100
3	H	130/132 (98%)	126 (97%)	4 (3%)	0	100	100
3	J	128/132 (97%)	124 (97%)	4 (3%)	0	100	100
4	E	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
4	K	103/105 (98%)	95 (92%)	8 (8%)	0	100	100
4	L	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
All	All	2370/2601 (91%)	2193 (92%)	175 (7%)	2 (0%)	54	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	GLU
1	A	470	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/425 (93%)	392 (99%)	5 (1%)	69	81
1	F	397/425 (93%)	397 (100%)	0	100	100
1	G	397/425 (93%)	397 (100%)	0	100	100
2	B	106/128 (83%)	106 (100%)	0	100	100
2	C	103/128 (80%)	103 (100%)	0	100	100
2	I	105/128 (82%)	105 (100%)	0	100	100
3	D	116/116 (100%)	116 (100%)	0	100	100
3	H	116/116 (100%)	116 (100%)	0	100	100
3	J	116/116 (100%)	116 (100%)	0	100	100
4	E	88/88 (100%)	88 (100%)	0	100	100
4	K	88/88 (100%)	86 (98%)	2 (2%)	50	70
4	L	88/88 (100%)	88 (100%)	0	100	100
All	All	2117/2271 (93%)	2110 (100%)	7 (0%)	92	95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	ILE
1	A	167	ASP
1	A	240	LYS
1	A	300	ASN
1	A	502	LYS
4	K	50	ASN
4	K	51	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	A	302	ASN
2	C	656	ASN
1	F	99	ASN
3	D	39	GLN
4	E	38	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

54 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
5	NAG	M	1	1,5	14,14,15	0.48	0	17,19,21	0.97	2 (11%)
5	NAG	M	2	5	14,14,15	0.23	0	17,19,21	0.53	0
5	NAG	N	1	1,5	14,14,15	0.24	0	17,19,21	0.48	0
5	NAG	N	2	5	14,14,15	0.27	0	17,19,21	0.43	0
6	NAG	O	1	1,6	14,14,15	0.25	0	17,19,21	0.43	0
6	NAG	O	2	6	14,14,15	0.26	0	17,19,21	0.54	0
6	BMA	O	3	6	11,11,12	0.69	0	15,15,17	0.76	0
6	MAN	O	4	6	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
5	NAG	P	1	1,5	14,14,15	0.27	0	17,19,21	0.50	0
5	NAG	P	2	5	14,14,15	0.27	0	17,19,21	0.43	0
5	NAG	Q	1	1,5	14,14,15	0.33	0	17,19,21	0.73	1 (5%)
5	NAG	Q	2	5	14,14,15	0.32	0	17,19,21	0.44	0
7	NAG	R	1	7,1	14,14,15	0.59	0	17,19,21	0.96	0
7	NAG	R	2	7	14,14,15	0.20	0	17,19,21	0.59	0
7	BMA	R	3	7	11,11,12	0.68	0	15,15,17	0.85	1 (6%)
7	MAN	R	4	7	11,11,12	0.75	0	15,15,17	1.21	2 (13%)
7	MAN	R	5	7	11,11,12	0.73	0	15,15,17	0.92	1 (6%)
7	MAN	R	6	7	11,11,12	0.68	0	15,15,17	1.06	2 (13%)
5	NAG	S	1	1,5	14,14,15	0.47	0	17,19,21	0.95	2 (11%)
5	NAG	S	2	5	14,14,15	0.23	0	17,19,21	0.52	0
5	NAG	T	1	1,5	14,14,15	0.26	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	T	2	5	14,14,15	0.27	0	17,19,21	0.42	0
6	NAG	U	1	1,6	14,14,15	0.20	0	17,19,21	0.45	0
6	NAG	U	2	6	14,14,15	0.30	0	17,19,21	0.51	0
6	BMA	U	3	6	11,11,12	0.69	0	15,15,17	0.80	0
6	MAN	U	4	6	11,11,12	0.71	0	15,15,17	1.07	2 (13%)
5	NAG	V	1	1,5	14,14,15	0.22	0	17,19,21	0.49	0
5	NAG	V	2	5	14,14,15	0.29	0	17,19,21	0.47	0
5	NAG	W	1	1,5	14,14,15	0.31	0	17,19,21	0.75	1 (5%)
5	NAG	W	2	5	14,14,15	0.29	0	17,19,21	0.44	0
7	NAG	X	1	7,1	14,14,15	0.68	1 (7%)	17,19,21	1.12	2 (11%)
7	NAG	X	2	7	14,14,15	0.22	0	17,19,21	0.49	0
7	BMA	X	3	7	11,11,12	0.83	0	15,15,17	0.95	0
7	MAN	X	4	7	11,11,12	0.65	0	15,15,17	1.07	2 (13%)
7	MAN	X	5	7	11,11,12	0.71	0	15,15,17	1.00	2 (13%)
7	MAN	X	6	7	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
5	NAG	Y	1	1,5	14,14,15	0.41	0	17,19,21	0.92	2 (11%)
5	NAG	Y	2	5	14,14,15	0.23	0	17,19,21	0.52	0
5	NAG	Z	1	1,5	14,14,15	0.50	0	17,19,21	0.61	0
5	NAG	Z	2	5	14,14,15	0.28	0	17,19,21	0.39	0
6	NAG	a	1	1,6	14,14,15	0.28	0	17,19,21	0.43	0
6	NAG	a	2	6	14,14,15	0.30	0	17,19,21	0.50	0
6	BMA	a	3	6	11,11,12	0.70	0	15,15,17	0.75	0
6	MAN	a	4	6	11,11,12	0.70	0	15,15,17	1.07	2 (13%)
5	NAG	b	1	1,5	14,14,15	0.60	0	17,19,21	1.27	1 (5%)
5	NAG	b	2	5	14,14,15	0.39	0	17,19,21	0.33	0
5	NAG	c	1	1,5	14,14,15	0.29	0	17,19,21	0.74	1 (5%)
5	NAG	c	2	5	14,14,15	0.25	0	17,19,21	0.47	0
7	NAG	d	1	7,1	14,14,15	0.25	0	17,19,21	0.54	0
7	NAG	d	2	7	14,14,15	0.21	0	17,19,21	0.48	0
7	BMA	d	3	7	11,11,12	0.86	0	15,15,17	0.78	0
7	MAN	d	4	7	11,11,12	0.62	0	15,15,17	1.03	2 (13%)
7	MAN	d	5	7	11,11,12	0.77	0	15,15,17	0.85	1 (6%)
7	MAN	d	6	7	11,11,12	0.72	0	15,15,17	1.06	2 (13%)

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
5	NAG	M	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
6	NAG	O	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	MAN	O	4	6	-	0/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	NAG	Q	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
7	NAG	R	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	R	2	7	-	2/6/23/26	0/1/1/1
7	BMA	R	3	7	-	1/2/19/22	0/1/1/1
7	MAN	R	4	7	-	0/2/19/22	0/1/1/1
7	MAN	R	5	7	-	0/2/19/22	0/1/1/1
7	MAN	R	6	7	-	0/2/19/22	0/1/1/1
5	NAG	S	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	S	2	5	-	0/6/23/26	0/1/1/1
5	NAG	T	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
6	NAG	U	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	U	2	6	-	2/6/23/26	0/1/1/1
6	BMA	U	3	6	-	0/2/19/22	0/1/1/1
6	MAN	U	4	6	-	0/2/19/22	0/1/1/1
5	NAG	V	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	V	2	5	-	1/6/23/26	0/1/1/1
5	NAG	W	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
7	NAG	X	1	7,1	-	3/6/23/26	0/1/1/1
7	NAG	X	2	7	-	0/6/23/26	0/1/1/1
7	BMA	X	3	7	-	1/2/19/22	0/1/1/1
7	MAN	X	4	7	-	2/2/19/22	0/1/1/1
7	MAN	X	5	7	-	2/2/19/22	0/1/1/1
7	MAN	X	6	7	-	1/2/19/22	0/1/1/1
5	NAG	Y	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	NAG	Z	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	a	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	BMA	a	3	6	-	1/2/19/22	0/1/1/1
6	MAN	a	4	6	-	0/2/19/22	0/1/1/1
5	NAG	b	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	1/6/23/26	0/1/1/1
5	NAG	c	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
7	NAG	d	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	d	2	7	-	2/6/23/26	0/1/1/1
7	BMA	d	3	7	-	2/2/19/22	0/1/1/1
7	MAN	d	4	7	-	0/2/19/22	0/1/1/1
7	MAN	d	5	7	-	0/2/19/22	0/1/1/1
7	MAN	d	6	7	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	1	NAG	O5-C1	-2.33	1.40	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	1	NAG	C1-O5-C5	4.75	118.62	112.19
7	R	4	MAN	C1-O5-C5	3.00	116.26	112.19
7	X	4	MAN	C1-O5-C5	2.78	115.97	112.19
6	a	4	MAN	C1-O5-C5	2.72	115.88	112.19
6	U	4	MAN	C1-O5-C5	2.70	115.84	112.19
7	R	6	MAN	C1-O5-C5	2.62	115.74	112.19
7	d	6	MAN	C1-O5-C5	2.56	115.67	112.19
5	M	1	NAG	C1-O5-C5	2.55	115.64	112.19
6	O	4	MAN	C1-O5-C5	2.54	115.63	112.19
7	d	4	MAN	C1-O5-C5	2.46	115.52	112.19
5	S	1	NAG	C1-O5-C5	2.43	115.49	112.19
7	X	6	MAN	C1-O5-C5	2.40	115.44	112.19
7	X	5	MAN	C1-O5-C5	2.28	115.28	112.19
5	Y	1	NAG	C1-O5-C5	2.27	115.27	112.19
7	X	6	MAN	O2-C2-C3	-2.26	105.60	110.14
7	R	5	MAN	O2-C2-C3	-2.24	105.65	110.14
7	X	4	MAN	O2-C2-C3	-2.24	105.66	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	4	MAN	O2-C2-C3	-2.23	105.68	110.14
7	X	5	MAN	O2-C2-C3	-2.22	105.68	110.14
7	d	5	MAN	O2-C2-C3	-2.21	105.71	110.14
7	d	6	MAN	O2-C2-C3	-2.21	105.72	110.14
7	R	6	MAN	O2-C2-C3	-2.21	105.72	110.14
7	d	4	MAN	O2-C2-C3	-2.20	105.74	110.14
6	a	4	MAN	O2-C2-C3	-2.19	105.75	110.14
7	X	1	NAG	O4-C4-C5	-2.18	103.88	109.30
6	O	4	MAN	O2-C2-C3	-2.18	105.76	110.14
7	R	4	MAN	O2-C2-C3	-2.17	105.79	110.14
5	W	1	NAG	C2-N2-C7	2.13	125.94	122.90
5	c	1	NAG	C2-N2-C7	2.13	125.93	122.90
7	X	1	NAG	C2-N2-C7	2.12	125.92	122.90
5	Y	1	NAG	C2-N2-C7	2.11	125.91	122.90
7	R	3	BMA	O2-C2-C3	-2.09	105.95	110.14
5	S	1	NAG	C2-N2-C7	2.08	125.86	122.90
5	Q	1	NAG	C2-N2-C7	2.08	125.86	122.90
5	M	1	NAG	C2-N2-C7	2.07	125.86	122.90

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	2	NAG	O5-C5-C6-O6
7	X	1	NAG	O5-C5-C6-O6
7	X	5	MAN	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6
7	d	3	BMA	O5-C5-C6-O6
5	Q	2	NAG	C4-C5-C6-O6
7	X	1	NAG	C4-C5-C6-O6
7	X	5	MAN	C4-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
5	Y	1	NAG	C4-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6
6	a	1	NAG	O5-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6

Continued on next page...



*Continued from previous page...*

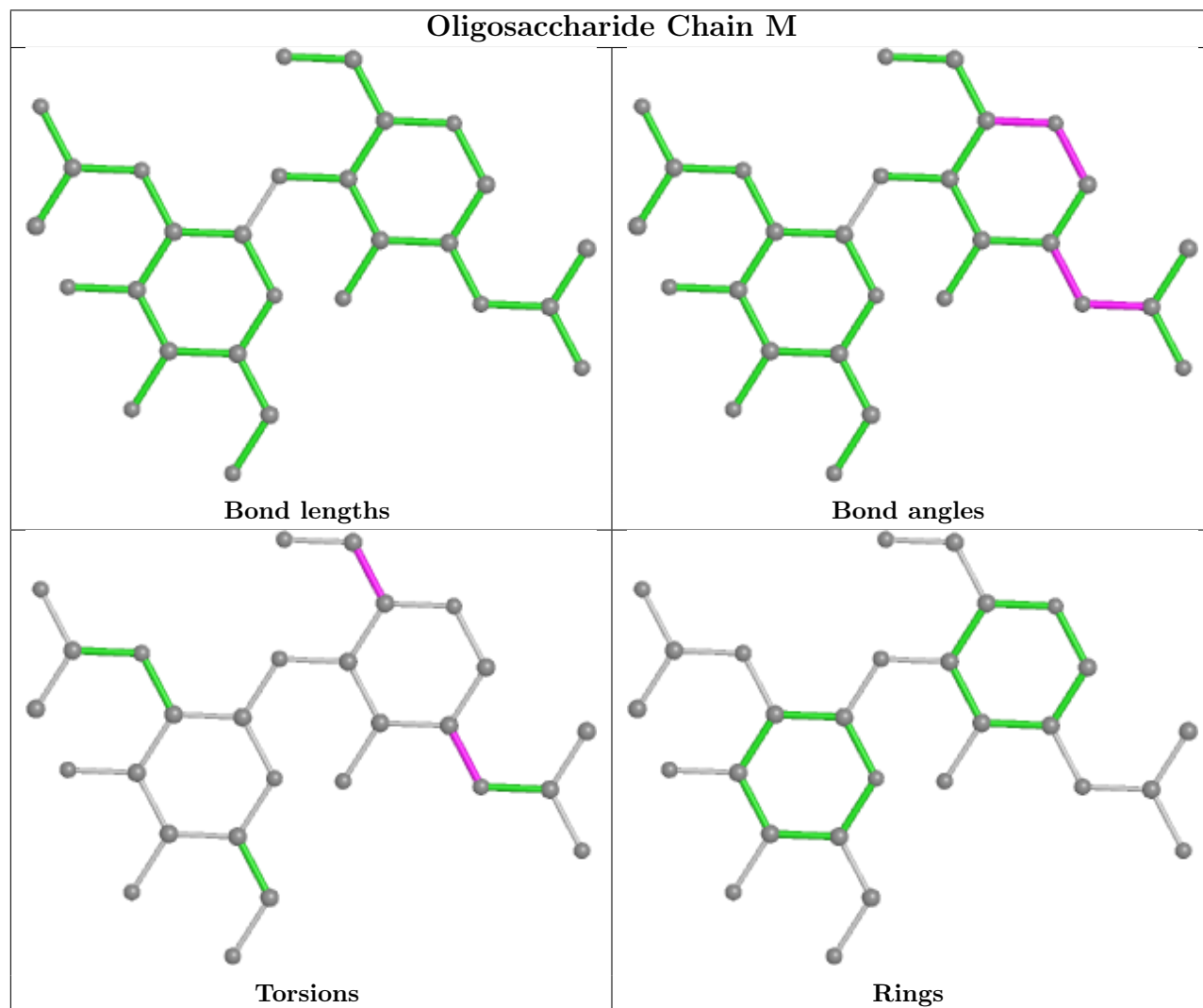
Mol	Chain	Res	Type	Atoms
6	a	1	NAG	C4-C5-C6-O6
7	d	1	NAG	C8-C7-N2-C2
7	d	1	NAG	O7-C7-N2-C2
5	c	1	NAG	O5-C5-C6-O6
5	c	2	NAG	C4-C5-C6-O6
5	W	2	NAG	C4-C5-C6-O6
6	O	1	NAG	C4-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
7	d	2	NAG	C4-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
7	R	2	NAG	C4-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
7	d	3	BMA	C4-C5-C6-O6
7	d	2	NAG	O5-C5-C6-O6
6	a	2	NAG	C4-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
6	U	1	NAG	O5-C5-C6-O6
7	R	3	BMA	O5-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
6	a	3	BMA	O5-C5-C6-O6
7	X	3	BMA	O5-C5-C6-O6
7	X	6	MAN	O5-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
5	Z	1	NAG	C4-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
5	M	1	NAG	C3-C2-N2-C7
5	Q	1	NAG	C3-C2-N2-C7
5	c	1	NAG	C3-C2-N2-C7
7	R	1	NAG	C3-C2-N2-C7
7	X	1	NAG	C3-C2-N2-C7
5	Z	1	NAG	O5-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	S	1	NAG	C3-C2-N2-C7
5	W	1	NAG	C3-C2-N2-C7
5	Y	1	NAG	C3-C2-N2-C7
7	X	4	MAN	C4-C5-C6-O6
7	X	4	MAN	O5-C5-C6-O6

