



## Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 12:11 PM EST

PDB ID : 7T74  
EMDB ID : EMD-25733  
Title : HIV-1 Envelope ApexGT2 in complex with PCT64.35S Fab and RM20A3 Fab  
Authors : Berndsen, Z.T.  
Deposited on : 2021-12-14  
Resolution : 3.35 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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>.

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

EMDB validation analysis : 0.0.1.dev43  
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 : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

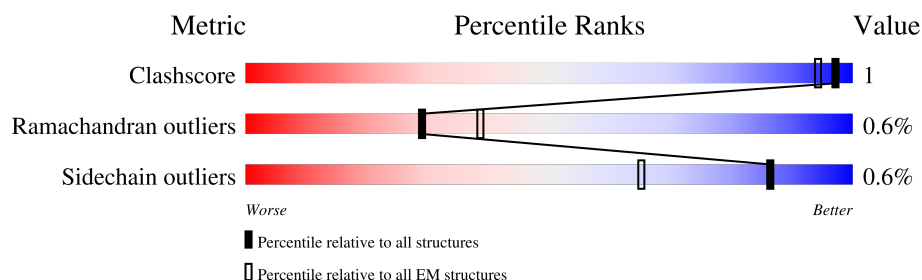
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.35 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	504	78% 5% 17%
1	C	504	80% 17%
1	E	504	79% 17%
2	B	162	72% 26%
2	D	162	72% 26%
2	F	162	70% 26%
3	I	125	92% 7% 1%
3	K	125	94% 5% 1%

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Mol	Chain	Length	Quality of chain
3	M	125	
4	G	128	
4	J	128	
4	N	128	
5	L	107	
6	H	134	
7	O	7	
8	P	2	
8	Q	2	
8	W	2	
8	X	2	
8	Z	2	
8	c	2	
8	d	2	
8	e	2	
8	g	2	
9	R	4	
9	S	4	
9	Y	4	
9	f	4	
10	T	2	
10	U	2	
10	a	2	
10	b	2	
10	h	2	

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Mol	Chain	Length	Quality of chain
10	i	2	<div> <div>50%</div> <div>100%</div> </div>
11	V	3	<div> <div>33%</div> <div>33%</div> <div>67%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	FUC	i	2	X	-	-	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21199 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 HIV Envelope ApexGT2 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	419	Total	C	N	O	S	0	0
			3305	2080	580	619	26		
1	C	419	Total	C	N	O	S	0	0
			3305	2080	580	619	26		
1	E	419	Total	C	N	O	S	0	0
			3305	2080	580	619	26		

- Molecule 2 is a protein called HIV Envelope ApexGT2 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	S	0	0
			958	604	167	181	6		
2	D	120	Total	C	N	O	S	0	0
			958	604	167	181	6		
2	F	120	Total	C	N	O	S	0	0
			962	606	167	183	6		

- Molecule 3 is a protein called RM20A3 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	124	Total	C	N	O	S	0	0
			943	595	161	182	5		
3	M	124	Total	C	N	O	S	0	0
			943	595	161	182	5		
3	I	124	Total	C	N	O	S	0	0
			943	595	161	182	5		

- Molecule 4 is a protein called RM20A3 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	109	Total	C	N	O	S	0	0
			811	505	136	167	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	109	Total	C	N	O	S	0	0
			811	505	136	167	3		
4	J	109	Total	C	N	O	S	0	0
			811	505	136	167	3		

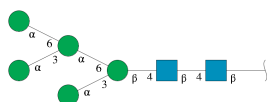
- Molecule 5 is a protein called PCT64.35S Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	106	Total	C	N	O	S	0	0
			820	515	141	162	2		

- Molecule 6 is a protein called PCT64.35S Fab Heavy Chain.

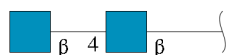
Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	130	Total	C	N	O	S	0	0
			1018	641	172	198	7		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
7	O	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 8 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
8	P	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	Q	2	Total	C	N	O	0	0
			28	16	2	10		
8	W	2	Total	C	N	O	0	0
			28	16	2	10		
8	X	2	Total	C	N	O	0	0
			28	16	2	10		
8	Z	2	Total	C	N	O	0	0
			28	16	2	10		
8	c	2	Total	C	N	O	0	0
			28	16	2	10		
8	d	2	Total	C	N	O	0	0
			28	16	2	10		
8	e	2	Total	C	N	O	0	0
			28	16	2	10		
8	g	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 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.



