



Full wwPDB EM Validation Report ⓘ

Jan 12, 2022 – 06:20 pm GMT

PDB ID : 7QO7
EMDB ID : EMD-14086
Title : SARS-CoV-2 S Omicron Spike B.1.1.529
Authors : Ni, D.; Lau, K.; Turelli, P.; Beckert, B.; Nazarov, S.; Pojer, F.; Myasnikov, A.; Stahlberg, H.; Trono, D.
Deposited on : 2021-12-23
Resolution : 3.02 Å(reported)
Based on initial model : 6XM3

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

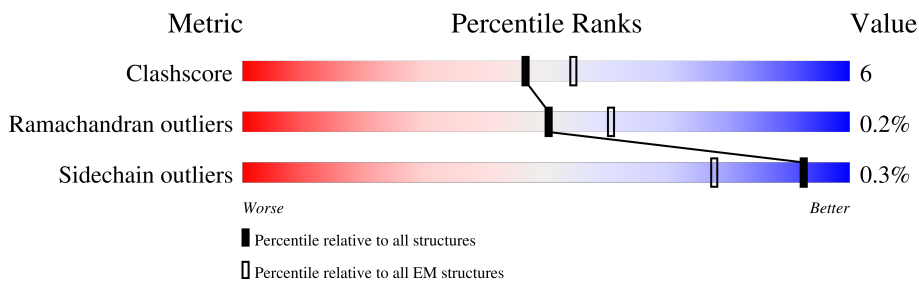
EMDB validation analysis : 0.0.0.dev97
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.24

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 3.02 Å.

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



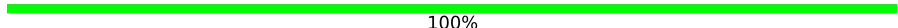
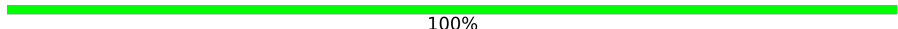

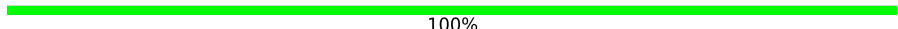
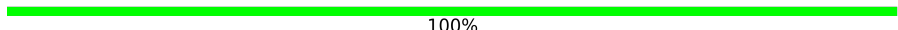
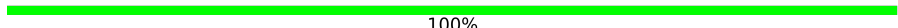


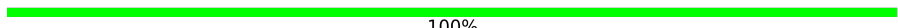





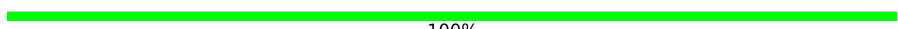
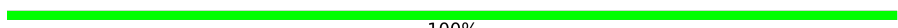
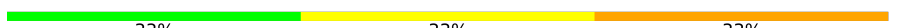
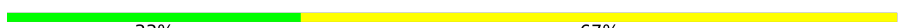
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1285	
1	B	1285	
1	C	1285	
2	D	4	
3	E	2	
3	H	2	
3	M	2	
4	F	3	

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Mol	Chain	Length	Quality of chain
4	G	3	 100%
4	I	3	 100%
4	J	3	 67% 33%
4	K	3	 100%
4	L	3	 100%
4	N	3	 100%
4	O	3	 100%
4	P	3	 100%
4	Q	3	 100%
4	R	3	 67% 33%
4	S	3	 67% 33%
4	T	3	 67% 33%
4	U	3	 33% 67%
4	V	3	 33% 67%
4	W	3	 100%
4	X	3	 100%
4	Z	3	 33% 33% 33%
5	Y	3	 33% 67%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 26865 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 Surface glycoprotein, Fibritin, SARS-CoV-2 S Omicron Spike B.1.1.529.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1101	8610	5502	1440	1629	39	0	0
1	B	1096	8589	5490	1435	1625	39	0	0
1	C	1098	8596	5494	1437	1626	39	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	conflict	UNP A0A8A4XEV3
A	?	-	HIS	deletion	UNP A0A8A4XEV3
A	?	-	VAL	deletion	UNP A0A8A4XEV3
A	93	ILE	THR	conflict	UNP A0A8A4XEV3
A	206	ILE	-	insertion	UNP A0A8A4XEV3
A	207	VAL	-	insertion	UNP A0A8A4XEV3
A	208	ARG	ASN	conflict	UNP A0A8A4XEV3
A	209	GLU	LEU	conflict	UNP A0A8A4XEV3
A	210	PRO	VAL	conflict	UNP A0A8A4XEV3
A	211	GLU	ARG	conflict	UNP A0A8A4XEV3
A	336	ASP	GLY	conflict	UNP A0A8A4XEV3
A	368	LEU	SER	conflict	UNP A0A8A4XEV3
A	370	PRO	SER	conflict	UNP A0A8A4XEV3
A	372	PHE	SER	conflict	UNP A0A8A4XEV3
A	414	ASN	LYS	conflict	UNP A0A8A4XEV3
A	437	LYS	ASN	conflict	UNP A0A8A4XEV3
A	443	SER	GLY	conflict	UNP A0A8A4XEV3
A	474	ASN	SER	conflict	UNP A0A8A4XEV3
A	475	LYS	THR	conflict	UNP A0A8A4XEV3
A	481	ALA	ARG	conflict	UNP A0A8A4XEV3
A	490	ARG	GLN	conflict	UNP A0A8A4XEV3
A	493	SER	GLY	conflict	UNP A0A8A4XEV3
A	495	ARG	GLN	conflict	UNP A0A8A4XEV3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	498	TYR	ASN	conflict	UNP A0A8A4XEV3
A	502	HIS	TYR	conflict	UNP A0A8A4XEV3
A	544	LYS	THR	conflict	UNP A0A8A4XEV3
A	652	TYR	HIS	conflict	UNP A0A8A4XEV3
A	676	LYS	ASN	conflict	UNP A0A8A4XEV3
A	678	HIS	PRO	conflict	UNP A0A8A4XEV3
A	679	GLY	ARG	conflict	UNP A0A8A4XEV3
A	680	SER	ARG	conflict	UNP A0A8A4XEV3
A	682	SER	ARG	conflict	UNP A0A8A4XEV3
A	761	LYS	ASN	conflict	UNP A0A8A4XEV3
A	793	TYR	ASP	conflict	UNP A0A8A4XEV3
A	853	LYS	ASN	conflict	UNP A0A8A4XEV3
A	951	HIS	GLN	conflict	UNP A0A8A4XEV3
A	966	LYS	ASN	conflict	UNP A0A8A4XEV3
A	978	PHE	LEU	conflict	UNP A0A8A4XEV3
A	983	PRO	LYS	conflict	UNP A0A8A4XEV3
A	984	PRO	VAL	conflict	UNP A0A8A4XEV3
A	1206	GLY	-	linker	UNP A0A8A4XEV3
A	1207	SER	-	linker	UNP A0A8A4XEV3
B	67	VAL	ALA	conflict	UNP A0A8A4XEV3
B	?	-	HIS	deletion	UNP A0A8A4XEV3
B	?	-	VAL	deletion	UNP A0A8A4XEV3
B	93	ILE	THR	conflict	UNP A0A8A4XEV3
B	206	ILE	-	insertion	UNP A0A8A4XEV3
B	207	VAL	-	insertion	UNP A0A8A4XEV3
B	208	ARG	ASN	conflict	UNP A0A8A4XEV3
B	209	GLU	LEU	conflict	UNP A0A8A4XEV3
B	210	PRO	VAL	conflict	UNP A0A8A4XEV3
B	211	GLU	ARG	conflict	UNP A0A8A4XEV3
B	336	ASP	GLY	conflict	UNP A0A8A4XEV3
B	368	LEU	SER	conflict	UNP A0A8A4XEV3
B	370	PRO	SER	conflict	UNP A0A8A4XEV3
B	372	PHE	SER	conflict	UNP A0A8A4XEV3
B	414	ASN	LYS	conflict	UNP A0A8A4XEV3
B	437	LYS	ASN	conflict	UNP A0A8A4XEV3
B	443	SER	GLY	conflict	UNP A0A8A4XEV3
B	474	ASN	SER	conflict	UNP A0A8A4XEV3
B	475	LYS	THR	conflict	UNP A0A8A4XEV3
B	481	ALA	ARG	conflict	UNP A0A8A4XEV3
B	490	ARG	GLN	conflict	UNP A0A8A4XEV3
B	493	SER	GLY	conflict	UNP A0A8A4XEV3
B	495	ARG	GLN	conflict	UNP A0A8A4XEV3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	498	TYR	ASN	conflict	UNP A0A8A4XEV3
B	502	HIS	TYR	conflict	UNP A0A8A4XEV3
B	544	LYS	THR	conflict	UNP A0A8A4XEV3
B	652	TYR	HIS	conflict	UNP A0A8A4XEV3
B	676	LYS	ASN	conflict	UNP A0A8A4XEV3
B	678	HIS	PRO	conflict	UNP A0A8A4XEV3
B	679	GLY	ARG	conflict	UNP A0A8A4XEV3
B	680	SER	ARG	conflict	UNP A0A8A4XEV3
B	682	SER	ARG	conflict	UNP A0A8A4XEV3
B	761	LYS	ASN	conflict	UNP A0A8A4XEV3
B	793	TYR	ASP	conflict	UNP A0A8A4XEV3
B	853	LYS	ASN	conflict	UNP A0A8A4XEV3
B	951	HIS	GLN	conflict	UNP A0A8A4XEV3
B	966	LYS	ASN	conflict	UNP A0A8A4XEV3
B	978	PHE	LEU	conflict	UNP A0A8A4XEV3
B	983	PRO	LYS	conflict	UNP A0A8A4XEV3
B	984	PRO	VAL	conflict	UNP A0A8A4XEV3
B	1206	GLY	-	linker	UNP A0A8A4XEV3
B	1207	SER	-	linker	UNP A0A8A4XEV3
C	67	VAL	ALA	conflict	UNP A0A8A4XEV3
C	?	-	HIS	deletion	UNP A0A8A4XEV3
C	?	-	VAL	deletion	UNP A0A8A4XEV3
C	93	ILE	THR	conflict	UNP A0A8A4XEV3
C	206	ILE	-	insertion	UNP A0A8A4XEV3
C	207	VAL	-	insertion	UNP A0A8A4XEV3
C	208	ARG	ASN	conflict	UNP A0A8A4XEV3
C	209	GLU	LEU	conflict	UNP A0A8A4XEV3
C	210	PRO	VAL	conflict	UNP A0A8A4XEV3
C	211	GLU	ARG	conflict	UNP A0A8A4XEV3
C	336	ASP	GLY	conflict	UNP A0A8A4XEV3
C	368	LEU	SER	conflict	UNP A0A8A4XEV3
C	370	PRO	SER	conflict	UNP A0A8A4XEV3
C	372	PHE	SER	conflict	UNP A0A8A4XEV3
C	414	ASN	LYS	conflict	UNP A0A8A4XEV3
C	437	LYS	ASN	conflict	UNP A0A8A4XEV3
C	443	SER	GLY	conflict	UNP A0A8A4XEV3
C	474	ASN	SER	conflict	UNP A0A8A4XEV3
C	475	LYS	THR	conflict	UNP A0A8A4XEV3
C	481	ALA	ARG	conflict	UNP A0A8A4XEV3
C	490	ARG	GLN	conflict	UNP A0A8A4XEV3
C	493	SER	GLY	conflict	UNP A0A8A4XEV3
C	495	ARG	GLN	conflict	UNP A0A8A4XEV3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	498	TYR	ASN	conflict	UNP A0A8A4XEV3
C	502	HIS	TYR	conflict	UNP A0A8A4XEV3
C	544	LYS	THR	conflict	UNP A0A8A4XEV3
C	652	TYR	HIS	conflict	UNP A0A8A4XEV3
C	676	LYS	ASN	conflict	UNP A0A8A4XEV3
C	678	HIS	PRO	conflict	UNP A0A8A4XEV3
C	679	GLY	ARG	conflict	UNP A0A8A4XEV3
C	680	SER	ARG	conflict	UNP A0A8A4XEV3
C	682	SER	ARG	conflict	UNP A0A8A4XEV3
C	761	LYS	ASN	conflict	UNP A0A8A4XEV3
C	793	TYR	ASP	conflict	UNP A0A8A4XEV3
C	853	LYS	ASN	conflict	UNP A0A8A4XEV3
C	951	HIS	GLN	conflict	UNP A0A8A4XEV3
C	966	LYS	ASN	conflict	UNP A0A8A4XEV3
C	978	PHE	LEU	conflict	UNP A0A8A4XEV3
C	983	PRO	LYS	conflict	UNP A0A8A4XEV3
C	984	PRO	VAL	conflict	UNP A0A8A4XEV3
C	1206	GLY	-	linker	UNP A0A8A4XEV3
C	1207	SER	-	linker	UNP A0A8A4XEV3

- Molecule 2 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
2	D	4	50	28	2	20	0	0

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



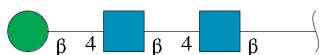
Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
3	E	2	28	16	2	10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	H	2	28	16	2	10	0	0
3	M	2	28	16	2	10	0	0

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



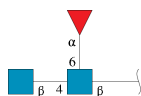
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	F	3	39	22	2	15	0	0
4	G	3	39	22	2	15	0	0
4	I	3	39	22	2	15	0	0
4	J	3	39	22	2	15	0	0
4	K	3	39	22	2	15	0	0
4	L	3	39	22	2	15	0	0
4	N	3	39	22	2	15	0	0
4	O	3	39	22	2	15	0	0
4	P	3	39	22	2	15	0	0
4	Q	3	39	22	2	15	0	0
4	R	3	39	22	2	15	0	0
4	S	3	39	22	2	15	0	0
4	T	3	39	22	2	15	0	0
4	U	3	39	22	2	15	0	0
4	V	3	39	22	2	15	0	0

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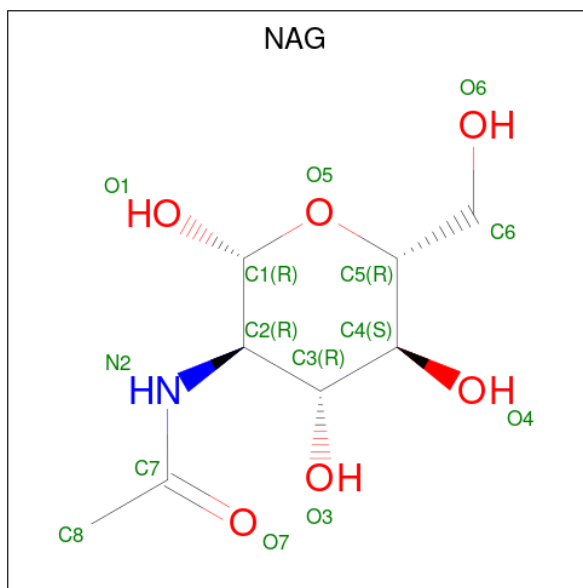
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	W	3	Total 39	C 22	N 2	O 15	0	0
4	X	3	Total 39	C 22	N 2	O 15	0	0
4	Z	3	Total 39	C 22	N 2	O 15	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	Y	3	Total 38	C 22	N 2	O 14	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	Total 70	C 40	N 5	O 25	0
6	A	1	Total 70	C 40	N 5	O 25	0

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Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total 70	C 40	N 5	O 25	0
6	A	1	Total 70	C 40	N 5	O 25	0
6	A	1	Total 70	C 40	N 5	O 25	0
6	B	1	Total 70	C 40	N 5	O 25	0
6	B	1	Total 70	C 40	N 5	O 25	0
6	B	1	Total 70	C 40	N 5	O 25	0
6	B	1	Total 70	C 40	N 5	O 25	0
6	B	1	Total 70	C 40	N 5	O 25	0
6	B	1	Total 70	C 40	N 5	O 25	0
6	C	1	Total 56	C 32	N 4	O 20	0
6	C	1	Total 56	C 32	N 4	O 20	0
6	C	1	Total 56	C 32	N 4	O 20	0
6	C	1	Total 56	C 32	N 4	O 20	0



MAG1
MAG2

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

Chain M:  100%



MAG1
MAG2

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

Chain F:  33% 33% 33%



MAG1
MAG2
BMAS

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

Chain G:  100%



MAG1
MAG2
BMAS

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

Chain I:  100%



MAG1
MAG2
BMAS

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

Chain J:  67% 33%



MAG1
MAG2
BMAS

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

Chain K: 100%



MAG1
MAG2
BMAS

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

Chain L:  100%

MAG1
MAG2
BMA3

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

Chain N:  100%

MAG1
MAG2
BMA3

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

Chain O:  100%

MAG1
MAG2
BMA3

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

Chain P:  100%

MAG1
MAG2
BMA3

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

Chain Q:  100%

MAG1
MAG2
BMA3

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

Chain R:  67% 33%

MAG1
MAG2
BMA3

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

Chain S:  67% 33%



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

Chain T: 67% 33%



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

Chain U: 33% 67%



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

Chain V: 33% 67%



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

Chain W: 100%



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

Chain X: 100%




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

Chain Z: 33% 33% 33%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  33% 67%

MAG1
MAG2
FUC3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76450	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.689	Depositor
Minimum map value	-0.291	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0528	Depositor
Map size (\AA)	373.48502, 373.48502, 373.48502	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0671, 1.0671, 1.0671	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, NAG, FUC, MAN

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	0.25	0/8813	0.48	0/11987
1	B	0.25	0/8793	0.48	0/11961
1	C	0.25	0/8799	0.47	0/11968
All	All	0.25	0/26405	0.48	0/35916