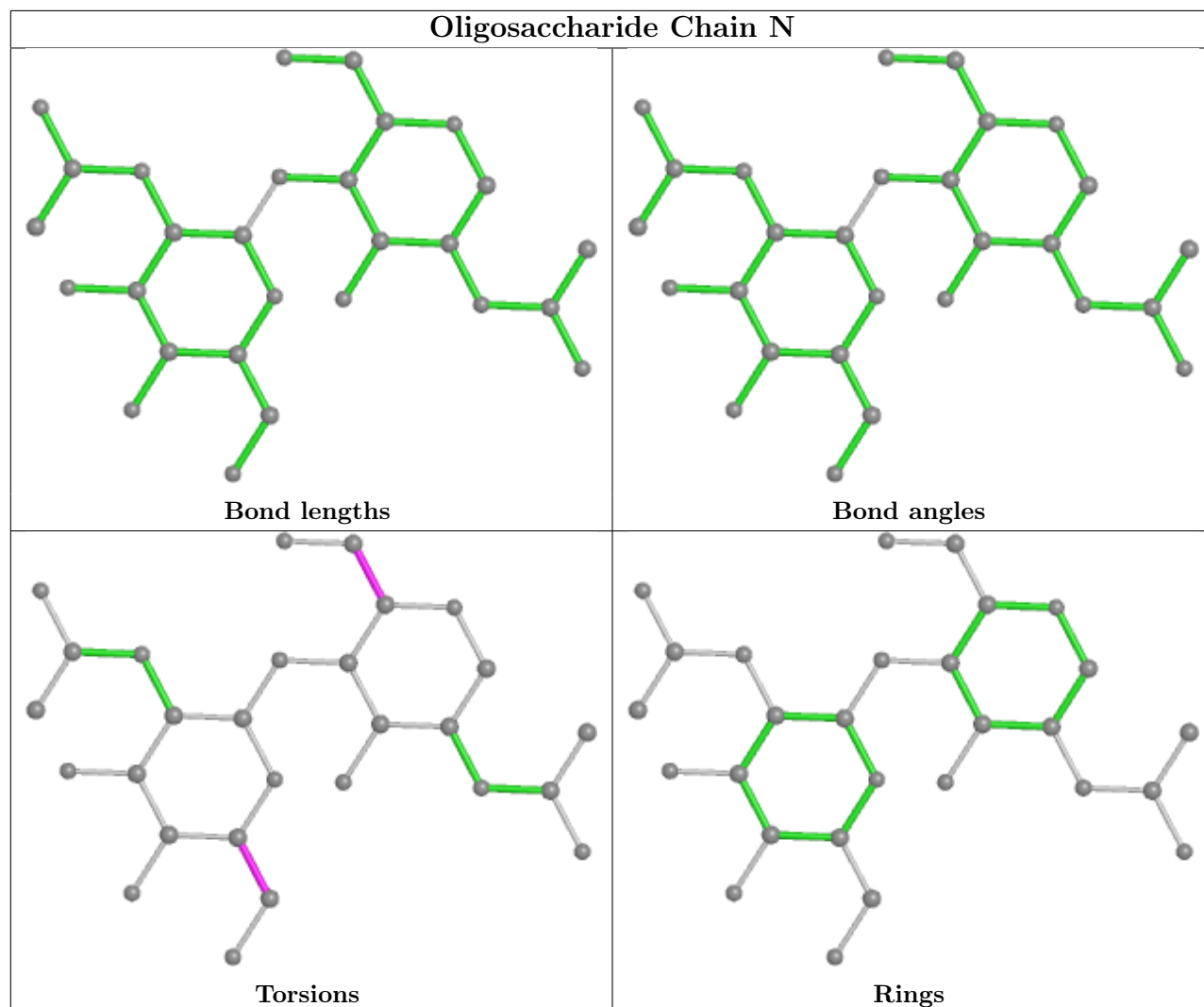
There are no ring outliers.

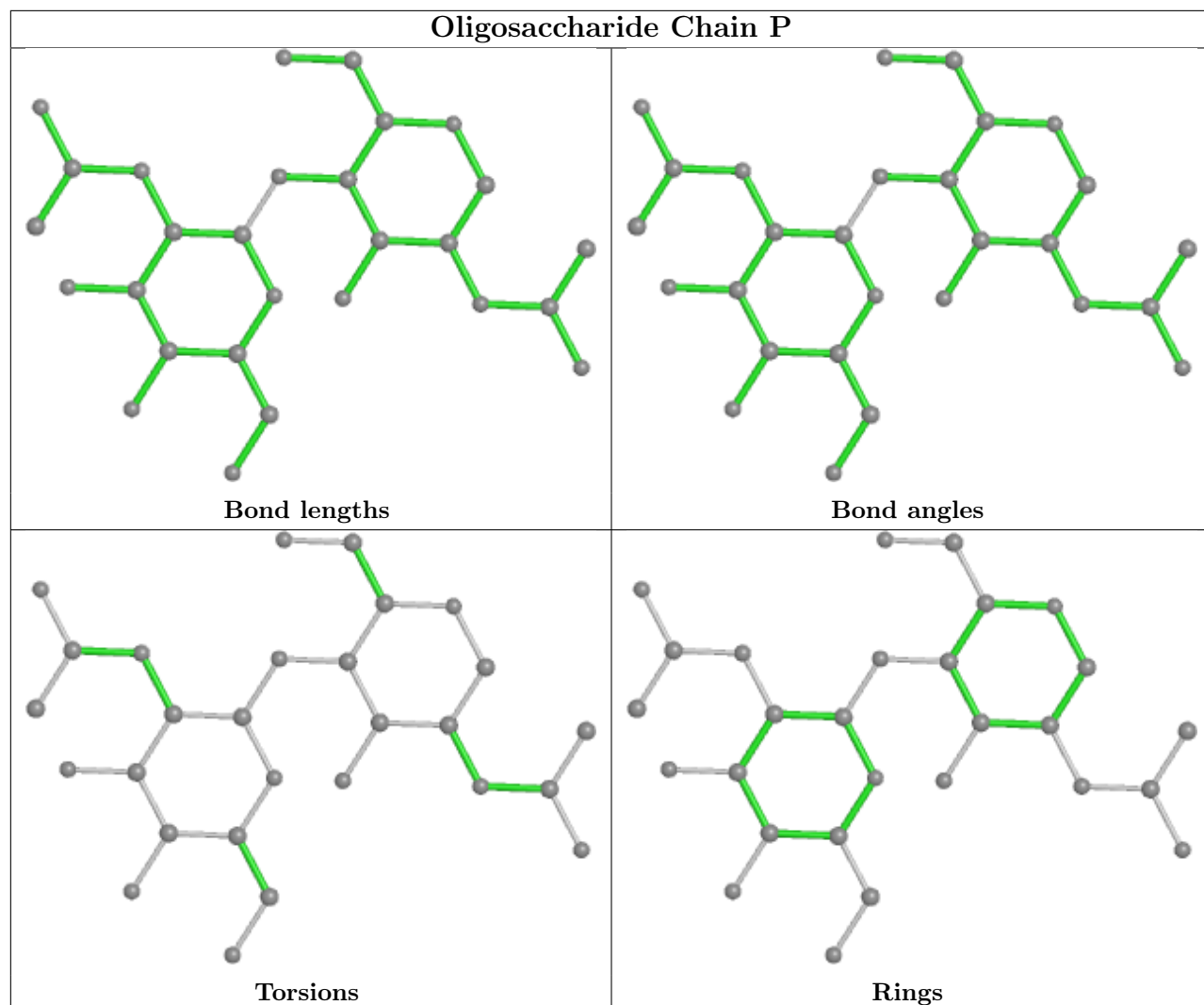
3 monomers are involved in 2 short contacts:

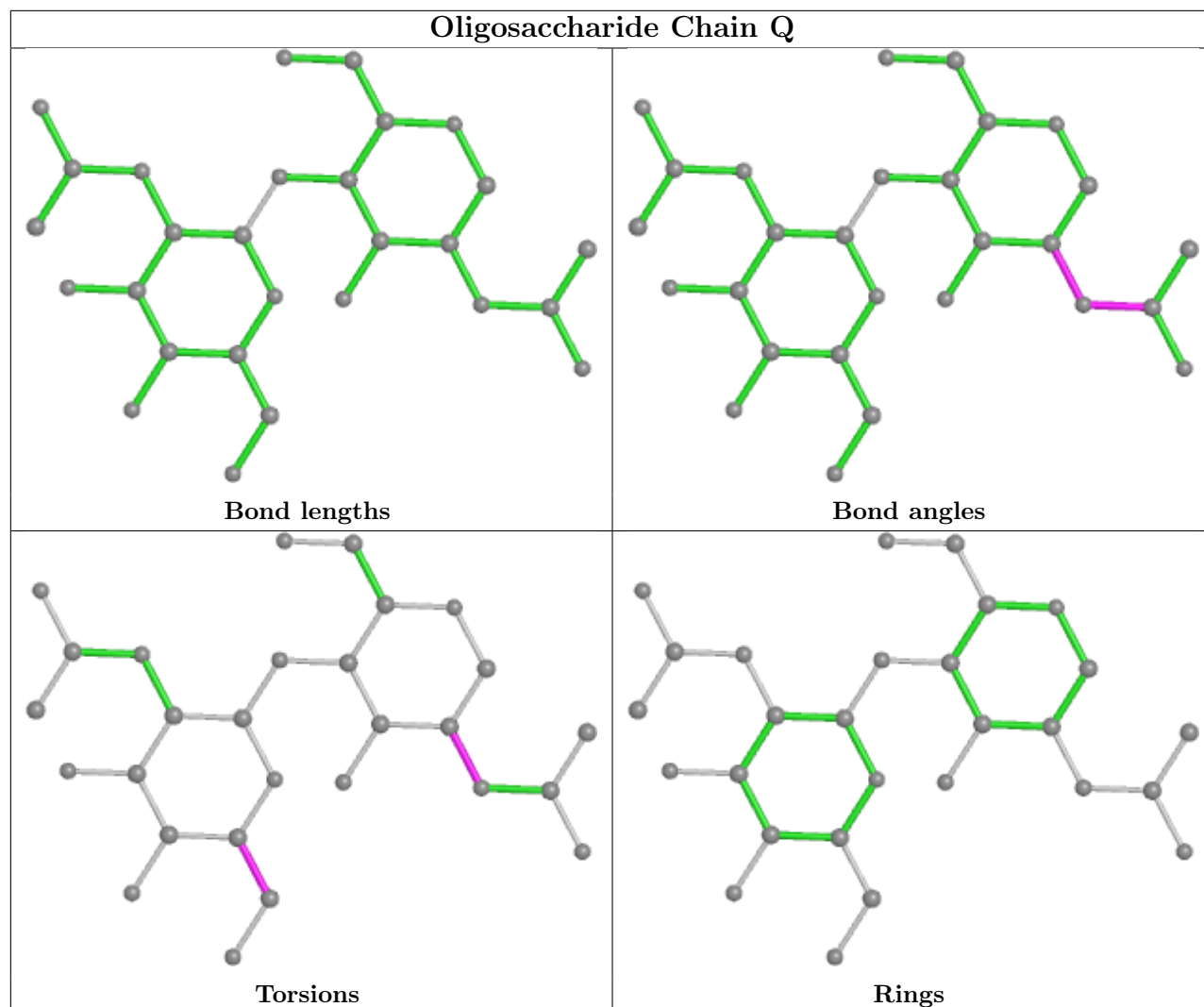
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	3	BMA	1	0
6	U	1	NAG	1	0
5	W	1	NAG	1	0

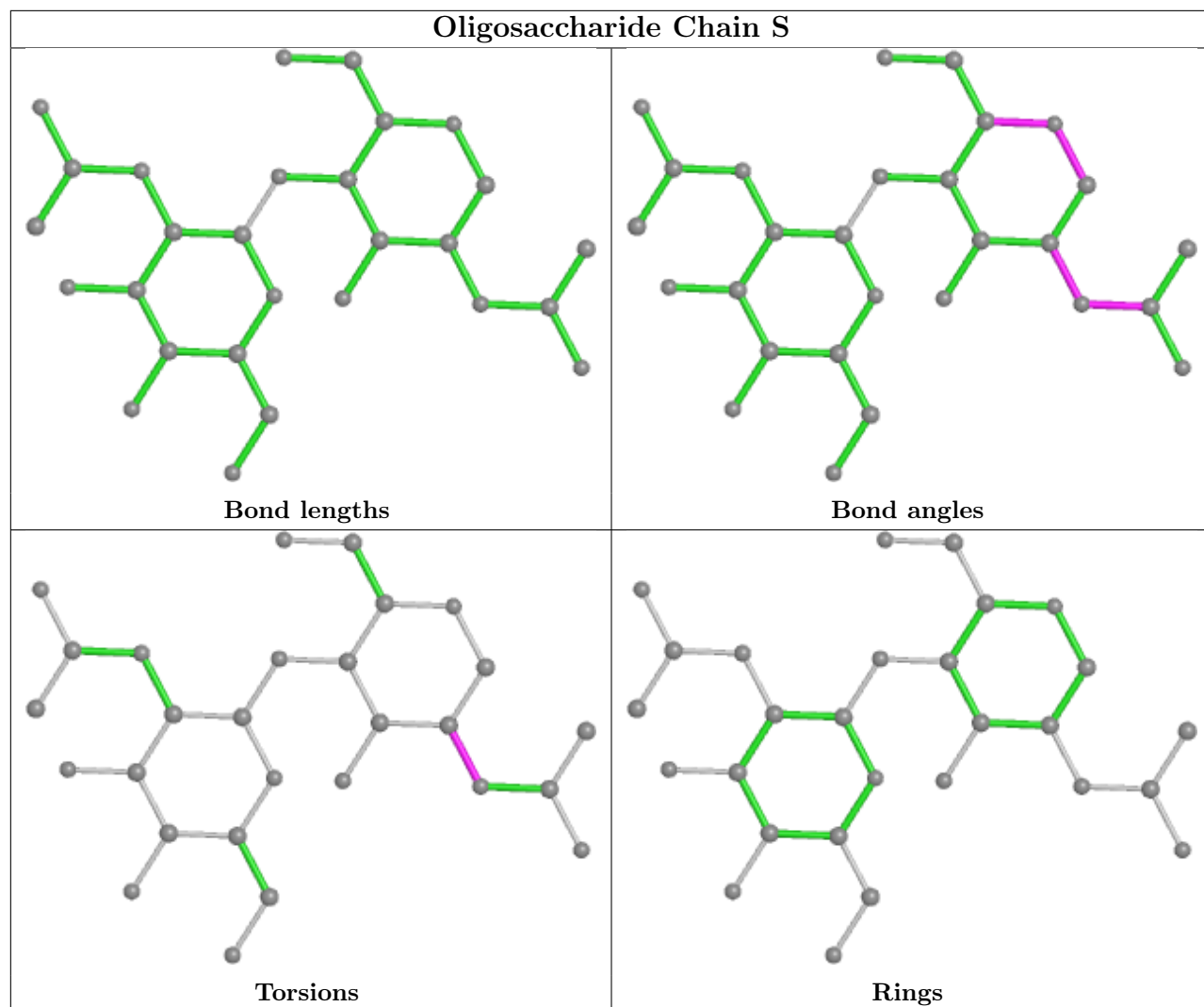
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