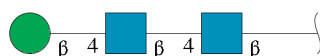
Mol	Chain	Residues	Atoms				AltConf	Trace
9	R	4	Total	C	N	O	0	0
			50	28	2	20		
9	S	4	Total	C	N	O	0	0
			50	28	2	20		
9	Y	4	Total	C	N	O	0	0
			50	28	2	20		
9	f	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 10 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



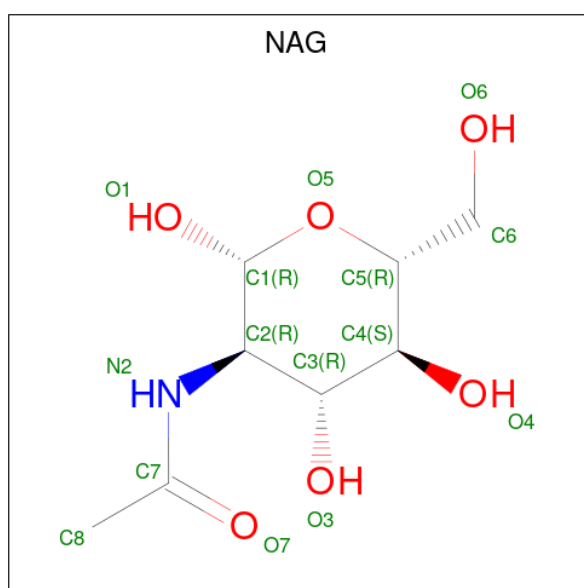
Mol	Chain	Residues	Atoms				AltConf	Trace
10	T	2	Total	C	N	O	0	0
			24	14	1	9		
10	U	2	Total	C	N	O	0	0
			24	14	1	9		
10	a	2	Total	C	N	O	0	0
			24	14	1	9		
10	b	2	Total	C	N	O	0	0
			24	14	1	9		
10	h	2	Total	C	N	O	0	0
			24	14	1	9		
10	i	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 11 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
11	V	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





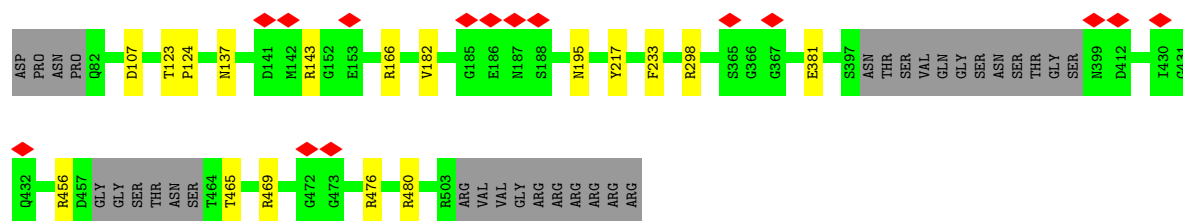
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	B	1	Total	C	N	O	0
			28	16	2	10	
12	B	1	Total	C	N	O	0
			28	16	2	10	
12	C	1	Total	C	N	O	0
			168	96	12	60	
12	C	1	Total	C	N	O	0
			168	96	12	60	
12	C	1	Total	C	N	O	0
			168	96	12	60	
12	C	1	Total	C	N	O	0
			168	96	12	60	
12	C	1	Total	C	N	O	0
			168	96	12	60	
12	C	1	Total	C	N	O	0
			168	96	12	60	
12	C	1	Total	C	N	O	0
			168	96	12	60	

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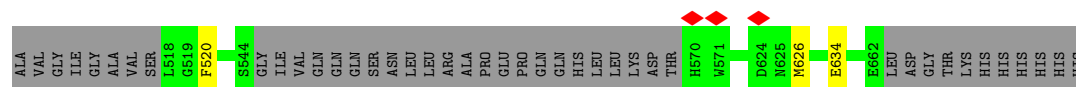
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Mol	Chain	Residues	Atoms				AltConf
12	C	1	Total 168	C 96	N 12	O 60	0
12	C	1	Total 168	C 96	N 12	O 60	0
12	C	1	Total 168	C 96	N 12	O 60	0
12	C	1	Total 168	C 96	N 12	O 60	0
12	D	1	Total 28	C 16	N 2	O 10	0
12	D	1	Total 28	C 16	N 2	O 10	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	F	1	Total 28	C 16	N 2	O 10	0
12	F	1	Total 28	C 16	N 2	O 10	0