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	8610	0	8389	107	0
1	B	8589	0	8390	127	0
1	C	8596	0	8383	122	0
2	D	50	0	43	1	0
3	E	28	0	25	1	0
3	H	28	0	25	0	0
3	M	28	0	25	0	0
4	F	39	0	34	1	0
4	G	39	0	34	0	0
4	I	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	39	0	34	1	0
4	K	39	0	34	0	0
4	L	39	0	34	0	0
4	N	39	0	34	0	0
4	O	39	0	34	0	0
4	P	39	0	34	0	0
4	Q	39	0	34	0	0
4	R	39	0	34	1	0
4	S	39	0	34	1	0
4	T	39	0	34	1	0
4	U	39	0	34	1	0
4	V	39	0	34	1	0
4	W	39	0	34	0	0
4	X	39	0	34	0	0
4	Z	39	0	34	1	0
5	Y	38	0	34	0	0
6	A	70	0	65	0	0
6	B	70	0	65	1	0
6	C	56	0	52	1	0
All	All	26865	0	26108	342	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 (342) 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:B:449:LEU:HD22	1:B:489:LEU:HD13	1.63	0.80
1:A:631:ARG:HG2	1:A:633:TYR:H	1.53	0.74
1:B:141:HIS:HB3	1:B:240:ALA:HB1	1.74	0.70
1:B:477:CYS:HB3	1:B:483:PHE:HB2	1.75	0.69
1:B:41:LYS:NZ	1:C:559:PHE:O	2.23	0.68
1:C:770:GLU:OE2	1:C:1016:ARG:NH1	2.27	0.67
1:C:739:ILE:O	1:C:997:ARG:NH1	2.28	0.67
1:C:421:LYS:HB3	1:C:458:LEU:HD13	1.78	0.64
1:A:388:CYS:HA	1:A:522:CYS:HB3	1.80	0.64
1:C:207:VAL:HG22	1:C:209:GLU:H	1.63	0.64
1:C:454:ARG:HH22	1:C:458:LEU:HG	1.63	0.63
1:A:244:SER:HG	1:A:253:SER:N	1.97	0.63
1:B:739:ILE:O	1:B:997:ARG:NH1	2.30	0.63
1:C:423:PRO:HG2	1:C:426:PHE:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ARG:HD2	1:B:119:ASN:HB3	1.81	0.62
1:A:334:PRO:HB2	1:A:337:GLU:HB2	1.80	0.62
1:B:241:LEU:HB3	1:B:255:TRP:HB3	1.82	0.62
2:D:2:NAG:H82	2:D:4:MAN:H2	1.81	0.61
1:B:388:CYS:SG	1:B:523:GLY:N	2.69	0.61
1:B:454:ARG:HD3	1:B:455:LYS:H	1.64	0.61
1:A:433:TRP:HE1	1:A:506:ARG:HH21	1.47	0.61
1:A:567:ALA:HB2	1:C:849:ALA:HB1	1.82	0.61
1:A:343:ARG:NH2	1:A:438:LEU:O	2.33	0.61
1:B:967:PHE:O	1:B:992:ARG:NH1	2.34	0.61
1:B:784:GLN:OE1	1:C:700:ASN:ND2	2.31	0.60
1:B:143:ASN:O	1:B:145:LYS:NZ	2.34	0.60
1:C:970:ILE:HD12	1:C:981:LEU:HD11	1.83	0.60
1:A:126:ILE:HB	1:A:165:TYR:HB3	1.83	0.60
4:F:2:NAG:H3	4:F:2:NAG:H83	1.83	0.60
1:A:990:ILE:O	1:A:994:ILE:HG12	2.02	0.60
1:C:421:LYS:HD3	1:C:458:LEU:HD22	1.83	0.60
1:C:801:GLN:NE2	1:C:932:GLN:OE1	2.32	0.60
1:B:329:ILE:HB	1:B:359:VAL:HG23	1.83	0.59
1:A:173:ASP:OD1	1:A:202:HIS:ND1	2.35	0.59
1:B:480:VAL:HA	1:B:485:CYS:HB2	1.83	0.59
1:C:574:ARG:HD3	1:C:581:ILE:HG22	1.85	0.59
1:C:538:PHE:HD1	1:C:540:PHE:H	1.49	0.59
1:C:243:ARG:NH1	1:C:244:SER:OG	2.35	0.59
1:C:278:GLU:HB3	4:Z:1:NAG:H82	1.85	0.59
1:A:627:THR:HB	1:A:630:TRP:CD1	2.37	0.58
1:C:81:VAL:HB	1:C:234:ARG:HD3	1.85	0.58
1:C:325:ARG:HG2	1:C:576:PRO:HD2	1.85	0.58
1:B:41:LYS:HZ2	1:C:561:GLN:HG2	1.69	0.58
1:A:106:THR:OG1	1:A:231:ASN:O	2.22	0.58
1:A:753:TYR:OH	1:A:991:ASP:OD1	2.17	0.58
1:B:981:LEU:HG	1:B:986:ALA:HB2	1.86	0.57
1:C:383:LYS:HG2	1:C:386:ASP:HB2	1.86	0.57
1:B:292:PRO:HG3	1:B:630:TRP:HE1	1.69	0.57
1:A:299:THR:HG23	1:A:300:LEU:HD12	1.86	0.57
1:B:386:ASP:O	1:B:525:LYS:NZ	2.38	0.57
1:C:969:ALA:HA	1:C:992:ARG:HH21	1.69	0.57
1:A:128:VAL:HG13	1:A:230:ILE:HD11	1.87	0.57
1:C:716:THR:HA	1:C:923:GLN:HE22	1.69	0.57
1:A:410:GLY:H	1:A:424:ASP:HA	1.70	0.57
1:B:79:ASN:ND2	1:B:237:THR:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:LEU:HD13	1:B:489:LEU:HB2	1.87	0.56
1:B:479:GLY:O	1:B:481:ALA:N	2.36	0.56
1:B:834:TYR:HE2	6:C:1303:NAG:H81	1.71	0.56
1:A:171:LEU:HD13	1:A:185:ARG:HH21	1.70	0.56
1:B:716:THR:HA	1:B:923:GLN:HE22	1.69	0.56
1:C:525:LYS:HD2	1:C:526:LYS:HG3	1.88	0.56
4:S:1:NAG:O4	4:S:1:NAG:O7	2.23	0.56
1:A:79:ASN:ND2	1:A:237:THR:O	2.34	0.56
1:A:205:ILE:O	1:A:208:ARG:NH2	2.38	0.56
1:B:495:ARG:HD3	1:B:496:PRO:HD2	1.87	0.56
1:A:27:ALA:HB3	1:A:64:TRP:HB3	1.88	0.56
1:A:983:PRO:O	1:A:987:GLU:HG2	2.06	0.56
1:C:454:ARG:HH12	1:C:458:LEU:HG	1.69	0.56
1:A:354:ARG:NH1	1:A:355:ILE:O	2.39	0.56
1:B:435:SER:HB3	1:B:439:ASP:HB2	1.87	0.56
1:A:400:ARG:HA	1:A:504:PRO:HA	1.88	0.55
6:B:1301:NAG:H3	6:B:1301:NAG:H83	1.87	0.55
1:B:377:TYR:OH	1:B:409:PRO:O	2.19	0.55
1:B:1100:PHE:HZ	4:R:1:NAG:H62	1.70	0.55
1:B:1113:THR:OG1	1:B:1115:ASP:OD1	2.16	0.55
1:C:1025:LYS:NZ	1:C:1039:PHE:O	2.39	0.55
1:A:469:ILE:O	1:A:471:GLN:NE2	2.40	0.55
1:C:241:LEU:HD22	1:C:256:THR:HA	1.89	0.55
1:A:125:VAL:HA	1:A:166:VAL:HG12	1.88	0.55
1:B:409:PRO:HB3	1:B:422:LEU:HD22	1.89	0.54
1:C:333:CYS:HB3	1:C:360:ALA:HB2	1.88	0.54
1:C:34:ARG:NH1	1:C:216:GLY:O	2.40	0.54
1:A:274:LEU:HD23	1:A:282:ILE:HD13	1.89	0.54
1:C:449:LEU:HD21	1:C:489:LEU:HA	1.88	0.54
1:A:21:ARG:HE	1:A:77:PHE:HB3	1.73	0.54
1:A:710:ALA:HB3	1:C:891:LEU:HB3	1.90	0.54
1:C:638:ASN:O	1:C:638:ASN:ND2	2.38	0.54
1:C:196:PHE:HB3	1:C:226:LEU:HB2	1.89	0.54
1:B:196:PHE:HB3	1:B:226:LEU:HB2	1.89	0.54
1:C:408:ALA:HA	1:C:422:LEU:HD12	1.88	0.53
1:A:1025:LYS:NZ	1:A:1039:PHE:O	2.41	0.53
1:C:520:THR:HG23	1:C:521:VAL:HG23	1.91	0.53
1:B:93:ILE:O	1:B:208:ARG:NH1	2.42	0.53
1:C:126:ILE:HB	1:C:165:TYR:HB3	1.89	0.53
1:A:181:PHE:HA	1:A:208:ARG:HH22	1.74	0.53
1:B:1123:CYS:HB2	1:B:1129:ILE:HD13	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:ILE:O	1:A:997:ARG:NH1	2.42	0.53
1:C:552:SER:OG	1:C:581:ILE:HG13	2.08	0.53
1:B:760:LEU:HD22	1:B:1005:VAL:HG21	1.90	0.53
1:B:92:SER:OG	1:B:94:GLU:HG3	2.08	0.53
1:B:97:ASN:HB3	1:B:100:ARG:HH11	1.74	0.53
1:B:181:PHE:HA	1:B:206:ILE:HA	1.91	0.53
1:B:326:PHE:O	1:B:577:GLN:NE2	2.36	0.53
1:C:471:GLN:HE22	1:C:476:PRO:HA	1.74	0.53
1:B:379:VAL:HG21	1:B:512:PHE:HZ	1.75	0.52
1:B:34:ARG:NH1	1:B:216:GLY:O	2.42	0.52
1:C:327:PRO:HD3	1:C:526:LYS:HB2	1.91	0.52
1:A:82:LEU:O	1:A:235:PHE:N	2.42	0.52
1:A:755:SER:OG	1:B:961:LYS:NZ	2.42	0.52
1:C:977:ILE:HD11	1:C:989:GLN:HB3	1.92	0.52
1:B:755:SER:OG	1:C:961:LYS:NZ	2.38	0.52
1:C:362:TYR:HB2	1:C:385:ASN:HB3	1.91	0.52
1:B:980:ARG:HG2	1:B:980:ARG:O	2.11	0.51
1:C:760:LEU:HG	1:C:1005:VAL:HG21	1.93	0.51
1:B:226:LEU:HB3	1:B:228:ILE:HD12	1.92	0.51
1:C:67:VAL:HB	1:C:260:ALA:HB3	1.93	0.51
1:C:116:LEU:HD21	1:C:127:LYS:HB3	1.92	0.51
1:A:561:GLN:OE1	1:A:574:ARG:NH2	2.43	0.51
1:B:660:ASP:H	1:B:668:CYS:HB3	1.75	0.51
1:A:358:CYS:H	1:A:521:VAL:HG12	1.76	0.51
1:C:67:VAL:O	1:C:260:ALA:N	2.42	0.51
1:B:129:CYS:HB2	1:B:131:PHE:CE2	2.46	0.51
1:B:277:ASN:OD1	1:B:281:THR:N	2.36	0.51
1:A:338:VAL:HA	1:A:353:LYS:HE2	1.92	0.50
1:A:371:PHE:HE2	1:A:374:PHE:HB3	1.76	0.50
1:B:348:TYR:HD1	1:B:449:LEU:HD11	1.76	0.50
1:B:762:ARG:NH1	1:C:954:GLN:OE1	2.44	0.50
1:B:805:ASP:OD1	1:B:805:ASP:N	2.44	0.50
1:C:142:LYS:HB2	1:C:242:HIS:CG	2.47	0.50
1:A:196:PHE:HB3	1:A:226:LEU:HB2	1.93	0.50
1:B:168:GLN:HG3	1:B:169:PRO:HD2	1.93	0.50
1:A:1088:ARG:NH1	1:A:1115:ASP:O	2.43	0.50
1:C:712:PRO:HA	1:C:1069:GLU:HA	1.94	0.50
1:B:789:PRO:HG2	1:C:704:TYR:HB3	1.94	0.50
1:C:345:ALA:HB3	1:C:396:SER:HB2	1.94	0.50
1:B:969:ALA:HA	1:B:992:ARG:HH22	1.76	0.50
1:C:1139:GLN:HG3	1:C:1140:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:ALA:HA	1:A:583:ASP:HA	1.93	0.50
1:A:381:PRO:HA	1:A:384:LEU:HB2	1.94	0.49
1:B:836:ASP:OD1	1:B:836:ASP:N	2.44	0.49
1:B:969:ALA:N	1:B:992:ARG:HH12	2.10	0.49
1:A:108:LEU:HD12	1:A:234:ARG:HE	1.77	0.49
1:B:98:ILE:O	1:B:240:ALA:N	2.45	0.49
1:B:103:ILE:HD12	1:B:103:ILE:H	1.77	0.49
1:C:29:THR:OG1	1:C:212:ASP:OD1	2.31	0.49
1:A:730:LYS:HD2	1:A:768:ALA:HB1	1.94	0.49
1:B:639:VAL:HG12	1:B:648:ILE:HG12	1.93	0.49
1:B:94:GLU:HB3	1:B:96:SER:O	2.12	0.49
1:C:140:ASP:OD1	1:C:153:ARG:NH2	2.44	0.49
1:C:106:THR:O	1:C:234:ARG:NH1	2.46	0.49
1:B:977:ILE:O	1:B:981:LEU:HB3	2.13	0.48
1:B:95:LYS:HG3	1:B:182:LYS:HE3	1.94	0.48
1:C:184:LEU:HD21	1:C:205:ILE:HD12	1.94	0.48
1:C:1100:PHE:HZ	4:T:1:NAG:H62	1.77	0.48
1:B:343:ARG:HH21	1:B:441:LYS:HD3	1.79	0.48
1:C:823:VAL:HB	1:C:1054:PRO:HG2	1.95	0.48
1:B:205:ILE:O	1:B:207:VAL:N	2.47	0.48
1:B:613:ASN:HB3	1:B:616:GLU:OE1	2.13	0.48
1:B:819:LEU:HD22	1:B:942:LEU:HD21	1.95	0.48
1:B:1139:GLN:HG3	1:B:1140:PRO:HD3	1.95	0.48
1:B:107:THR:OG1	1:B:109:ASP:OD1	2.30	0.48
1:B:1083:LYS:HD2	1:B:1119:VAL:HG11	1.95	0.48
1:C:407:ILE:HG22	1:C:416:ALA:HB2	1.94	0.48
1:B:454:ARG:HD3	1:B:455:LYS:N	2.29	0.48
1:C:375:LYS:HA	1:C:381:PRO:HB3	1.95	0.48
1:C:561:GLN:OE1	1:C:574:ARG:HG3	2.14	0.48
1:C:43:PHE:HE1	1:C:280:GLY:HA3	1.79	0.47
1:C:819:LEU:HD22	1:C:942:LEU:HD21	1.95	0.47
1:B:465:ILE:HD12	1:B:465:ILE:H	1.80	0.47
1:B:1050:PRO:O	1:B:1051:GLN:NE2	2.41	0.47
1:C:805:ASP:OD1	1:C:805:ASP:N	2.47	0.47
1:A:359:VAL:HB	1:A:524:PRO:HD3	1.95	0.47
1:C:142:LYS:HE2	1:C:242:HIS:CD2	2.50	0.47
1:A:1100:PHE:HZ	4:J:1:NAG:H61	1.78	0.47
1:B:348:TYR:HB2	1:B:464:ASP:HB3	1.96	0.47
1:C:139:LEU:O	1:C:241:LEU:N	2.45	0.47
1:A:631:ARG:H	1:A:631:ARG:HD3	1.80	0.47
1:B:348:TYR:O	1:B:464:ASP:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ASP:OD1	1:C:78:ASP:N	2.47	0.47
1:B:140:ASP:HB2	1:B:151:GLU:HG2	1.97	0.47
1:B:419:ASN:HA	1:B:458:LEU:HD23	1.97	0.47
1:B:851:LYS:HG3	1:B:852:PHE:H	1.79	0.47
1:C:900:ALA:HB1	1:C:910:GLN:HB2	1.96	0.47
1:A:141:HIS:CD2	1:A:142:LYS:HG2	2.50	0.47
1:A:292:PRO:HA	1:A:630:TRP:CH2	2.49	0.47
1:A:333:CYS:HB2	1:A:358:CYS:HB2	1.68	0.47
1:B:557:LEU:HB2	1:B:560:GLN:HG3	1.95	0.47
1:A:789:PRO:HG2	1:B:704:TYR:HB3	1.97	0.47
1:C:97:ASN:HD21	1:C:100:ARG:HD2	1.80	0.47
1:A:323:ILE:HG21	1:A:530:LEU:HA	1.96	0.47
1:A:413:GLY:H	1:A:416:ALA:HB3	1.80	0.46
1:B:174:LEU:HG	1:B:176:GLY:H	1.80	0.46
1:B:395:ASP:OD1	1:B:509:VAL:N	2.36	0.46
1:B:734:ASP:OD2	1:C:314:ASN:ND2	2.47	0.46
1:A:347:VAL:HG23	1:A:397:PHE:HB2	1.98	0.46
1:A:617:VAL:HG13	1:A:621:ILE:HD11	1.97	0.46
1:B:489:LEU:HD12	1:B:490:ARG:HB2	1.97	0.46
1:A:95:LYS:HB2	1:A:182:LYS:HG2	1.96	0.46
1:A:131:PHE:HB2	1:A:133:PHE:CE1	2.50	0.46
1:A:824:THR:HA	1:A:827:ASP:HB3	1.97	0.46
1:C:34:ARG:HH12	1:C:216:GLY:H	1.61	0.46
1:A:559:PHE:O	1:C:41:LYS:HD2	2.16	0.46
1:A:1091:VAL:HG12	1:C:901:TYR:OH	2.16	0.46
1:C:113:GLN:HG2	1:C:230:ILE:HD12	1.97	0.46
1:A:320:THR:OG1	1:A:321:GLU:OE1	2.32	0.46
1:B:981:LEU:HD12	1:B:982:ASP:N	2.30	0.46
1:A:34:ARG:NH1	1:A:216:GLY:O	2.49	0.46
1:A:883:TRP:HZ3	1:A:898:GLN:HG3	1.80	0.46
1:A:421:LYS:H	1:A:458:LEU:HD11	1.81	0.46
1:C:142:LYS:O	1:C:242:HIS:ND1	2.48	0.46
1:A:135:ASN:OD1	1:A:136:ASP:N	2.49	0.46
1:A:830:PHE:HD2	1:A:832:LYS:H	1.63	0.46
1:C:182:LYS:HG3	1:C:208:ARG:HH11	1.80	0.46
1:A:832:LYS:O	1:A:832:LYS:HG3	2.17	0.45
1:A:880:THR:HG23	1:B:704:TYR:HB2	1.98	0.45
1:A:1083:LYS:HD3	1:A:1119:VAL:HG11	1.98	0.45
1:B:139:LEU:O	1:B:241:LEU:N	2.44	0.45
1:C:819:LEU:O	1:C:823:VAL:HG23	2.16	0.45
1:B:108:LEU:HG	1:B:234:ARG:HH12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1:NAG:H62	3:E:2:NAG:N2	2.31	0.45
1:C:403:GLU:O	1:C:407:ILE:HG23	2.16	0.45
1:A:373:THR:HB	1:A:432:ALA:H	1.81	0.45
1:A:394:ALA:HA	1:A:510:LEU:HG	1.98	0.45
1:A:712:PRO:HA	1:A:1069:GLU:HA	1.99	0.45
1:C:127:LYS:HD2	1:C:164:GLU:OE1	2.17	0.45
1:C:556:PHE:CD2	1:C:581:ILE:HG21	2.52	0.45
1:A:424:ASP:OD1	1:A:424:ASP:N	2.50	0.45
1:B:82:LEU:O	1:B:235:PHE:N	2.47	0.45
1:A:483:PHE:HB3	1:C:372:PHE:HB2	1.99	0.44
1:A:744:THR:O	1:A:748:ASN:ND2	2.49	0.44
1:C:277:ASN:OD1	1:C:281:THR:N	2.49	0.44
1:B:1079:CYS:HB2	1:B:1123:CYS:HB2	1.97	0.44
1:A:81:VAL:HB	1:A:234:ARG:HD2	1.99	0.44
1:A:277:ASN:OD1	1:A:281:THR:N	2.44	0.44
1:B:73:GLY:HA2	1:B:256:THR:HG21	1.98	0.44
1:B:88:VAL:HG12	1:B:90:PHE:H	1.82	0.44
1:B:321:GLU:HG3	1:B:536:VAL:HG23	1.98	0.44
1:B:348:TYR:CE1	1:B:449:LEU:HD21	2.53	0.44
1:A:75:LYS:HD2	1:A:255:TRP:HD1	1.83	0.44
1:A:1140:PRO:HG2	1:A:1141:GLU:OE1	2.17	0.44
1:A:129:CYS:HB2	1:A:131:PHE:CE1	2.53	0.44
1:A:454:ARG:HG2	1:A:455:LYS:H	1.83	0.44
1:B:182:LYS:HG2	1:B:208:ARG:HD3	1.98	0.44
4:U:1:NAG:H61	4:U:2:NAG:O5	2.18	0.44
1:A:185:ARG:HA	1:A:202:HIS:HD2	1.83	0.44
1:A:490:ARG:HG2	1:A:491:SER:N	2.33	0.44
1:B:41:LYS:NZ	1:C:561:GLN:HG2	2.32	0.44
1:A:292:PRO:HB2	1:A:605:VAL:HG21	2.00	0.43
1:B:142:LYS:HB2	1:B:242:HIS:CG	2.53	0.43
1:A:318:GLN:NE2	1:A:626:LEU:HD12	2.32	0.43
1:B:349:ALA:HA	1:B:463:ARG:HB3	2.00	0.43
1:B:141:HIS:CE1	1:B:142:LYS:HG2	2.53	0.43
1:C:480:VAL:HG22	1:C:481:ALA:H	1.83	0.43
1:C:316:ARG:H	1:C:626:LEU:HB2	1.83	0.43
1:C:454:ARG:NE	1:C:456:SER:O	2.51	0.43
1:B:287:ASP:O	1:B:294:SER:HB3	2.18	0.43
1:B:966:LYS:HB2	1:B:966:LYS:HE2	1.72	0.43
1:C:333:CYS:HB2	1:C:358:CYS:HB3	1.82	0.43
1:A:287:ASP:OD1	1:A:288:CYS:N	2.51	0.43
1:B:453:PHE:HB3	1:B:488:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:LEU:O	1:C:235:PHE:N	2.44	0.43
1:B:487:PHE:HA	1:B:488:PRO:HD3	1.93	0.43
1:C:70:GLY:O	1:C:74:THR:N	2.36	0.43
1:C:535:CYS:HB3	1:C:587:CYS:HB3	1.88	0.43
1:B:126:ILE:HD12	1:B:165:TYR:HD2	1.83	0.42
1:B:901:TYR:OH	1:C:1091:VAL:HG12	2.19	0.42
1:C:706:ASN:HB2	4:V:1:NAG:H2	2.00	0.42
1:A:805:ASP:OD1	1:A:805:ASP:N	2.50	0.42
1:B:371:PHE:HB3	1:B:433:TRP:CD1	2.54	0.42
1:C:100:ARG:HG2	1:C:119:ASN:HB3	2.00	0.42
1:A:451:ARG:HD3	1:A:488:PRO:HG3	2.02	0.42
1:B:656:SER:HB3	1:B:695:SER:HB3	2.02	0.42
1:A:148:MET:SD	1:A:149:GLU:HG3	2.59	0.42
1:A:386:ASP:HB3	1:A:525:LYS:HE2	2.02	0.42
1:B:712:PRO:HA	1:B:1069:GLU:HA	2.01	0.42
1:C:421:LYS:HE3	1:C:462:GLU:H	1.84	0.42
1:A:446:TYR:HB3	1:A:491:SER:HA	2.00	0.42
1:B:79:ASN:HB3	1:B:236:GLN:HE21	1.84	0.42
1:B:428:GLY:HA2	1:B:512:PHE:CE1	2.54	0.42
1:A:384:LEU:HD23	1:A:387:LEU:HD12	2.01	0.42
1:B:505:TYR:O	1:B:507:VAL:HG23	2.20	0.42
1:C:305:VAL:HB	1:C:599:THR:HG23	2.01	0.42
1:C:535:CYS:HB3	1:C:548:VAL:HG22	2.02	0.42
1:C:903:PHE:CD2	1:C:913:LEU:HB2	2.54	0.42
1:A:968:GLY:O	1:A:992:ARG:NH2	2.52	0.42
1:C:326:PHE:CD2	1:C:327:PRO:HD2	2.55	0.42
1:C:403:GLU:HG3	1:C:415:ILE:HG22	2.00	0.42
1:C:436:ASN:HB2	1:C:503:GLN:OE1	2.19	0.42
1:C:982:ASP:HB2	1:C:984:PRO:HD2	2.00	0.42
1:B:494:PHE:O	1:B:494:PHE:CG	2.72	0.42
1:C:71:THR:O	1:C:71:THR:HG22	2.19	0.42
1:C:618:PRO:O	1:C:621:ILE:HG12	2.19	0.42
1:C:756:PHE:HA	1:C:759:GLN:NE2	2.34	0.42
1:A:453:PHE:HZ	1:C:375:LYS:HD3	1.83	0.42
1:A:801:GLN:NE2	1:A:932:GLN:OE1	2.31	0.42
1:A:819:LEU:HD22	1:A:942:LEU:HD21	2.02	0.42
1:A:951:HIS:O	1:A:954:GLN:HG3	2.19	0.42
1:B:740:CYS:HB3	1:B:746:CYS:HB3	1.90	0.42
1:A:170:PHE:CE1	1:A:171:LEU:HD23	2.55	0.41
1:A:379:VAL:HG21	1:C:980:ARG:CZ	2.50	0.41
1:B:102:TRP:HB3	1:B:104:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:THR:HB	1:C:74:THR:HB	2.02	0.41
1:C:182:LYS:H	1:C:208:ARG:HH12	1.67	0.41
1:C:205:ILE:O	1:C:208:ARG:NH2	2.48	0.41
1:C:480:VAL:HG13	1:C:481:ALA:N	2.35	0.41
1:A:1070:LYS:HB3	1:A:1070:LYS:HE3	1.79	0.41
1:B:19:THR:HG23	1:B:75:LYS:HD3	2.02	0.41
1:B:819:LEU:O	1:B:823:VAL:HG23	2.20	0.41
1:B:981:LEU:HD12	1:B:982:ASP:H	1.84	0.41
1:B:428:GLY:HA2	1:B:512:PHE:HE1	1.84	0.41
1:C:433:TRP:HE1	1:C:506:ARG:HD2	1.86	0.41
1:C:700:ASN:OD1	1:C:701:SER:N	2.53	0.41
1:C:638:ASN:C	1:C:638:ASN:HD22	2.14	0.41
1:C:1050:PRO:O	1:C:1051:GLN:NE2	2.48	0.41
1:B:660:ASP:HB3	1:B:669:ALA:O	2.21	0.41
1:C:419:ASN:HD21	1:C:451:ARG:N	2.18	0.41
1:A:205:ILE:HB	1:A:208:ARG:HH21	1.85	0.41
1:A:686:SER:OG	1:A:687:GLN:N	2.53	0.41
1:B:292:PRO:HG3	1:B:630:TRP:NE1	2.33	0.41
1:B:512:PHE:CD2	1:B:513:GLU:HG2	2.56	0.41
1:B:1142:LEU:HD13	1:C:1138:LEU:HD22	2.02	0.41
1:B:390:THR:HG22	1:B:519:ALA:HA	2.03	0.41
1:A:129:CYS:HB2	1:A:131:PHE:CZ	2.56	0.40
1:A:139:LEU:O	1:A:241:LEU:N	2.54	0.40
1:A:207:VAL:HG22	1:A:209:GLU:H	1.86	0.40
1:A:803:LEU:HD23	1:A:803:LEU:HA	1.95	0.40
1:B:93:ILE:O	1:B:93:ILE:HG22	2.20	0.40
1:B:431:ILE:O	1:B:507:VAL:HA	2.21	0.40
1:A:270:ARG:NH1	1:A:287:ASP:OD2	2.54	0.40
1:B:173:ASP:HB2	1:B:185:ARG:HH21	1.85	0.40
1:C:994:ILE:O	1:C:998:LEU:HD23	2.21	0.40
1:B:124:VAL:HG22	1:B:167:SER:H	1.86	0.40
1:B:154:VAL:HG23	1:B:155:TYR:HD1	1.86	0.40
1:B:986:ALA:O	1:B:990:ILE:HD12	2.21	0.40
1:C:373:THR:OG1	1:C:432:ALA:N	2.54	0.40
1:C:753:TYR:HB3	1:C:756:PHE:CE2	2.56	0.40
1:C:220:LEU:HD23	1:C:220:LEU:HA	1.95	0.40
1:C:372:PHE:CE2	1:C:373:THR:HG23	2.56	0.40
1:A:903:PHE:CD2	1:A:913:LEU:HB2	2.57	0.40
1:B:783:LYS:H	1:B:783:LYS:HG2	1.71	0.40
1:C:208:ARG:HD3	1:C:208:ARG:HA	1.90	0.40
1:C:376:CYS:SG	1:C:381:PRO:HA	2.61	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	1089/1285 (85%)	1023 (94%)	66 (6%)	0	100	100
1	B	1086/1285 (84%)	1004 (92%)	78 (7%)	4 (0%)	34	71
1	C	1086/1285 (84%)	1032 (95%)	51 (5%)	3 (0%)	41	75
All	All	3261/3855 (85%)	3059 (94%)	195 (6%)	7 (0%)	50	81