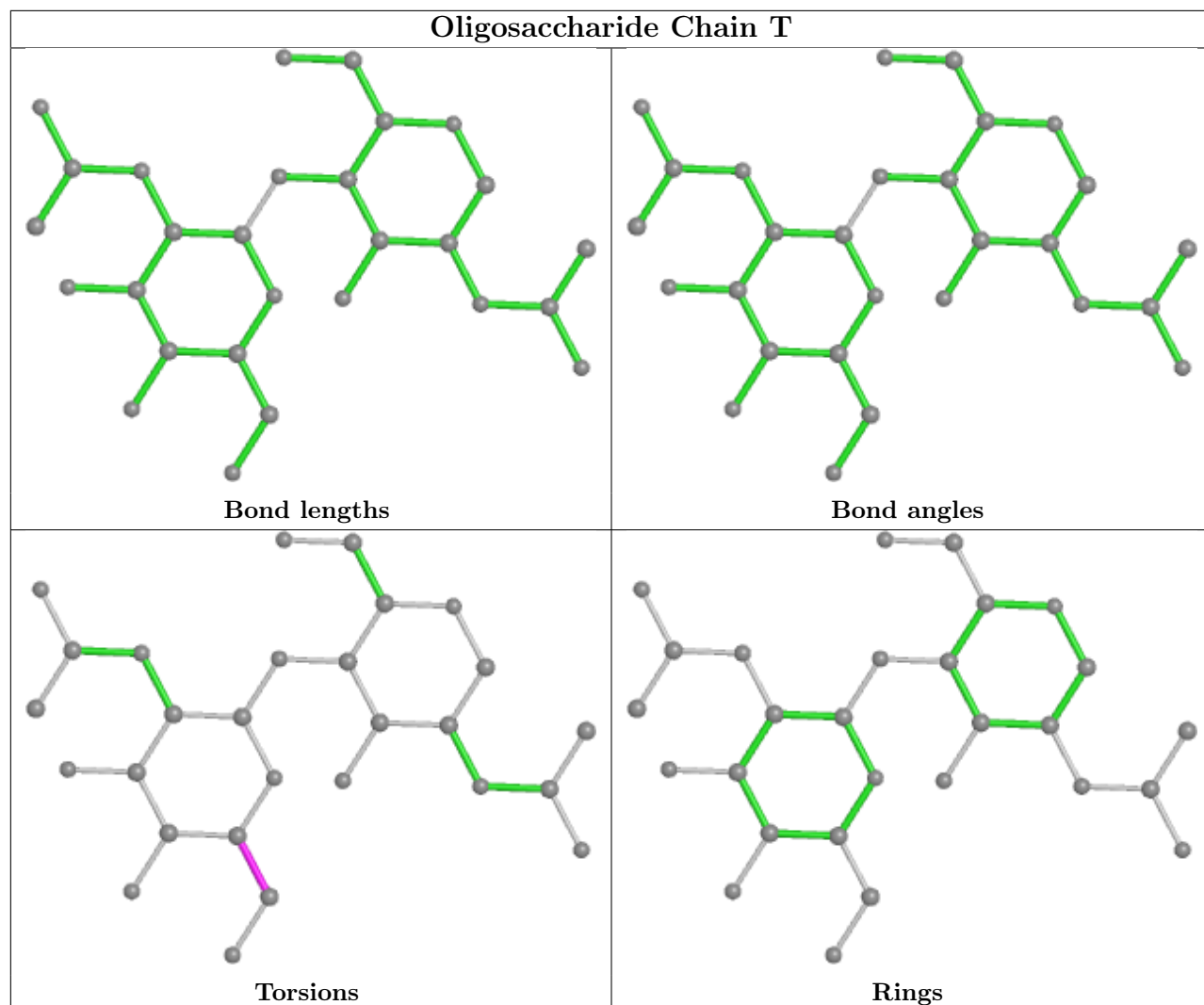


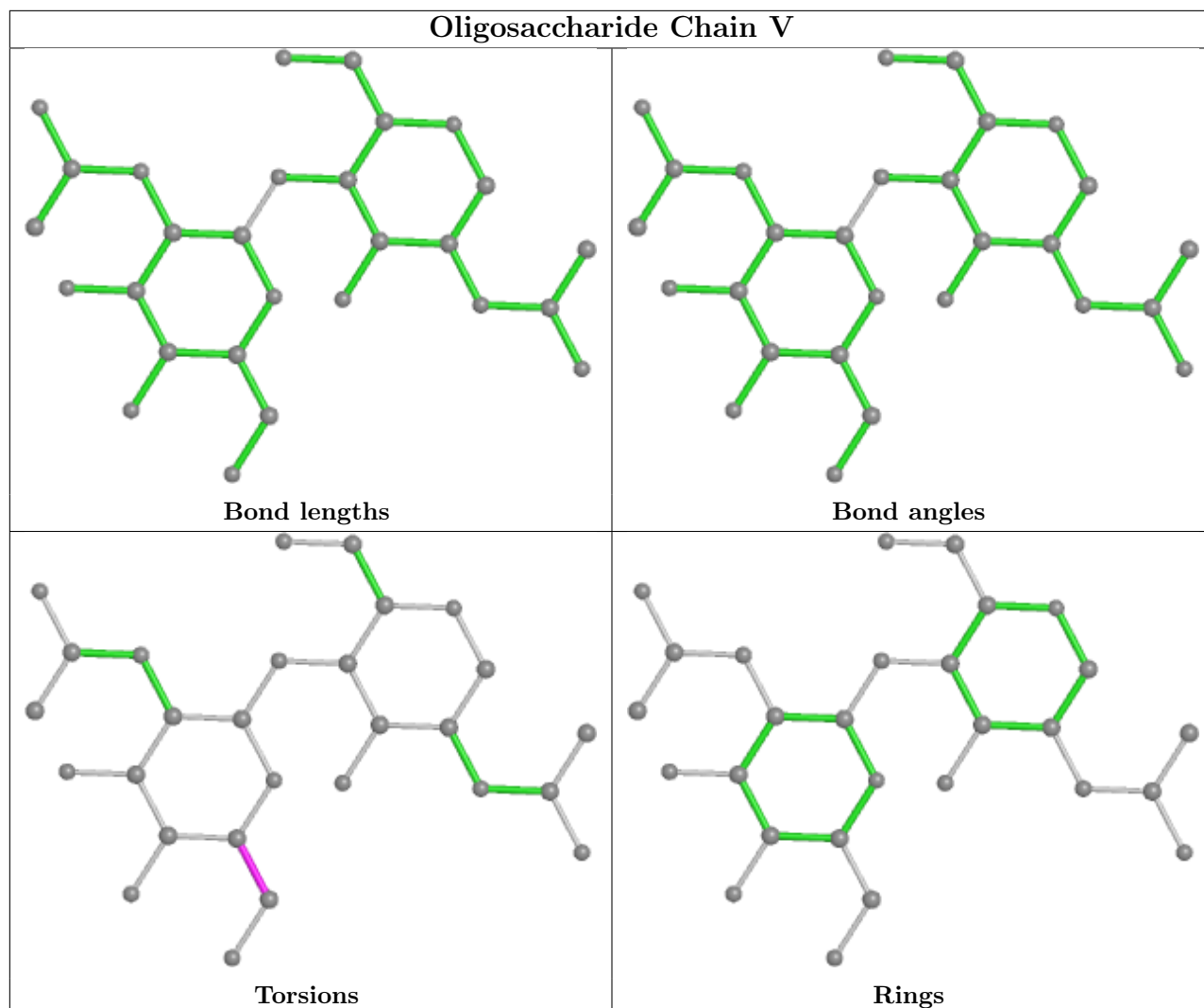




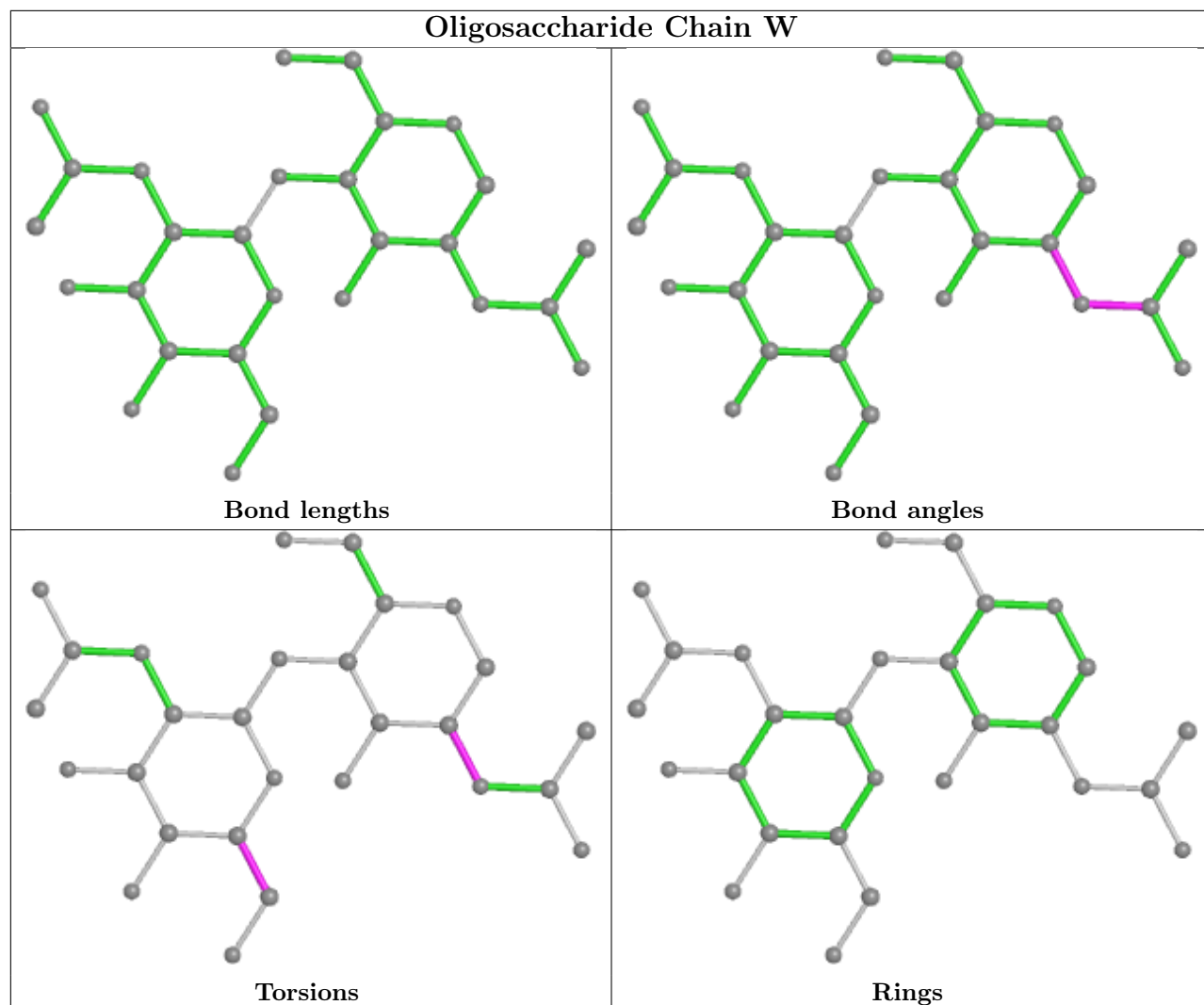


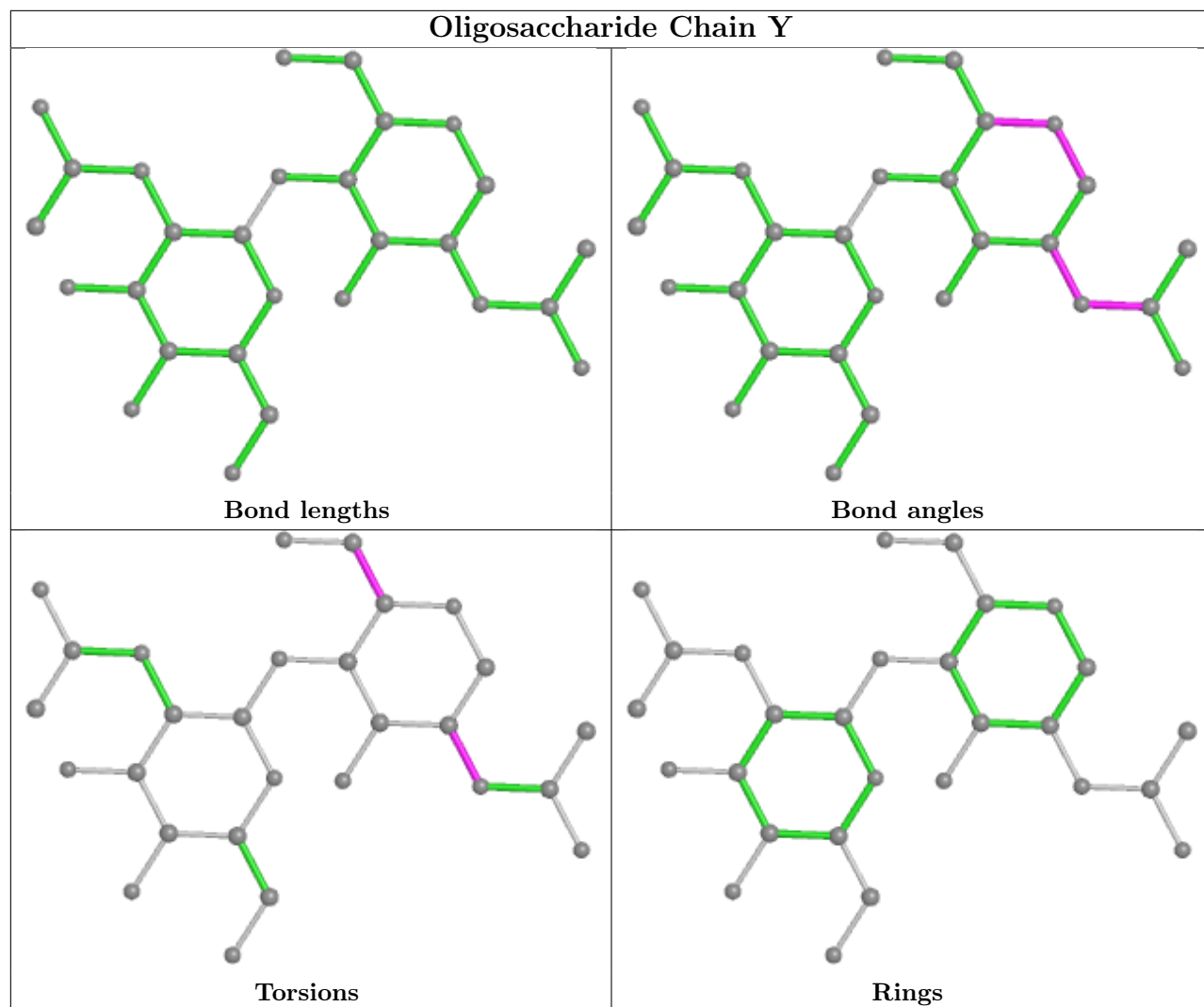


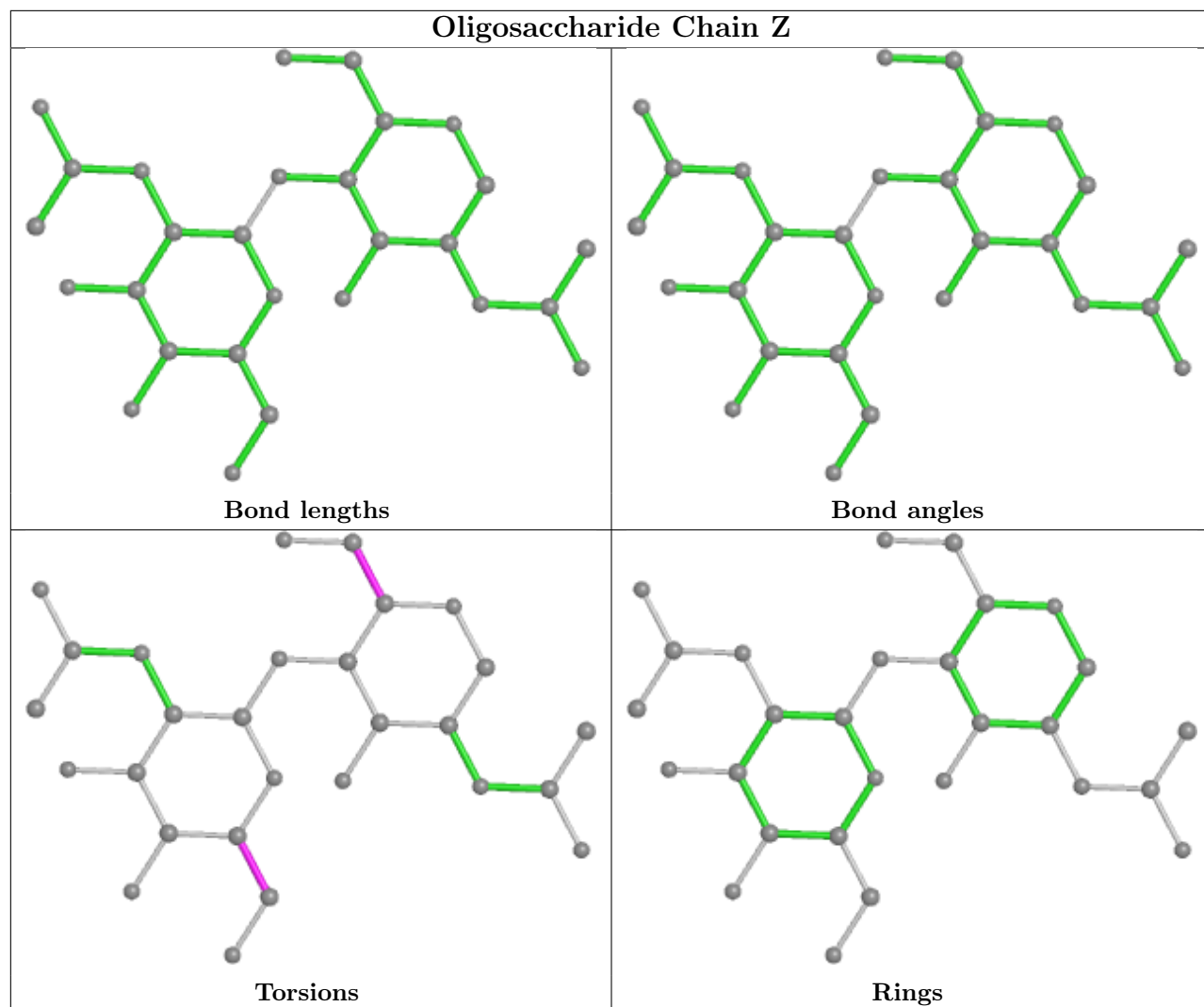


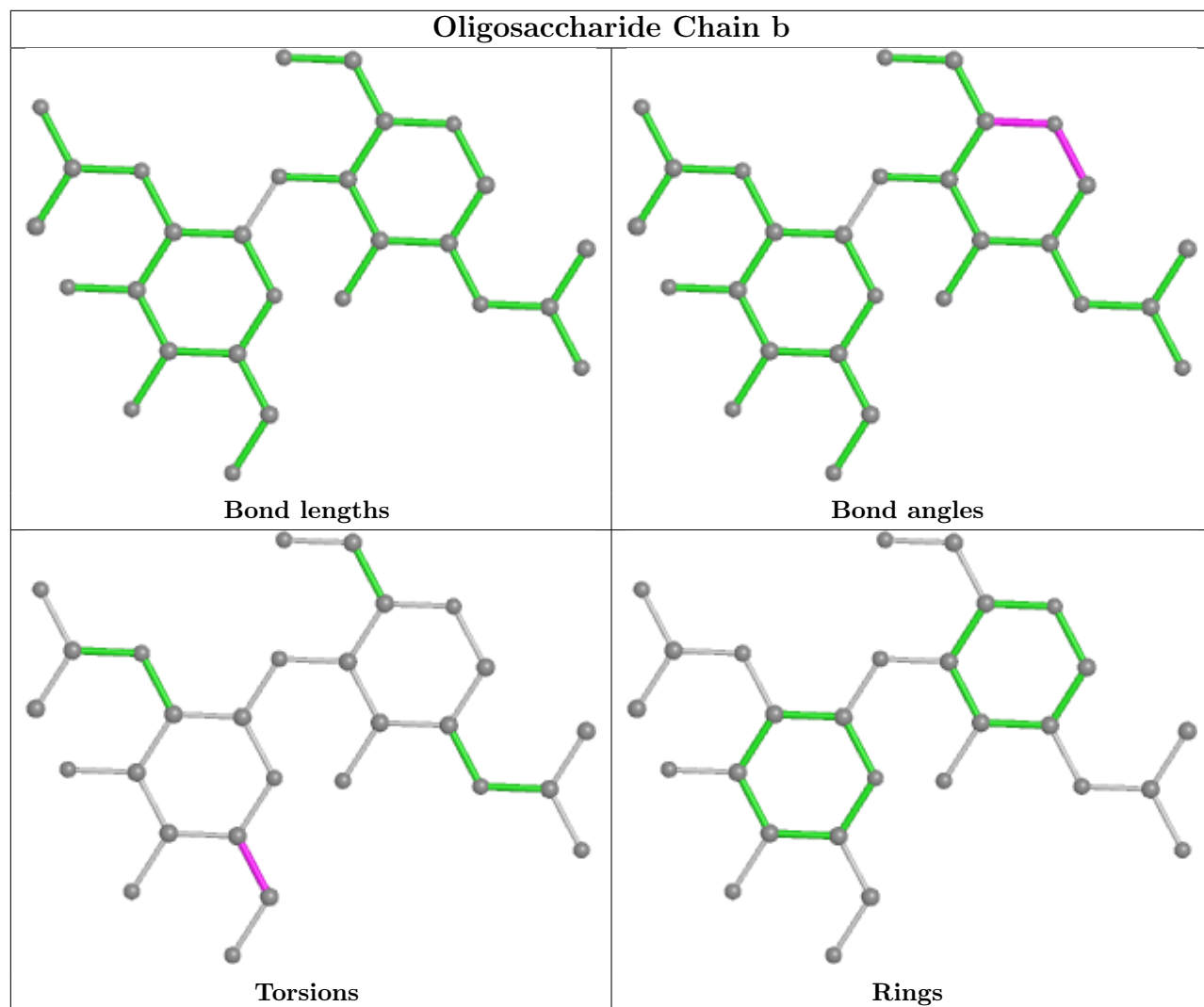


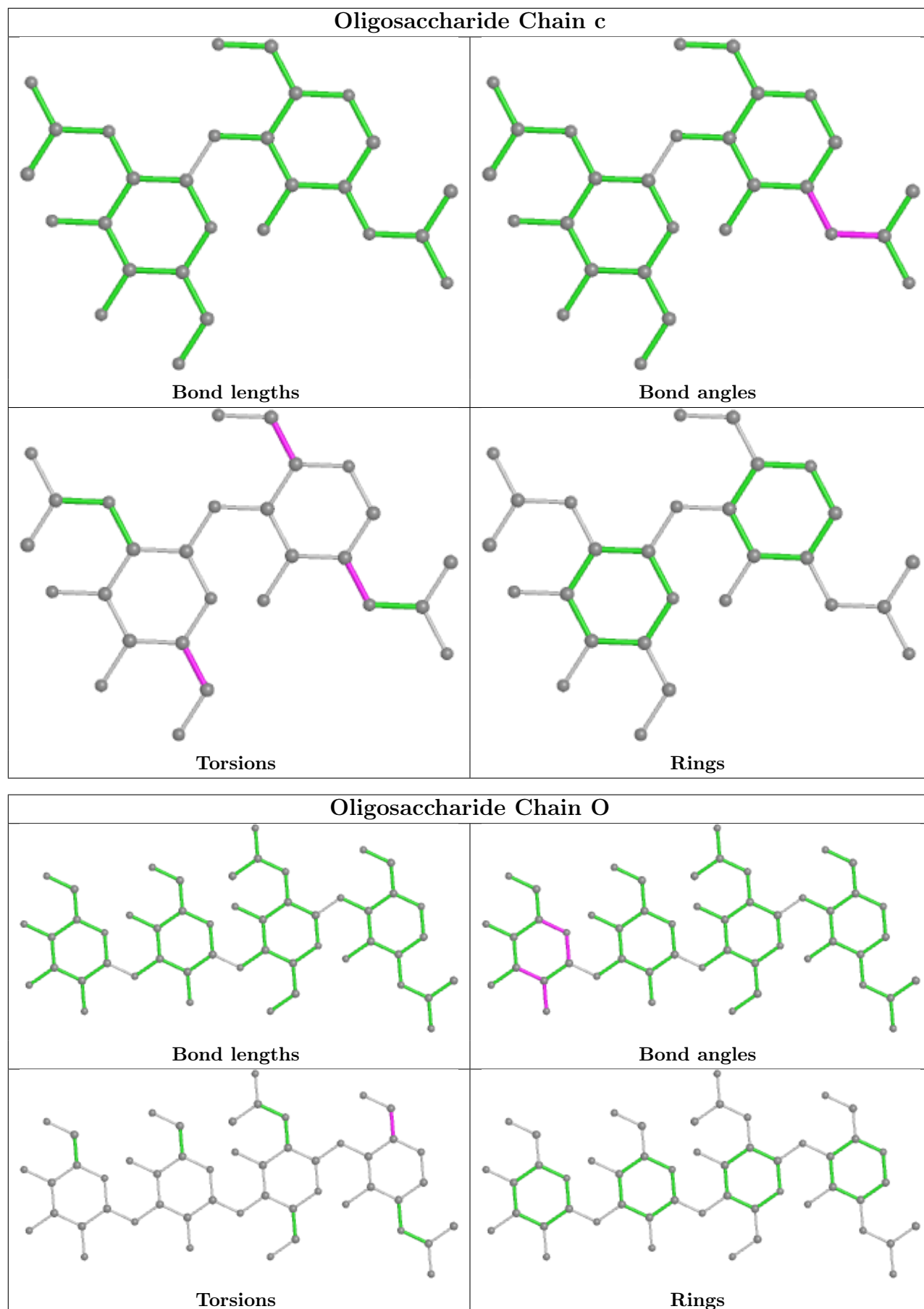


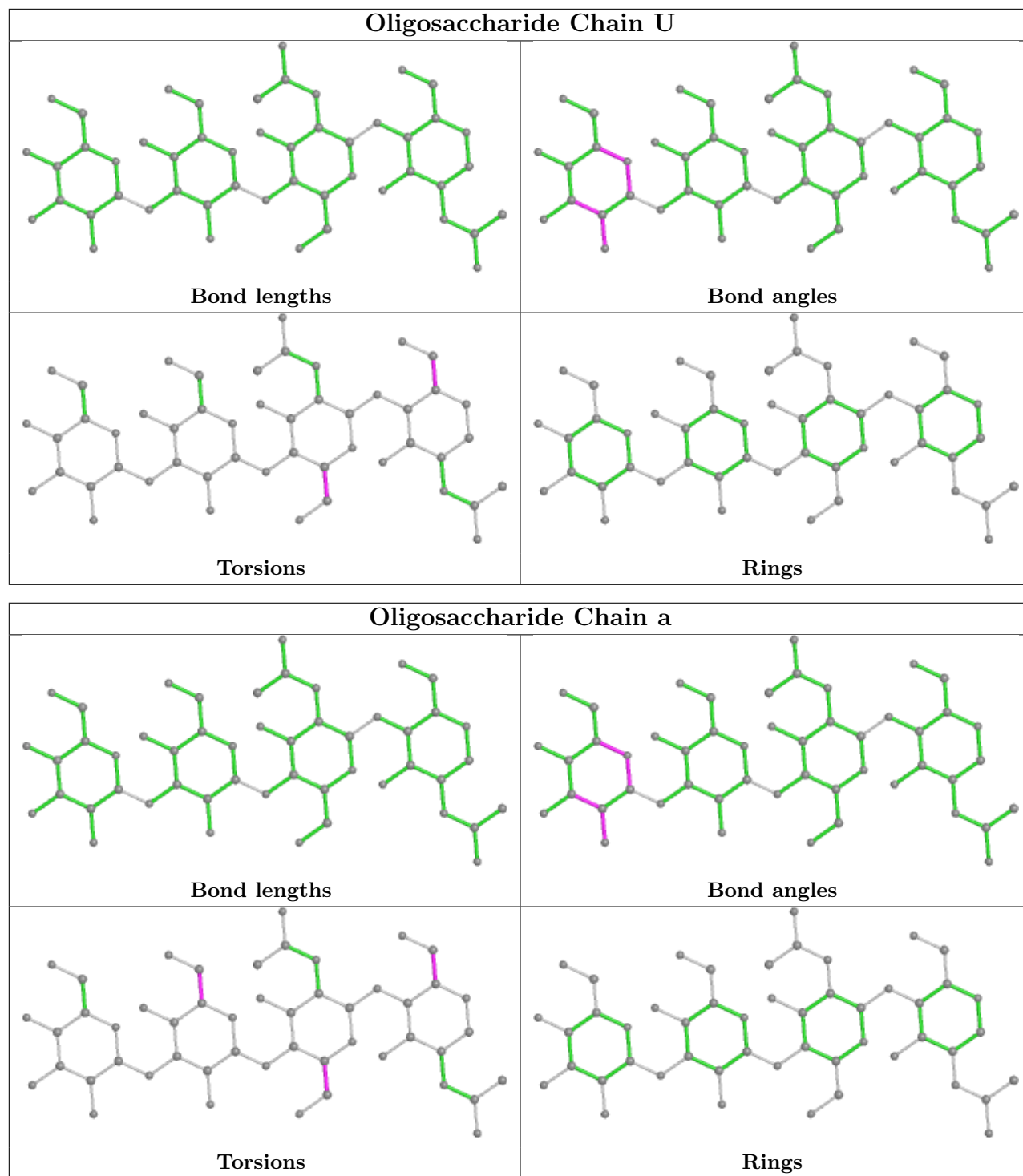


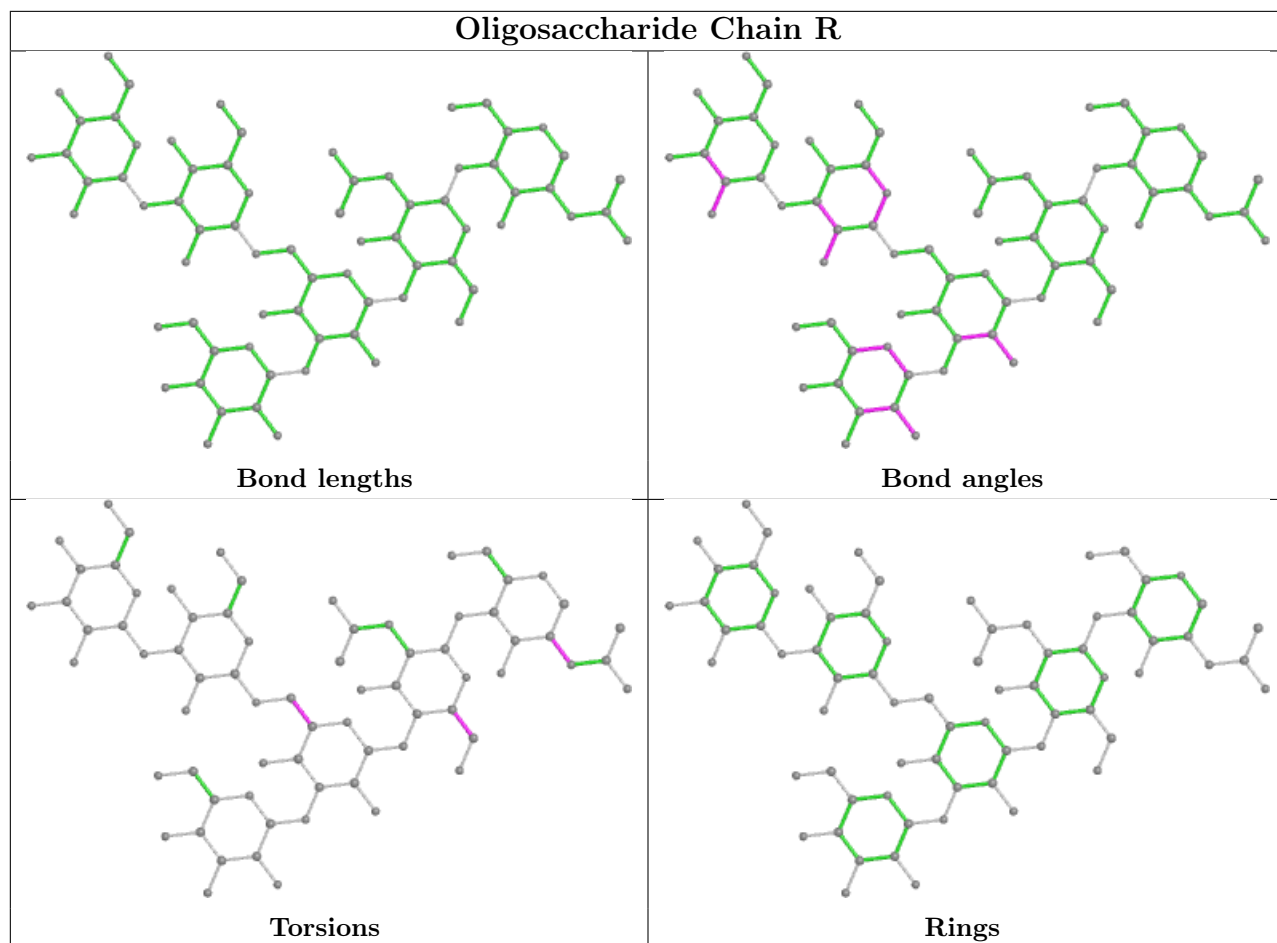


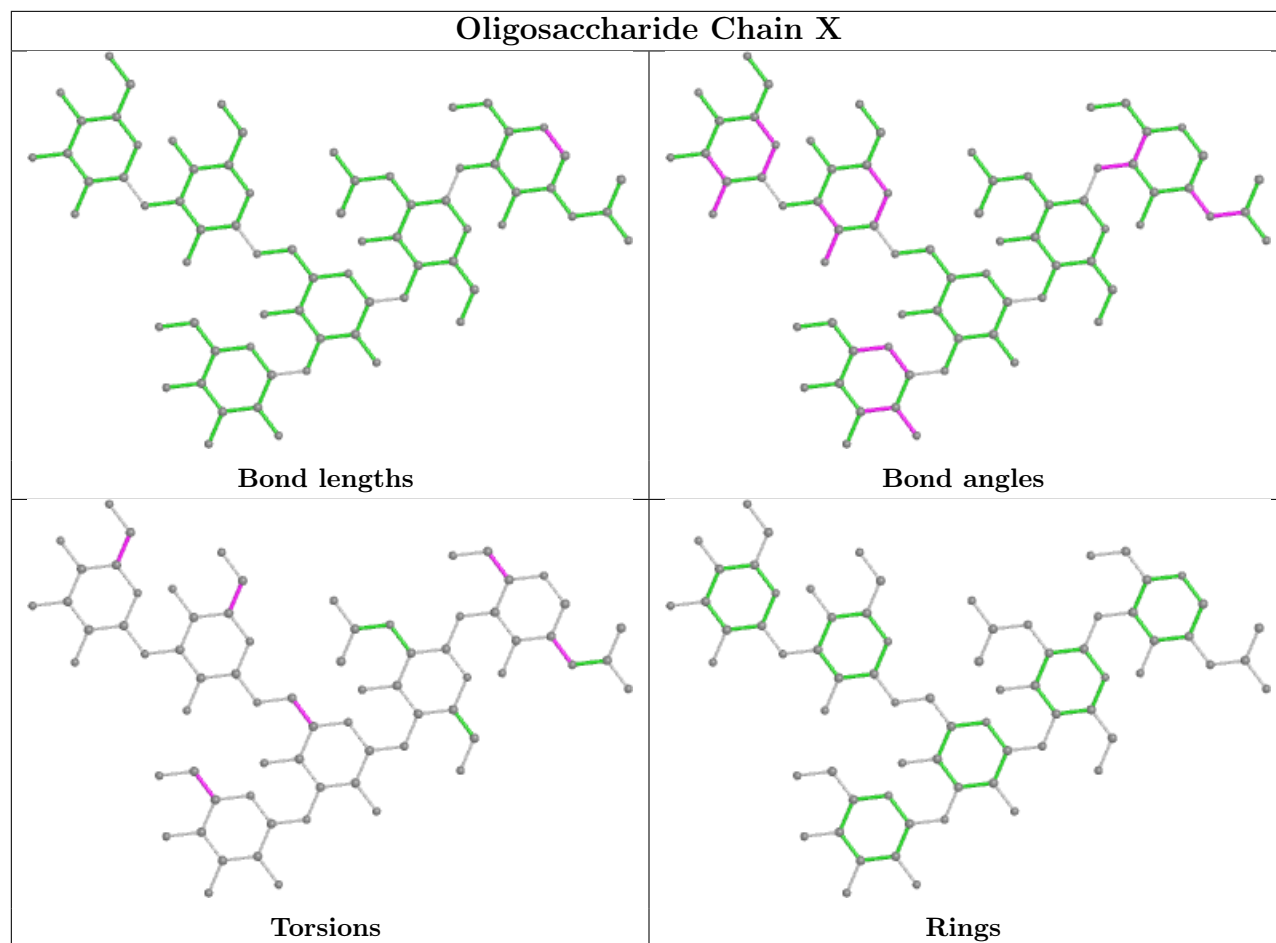




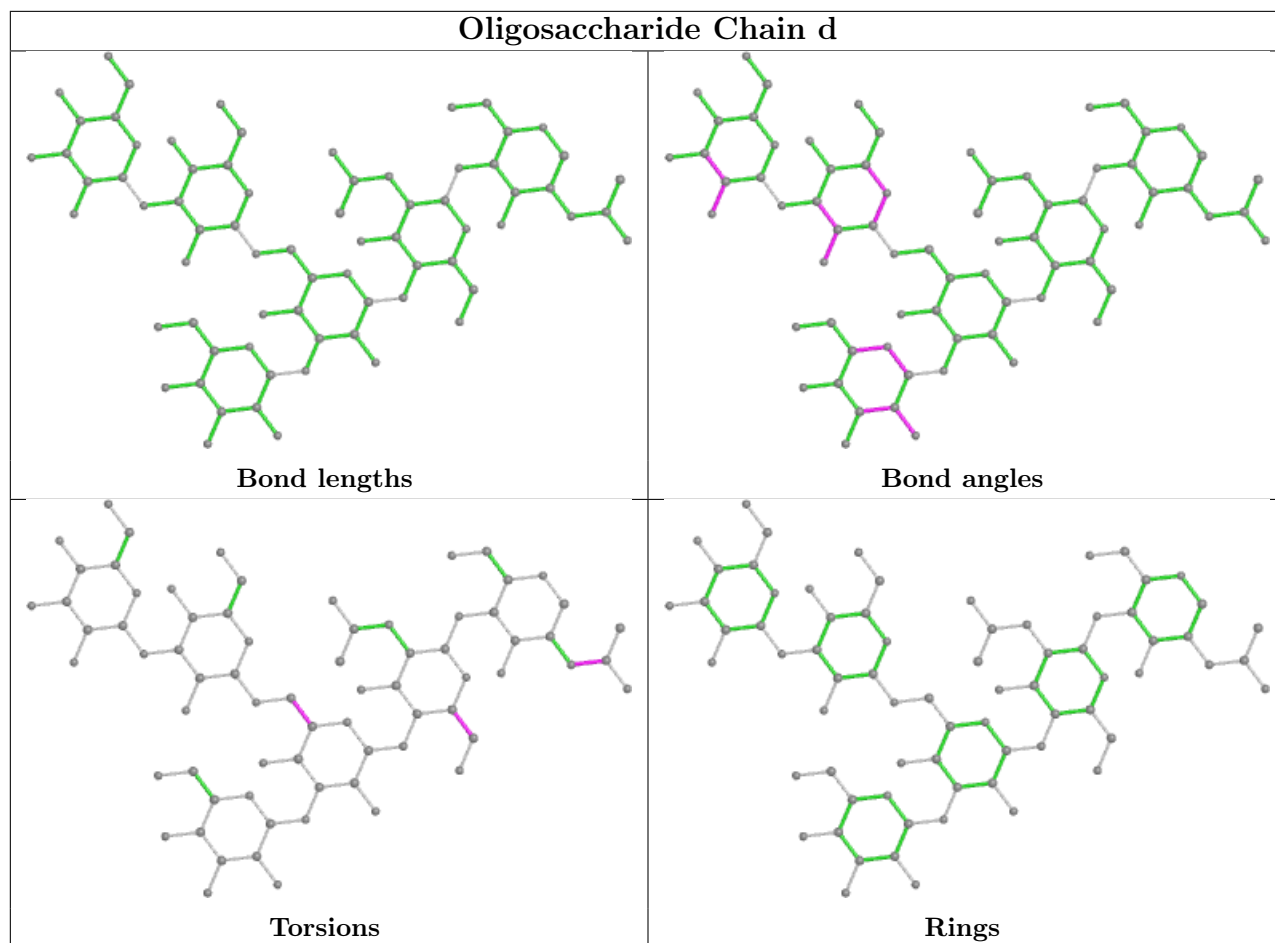












## 5.6 Ligand geometry [i](#)

46 ligands 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
8	NAG	A	605	1	14,14,15	0.28	0	17,19,21	0.41	0
8	NAG	A	601	1	14,14,15	0.25	0	17,19,21	0.42	0
8	NAG	C	704	2	14,14,15	0.50	0	17,19,21	0.45	0
8	NAG	G	602	1	14,14,15	0.31	0	17,19,21	0.42	0
8	NAG	I	703	2	14,14,15	0.26	0	17,19,21	0.47	0
8	NAG	I	701	-	14,14,15	0.45	0	17,19,21	0.36	0
8	NAG	F	608	1	14,14,15	0.25	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	G	606	1	14,14,15	0.25	0	17,19,21	0.45	0
8	NAG	G	610	1	14,14,15	0.23	0	17,19,21	0.48	0
8	NAG	F	607	1	14,14,15	0.23	0	17,19,21	0.45	0
8	NAG	G	608	1	14,14,15	0.23	0	17,19,21	0.42	0
8	NAG	A	612	1	14,14,15	0.29	0	17,19,21	0.46	0
8	NAG	F	610	1	14,14,15	0.24	0	17,19,21	0.47	0
8	NAG	A	606	1	14,14,15	0.25	0	17,19,21	0.44	0
8	NAG	B	703	2	14,14,15	0.28	0	17,19,21	0.46	0
8	NAG	A	608	1	14,14,15	0.26	0	17,19,21	0.45	0
8	NAG	A	602	1	14,14,15	0.29	0	17,19,21	0.43	0
8	NAG	F	602	1	14,14,15	0.28	0	17,19,21	0.42	0
8	NAG	F	603	1	14,14,15	0.27	0	17,19,21	0.48	0
8	NAG	C	703	2	14,14,15	0.25	0	17,19,21	0.43	0
8	NAG	A	611	1	14,14,15	0.45	0	17,19,21	0.76	1 (5%)
8	NAG	A	607	1	14,14,15	0.25	0	17,19,21	0.43	0
8	NAG	G	612	1	14,14,15	0.33	0	17,19,21	0.45	0