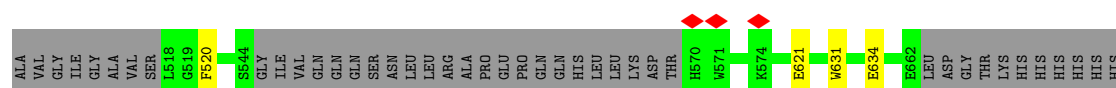




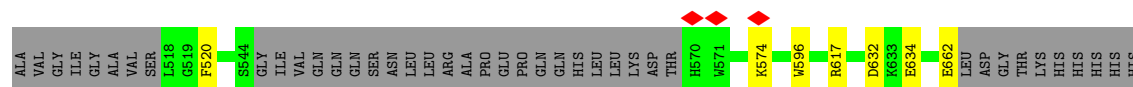
- Molecule 2: HIV Envelope ApexGT2 gp41



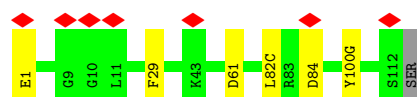
- Molecule 2: HIV Envelope ApexGT2 gp41



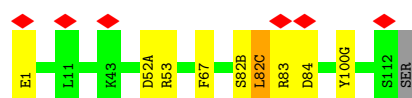
- Molecule 2: HIV Envelope ApexGT2 gp41



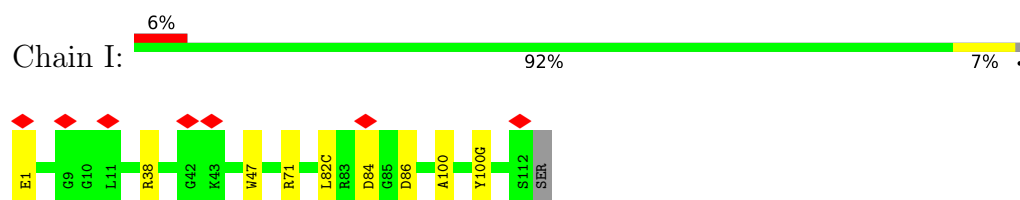
- Molecule 3: RM20A3 Fab Heavy Chain



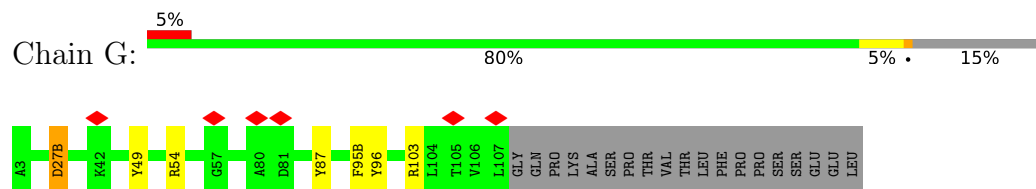
- Molecule 3: RM20A3 Fab Heavy Chain



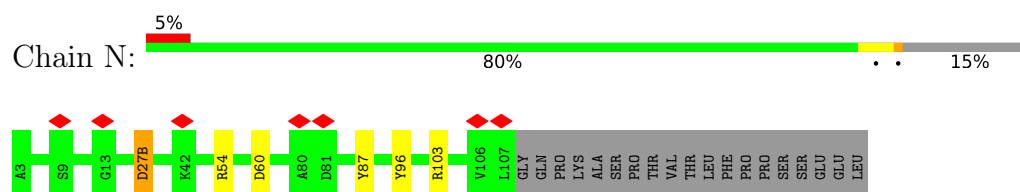
- Molecule 3: RM20A3 Fab Heavy Chain



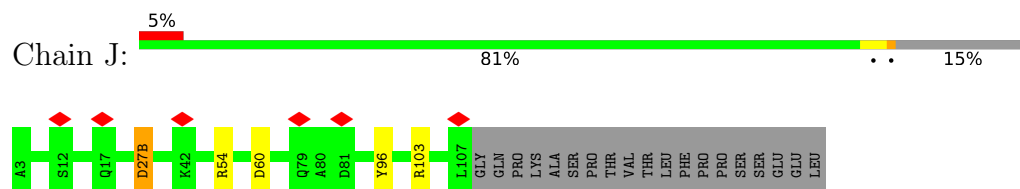
• Molecule 4: RM20A3 Fab Light Chain



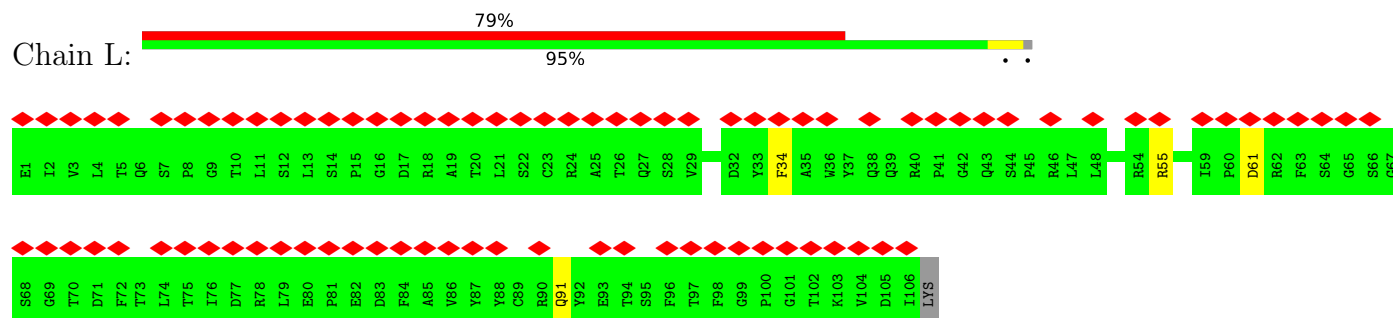
• Molecule 4: RM20A3 Fab Light Chain



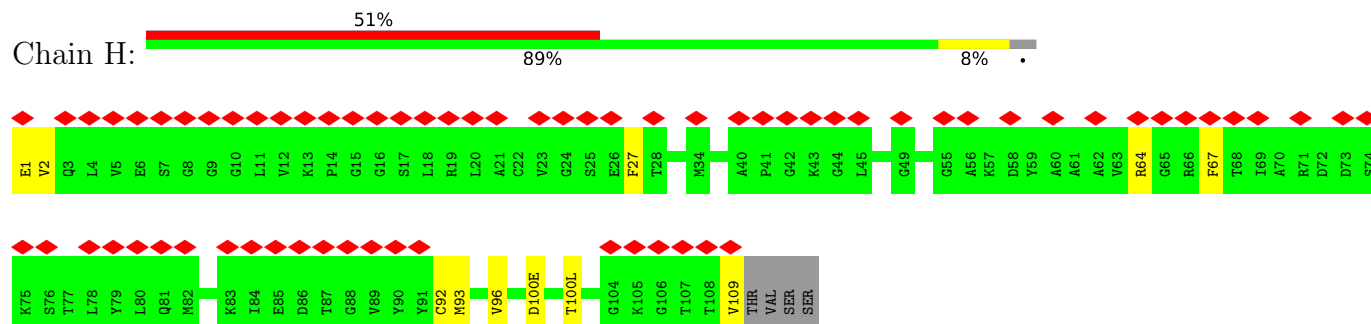
• Molecule 4: RM20A3 Fab Light Chain



• Molecule 5: PCT64.35S Fab Light Chain



• Molecule 6: PCT64.35S Fab Heavy Chain



- Molecule 7:  $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-6)] $\alpha$ -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 O: 



- Molecule 8: 2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain P: 



- Molecule 8: 2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain Q: 



- Molecule 8: 2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain W: 



- Molecule 8: 2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain X: 



- Molecule 8: 2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain Z: 



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



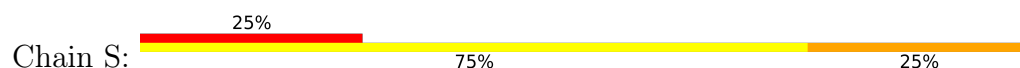
- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 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



- Molecule 9: 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





- Molecule 9: 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



- Molecule 9: 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



- Molecule 10: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose







- Molecule 10: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38081	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.156	Depositor
Minimum map value	-0.523	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	360.5, 360.5, 360.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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: MAN, FUC, BMA, TYS, 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	1.10	2/3371 (0.1%)	0.92	11/4575 (0.2%)