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	373	THR
1	B	369	ALA
1	B	502	HIS
1	C	480	VAL
1	C	160	ASN
1	B	206	ILE
1	C	125	VAL

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	954/1113 (86%)	949 (100%)	5 (0%)	88	96
1	B	956/1113 (86%)	956 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	954/1113 (86%)	950 (100%)	4 (0%)	91	97
All	All	2864/3339 (86%)	2855 (100%)	9 (0%)	92	97

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	132	GLN
1	A	405	ARG
1	A	475	LYS
1	A	631	ARG
1	C	21	ARG
1	C	375	LYS
1	C	631	ARG
1	C	638	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	236	GLN
1	B	923	GLN
1	C	638	ASN
1	C	923	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](#)

67 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
2	NAG	D	1	2,1	14,14,15	0.35	0	17,19,21	1.30	1 (5%)
2	NAG	D	2	2	14,14,15	0.61	1 (7%)	17,19,21	1.25	1 (5%)
2	BMA	D	3	2	11,11,12	1.03	0	15,15,17	1.55	2 (13%)
2	MAN	D	4	2	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
3	NAG	E	1	3,1	14,14,15	0.26	0	17,19,21	0.51	0
3	NAG	E	2	3	14,14,15	0.32	0	17,19,21	0.57	0
4	NAG	F	1	4,1	14,14,15	0.47	0	17,19,21	0.47	0
4	NAG	F	2	4	14,14,15	0.41	0	17,19,21	1.31	2 (11%)
4	BMA	F	3	4	11,11,12	1.41	2 (18%)	15,15,17	0.96	1 (6%)
4	NAG	G	1	4,1	14,14,15	0.27	0	17,19,21	0.49	0
4	NAG	G	2	4	14,14,15	0.21	0	17,19,21	0.43	0
4	BMA	G	3	4	11,11,12	0.61	0	15,15,17	0.77	0
3	NAG	H	1	3,1	14,14,15	0.33	0	17,19,21	0.58	0
3	NAG	H	2	3	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	I	1	4,1	14,14,15	0.25	0	17,19,21	0.57	0
4	NAG	I	2	4	14,14,15	0.30	0	17,19,21	0.45	0
4	BMA	I	3	4	11,11,12	0.56	0	15,15,17	0.75	0
4	NAG	J	1	4,1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	J	2	4	14,14,15	0.21	0	17,19,21	0.41	0
4	BMA	J	3	4	11,11,12	0.58	0	15,15,17	0.73	0
4	NAG	K	1	4,1	14,14,15	0.24	0	17,19,21	0.46	0
4	NAG	K	2	4	14,14,15	0.21	0	17,19,21	0.39	0
4	BMA	K	3	4	11,11,12	0.59	0	15,15,17	0.77	0
4	NAG	L	1	4,1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	L	2	4	14,14,15	0.22	0	17,19,21	0.40	0
4	BMA	L	3	4	11,11,12	0.56	0	15,15,17	0.72	0
3	NAG	M	1	3,1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	M	2	3	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	N	1	4,1	14,14,15	0.27	0	17,19,21	0.42	0
4	NAG	N	2	4	14,14,15	0.26	0	17,19,21	0.51	0
4	BMA	N	3	4	11,11,12	0.64	0	15,15,17	0.76	0
4	NAG	O	1	4,1	14,14,15	0.24	0	17,19,21	0.48	0
4	NAG	O	2	4	14,14,15	0.22	0	17,19,21	0.39	0
4	BMA	O	3	4	11,11,12	0.61	0	15,15,17	0.75	0
4	NAG	P	1	4,1	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	P	2	4	14,14,15	0.20	0	17,19,21	0.45	0
4	BMA	P	3	4	11,11,12	0.57	0	15,15,17	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	Q	1	4,1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	Q	2	4	14,14,15	0.22	0	17,19,21	0.39	0
4	BMA	Q	3	4	11,11,12	0.60	0	15,15,17	0.74	0
4	NAG	R	1	4,1	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	R	2	4	14,14,15	0.25	0	17,19,21	0.50	0
4	BMA	R	3	4	11,11,12	0.61	0	15,15,17	0.75	0
4	NAG	S	1	4,1	14,14,15	0.71	1 (7%)	17,19,21	0.77	0
4	NAG	S	2	4	14,14,15	0.24	0	17,19,21	0.40	0
4	BMA	S	3	4	11,11,12	0.82	0	15,15,17	0.91	0
4	NAG	T	1	4,1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	T	2	4	14,14,15	0.22	0	17,19,21	0.38	0
4	BMA	T	3	4	11,11,12	0.57	0	15,15,17	0.76	0
4	NAG	U	1	4,1	14,14,15	0.28	0	17,19,21	0.43	0
4	NAG	U	2	4	14,14,15	0.38	0	17,19,21	0.39	0
4	BMA	U	3	4	11,11,12	0.64	0	15,15,17	0.71	0
4	NAG	V	1	4,1	14,14,15	0.43	0	17,19,21	0.43	0
4	NAG	V	2	4	14,14,15	0.25	0	17,19,21	0.36	0
4	BMA	V	3	4	11,11,12	1.08	2 (18%)	15,15,17	1.60	3 (20%)
4	NAG	W	1	4,1	14,14,15	0.21	0	17,19,21	0.46	0
4	NAG	W	2	4	14,14,15	0.23	0	17,19,21	0.41	0
4	BMA	W	3	4	11,11,12	0.59	0	15,15,17	0.71	0
4	NAG	X	1	4,1	14,14,15	0.23	0	17,19,21	0.50	0
4	NAG	X	2	4	14,14,15	0.22	0	17,19,21	0.38	0
4	BMA	X	3	4	11,11,12	0.59	0	15,15,17	0.77	0
5	NAG	Y	1	5,1	14,14,15	0.27	0	17,19,21	0.64	1 (5%)
5	NAG	Y	2	5	14,14,15	0.25	0	17,19,21	0.43	0
5	FUC	Y	3	5	10,10,11	0.95	0	14,14,16	1.24	2 (14%)
4	NAG	Z	1	4,1	14,14,15	0.38	0	17,19,21	0.74	1 (5%)
4	NAG	Z	2	4	14,14,15	0.31	0	17,19,21	0.72	1 (5%)
4	BMA	Z	3	4	11,11,12	0.61	0	15,15,17	0.75	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
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	1/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	3/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	1/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	BMA	K	3	4	-	1/2/19/22	0/1/1/1
4	NAG	L	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	BMA	L	3	4	-	1/2/19/22	0/1/1/1
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	3/6/23/26	0/1/1/1
4	BMA	N	3	4	-	1/2/19/22	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	1/6/23/26	0/1/1/1
4	BMA	O	3	4	-	0/2/19/22	0/1/1/1
4	NAG	P	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	1/6/23/26	0/1/1/1
4	BMA	P	3	4	-	0/2/19/22	0/1/1/1
4	NAG	Q	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	BMA	Q	3	4	-	0/2/19/22	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	R	3	4	-	0/2/19/22	0/1/1/1
4	NAG	S	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	S	2	4	-	1/6/23/26	0/1/1/1
4	BMA	S	3	4	-	0/2/19/22	0/1/1/1
4	NAG	T	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	BMA	T	3	4	-	0/2/19/22	0/1/1/1
4	NAG	U	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	3/6/23/26	0/1/1/1
4	BMA	U	3	4	-	0/2/19/22	0/1/1/1
4	NAG	V	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	BMA	V	3	4	-	0/2/19/22	0/1/1/1
4	NAG	W	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	0/6/23/26	0/1/1/1
4	BMA	W	3	4	-	0/2/19/22	0/1/1/1
4	NAG	X	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	BMA	X	3	4	-	1/2/19/22	0/1/1/1
5	NAG	Y	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	2/6/23/26	0/1/1/1
5	FUC	Y	3	5	-	-	0/1/1/1
4	NAG	Z	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	1/6/23/26	0/1/1/1
4	BMA	Z	3	4	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3	BMA	C1-C2	3.73	1.60	1.52
4	S	1	NAG	O5-C1	-2.51	1.39	1.43
4	F	3	BMA	O5-C1	2.33	1.47	1.43
4	V	3	BMA	C4-C5	2.27	1.57	1.53
4	V	3	BMA	O5-C5	2.14	1.47	1.43
2	D	2	NAG	O5-C1	2.09	1.47	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	4.74	118.61	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	4.71	118.58	112.19
4	V	3	BMA	C1-O5-C5	4.51	118.31	112.19
4	F	2	NAG	C2-N2-C7	4.39	129.15	122.90
2	D	3	BMA	C1-O5-C5	4.28	117.99	112.19
2	D	4	MAN	C1-O5-C5	3.03	116.30	112.19
5	Y	3	FUC	O5-C5-C4	2.97	114.86	109.52
4	Z	1	NAG	C1-O5-C5	2.34	115.36	112.19
4	F	3	BMA	O2-C2-C3	-2.32	105.49	110.14
4	V	3	BMA	C3-C4-C5	2.27	114.29	110.24
2	D	4	MAN	O2-C2-C3	-2.23	105.66	110.14
5	Y	3	FUC	C3-C4-C5	2.23	113.25	109.77
4	Z	2	NAG	C1-O5-C5	2.21	115.19	112.19
5	Y	1	NAG	C1-O5-C5	2.20	115.17	112.19
2	D	3	BMA	C3-C4-C5	2.15	114.08	110.24
4	V	3	BMA	O5-C5-C6	2.07	110.44	107.20
4	F	2	NAG	C1-C2-N2	2.02	113.93	110.49

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1	NAG	O5-C5-C6-O6
5	Y	2	NAG	C4-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	V	1	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	X	3	BMA	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
4	F	1	NAG	C1-C2-N2-C7
4	P	2	NAG	O5-C5-C6-O6
4	L	3	BMA	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6

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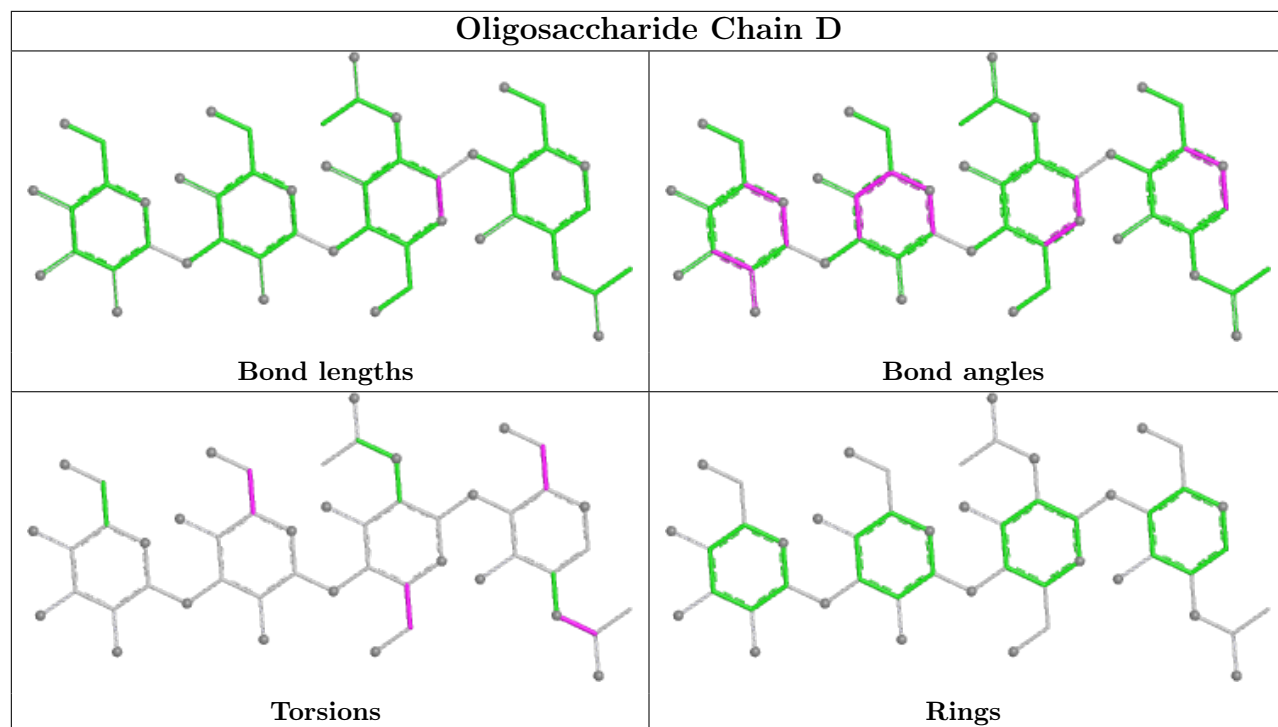
Mol	Chain	Res	Type	Atoms
4	U	2	NAG	C1-C2-N2-C7
4	R	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
3	E	2	NAG	C3-C2-N2-C7
3	H	1	NAG	C3-C2-N2-C7
4	F	2	NAG	C3-C2-N2-C7
4	G	1	NAG	C3-C2-N2-C7
4	I	1	NAG	C3-C2-N2-C7
4	R	2	NAG	C3-C2-N2-C7
4	S	1	NAG	C3-C2-N2-C7
4	Z	2	NAG	C3-C2-N2-C7
3	E	2	NAG	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	V	1	NAG	C1-C2-N2-C7
4	F	1	NAG	C3-C2-N2-C7
4	N	2	NAG	C3-C2-N2-C7
4	V	2	NAG	O5-C5-C6-O6
4	S	1	NAG	C1-C2-N2-C7

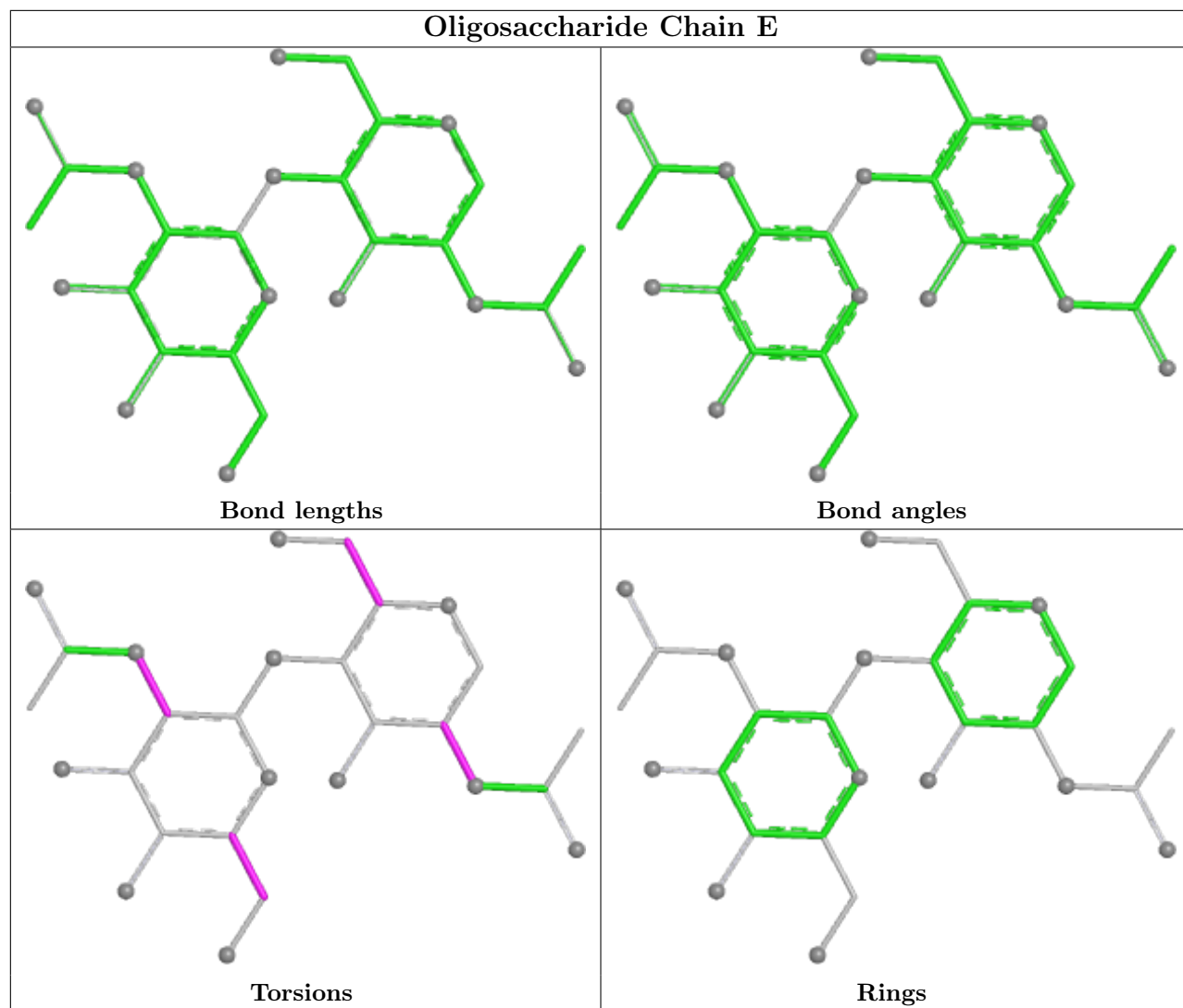
There are no ring outliers.