8	NAG	A	610	1	14,14,15	0.40	0	17,19,21	0.37	0
8	NAG	F	601	1	14,14,15	0.27	0	17,19,21	0.41	0
8	NAG	A	603	1	14,14,15	0.30	0	17,19,21	0.48	0
8	NAG	F	604	1	14,14,15	0.23	0	17,19,21	0.48	0
8	NAG	B	702	2	14,14,15	0.23	0	17,19,21	0.45	0
8	NAG	G	609	1	14,14,15	0.58	0	17,19,21	0.89	1 (5%)
8	NAG	A	604	1	14,14,15	0.27	0	17,19,21	0.46	0
8	NAG	G	611	1	14,14,15	0.41	0	17,19,21	0.74	1 (5%)
8	NAG	F	611	1	14,14,15	0.33	0	17,19,21	0.46	0
8	NAG	G	605	1	14,14,15	0.26	0	17,19,21	0.42	0
8	NAG	G	607	1	14,14,15	0.26	0	17,19,21	0.44	0
8	NAG	C	702	2	14,14,15	0.48	0	17,19,21	0.44	0
8	NAG	F	609	1	14,14,15	0.26	0	17,19,21	0.38	0
8	NAG	F	605	1	14,14,15	0.24	0	17,19,21	0.45	0
8	NAG	B	701	2	14,14,15	0.37	0	17,19,21	0.35	0
9	SO4	A	613	-	4,4,4	0.14	0	6,6,6	0.04	0
8	NAG	G	601	1	14,14,15	0.30	0	17,19,21	0.44	0
8	NAG	C	701	2	14,14,15	0.23	0	17,19,21	0.45	0
8	NAG	G	603	1	14,14,15	0.30	0	17,19,21	0.55	0
8	NAG	G	604	1	14,14,15	0.21	0	17,19,21	0.45	0
8	NAG	F	606	1	14,14,15	0.23	0	17,19,21	0.42	0
8	NAG	I	702	2	14,14,15	0.31	0	17,19,21	0.50	0
8	NAG	A	609	1	14,14,15	0.31	0	17,19,21	0.41	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
8	NAG	A	605	1	-	1/6/23/26	0/1/1/1
8	NAG	A	601	1	-	2/6/23/26	0/1/1/1
8	NAG	C	704	2	-	2/6/23/26	0/1/1/1
8	NAG	G	602	1	-	1/6/23/26	0/1/1/1
8	NAG	I	703	2	-	2/6/23/26	0/1/1/1
8	NAG	I	701	-	-	2/6/23/26	0/1/1/1
8	NAG	F	608	1	-	1/6/23/26	0/1/1/1
8	NAG	G	606	1	-	2/6/23/26	0/1/1/1
8	NAG	G	610	1	-	4/6/23/26	0/1/1/1
8	NAG	F	607	1	-	2/6/23/26	0/1/1/1
8	NAG	G	608	1	-	1/6/23/26	0/1/1/1
8	NAG	A	612	1	-	0/6/23/26	0/1/1/1
8	NAG	F	610	1	-	4/6/23/26	0/1/1/1
8	NAG	A	606	1	-	2/6/23/26	0/1/1/1
8	NAG	B	703	2	-	2/6/23/26	0/1/1/1
8	NAG	A	608	1	-	2/6/23/26	0/1/1/1