1	C	1.09	2/3371 (0.1%)	0.86	5/4575 (0.1%)
1	E	1.08	4/3371 (0.1%)	0.89	8/4575 (0.2%)
2	B	1.28	3/977 (0.3%)	0.79	0/1325
2	D	1.26	4/977 (0.4%)	0.79	0/1325
2	F	1.25	4/981 (0.4%)	0.76	1/1330 (0.1%)
3	I	1.25	6/963 (0.6%)	1.00	3/1300 (0.2%)
3	K	1.20	5/963 (0.5%)	0.91	1/1300 (0.1%)
3	M	1.18	2/963 (0.2%)	0.93	2/1300 (0.2%)
4	G	1.19	5/830 (0.6%)	0.98	3/1129 (0.3%)
4	J	1.17	2/830 (0.2%)	0.98	2/1129 (0.2%)
4	N	1.15	3/830 (0.4%)	0.98	2/1129 (0.2%)
5	L	0.98	2/840 (0.2%)	0.97	1/1141 (0.1%)
6	H	0.94	3/1025 (0.3%)	0.90	2/1386 (0.1%)
All	All	1.13	47/20292 (0.2%)	0.90	41/27519 (0.1%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	27(B)	ASP	CB-CG	-7.10	1.36	1.51
1	A	501	CYS	CB-SG	-7.07	1.70	1.82
4	N	27(B)	ASP	CB-CG	-6.83	1.37	1.51
2	F	662	GLU	CB-CG	6.67	1.64	1.52
2	F	520	PHE	CB-CG	-6.64	1.40	1.51
4	G	27(B)	ASP	CB-CG	-6.64	1.37	1.51
4	N	96	TYR	CB-CG	-6.22	1.42	1.51
2	B	520	PHE	CB-CG	-6.15	1.40	1.51
3	K	100(G)	TYR	CG-CD1	-6.08	1.31	1.39
4	J	96	TYR	CB-CG	-6.06	1.42	1.51
2	D	520	PHE	CB-CG	-6.00	1.41	1.51
5	L	34	PHE	CB-CG	-5.98	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	100(G)	TYR	CB-CG	-5.67	1.43	1.51
4	G	96	TYR	CB-CG	-5.61	1.43	1.51
4	N	87	TYR	CB-CG	-5.61	1.43	1.51
4	G	95(B)	PHE	CB-CG	-5.51	1.42	1.51
2	D	634	GLU	CD-OE1	-5.50	1.19	1.25
3	K	29	PHE	CB-CG	-5.49	1.42	1.51
3	K	1	GLU	CB-CG	5.49	1.62	1.52
4	G	87	TYR	CB-CG	-5.45	1.43	1.51
2	F	634	GLU	CD-OE1	-5.42	1.19	1.25
1	E	233	PHE	CB-CG	-5.39	1.42	1.51
3	I	1	GLU	CB-CG	5.39	1.62	1.52
3	I	100(G)	TYR	CG-CD1	-5.37	1.32	1.39
4	G	49	TYR	CB-CG	-5.37	1.43	1.51
6	H	1	GLU	CB-CG	5.37	1.62	1.52
6	H	92	CYS	CB-SG	-5.36	1.73	1.81
2	D	621	GLU	CD-OE2	-5.35	1.19	1.25
3	K	100(G)	TYR	CD1-CE1	-5.29	1.31	1.39
3	I	47	TRP	CD2-CE2	-5.25	1.35	1.41
3	K	100(G)	TYR	CB-CG	-5.21	1.43	1.51
2	B	634	GLU	CD-OE1	-5.21	1.20	1.25
1	E	217	TYR	CB-CG	-5.20	1.43	1.51
6	H	109	VAL	CB-CG1	5.19	1.63	1.52
2	D	631	TRP	CD2-CE2	-5.19	1.35	1.41
1	E	42	VAL	CB-CG1	-5.17	1.42	1.52
3	I	38	ARG	CB-CG	-5.17	1.38	1.52
2	B	634	GLU	CD-OE2	-5.17	1.20	1.25
2	F	596	TRP	CD2-CE2	-5.17	1.35	1.41
1	C	91	GLU	CD-OE2	-5.15	1.20	1.25
1	C	233	PHE	CB-CG	-5.09	1.42	1.51
1	E	381	GLU	CD-OE1	-5.09	1.20	1.25
5	L	91	GLN	CG-CD	-5.08	1.39	1.51
3	M	1	GLU	CB-CG	5.04	1.61	1.52
1	A	42	VAL	CB-CG1	-5.04	1.42	1.52
3	I	100(G)	TYR	CD1-CE1	-5.02	1.31	1.39
3	M	100(G)	TYR	CG-CD1	-5.02	1.32	1.39