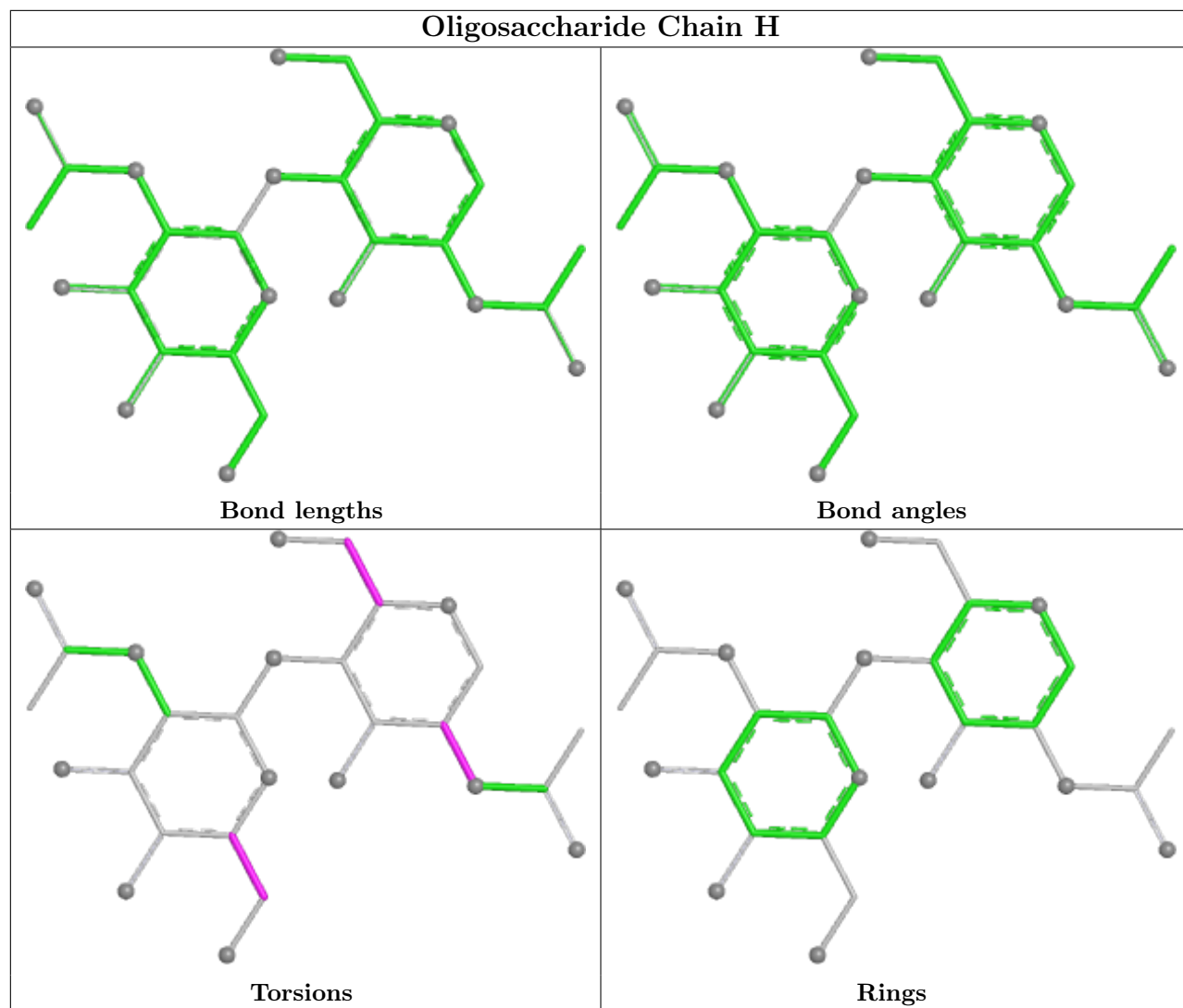
13 monomers are involved in 10 short contacts:

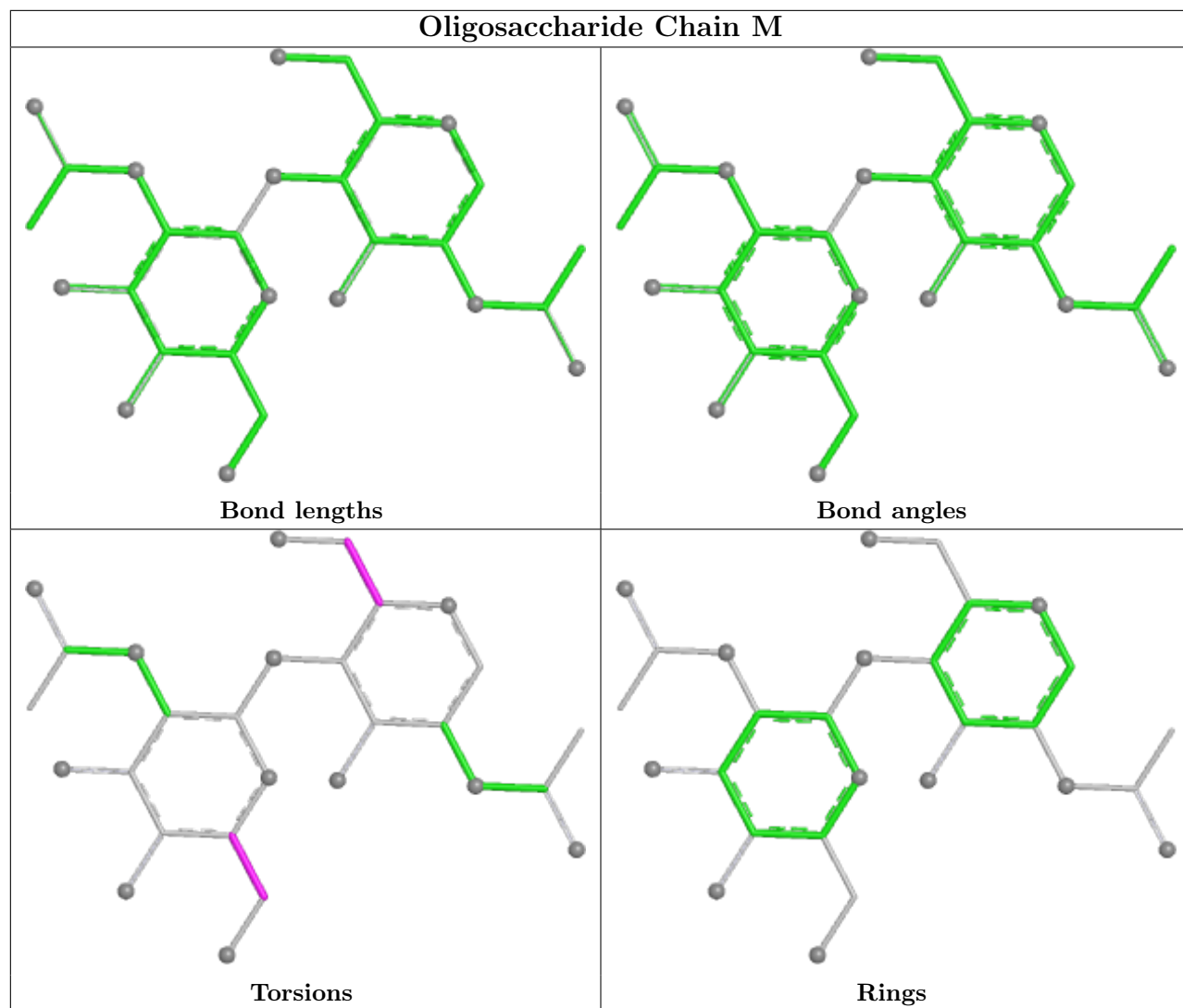
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	V	1	NAG	1	0
4	U	1	NAG	1	0
3	E	1	NAG	1	0
2	D	4	MAN	1	0
4	T	1	NAG	1	0
4	J	1	NAG	1	0
4	Z	1	NAG	1	0
4	F	2	NAG	1	0
4	R	1	NAG	1	0
4	S	1	NAG	1	0
2	D	2	NAG	1	0
4	U	2	NAG	1	0
3	E	2	NAG	1	0

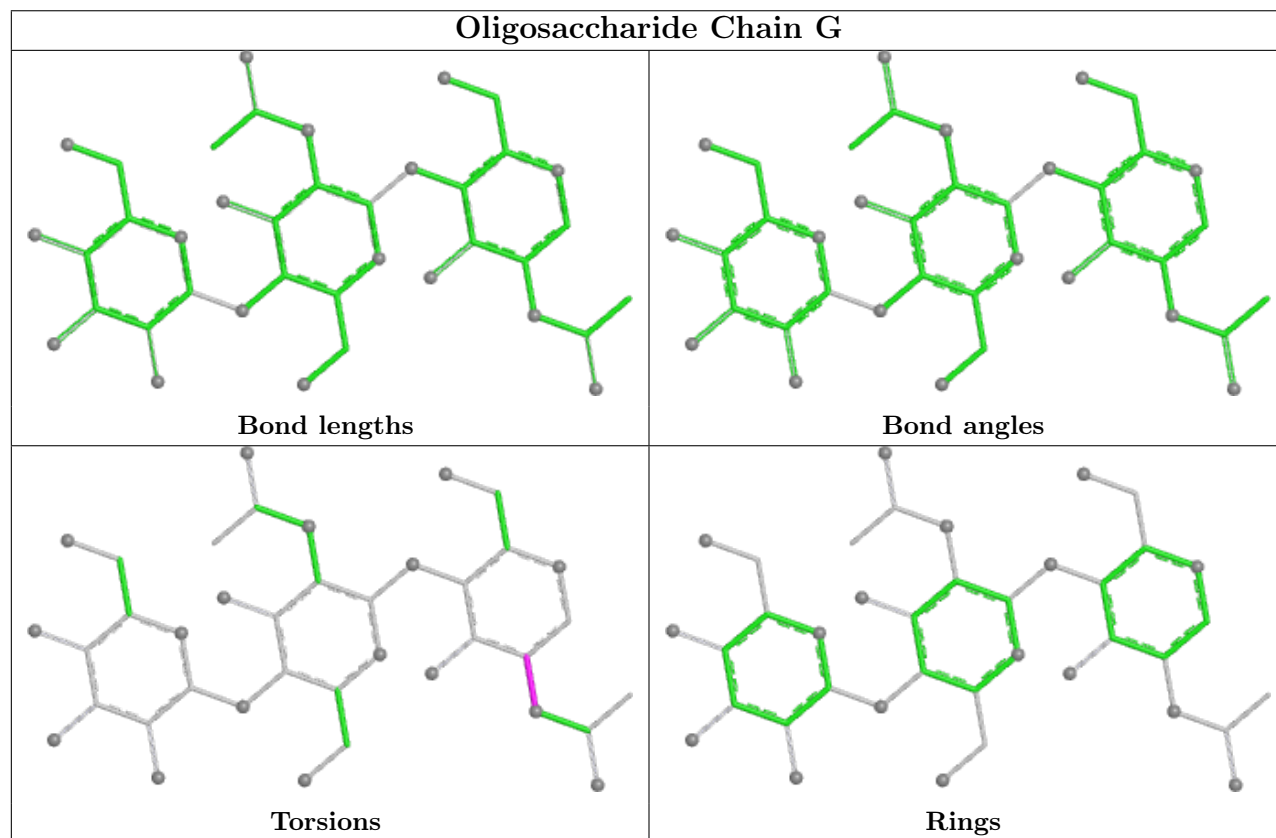
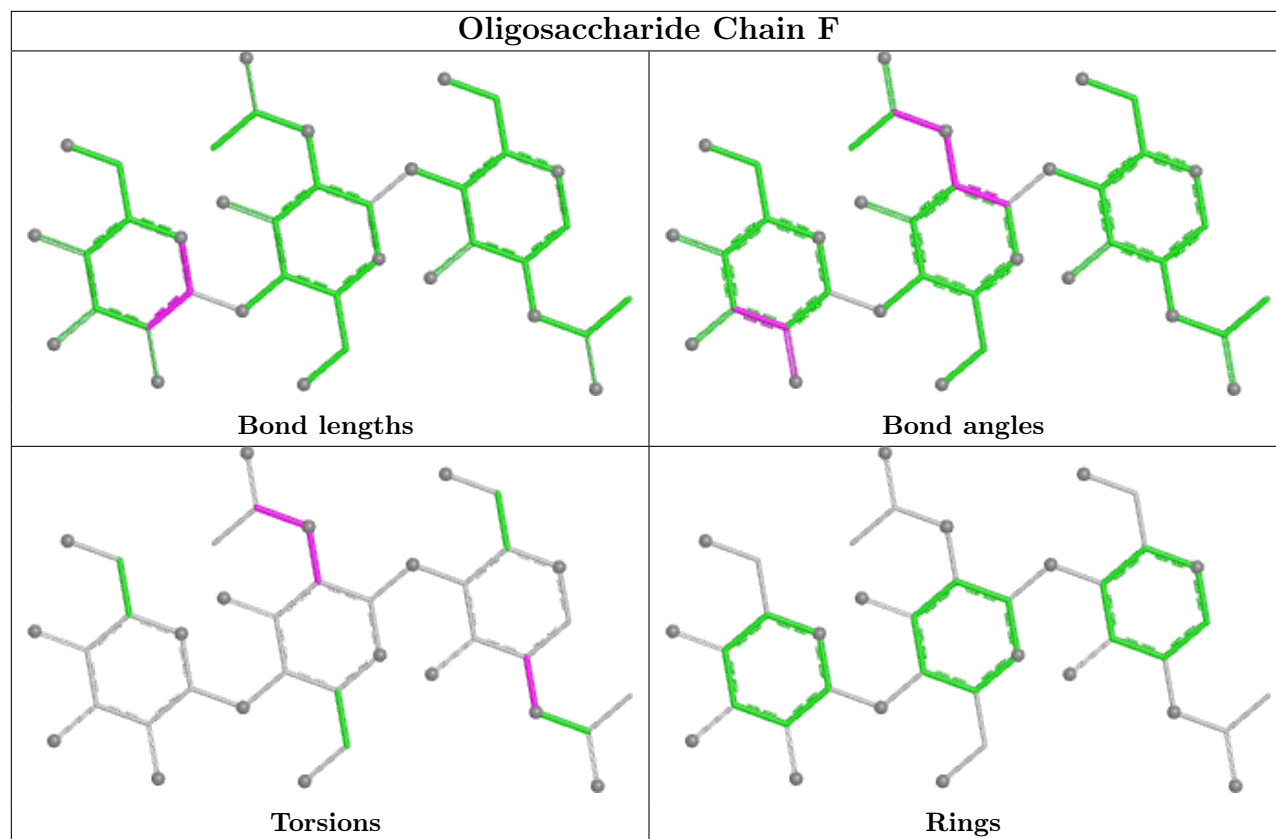
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

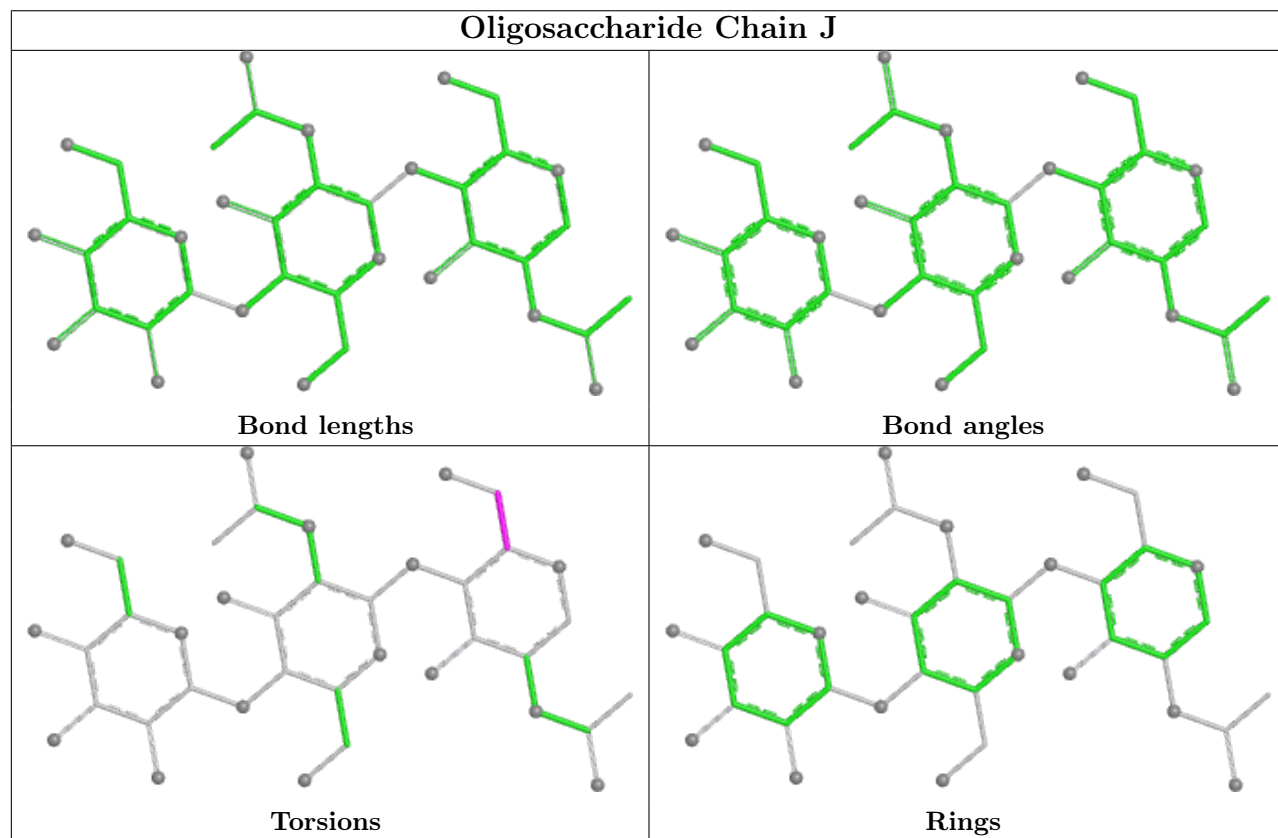
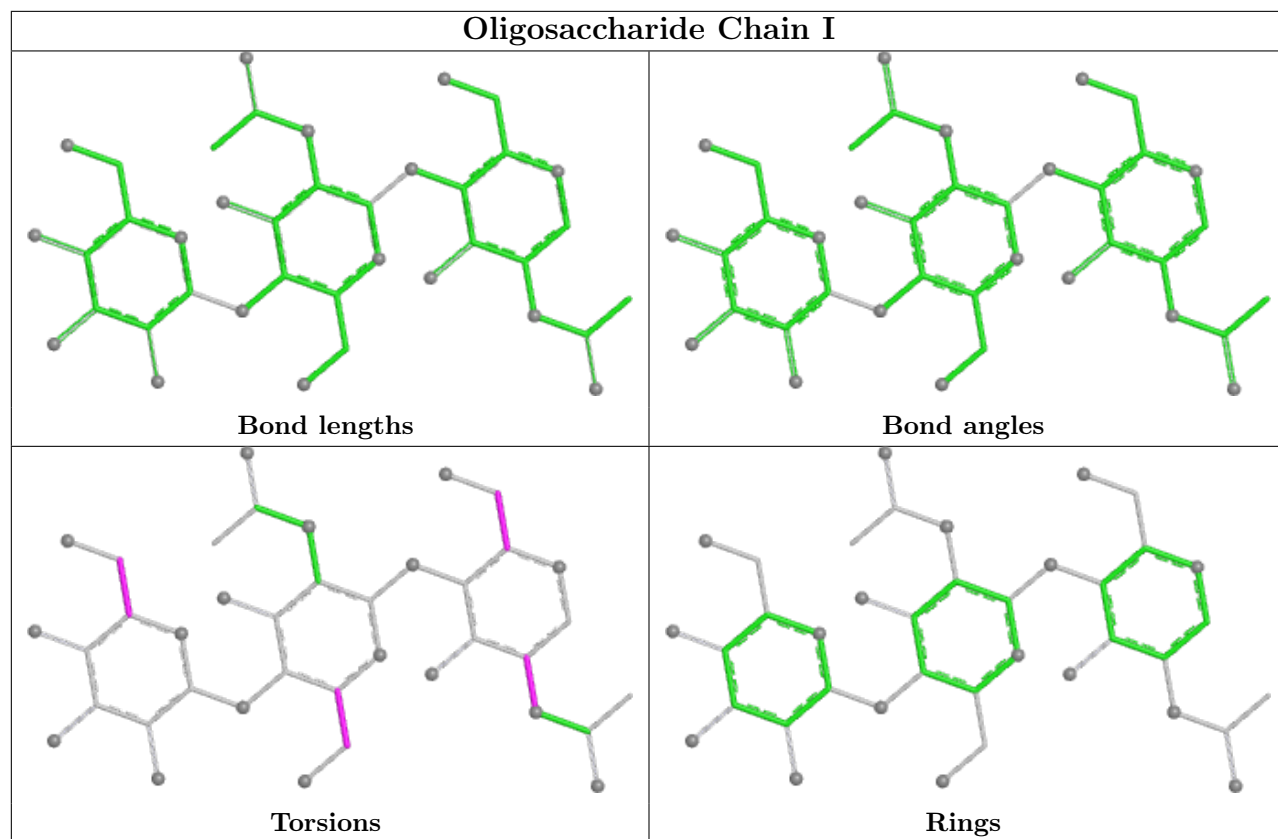