8	NAG	A	602	1	-	2/6/23/26	0/1/1/1
8	NAG	F	602	1	-	2/6/23/26	0/1/1/1
8	NAG	F	603	1	-	2/6/23/26	0/1/1/1
8	NAG	C	703	2	-	1/6/23/26	0/1/1/1
8	NAG	A	611	1	-	1/6/23/26	0/1/1/1
8	NAG	A	607	1	-	1/6/23/26	0/1/1/1
8	NAG	G	612	1	-	0/6/23/26	0/1/1/1
8	NAG	A	610	1	-	4/6/23/26	0/1/1/1
8	NAG	F	601	1	-	1/6/23/26	0/1/1/1
8	NAG	A	603	1	-	2/6/23/26	0/1/1/1
8	NAG	F	604	1	-	2/6/23/26	0/1/1/1
8	NAG	B	702	2	-	2/6/23/26	0/1/1/1
8	NAG	G	609	1	-	2/6/23/26	0/1/1/1
8	NAG	A	604	1	-	2/6/23/26	0/1/1/1
8	NAG	G	611	1	-	1/6/23/26	0/1/1/1
8	NAG	F	611	1	-	2/6/23/26	0/1/1/1
8	NAG	G	605	1	-	0/6/23/26	0/1/1/1
8	NAG	G	607	1	-	2/6/23/26	0/1/1/1
8	NAG	C	702	2	-	2/6/23/26	0/1/1/1

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	F	609	1	-	2/6/23/26	0/1/1/1
8	NAG	F	605	1	-	2/6/23/26	0/1/1/1
8	NAG	B	701	2	-	2/6/23/26	0/1/1/1
8	NAG	G	601	1	-	2/6/23/26	0/1/1/1
8	NAG	C	701	2	-	3/6/23/26	0/1/1/1
8	NAG	G	603	1	-	2/6/23/26	0/1/1/1
8	NAG	G	604	1	-	0/6/23/26	0/1/1/1
8	NAG	F	606	1	-	1/6/23/26	0/1/1/1
8	NAG	I	702	2	-	2/6/23/26	0/1/1/1
8	NAG	A	609	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	609	NAG	C1-O5-C5	3.13	116.44	112.19
8	G	611	NAG	C2-N2-C7	2.08	125.86	122.90
8	A	611	NAG	C2-N2-C7	2.05	125.83	122.90

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	702	NAG	C4-C5-C6-O6
8	G	603	NAG	O5-C5-C6-O6
8	G	610	NAG	O5-C5-C6-O6
8	A	609	NAG	O5-C5-C6-O6
8	A	603	NAG	O5-C5-C6-O6
8	C	702	NAG	O5-C5-C6-O6
8	I	702	NAG	O5-C5-C6-O6
8	B	703	NAG	C4-C5-C6-O6
8	A	601	NAG	C4-C5-C6-O6
8	G	601	NAG	O5-C5-C6-O6
8	F	603	NAG	O5-C5-C6-O6
8	F	610	NAG	O5-C5-C6-O6
8	G	606	NAG	C4-C5-C6-O6
8	A	606	NAG	O5-C5-C6-O6
8	C	704	NAG	O5-C5-C6-O6
8	F	607	NAG	O5-C5-C6-O6

Continued on next page...