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	71	ARG	NE-CZ-NH2	-11.06	114.77	120.30
1	A	503	ARG	NE-CZ-NH1	10.47	125.53	120.30
1	C	143	ARG	NE-CZ-NH2	-8.24	116.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	E	143	ARG	NE-CZ-NH2	-8.15	116.23	120.30
1	A	419	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	E	476	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	A	476	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	E	217	TYR	CB-CG-CD2	-7.43	116.54	121.00
6	H	64	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	C	217	TYR	CB-CG-CD2	-7.19	116.68	121.00
3	I	71	ARG	NE-CZ-NH1	7.12	123.86	120.30
5	L	55	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	E	456	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	456	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	C	469	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	E	469	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	469	ARG	NE-CZ-NH2	-6.27	117.17	120.30
4	J	54	ARG	NE-CZ-NH2	-6.12	117.24	120.30
4	G	87	TYR	CB-CG-CD2	-6.01	117.39	121.00
4	G	54	ARG	NE-CZ-NH2	-5.96	117.32	120.30
4	N	54	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	273	ARG	NE-CZ-NH1	5.89	123.25	120.30
4	J	103	ARG	NE-CZ-NH2	-5.82	117.39	120.30
4	N	103	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	166	ARG	NE-CZ-NH1	5.58	123.09	120.30
3	M	83	ARG	NE-CZ-NH2	-5.52	117.54	120.30
6	H	67	PHE	CB-CG-CD1	5.49	124.64	120.80
4	G	103	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	E	298	ARG	NE-CZ-NH2	5.35	122.98	120.30
3	I	86	ASP	CB-CG-OD1	5.30	123.07	118.30
1	E	469	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	E	480	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	469	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	217	TYR	CB-CG-CD2	-5.13	117.92	121.00
2	F	617	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	469	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	273	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	C	273	ARG	NE-CZ-NH1	5.04	122.82	120.30
3	K	100(G)	TYR	CB-CG-CD1	-5.03	117.98	121.00
3	M	67	PHE	CB-CG-CD1	5.01	124.31	120.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	3305	0	3257	7	0
1	C	3305	0	3256	4	0
1	E	3305	0	3256	2	0
2	B	958	0	921	0	0
2	D	958	0	920	0	0
2	F	962	0	924	2	0
3	I	943	0	915	1	0
3	K	943	0	915	2	0
3	M	943	0	915	4	0
4	G	811	0	767	0	0
4	J	811	0	767	1	0
4	N	811	0	767	1	0
5	L	820	0	784	1	0
6	H	1018	0	965	2	0
7	O	83	0	70	1	0
8	P	28	0	25	0	0
8	Q	28	0	24	0	0
8	W	28	0	25	0	0
8	X	28	0	25	0	0
8	Z	28	0	25	1	0
8	c	28	0	25	0	0
8	d	28	0	25	0	0
8	e	28	0	24	0	0
8	g	28	0	25	0	0
9	R	50	0	43	0	0
9	S	50	0	43	1	0
9	Y	50	0	43	0	0
9	f	50	0	43	0	0
10	T	24	0	22	0	0
10	U	24	0	22	0	0
10	a	24	0	22	0	0
10	b	24	0	21	0	0
10	h	24	0	22	0	0
10	i	24	0	22	0	0
11	V	39	0	34	0	0
12	A	168	0	156	1	0
12	B	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	168	0	156	0	0
12	D	28	0	25	0	0
12	E	168	0	156	0	0
12	F	28	0	26	0	0
All	All	21199	0	20503	25	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 1.