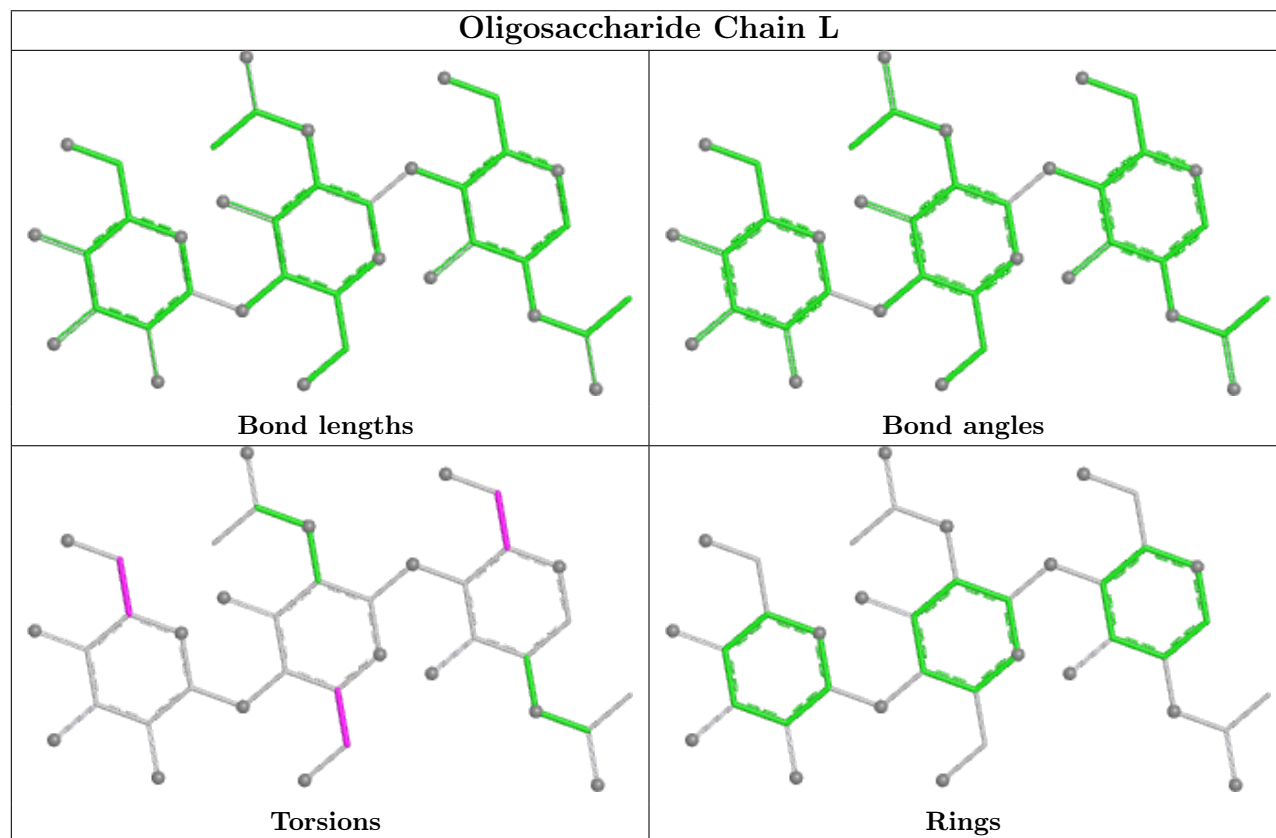
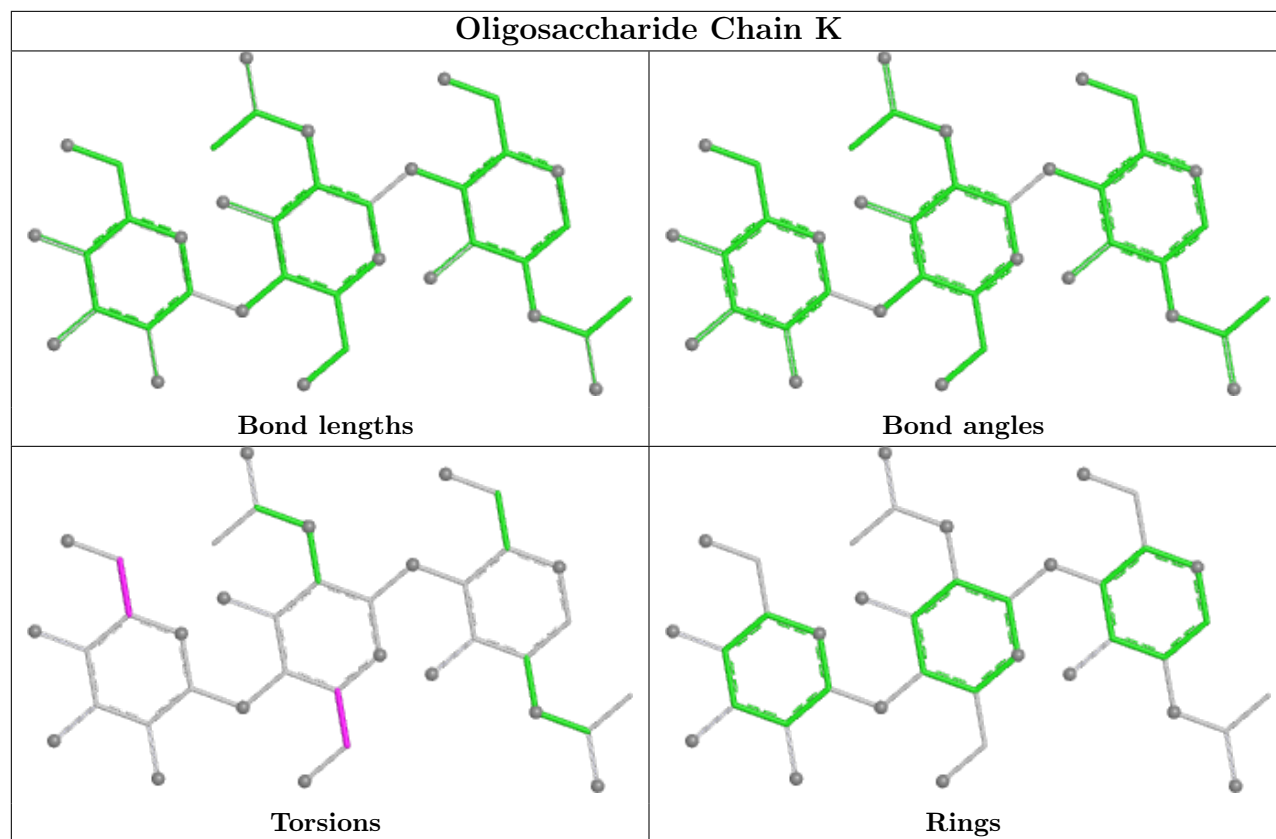


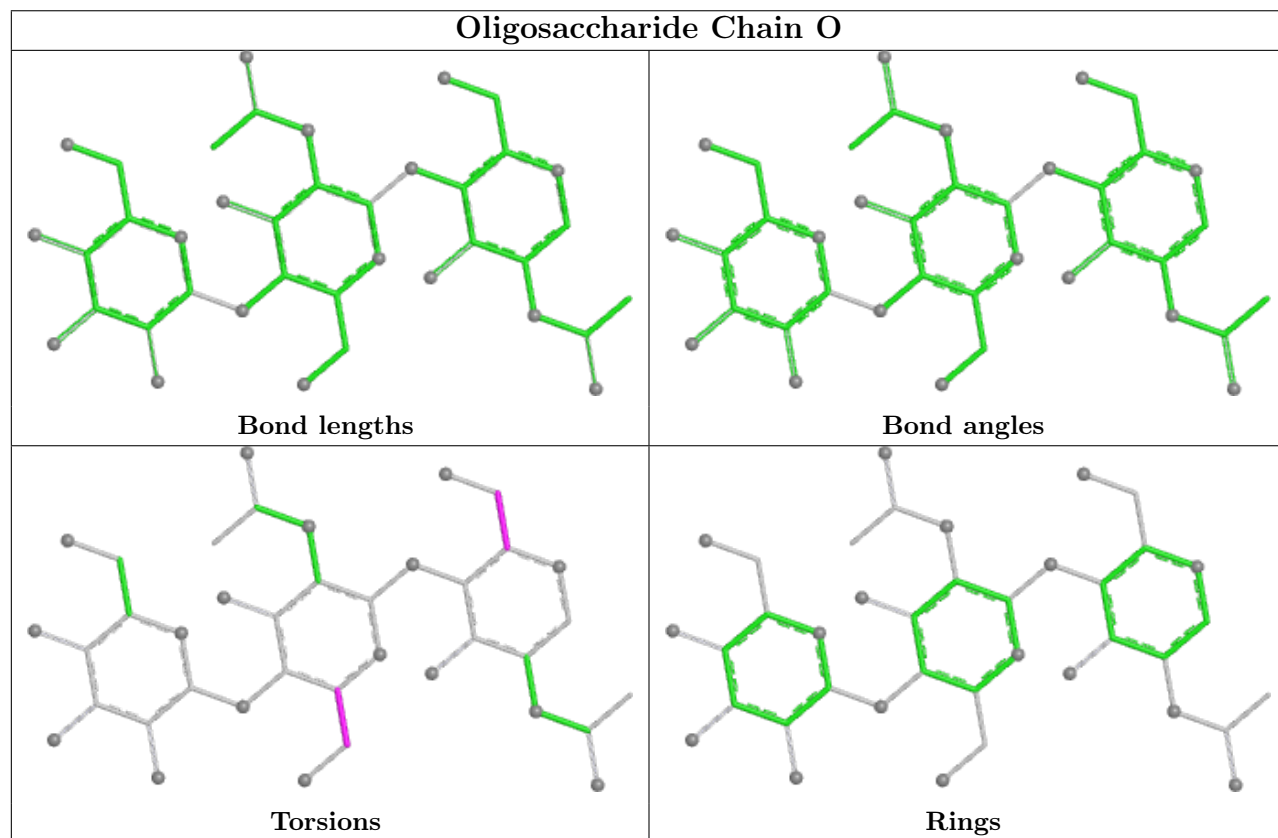
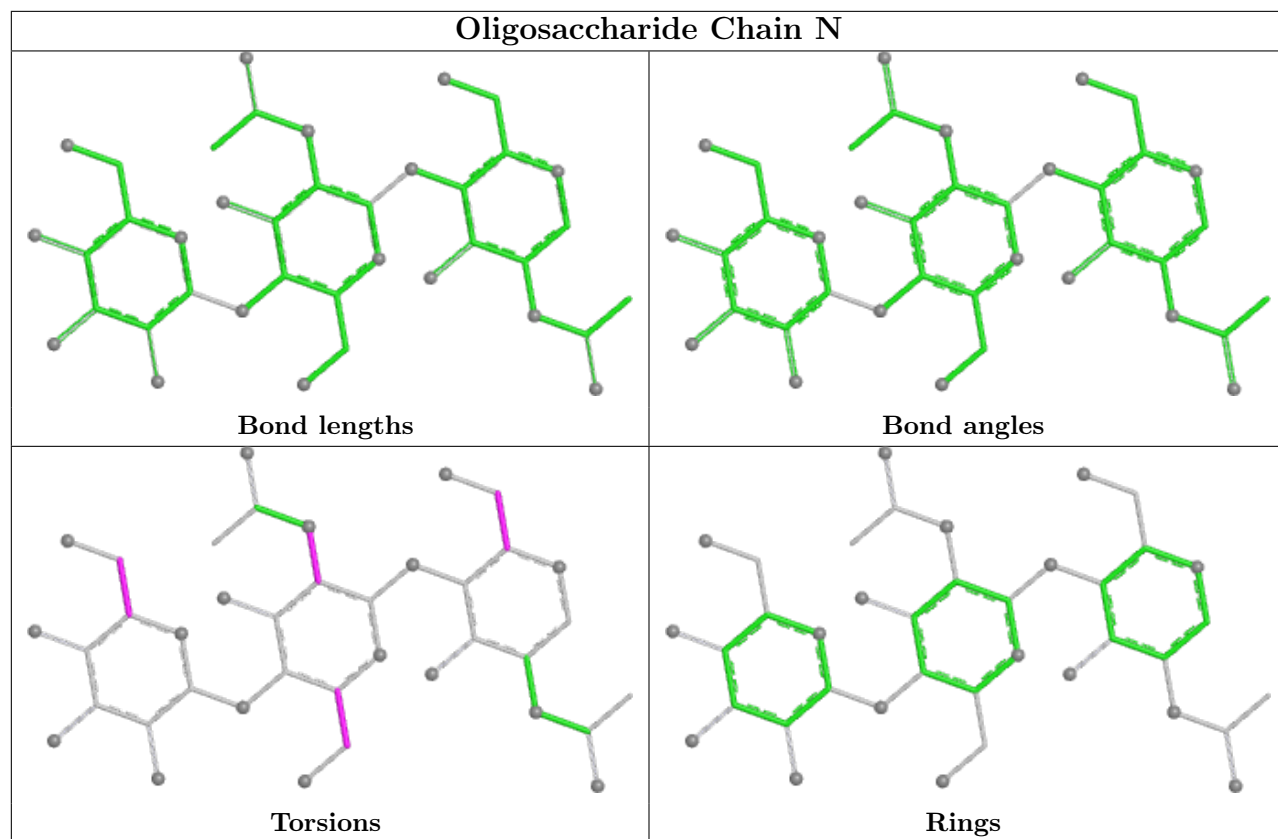


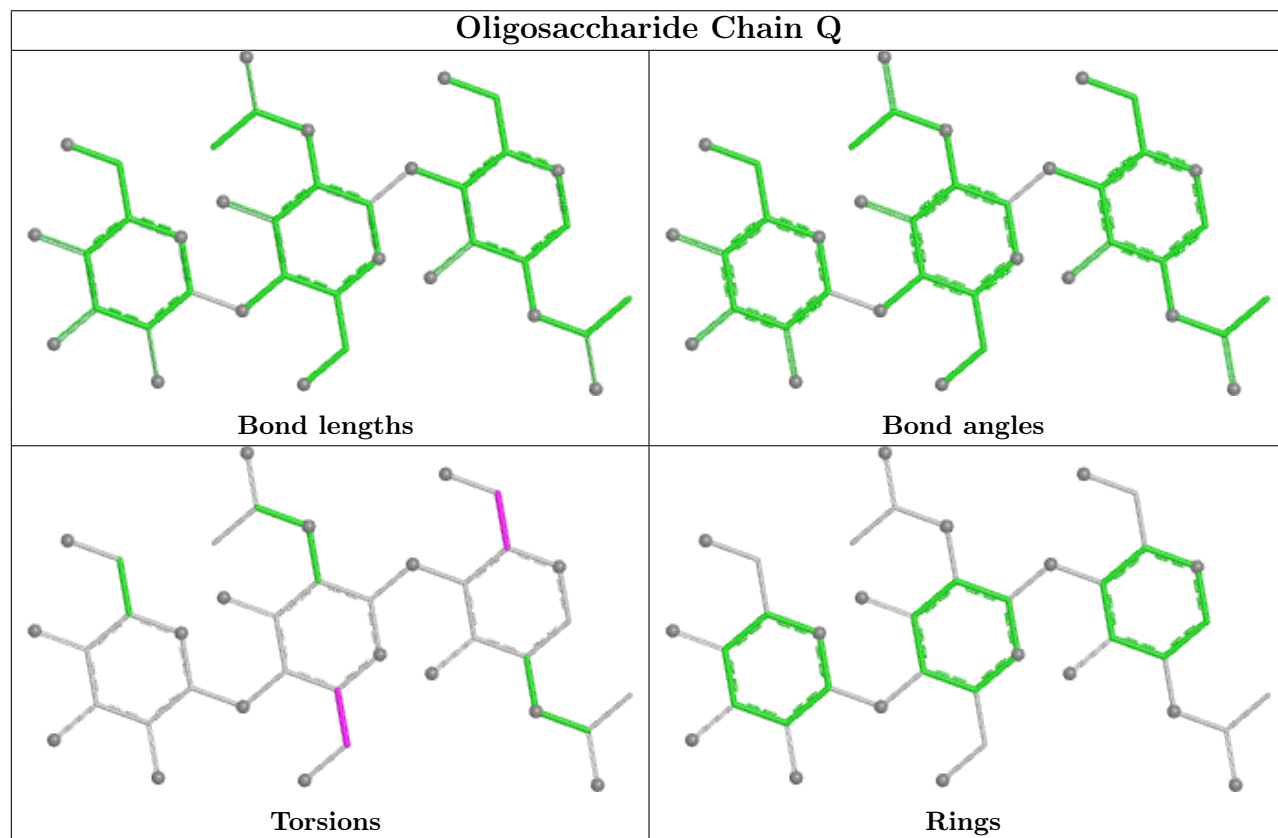
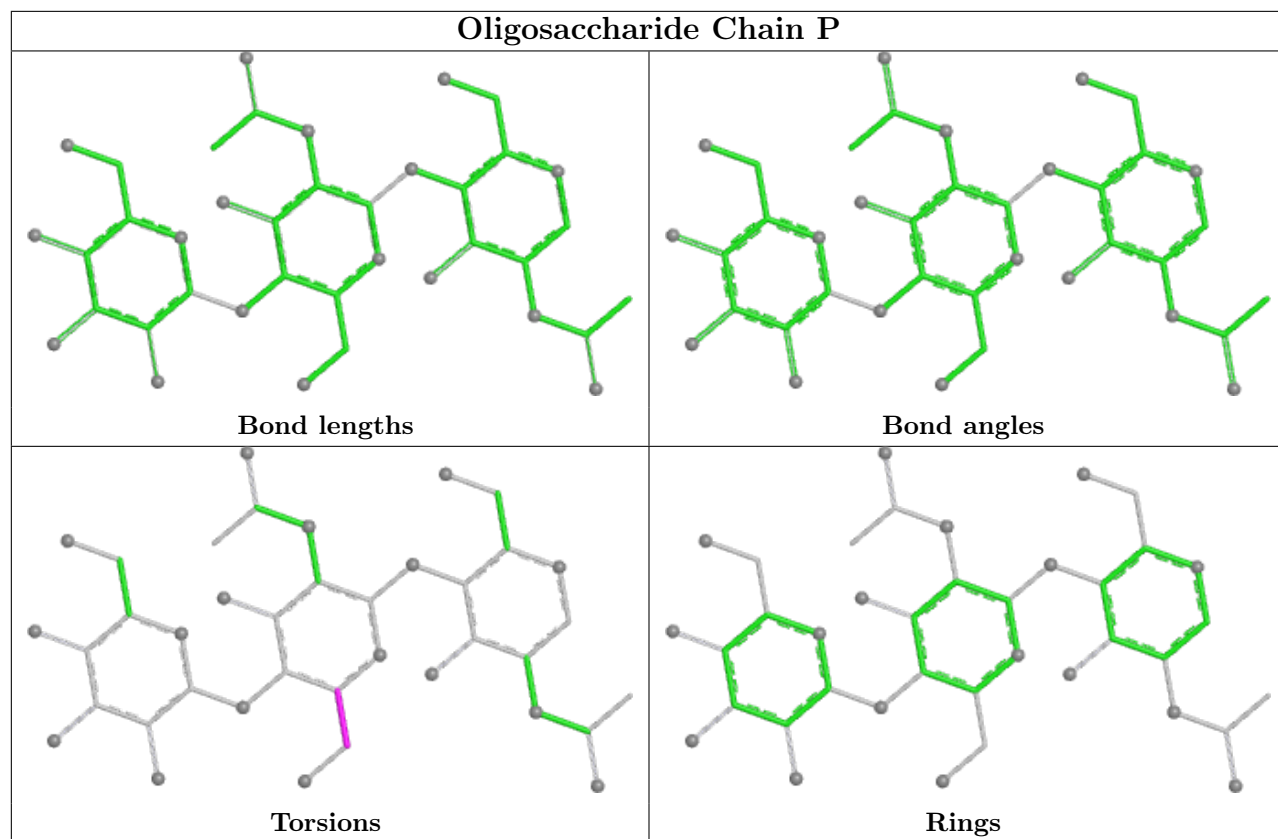