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
8	F	603	NAG	C4-C5-C6-O6
8	A	602	NAG	O5-C5-C6-O6
8	A	608	NAG	O5-C5-C6-O6
8	A	604	NAG	O5-C5-C6-O6
8	F	602	NAG	O5-C5-C6-O6
8	G	610	NAG	C4-C5-C6-O6
8	A	603	NAG	C4-C5-C6-O6
8	C	702	NAG	C4-C5-C6-O6
8	C	704	NAG	C4-C5-C6-O6
8	F	610	NAG	C4-C5-C6-O6
8	B	702	NAG	O5-C5-C6-O6
8	F	609	NAG	O5-C5-C6-O6
8	G	603	NAG	C4-C5-C6-O6
8	I	701	NAG	C4-C5-C6-O6
8	F	605	NAG	O5-C5-C6-O6
8	A	609	NAG	C4-C5-C6-O6
8	G	607	NAG	O5-C5-C6-O6
8	F	605	NAG	C4-C5-C6-O6
8	F	609	NAG	C4-C5-C6-O6
8	G	610	NAG	C8-C7-N2-C2
8	G	610	NAG	O7-C7-N2-C2
8	A	610	NAG	C8-C7-N2-C2
8	A	610	NAG	O7-C7-N2-C2
8	C	701	NAG	C8-C7-N2-C2
8	C	701	NAG	O7-C7-N2-C2
8	F	610	NAG	C8-C7-N2-C2
8	F	610	NAG	O7-C7-N2-C2
8	G	601	NAG	C4-C5-C6-O6
8	B	703	NAG	O5-C5-C6-O6
8	I	703	NAG	O5-C5-C6-O6
8	B	702	NAG	C4-C5-C6-O6
8	F	607	NAG	C4-C5-C6-O6
8	A	601	NAG	O5-C5-C6-O6
8	G	609	NAG	O5-C5-C6-O6
8	A	610	NAG	O5-C5-C6-O6
8	G	606	NAG	O5-C5-C6-O6
8	I	703	NAG	C4-C5-C6-O6
8	G	609	NAG	C4-C5-C6-O6
8	A	606	NAG	C4-C5-C6-O6
8	A	602	NAG	C4-C5-C6-O6
8	G	602	NAG	O5-C5-C6-O6
8	A	608	NAG	C4-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	A	604	NAG	C4-C5-C6-O6
8	I	701	NAG	O5-C5-C6-O6
8	F	602	NAG	C4-C5-C6-O6
8	F	601	NAG	O5-C5-C6-O6
8	G	608	NAG	O5-C5-C6-O6
8	F	606	NAG	O5-C5-C6-O6
8	C	701	NAG	O5-C5-C6-O6
8	F	611	NAG	C4-C5-C6-O6
8	F	608	NAG	O5-C5-C6-O6
8	A	605	NAG	O5-C5-C6-O6
8	A	607	NAG	O5-C5-C6-O6
8	F	604	NAG	C4-C5-C6-O6
8	A	610	NAG	C4-C5-C6-O6
8	G	607	NAG	C4-C5-C6-O6
8	F	611	NAG	O5-C5-C6-O6
8	B	701	NAG	C4-C5-C6-O6
8	B	701	NAG	O5-C5-C6-O6
8	C	703	NAG	C4-C5-C6-O6
8	F	604	NAG	O5-C5-C6-O6
8	G	611	NAG	C3-C2-N2-C7
8	A	611	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	603	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	J	1
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	102:VAL	C	103:TRP	N	3.20
1	F	309:ILE	C	312:GLY	N	3.19

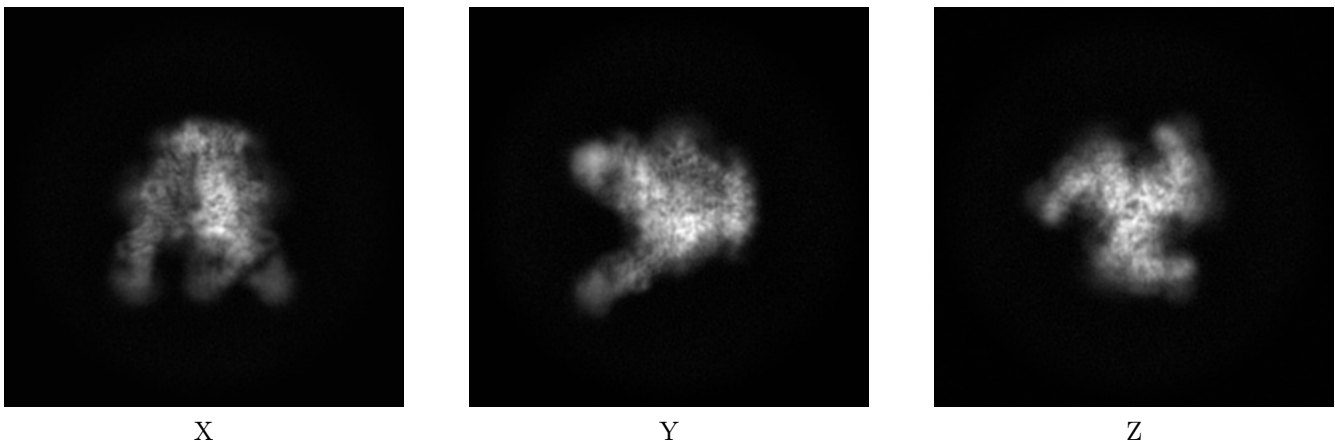
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44482. These allow visual inspection of the internal detail of the map and identification of artifacts.

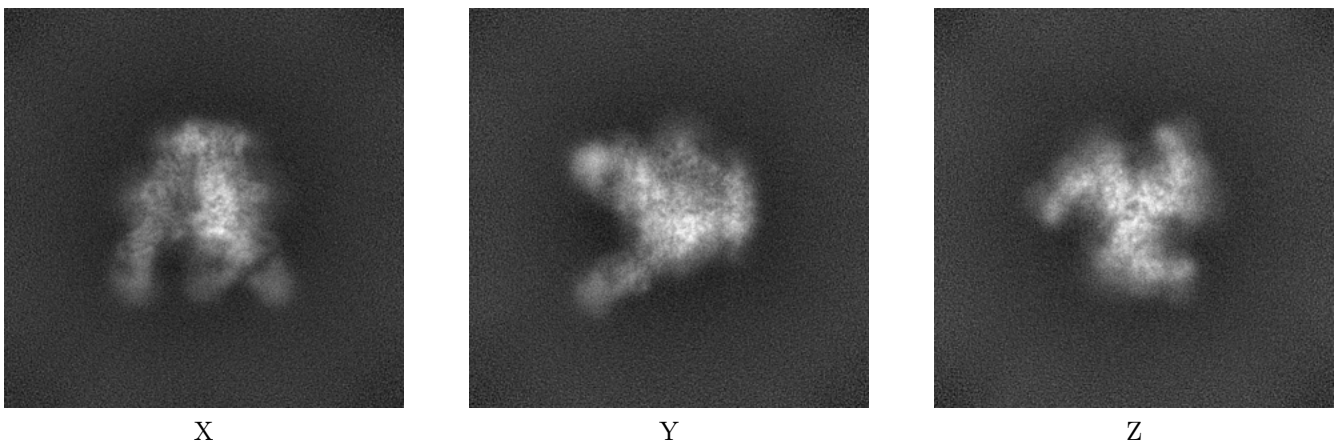
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



#### 6.1.2 Raw map

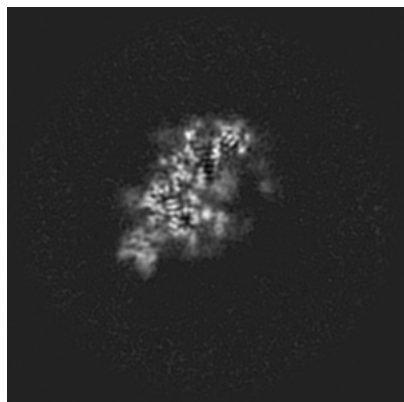


The images above show the map projected in three orthogonal directions.

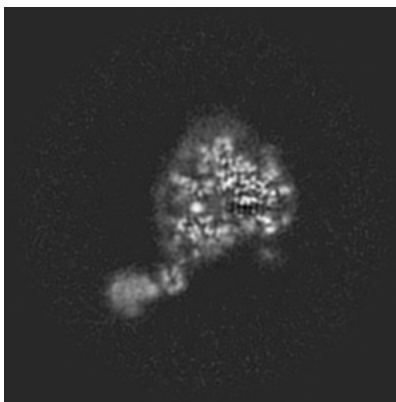


## 6.2 Central slices [i](#)

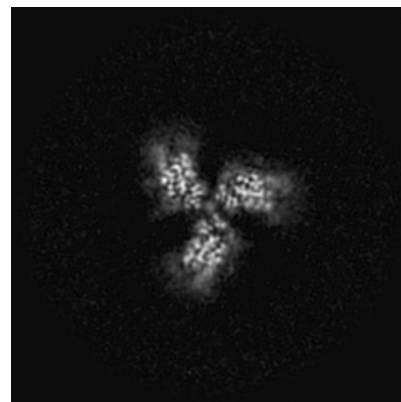
### 6.2.1 Primary map



X Index: 160

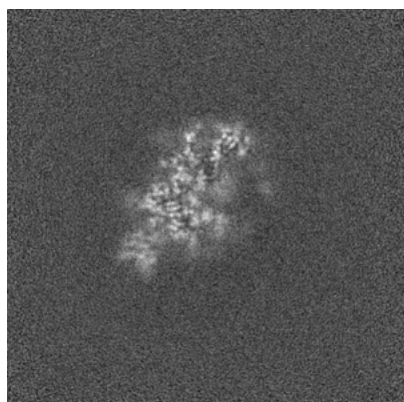


Y Index: 160

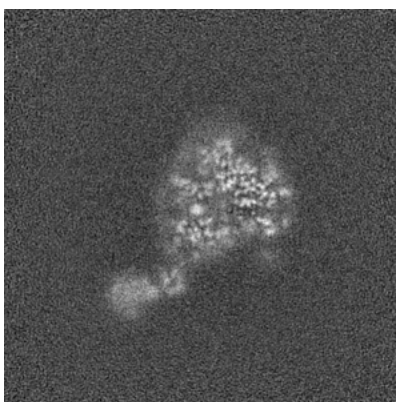


Z Index: 160

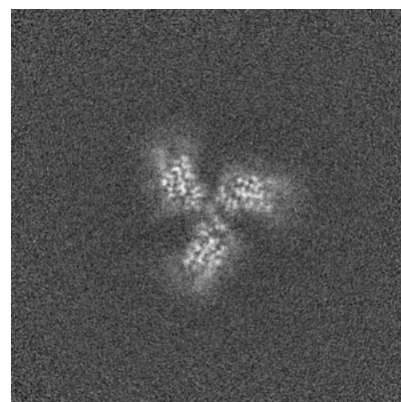
### 6.2.2 Raw map



X Index: 160



Y Index: 160

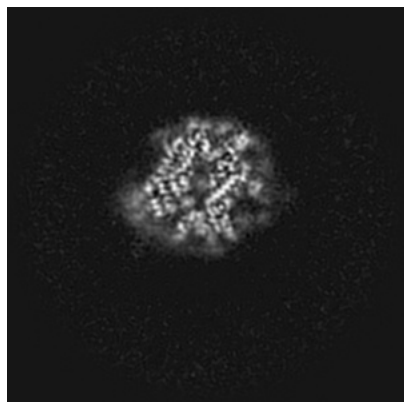


Z Index: 160

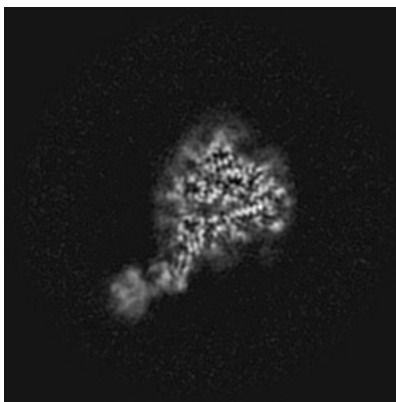
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

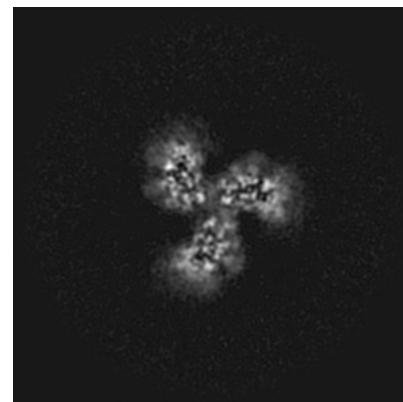
### 6.3.1 Primary map



X Index: 150

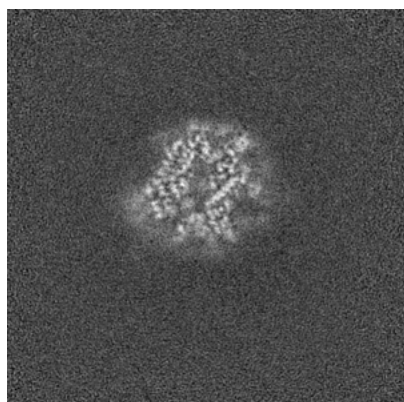


Y Index: 166

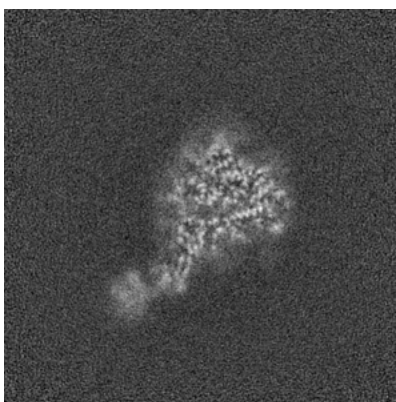


Z Index: 169

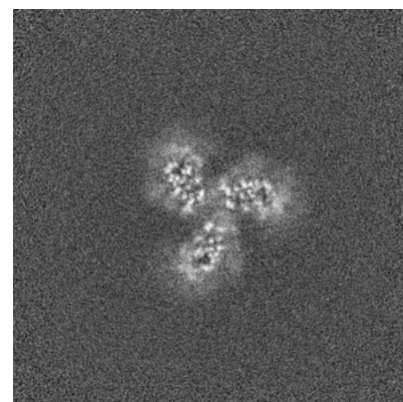
### 6.3.2 Raw map



X Index: 150



Y Index: 166

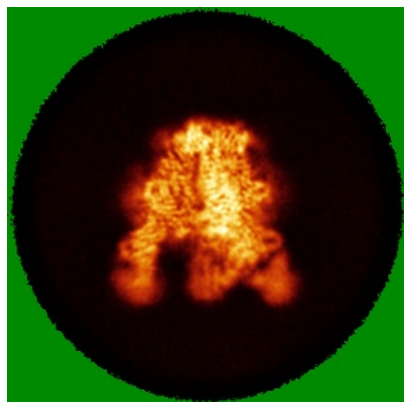


Z Index: 171

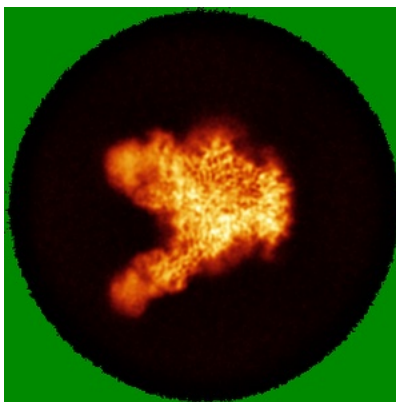
The images above show the largest variance slices of the map in three orthogonal directions.