All (25) 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)
6:H:2:VAL:HG11	6:H:96:VAL:HG21	1.79	0.64
3:M:84:ASP:N	3:M:84:ASP:OD1	2.36	0.58
1:A:130:GLN:HG2	7:O:1:NAG:H83	1.86	0.57
1:A:123:THR:N	1:A:124:PRO:CD	2.68	0.56
1:C:123:THR:N	1:C:124:PRO:CD	2.69	0.56
1:A:134:VAL:HG13	9:S:1:NAG:H81	1.88	0.56
3:I:84:ASP:N	3:I:84:ASP:OD1	2.36	0.55
3:K:84:ASP:N	3:K:84:ASP:OD1	2.36	0.55
1:E:107:ASP:OD1	2:F:574:LYS:NZ	2.42	0.53
1:E:46:LYS:NZ	2:F:632:ASP:OD2	2.45	0.49
1:C:232:LYS:NZ	1:C:268:GLU:OE1	2.49	0.46
6:H:2:VAL:HG13	6:H:27:PHE:HB3	1.96	0.46
1:C:134:VAL:HG13	8:Z:1:NAG:H81	1.98	0.45
1:A:122:LEU:HB2	1:A:201:ILE:HG23	2.00	0.44
4:N:60:ASP:N	4:N:60:ASP:OD1	2.46	0.44
3:M:52(A):ASP:N	3:M:52(A):ASP:OD1	2.46	0.44
5:L:61:ASP:OD1	5:L:61:ASP:N	2.48	0.44
4:J:60:ASP:N	4:J:60:ASP:OD1	2.47	0.43
1:A:87:GLU:HB3	12:A:601:NAG:H82	2.01	0.42
3:K:61:ASP:OD1	3:K:61:ASP:N	2.53	0.41
3:M:52(A):ASP:OD1	3:M:53:ARG:N	2.54	0.41
3:M:82(B):SER:O	3:M:82(C):LEU:C	2.60	0.40
1:A:117:LYS:N	1:A:118:PRO:CD	2.84	0.40
1:C:195:ASN:ND2	1:C:199:SER:O	2.53	0.40
1:A:95:MET:O	1:A:96:TRP:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/504 (82%)	397 (97%)	11 (3%)	3 (1%)	22	56
1	C	411/504 (82%)	398 (97%)	12 (3%)	1 (0%)	47	78
1	E	411/504 (82%)	398 (97%)	11 (3%)	2 (0%)	29	63
2	B	116/162 (72%)	115 (99%)	0	1 (1%)	17	51
2	D	116/162 (72%)	116 (100%)	0	0	100	100
2	F	116/162 (72%)	115 (99%)	1 (1%)	0	100	100
3	I	122/125 (98%)	118 (97%)	2 (2%)	2 (2%)	9	38
3	K	122/125 (98%)	118 (97%)	3 (2%)	1 (1%)	19	53
3	M	122/125 (98%)	117 (96%)	4 (3%)	1 (1%)	19	53
4	G	107/128 (84%)	101 (94%)	5 (5%)	1 (1%)	17	51
4	J	107/128 (84%)	101 (94%)	5 (5%)	1 (1%)	17	51
4	N	107/128 (84%)	101 (94%)	5 (5%)	1 (1%)	17	51
5	L	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
6	H	127/134 (95%)	126 (99%)	1 (1%)	0	100	100
All	All	2499/2998 (83%)	2423 (97%)	62 (2%)	14 (1%)	29	59

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	82(C)	LEU
3	M	82(C)	LEU
3	I	82(C)	LEU
1	A	185	GLY
4	N	27(B)	ASP
3	I	100	ALA
4	J	27(B)	ASP
1	A	465	THR
4	G	27(B)	ASP