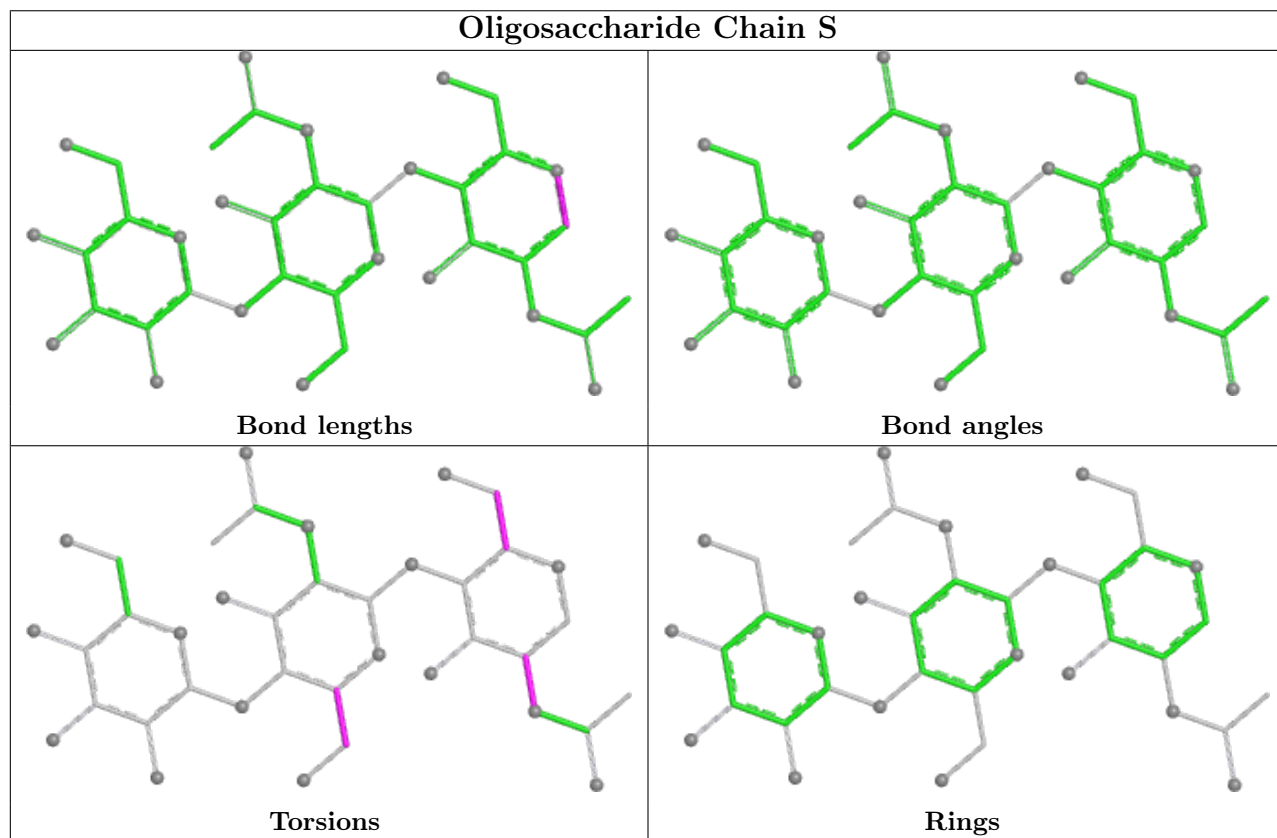
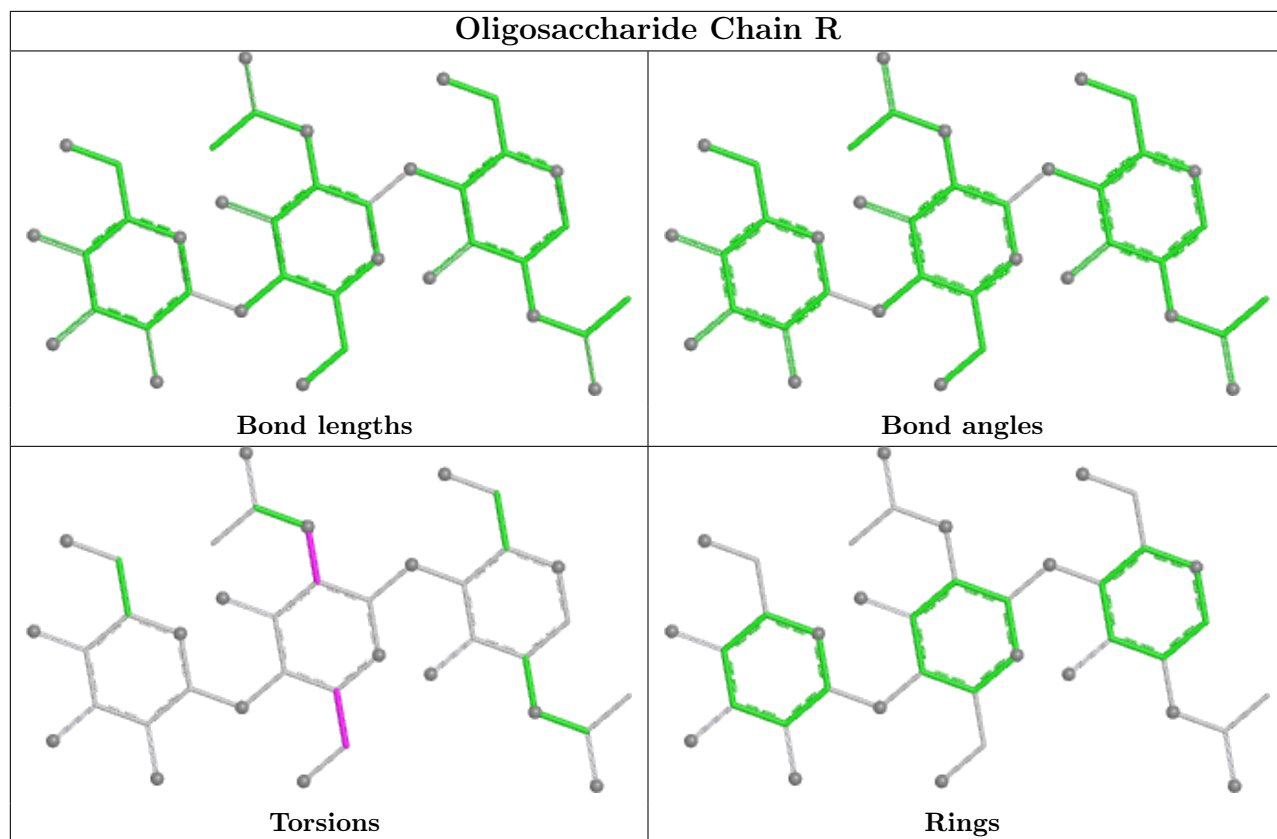


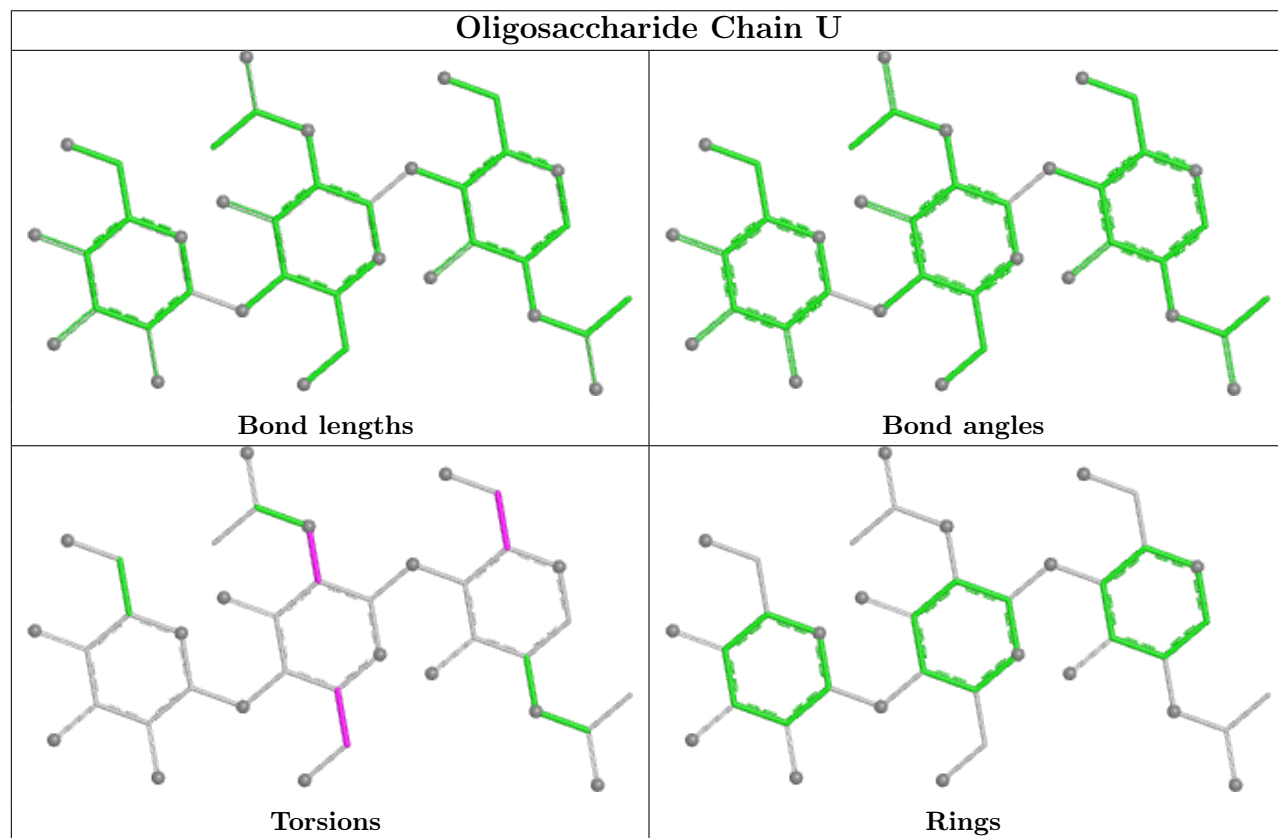
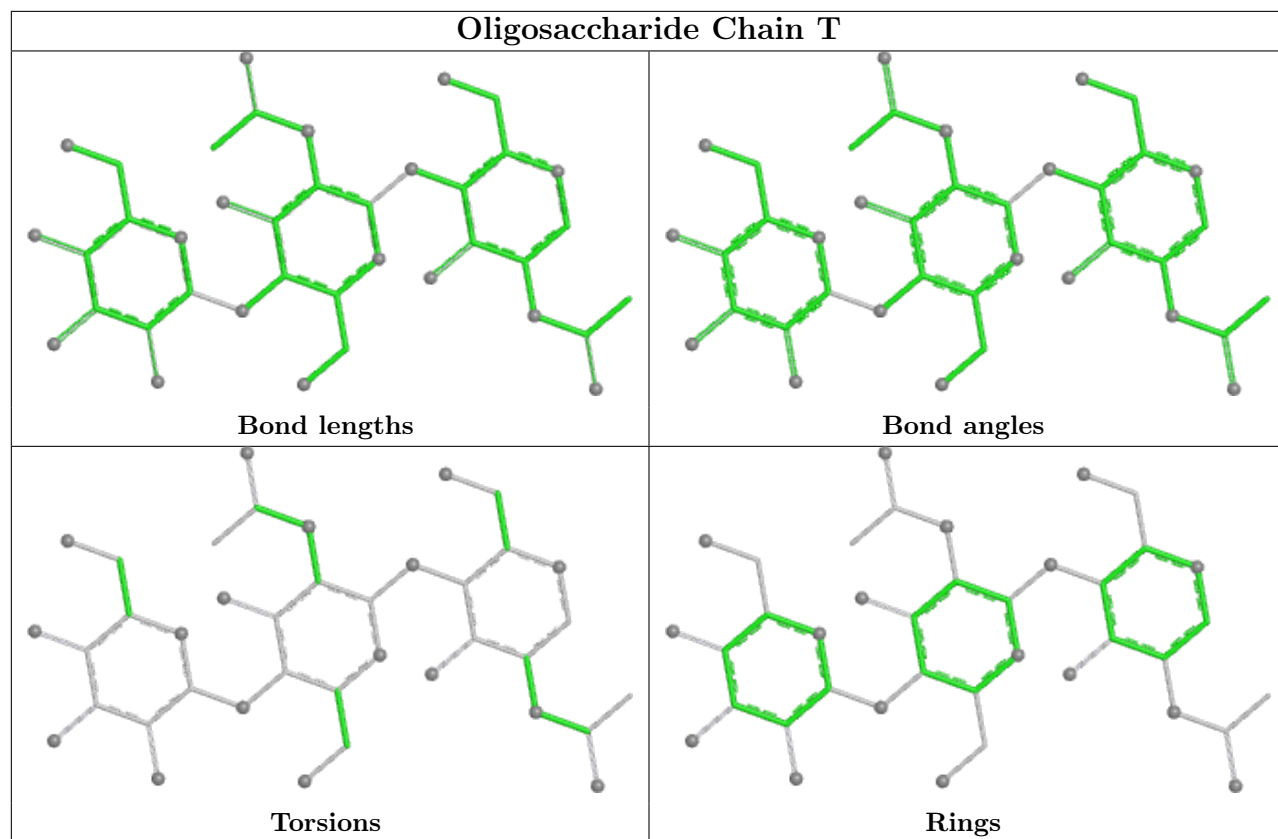


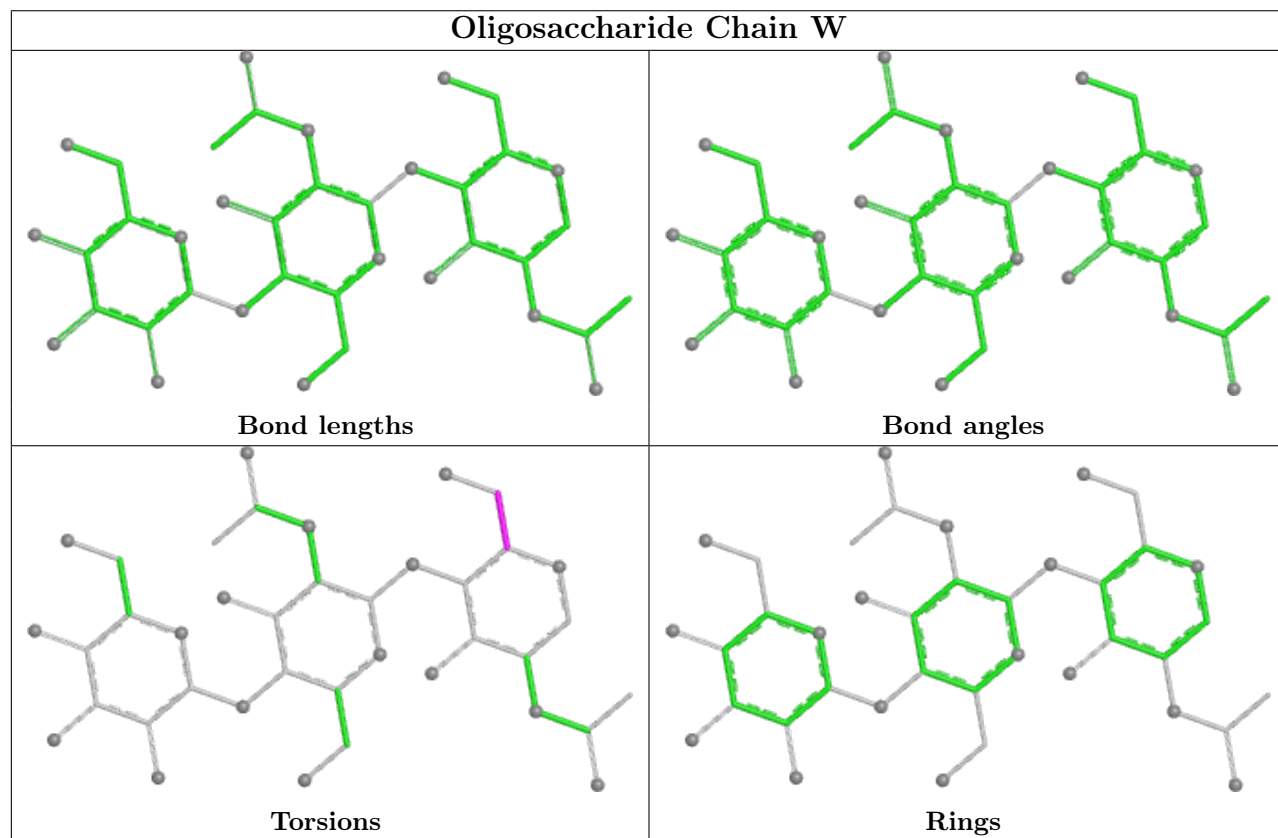
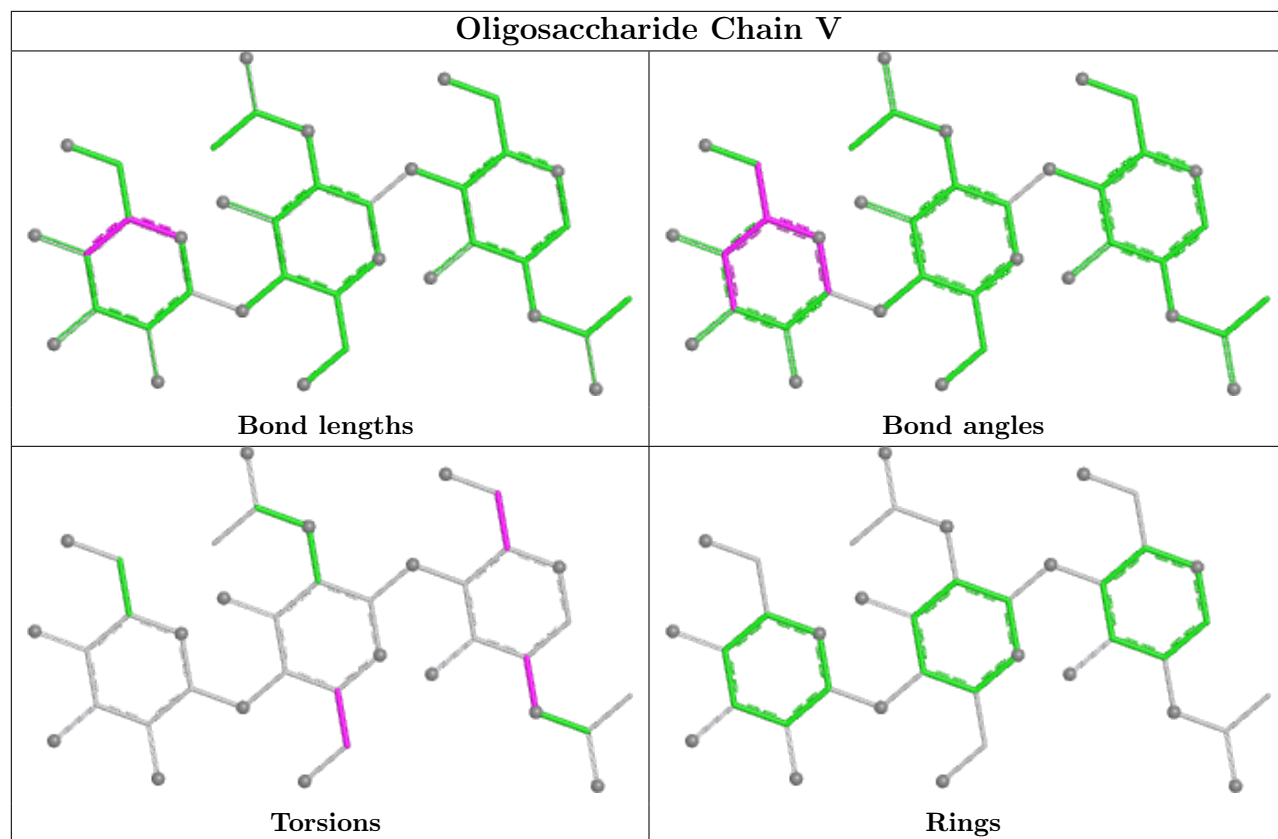