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

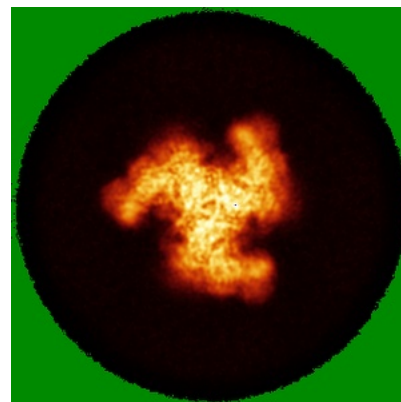
### 6.4.1 Primary map



X

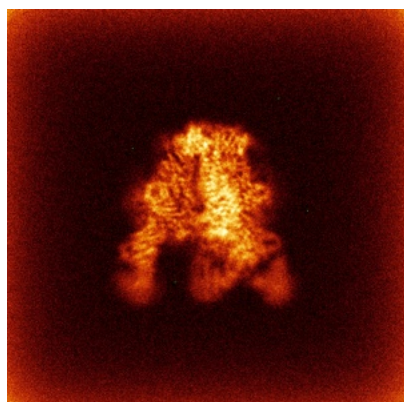


Y

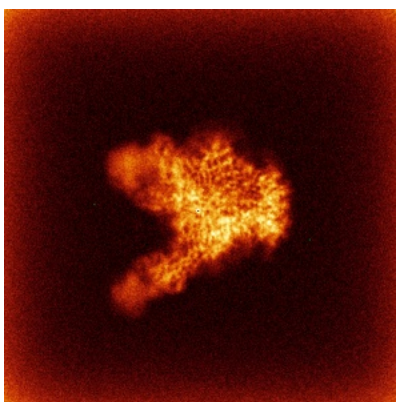


Z

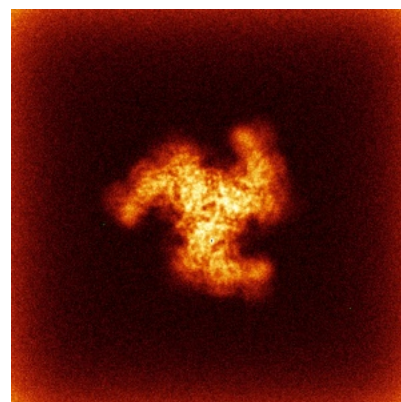
### 6.4.2 Raw map



X



Y

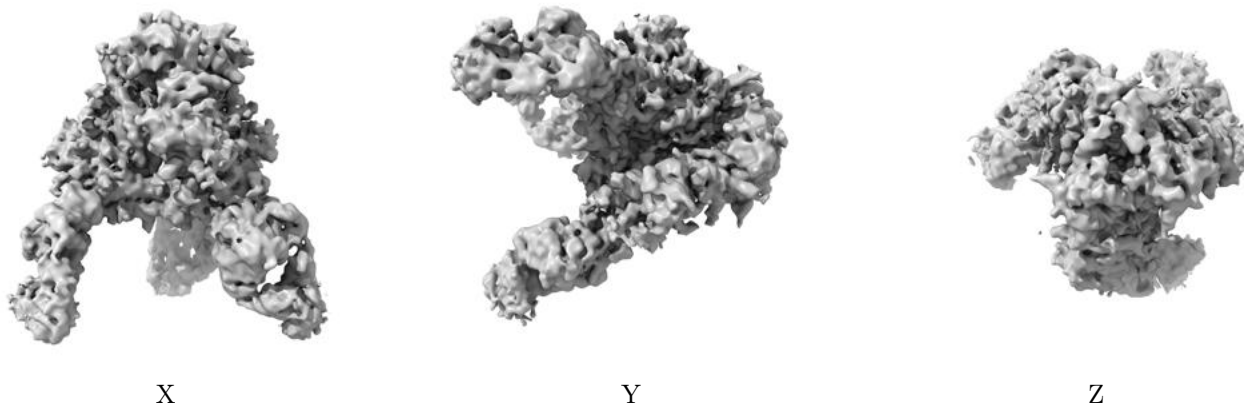


Z

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.

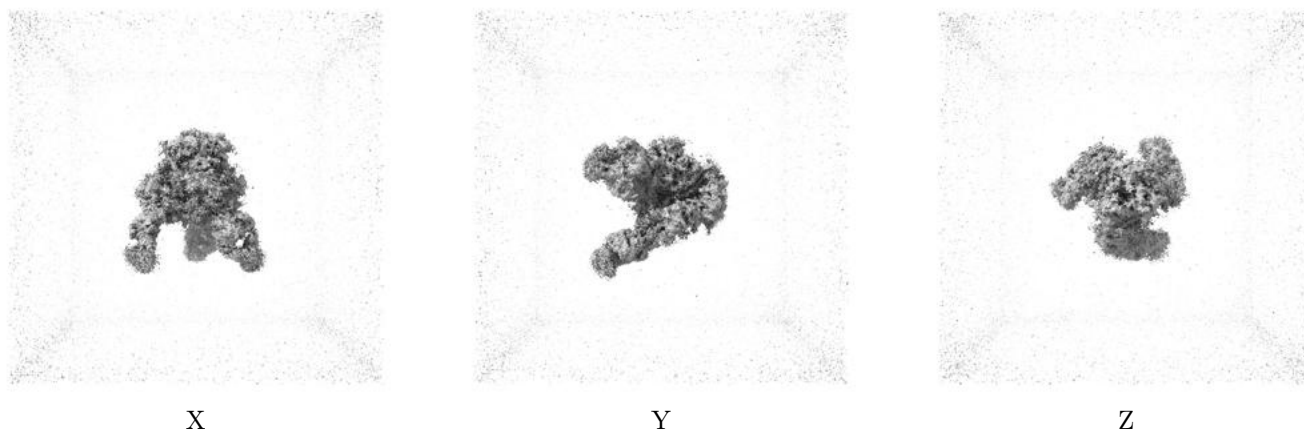
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

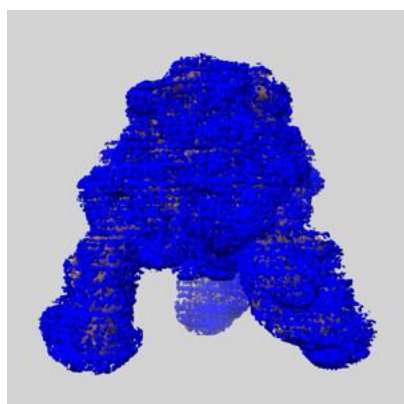
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

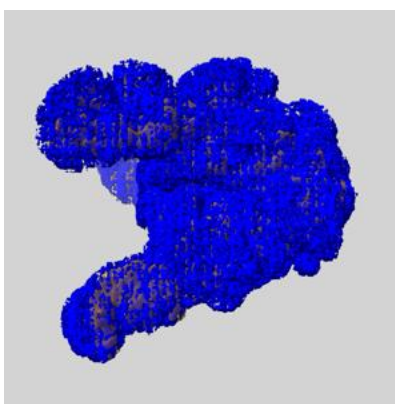
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

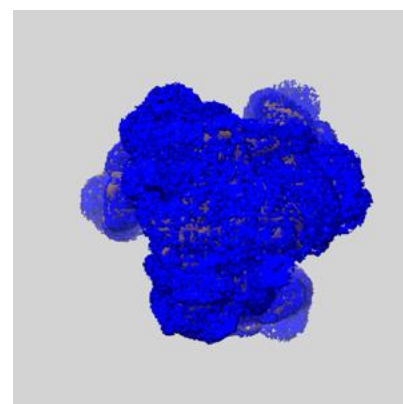
### 6.6.1 emd\_44482\_msk\_1.map [i](#)



X



Y

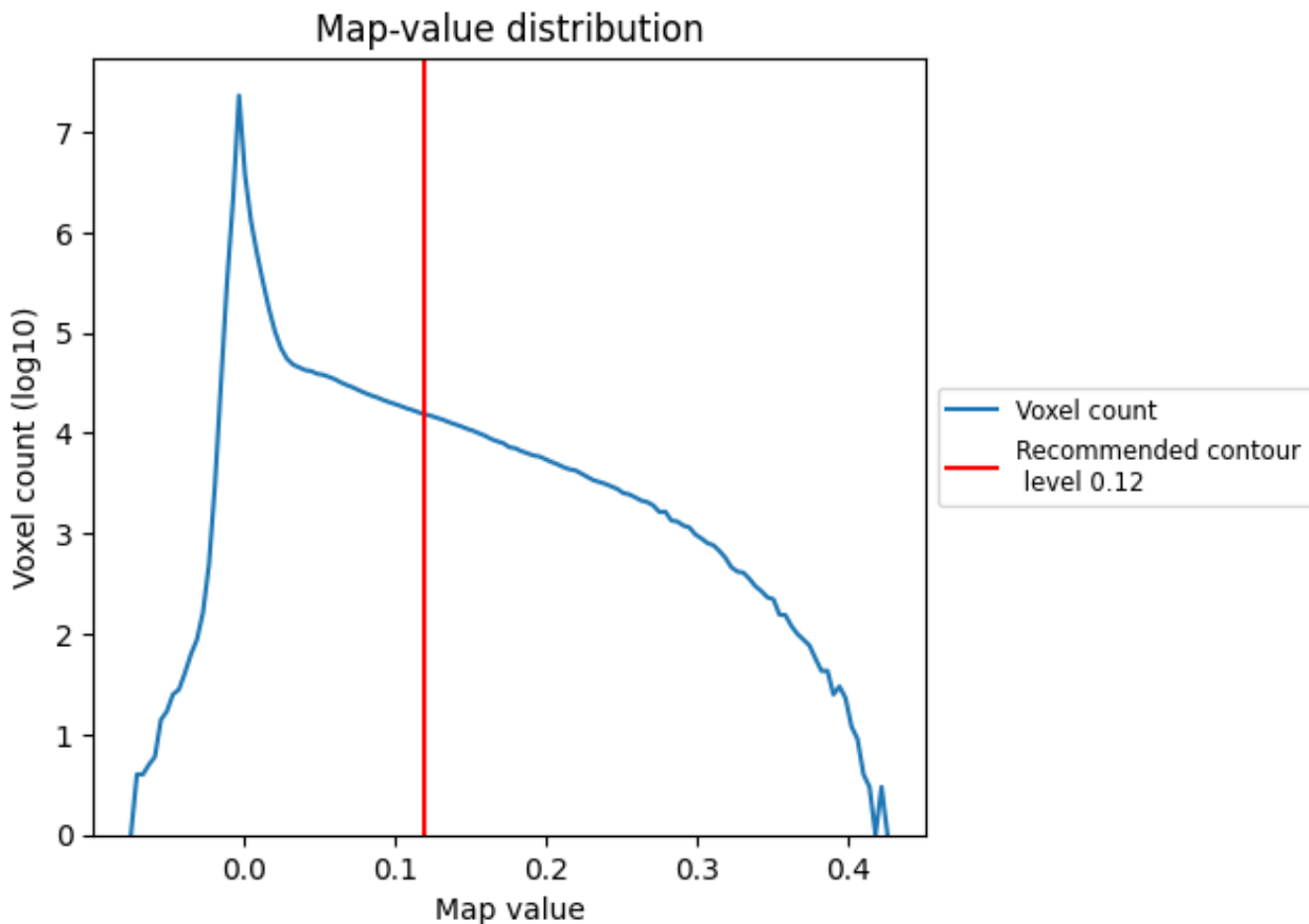


Z

## 7 Map analysis [i](#)

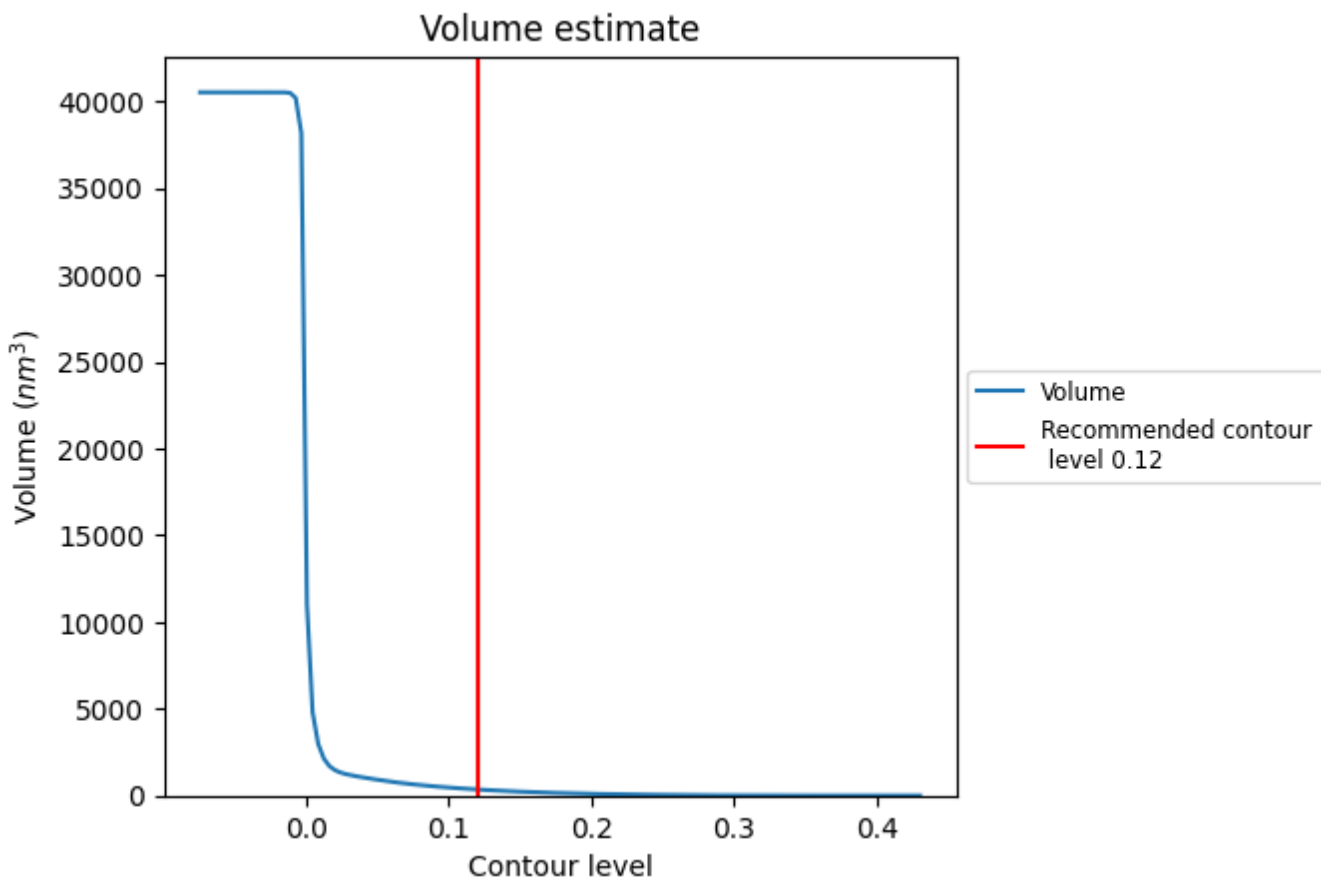
This section contains the results of statistical analysis of the map.