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Mol	Chain	Res	Type
1	E	465	THR
1	C	465	THR
1	A	184	MET
2	B	626	MET
1	E	124	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/445 (84%)	372 (99%)	4 (1%)	73	86
1	C	376/445 (84%)	374 (100%)	2 (0%)	88	94
1	E	376/445 (84%)	371 (99%)	5 (1%)	69	84
2	B	103/139 (74%)	103 (100%)	0	100	100
2	D	103/139 (74%)	103 (100%)	0	100	100
2	F	104/139 (75%)	104 (100%)	0	100	100
3	I	101/102 (99%)	101 (100%)	0	100	100
3	K	101/102 (99%)	101 (100%)	0	100	100
3	M	101/102 (99%)	101 (100%)	0	100	100
4	G	89/106 (84%)	89 (100%)	0	100	100
4	J	89/106 (84%)	89 (100%)	0	100	100
4	N	89/106 (84%)	89 (100%)	0	100	100
5	L	88/89 (99%)	88 (100%)	0	100	100
6	H	104/108 (96%)	101 (97%)	3 (3%)	42	70
All	All	2200/2573 (86%)	2186 (99%)	14 (1%)	86	93

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	MET
1	A	186	GLU

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Mol	Chain	Res	Type
1	A	190	ASN
1	A	198	THR
6	H	93	MET
6	H	100(E)	ASP
6	H	100(L)	THR
1	C	187	ASN
1	C	201	ILE
1	E	123	THR
1	E	137	ASN
1	E	166	ARG
1	E	182	VAL
1	E	195	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	187	ASN
1	E	187	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	TYS	H	100(F)	6	15,16,17	0.60	0	18,22,24	0.87	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	TYS	H	100(F)	6	-	2/10/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	100(F)	TYS	CE2-CZ-OH-S
6	H	100(F)	TYS	CE1-CZ-OH-S