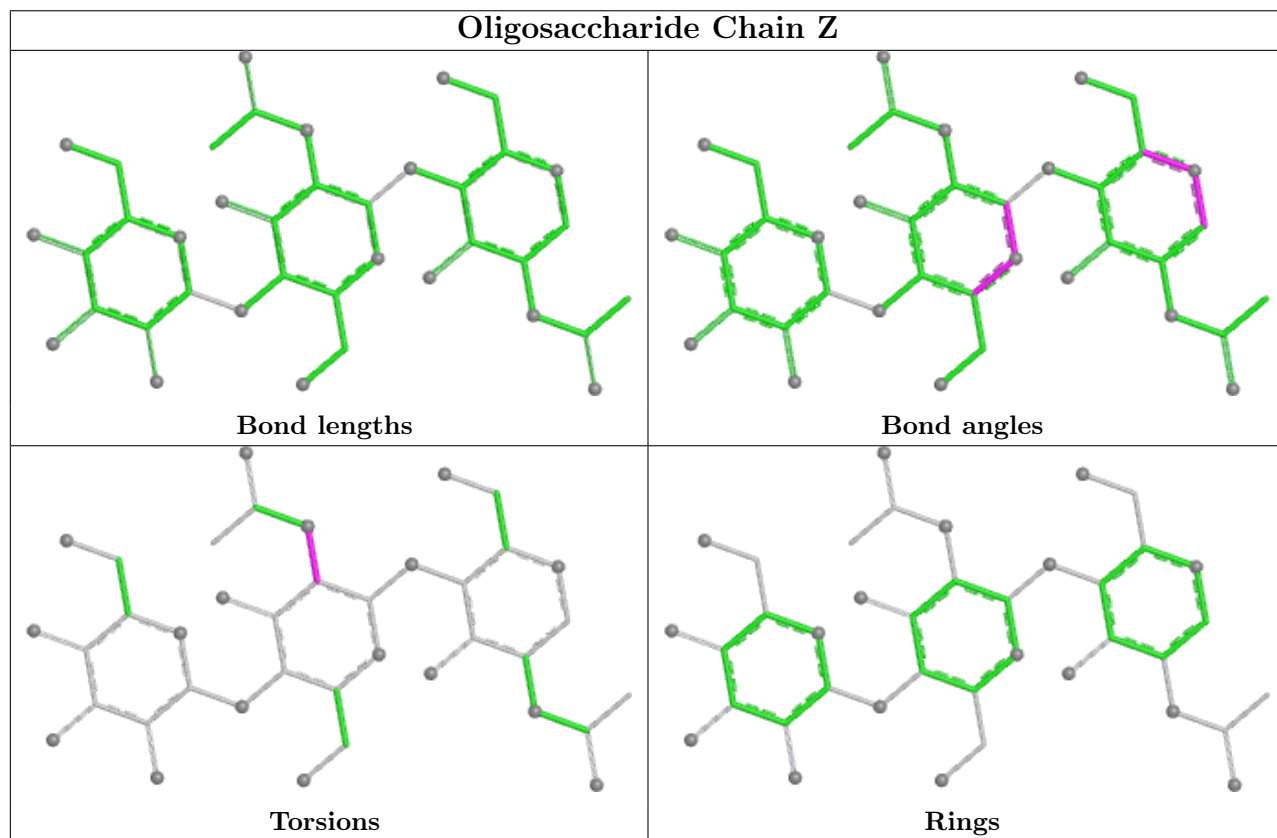
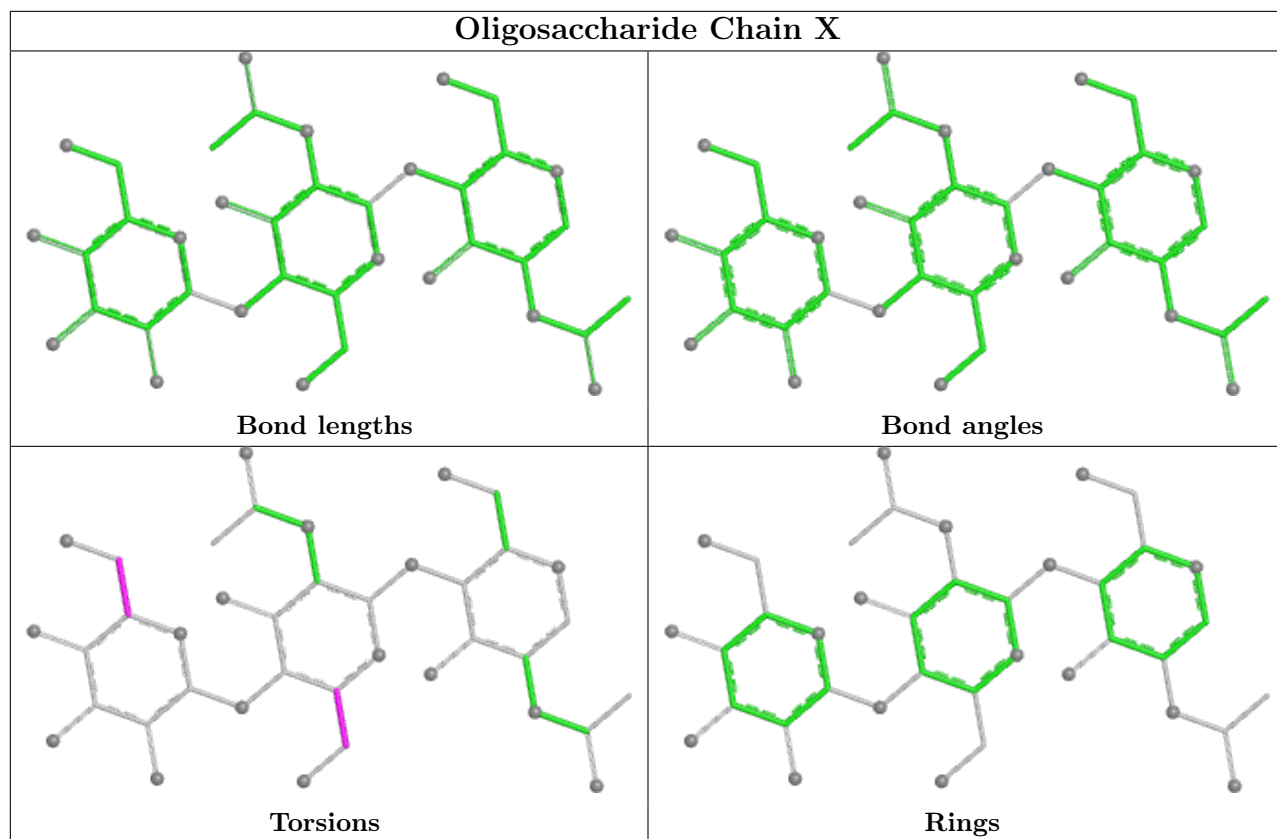


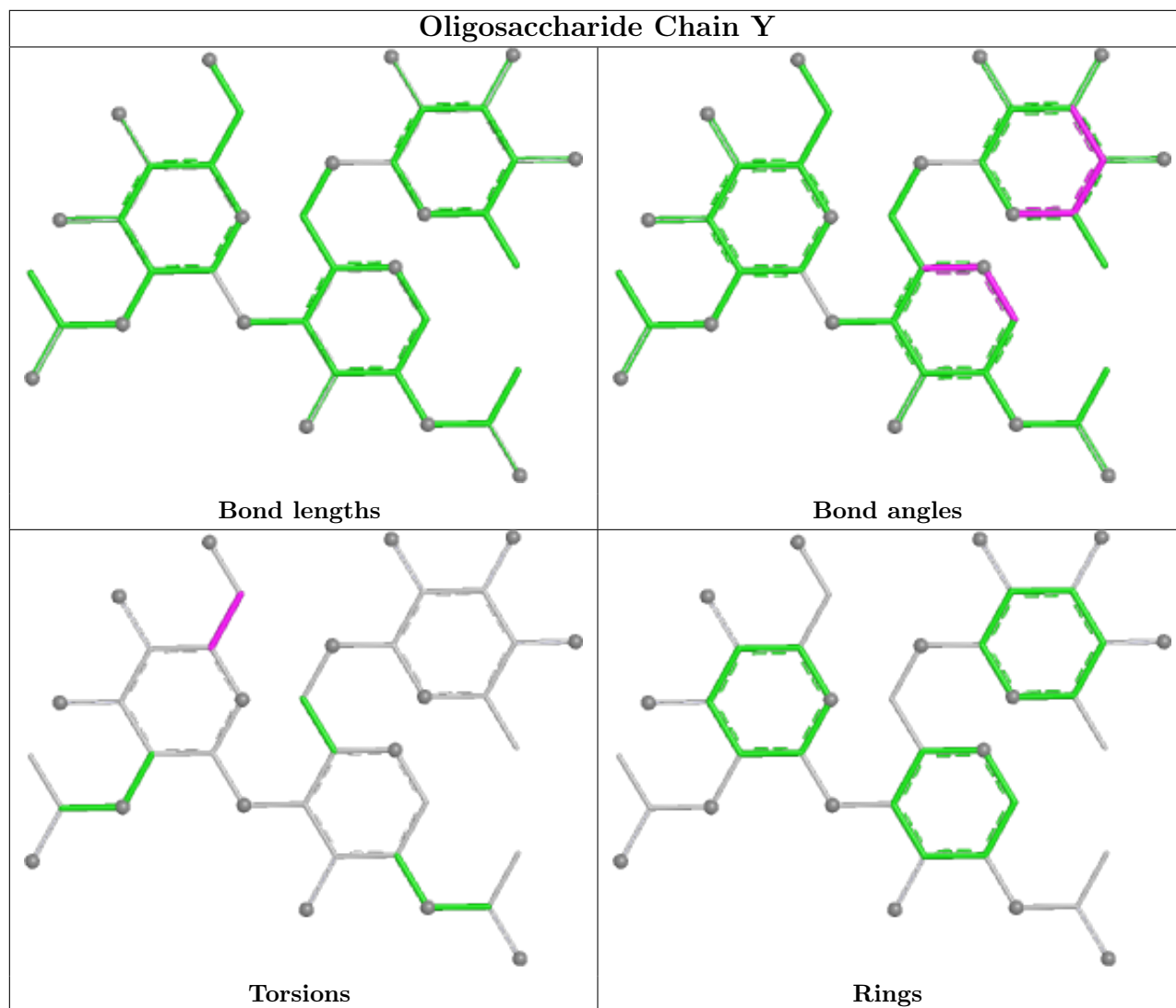












5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
6	NAG	B	1304	1	14,14,15	0.25	0	17,19,21	0.45	0
6	NAG	A	1303	1	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	A	1301	1	14,14,15	0.27	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	1302	1	14,14,15	0.26	0	17,19,21	0.44	0
6	NAG	A	1305	1	14,14,15	0.32	0	17,19,21	0.37	0
6	NAG	C	1303	1	14,14,15	0.27	0	17,19,21	0.46	0
6	NAG	B	1302	1	14,14,15	0.69	0	17,19,21	1.53	3 (17%)
6	NAG	B	1305	1	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	A	1304	1	14,14,15	0.45	0	17,19,21	1.25	1 (5%)
6	NAG	B	1301	1	14,14,15	0.43	0	17,19,21	1.24	1 (5%)
6	NAG	C	1304	1	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	C	1302	1	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	B	1303	1	14,14,15	0.45	0	17,19,21	1.24	1 (5%)
6	NAG	C	1301	1	14,14,15	0.21	0	17,19,21	0.43	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
6	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1302	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1301	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1301	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1304	NAG	C1-O5-C5	4.74	118.62	112.19
6	B	1303	NAG	C1-O5-C5	4.74	118.61	112.19

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1302	NAG	C1-O5-C5	4.73	118.60	112.19
6	B	1301	NAG	C2-N2-C7	4.28	129.00	122.90
6	B	1302	NAG	C2-N2-C7	2.40	126.31	122.90
6	B	1302	NAG	C1-C2-N2	2.12	114.10	110.49

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1301	NAG	O5-C5-C6-O6
6	B	1302	NAG	O5-C5-C6-O6
6	C	1303	NAG	O5-C5-C6-O6
6	C	1301	NAG	C4-C5-C6-O6
6	A	1301	NAG	O5-C5-C6-O6
6	B	1304	NAG	O5-C5-C6-O6
6	A	1301	NAG	C4-C5-C6-O6
6	A	1302	NAG	C8-C7-N2-C2
6	A	1302	NAG	O7-C7-N2-C2
6	A	1305	NAG	C8-C7-N2-C2
6	A	1305	NAG	O7-C7-N2-C2
6	B	1301	NAG	C8-C7-N2-C2
6	B	1301	NAG	O7-C7-N2-C2
6	C	1304	NAG	C8-C7-N2-C2
6	C	1304	NAG	O7-C7-N2-C2
6	B	1304	NAG	C4-C5-C6-O6
6	A	1304	NAG	O5-C5-C6-O6
6	B	1305	NAG	O5-C5-C6-O6
6	B	1305	NAG	C4-C5-C6-O6
6	A	1302	NAG	O5-C5-C6-O6
6	A	1302	NAG	C4-C5-C6-O6
6	B	1302	NAG	C4-C5-C6-O6
6	B	1303	NAG	O5-C5-C6-O6
6	A	1303	NAG	O5-C5-C6-O6
6	B	1302	NAG	C1-C2-N2-C7
6	C	1303	NAG	C4-C5-C6-O6
6	A	1301	NAG	C3-C2-N2-C7
6	B	1301	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1303	NAG	1	0
6	B	1301	NAG	1	0

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.

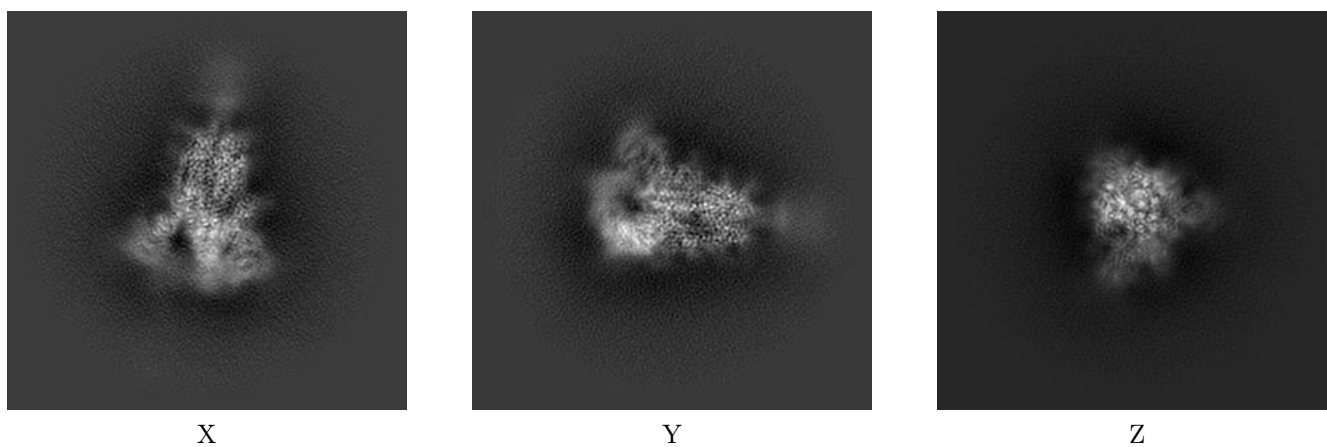
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14086. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

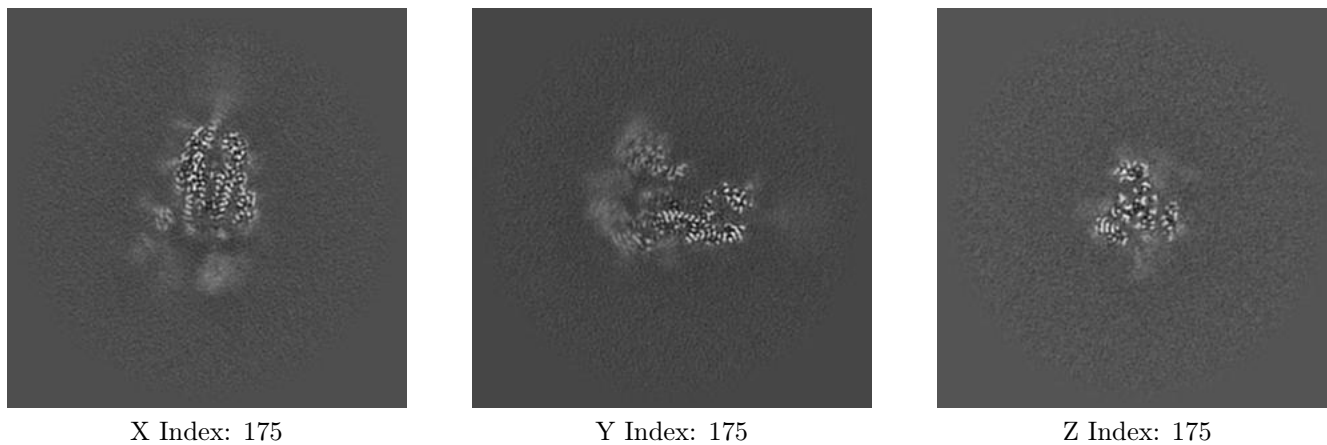
6.1.1 Primary map



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

6.2 Central slices [i](#)

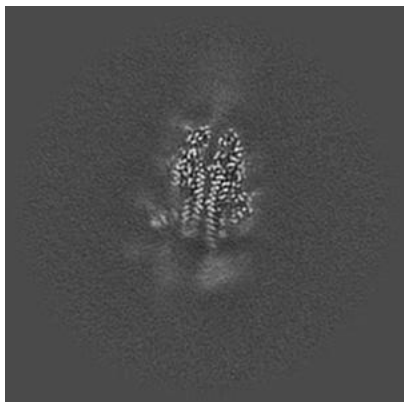
6.2.1 Primary map



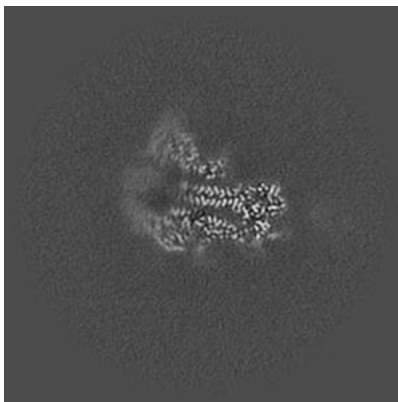
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

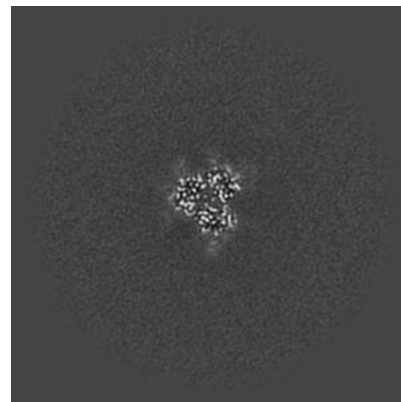
6.3.1 Primary map



X Index: 178



Y Index: 169



Z Index: 211

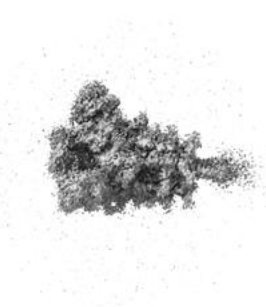
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0528. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