### 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.

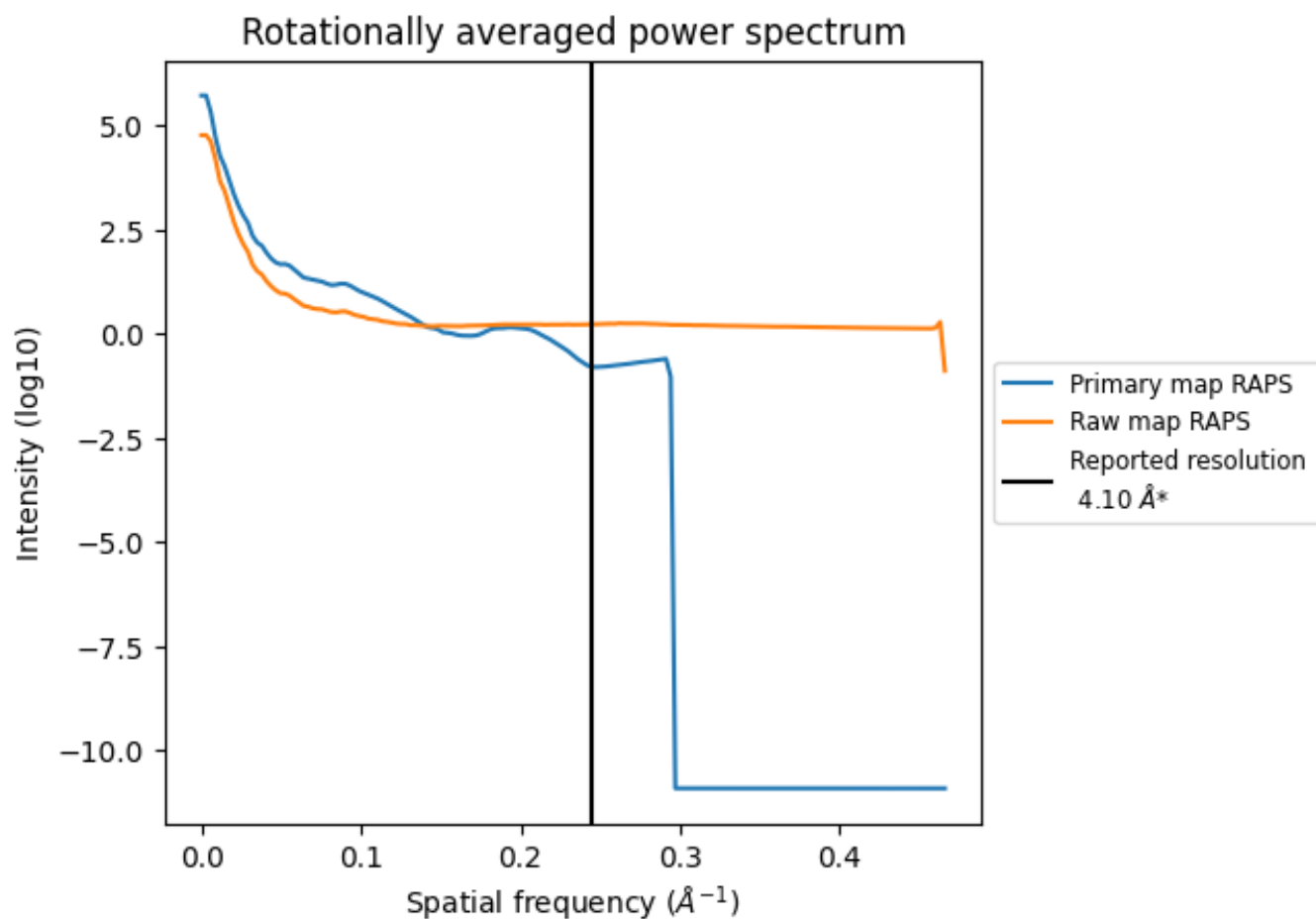
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 351  $\text{nm}^3$ ; this corresponds to an approximate mass of 317 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



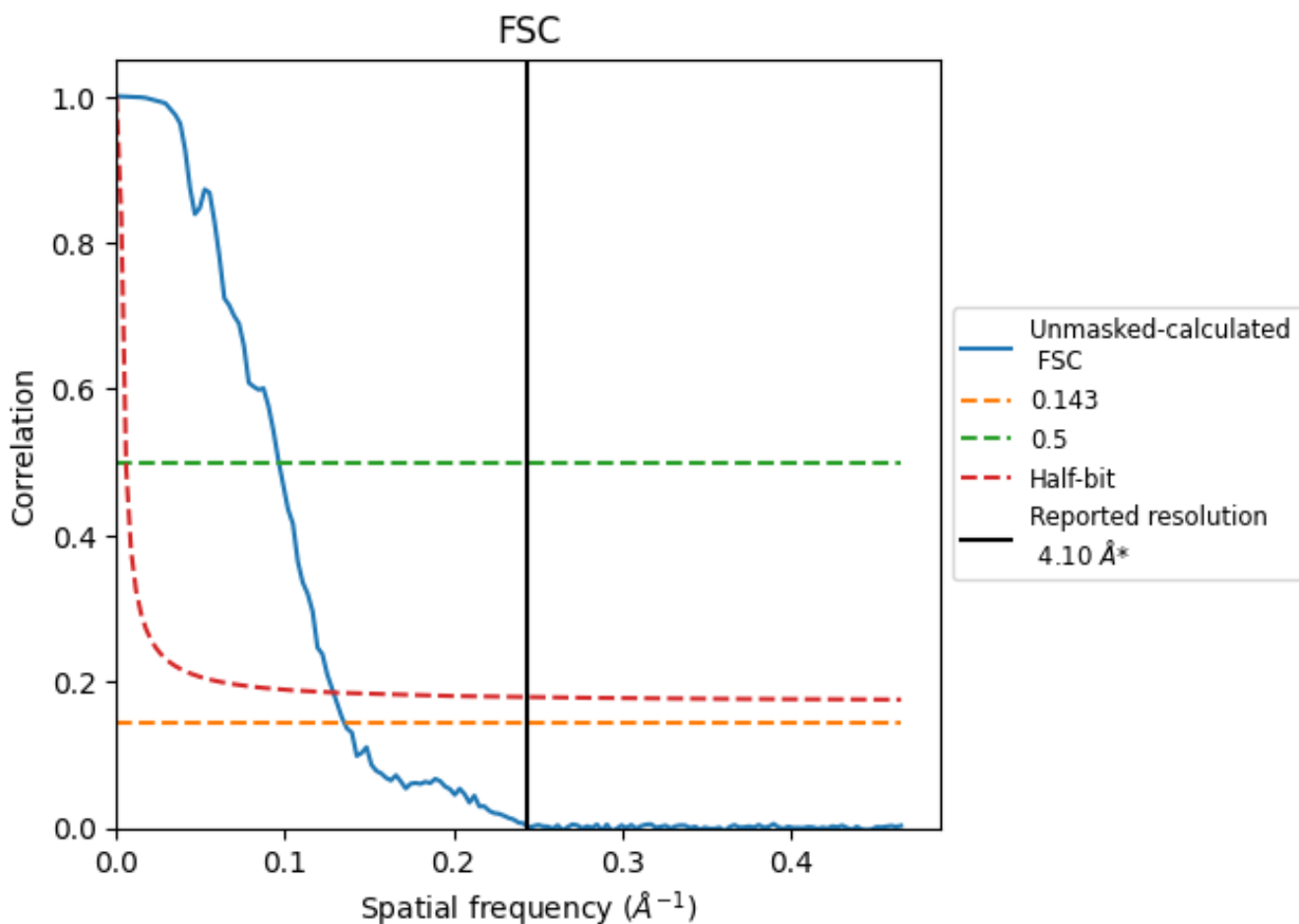
\*Reported resolution corresponds to spatial frequency of  $0.244 \text{ \AA}^{-1}$



## 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 0.244  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

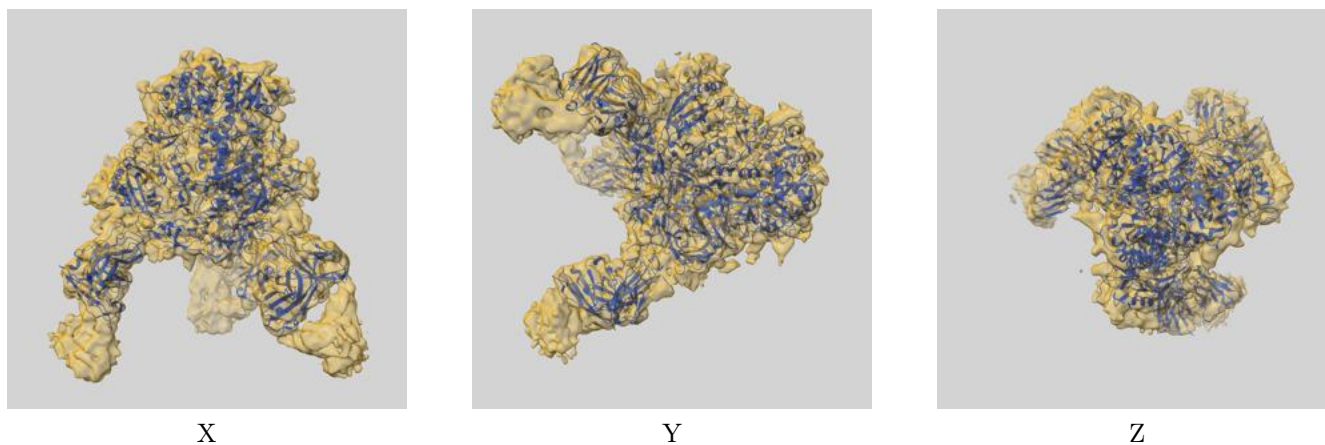
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.38	10.37	7.76

\*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 7.38 differs from the reported value 4.1 by more than 10 %

## 9 Map-model fit [i](#)

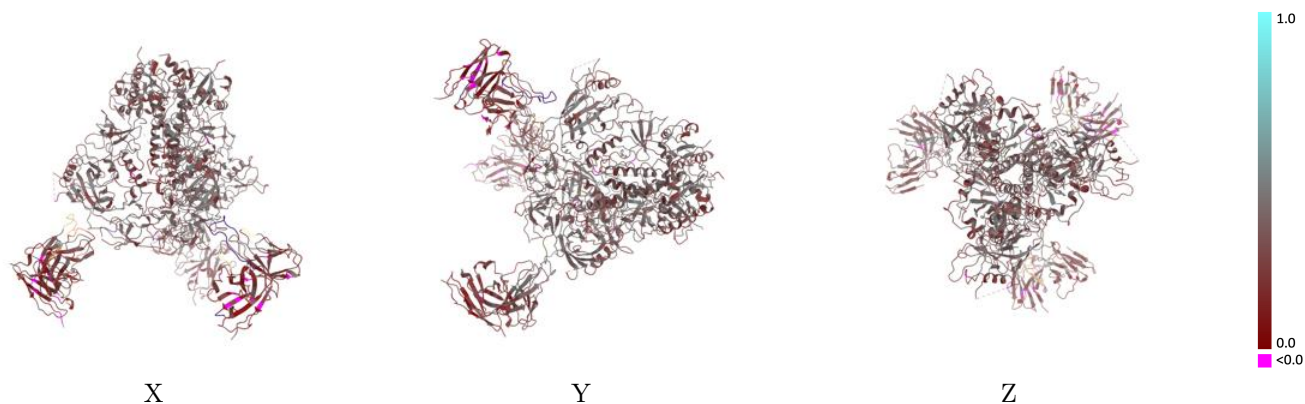
This section contains information regarding the fit between EMDB map EMD-44482 and PDB model 9BER. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.12 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 [\(i\)](#)



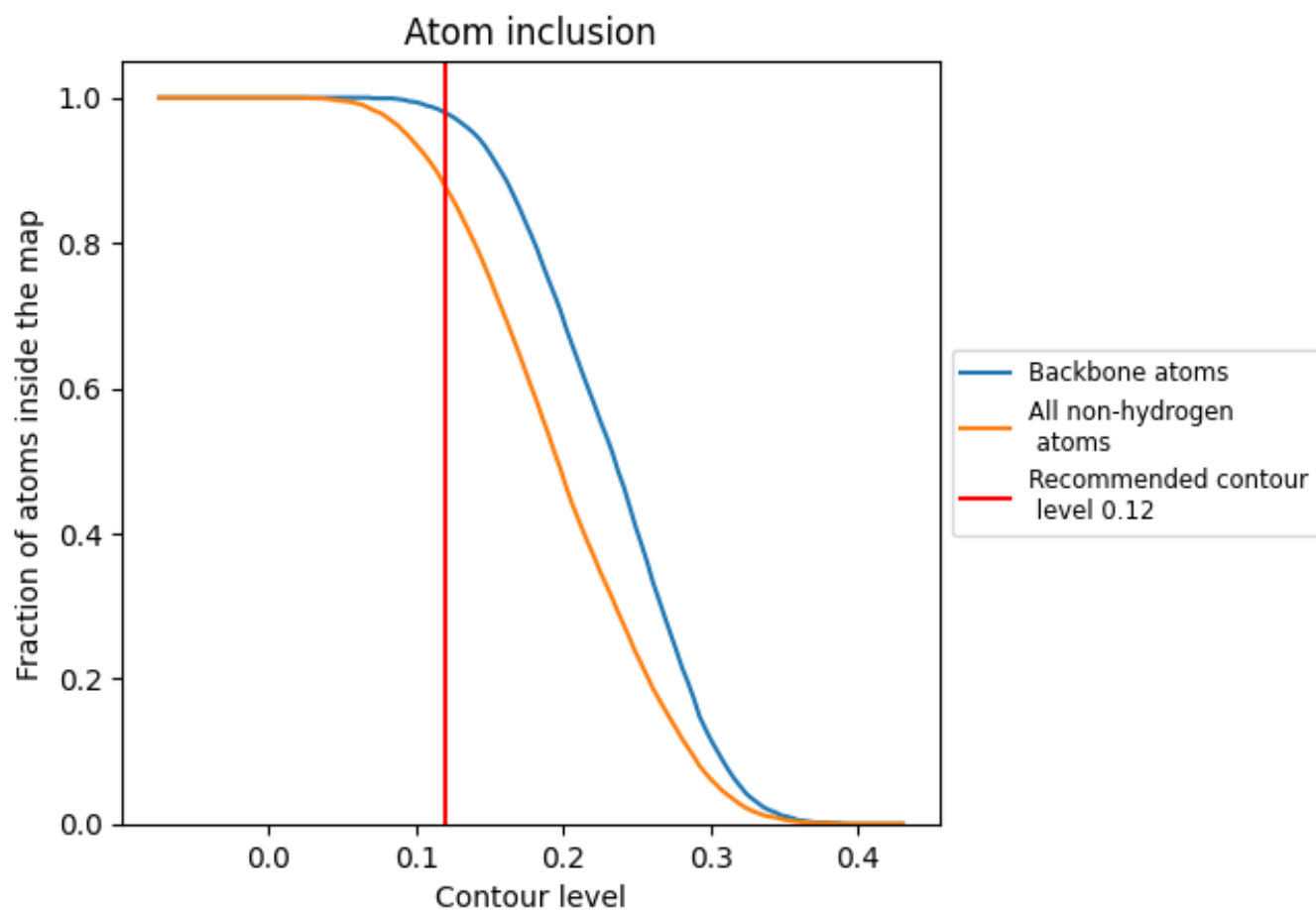
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 88% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.3270
A	 0.8850	 0.3420
B	 0.9000	 0.3590
C	 0.8690	 0.3240
D	 0.8300	 0.2270
E	 0.8200	 0.2630
F	 0.8910	 0.3560
G	 0.8990	 0.3740
H	 0.8560	 0.2690
I	 0.9080	 0.3560
J	 0.8130	 0.1920
K	 0.8480	 0.2720
L	 0.8530	 0.2990
M	 0.9640	 0.3130
N	 0.8930	 0.4430
O	 0.9000	 0.3840
P	 0.9290	 0.4370
Q	 0.8570	 0.3250
R	 0.9440	 0.4020
S	 0.9290	 0.3300
T	 0.8930	 0.3310
U	 0.8600	 0.3680
V	 0.9290	 0.3910
W	 0.8210	 0.3610
X	 0.9030	 0.4170
Y	 0.8930	 0.2840
Z	 0.7860	 0.3720
a	 0.9200	 0.3670
b	 0.8570	 0.3930
c	 0.8930	 0.4320
d	 0.9440	 0.3970