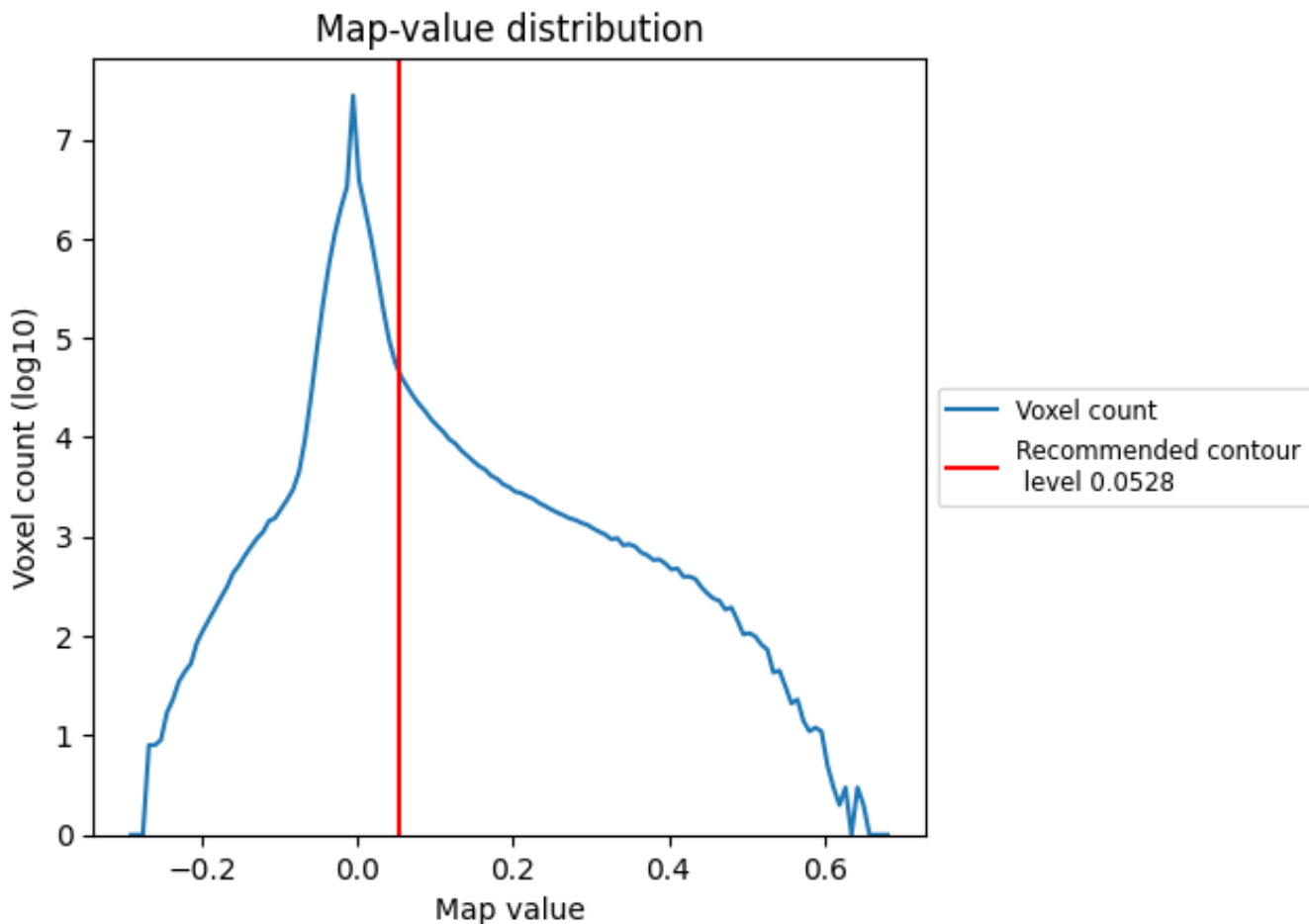
6.5 Mask visualisation

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

7 Map analysis [i](#)

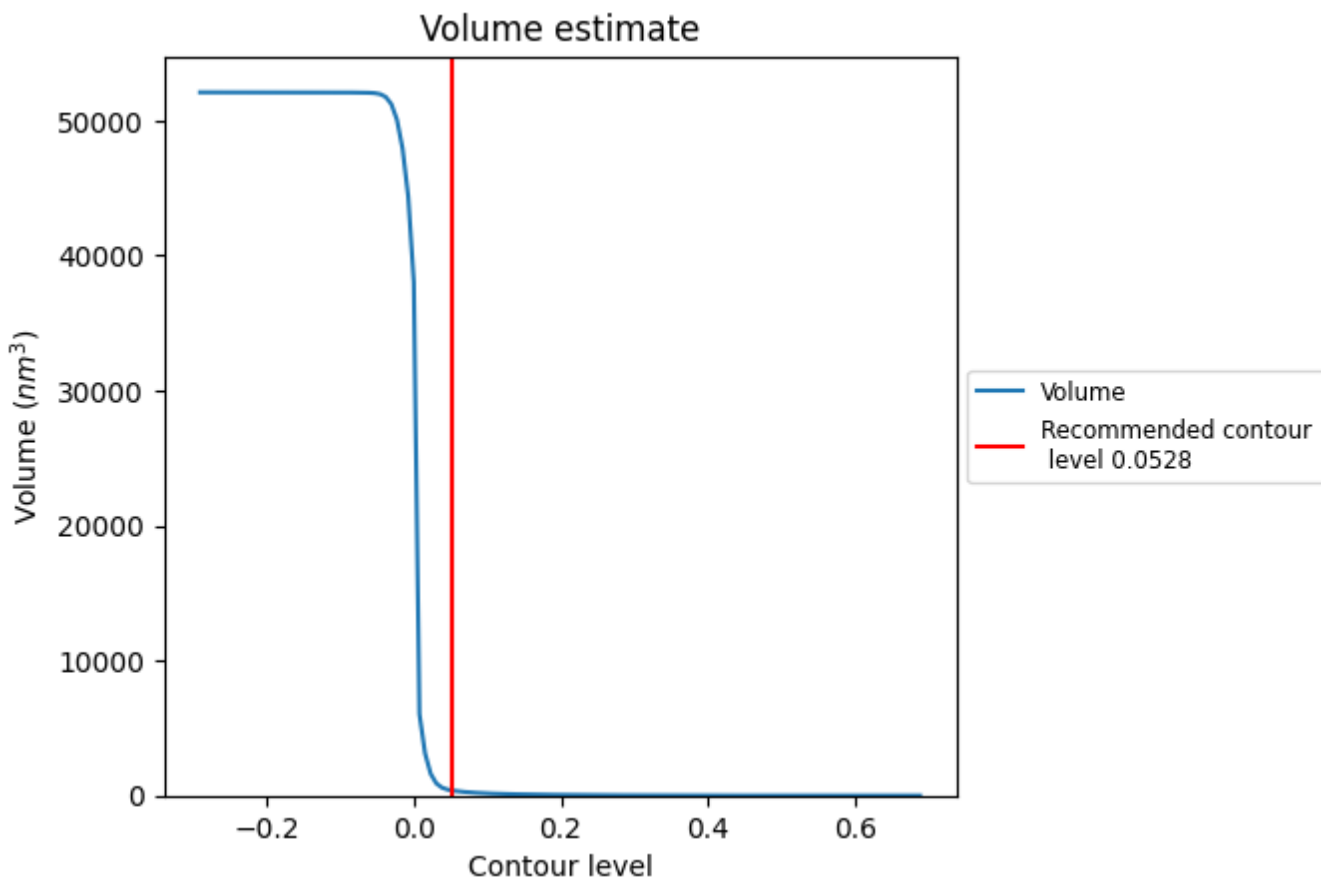
This section contains the results of statistical analysis of the map.

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.

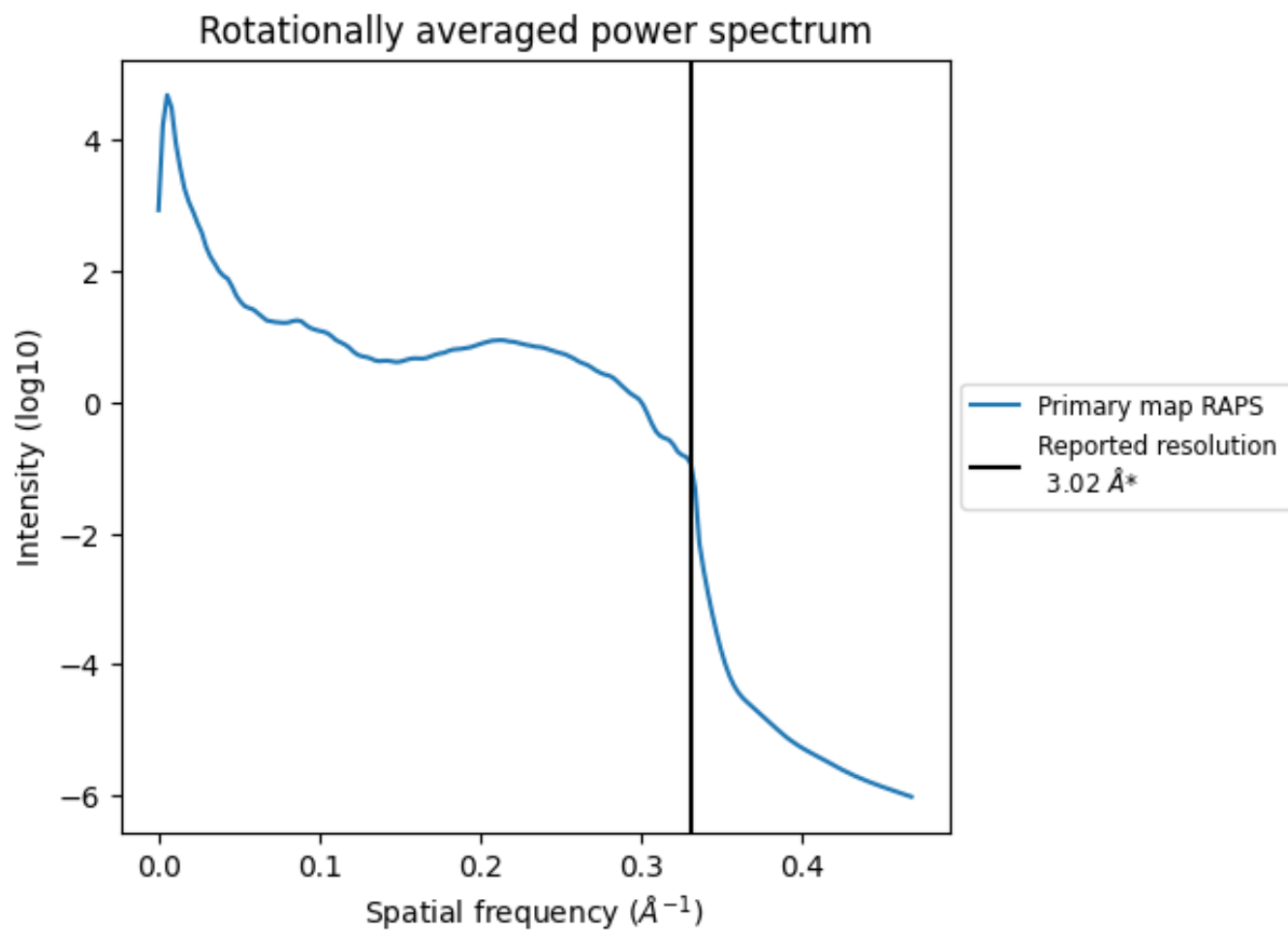
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 371 nm^3 ; this corresponds to an approximate mass of 335 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

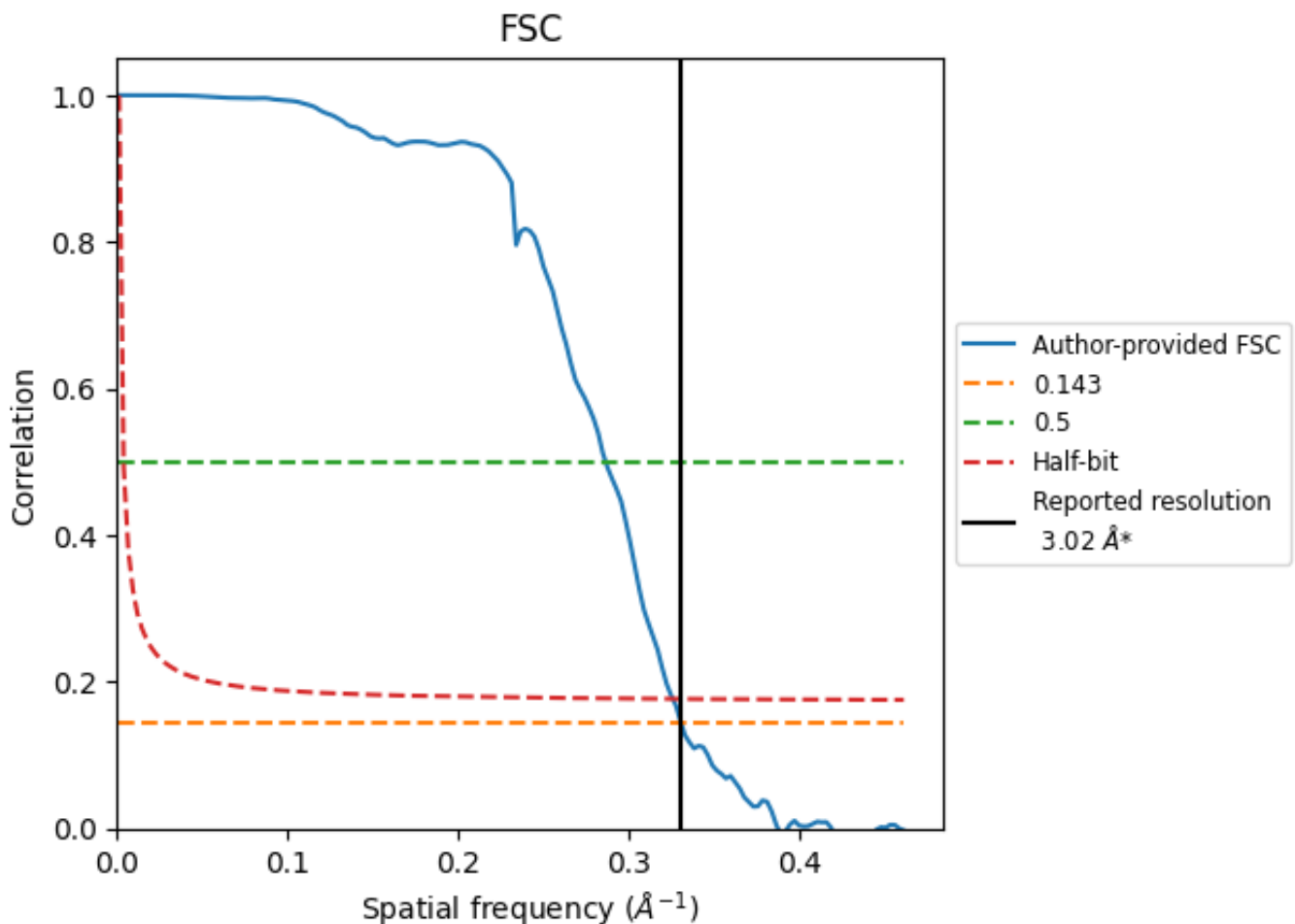


*Reported resolution corresponds to spatial frequency of 0.331 Å⁻¹

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 0.331 Å⁻¹

8.2 Resolution estimates [i](#)

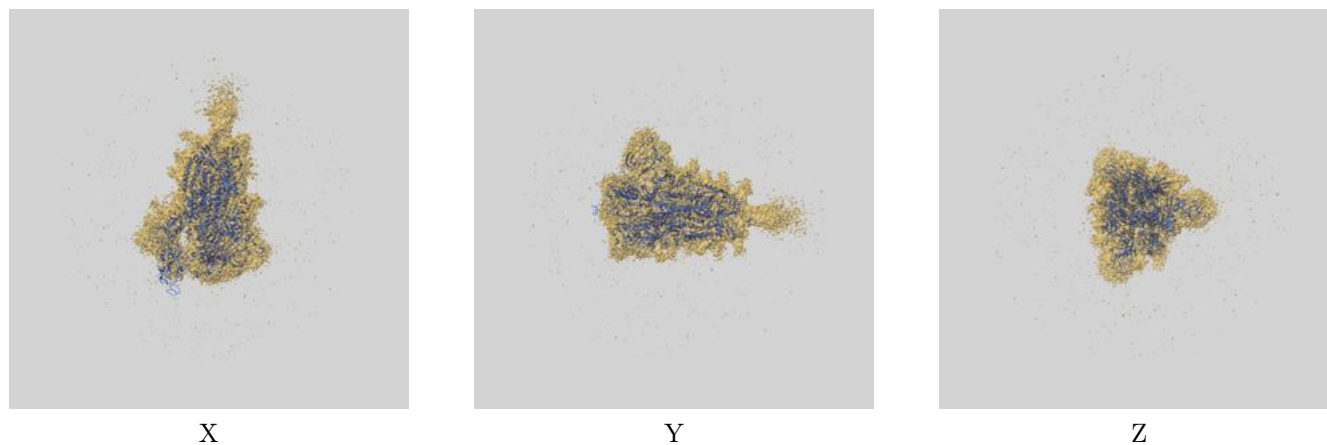
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.49	3.07
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

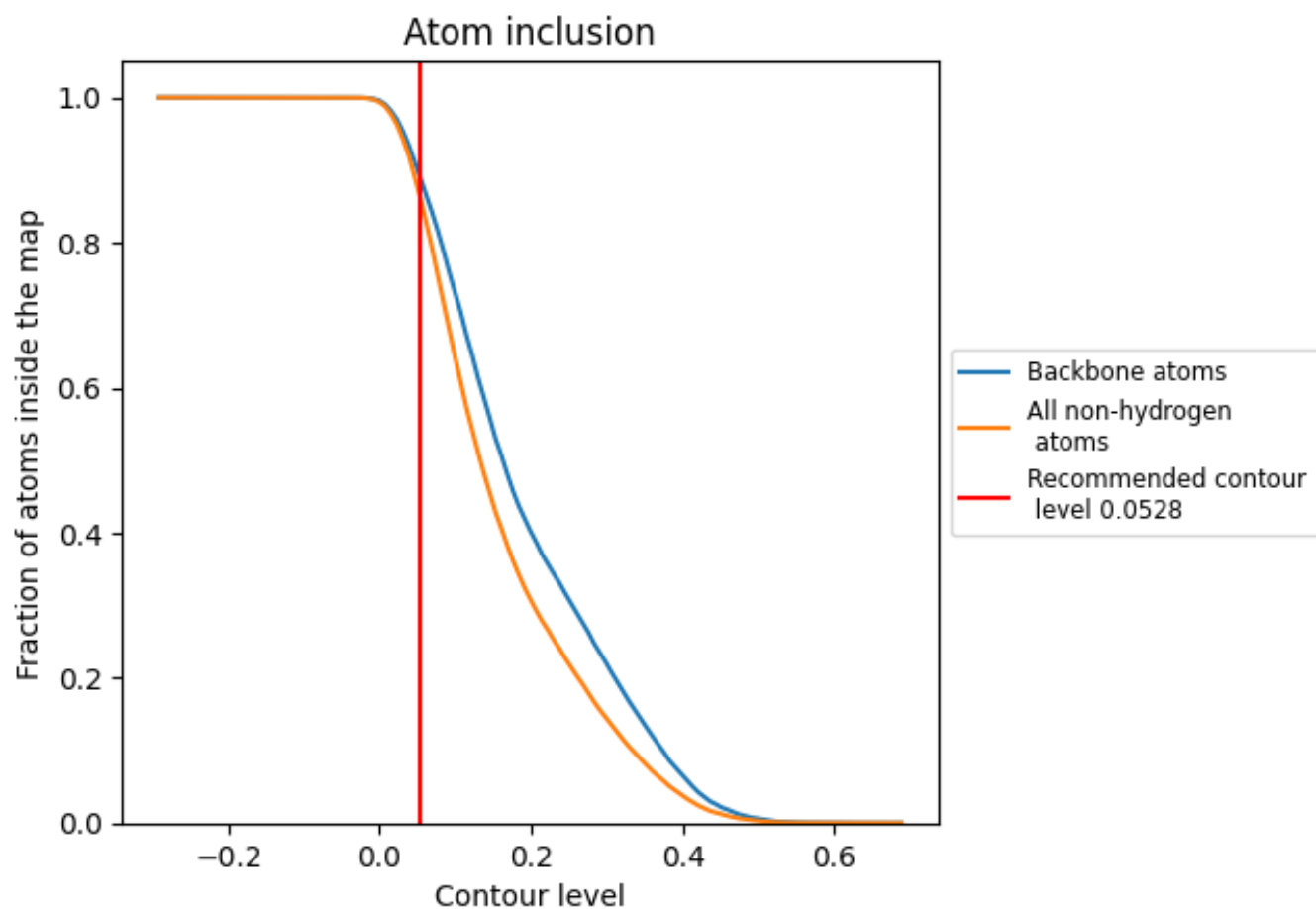
This section contains information regarding the fit between EMDB map EMD-14086 and PDB model 7QO7. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0528 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 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.