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

56 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
7	NAG	O	1	1,7	14,14,15	0.42	0	17,19,21	1.25	2 (11%)
7	NAG	O	2	7	14,14,15	0.40	0	17,19,21	0.90	0
7	BMA	O	3	7	11,11,12	0.25	0	15,15,17	1.09	1 (6%)
7	MAN	O	4	7	11,11,12	0.51	0	15,15,17	1.40	3 (20%)
7	MAN	O	5	7	11,11,12	0.25	0	15,15,17	0.80	0
7	MAN	O	6	7	11,11,12	0.26	0	15,15,17	0.66	0
7	MAN	O	7	7	11,11,12	0.20	0	15,15,17	0.59	0
8	NAG	P	1	1,8	14,14,15	1.98	5 (35%)	17,19,21	0.92	0
8	NAG	P	2	8	14,14,15	1.88	5 (35%)	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	Q	1	1,8	14,14,15	2.11	6 (42%)	17,19,21	6.76	4 (23%)
8	NAG	Q	2	8	14,14,15	1.89	5 (35%)	17,19,21	0.99	2 (11%)
9	NAG	R	1	1,9	14,14,15	1.94	4 (28%)	17,19,21	1.19	3 (17%)
9	NAG	R	2	9	14,14,15	1.80	5 (35%)	17,19,21	0.89	1 (5%)
9	BMA	R	3	9	11,11,12	0.71	0	15,15,17	0.87	1 (6%)
9	MAN	R	4	9	11,11,12	1.93	5 (45%)	15,15,17	0.66	0
9	NAG	S	1	1,9	14,14,15	1.77	4 (28%)	17,19,21	0.90	0
9	NAG	S	2	9	14,14,15	1.77	4 (28%)	17,19,21	0.90	0
9	BMA	S	3	9	11,11,12	0.71	0	15,15,17	0.97	1 (6%)
9	MAN	S	4	9	11,11,12	2.01	5 (45%)	15,15,17	0.84	0
10	NAG	T	1	2,10	14,14,15	1.94	4 (28%)	17,19,21	1.00	1 (5%)
10	FUC	T	2	10	10,10,11	2.06	6 (60%)	14,14,16	0.67	0
10	NAG	U	1	2,10	14,14,15	2.05	6 (42%)	17,19,21	1.15	2 (11%)
10	FUC	U	2	10	10,10,11	1.82	4 (40%)	14,14,16	0.58	0
11	NAG	V	1	1,11	14,14,15	0.59	0	17,19,21	1.18	2 (11%)
11	NAG	V	2	11	14,14,15	0.34	0	17,19,21	0.62	0
11	BMA	V	3	11	11,11,12	0.22	0	15,15,17	0.85	1 (6%)
8	NAG	W	1	1,8	14,14,15	2.09	4 (28%)	17,19,21	0.99	0
8	NAG	W	2	8	14,14,15	1.89	4 (28%)	17,19,21	0.94	2 (11%)
8	NAG	X	1	1,8	14,14,15	1.97	5 (35%)	17,19,21	1.16	2 (11%)
8	NAG	X	2	8	14,14,15	1.81	5 (35%)	17,19,21	0.94	1 (5%)
9	NAG	Y	1	1,9	14,14,15	1.92	4 (28%)	17,19,21	1.13	2 (11%)
9	NAG	Y	2	9	14,14,15	1.88	4 (28%)	17,19,21	0.97	2 (11%)
9	BMA	Y	3	9	11,11,12	0.70	0	15,15,17	0.88	1 (6%)
9	MAN	Y	4	9	11,11,12	1.94	6 (54%)	15,15,17	0.77	0
8	NAG	Z	1	1,8	14,14,15	1.91	4 (28%)	17,19,21	1.05	1 (5%)
8	NAG	Z	2	8	14,14,15	1.93	5 (35%)	17,19,21	0.91	1 (5%)
10	NAG	a	1	2,10	14,14,15	1.93	4 (28%)	17,19,21	0.98	0
10	FUC	a	2	10	10,10,11	2.07	6 (60%)	14,14,16	0.67	0
10	NAG	b	1	2,10	14,14,15	1.93	6 (42%)	17,19,21	6.85	3 (17%)
10	FUC	b	2	10	10,10,11	2.02	6 (60%)	14,14,16	0.64	0
8	NAG	c	1	1,8	14,14,15	0.44	0	17,19,21	1.14	2 (11%)
8	NAG	c	2	8	14,14,15	0.34	0	17,19,21	1.44	1 (5%)
8	NAG	d	1	1,8	14,14,15	1.96	3 (21%)	17,19,21	1.14	1 (5%)
8	NAG	d	2	8	14,14,15	1.94	5 (35%)	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	e	1	1,8	14,14,15	2.13	4 (28%)	17,19,21	7.02	3 (17%)
8	NAG	e	2	8	14,14,15	1.89	5 (35%)	17,19,21	0.94	1 (5%)
9	NAG	f	1	1,9	14,14,15	1.97	4 (28%)	17,19,21	1.17	3 (17%)
9	NAG	f	2	9	14,14,15	1.89	4 (28%)	17,19,21	0.89	1 (5%)
9	BMA	f	3	9	11,11,12	0.76	0	15,15,17	0.85	1 (6%)
9	MAN	f	4	9	11,11,12	1.95	5 (45%)	15,15,17	0.70	0
8	NAG	g	1	1,8	14,14,15	1.88	4 (28%)	17,19,21	1.00	1 (5%)
8	NAG	g	2	8	14,14,15	1.84	5 (35%)	17,19,21	0.91	1 (5%)
10	NAG	h	1	2,10	14,14,15	2.03	4 (28%)	17,19,21	1.02	1 (5%)
10	FUC	h	2	10	10,10,11	2.11	4 (40%)	14,14,16	0.82	0
10	NAG	i	1	2,10	14,14,15	2.04	5 (35%)	17,19,21	1.05	1 (5%)
10	FUC	i	2	10	10,10,11	1.92	5 (50%)	14,14,16	0.69	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
7	NAG	O	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	O	2	7	-	2/6/23/26	0/1/1/1
7	BMA	O	3	7	-	2/2/19/22	0/1/1/1
7	MAN	O	4	7	-	0/2/19/22	0/1/1/1
7	MAN	O	5	7	-	0/2/19/22	0/1/1/1
7	MAN	O	6	7	-	0/2/19/22	0/1/1/1
7	MAN	O	7	7	-	2/2/19/22	0/1/1/1
8	NAG	P	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	P	2	8	-	0/6/23/26	0/1/1/1
8	NAG	Q	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	0/6/23/26	0/1/1/1
9	NAG	R	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	R	2	9	-	0/6/23/26	0/1/1/1
9	BMA	R	3	9	-	1/2/19/22	0/1/1/1
9	MAN	R	4	9	-	0/2/19/22	0/1/1/1
9	NAG	S	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	S	2	9	-	0/6/23/26	0/1/1/1
9	BMA	S	3	9	-	0/2/19/22	0/1/1/1
9	MAN	S	4	9	-	0/2/19/22	0/1/1/1
10	NAG	T	1	2,10	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FUC	T	2	10	-	-	0/1/1/1
10	NAG	U	1	2,10	-	1/6/23/26	0/1/1/1
10	FUC	U	2	10	-	-	0/1/1/1
11	NAG	V	1	1,11	-	1/6/23/26	0/1/1/1
11	NAG	V	2	11	-	2/6/23/26	0/1/1/1
11	BMA	V	3	11	-	1/2/19/22	0/1/1/1
8	NAG	W	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	W	2	8	-	0/6/23/26	0/1/1/1
8	NAG	X	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	X	2	8	-	0/6/23/26	0/1/1/1
9	NAG	Y	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	0/6/23/26	0/1/1/1
9	BMA	Y	3	9	-	1/2/19/22	0/1/1/1
9	MAN	Y	4	9	-	1/2/19/22	0/1/1/1
8	NAG	Z	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	0/6/23/26	0/1/1/1
10	NAG	a	1	2,10	-	0/6/23/26	0/1/1/1
10	FUC	a	2	10	-	-	0/1/1/1
10	NAG	b	1	2,10	-	2/6/23/26	0/1/1/1
10	FUC	b	2	10	-	-	0/1/1/1
8	NAG	c	1	1,8	-	4/6/23/26	0/1/1/1
8	NAG	c	2	8	-	4/6/23/26	0/1/1/1
8	NAG	d	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	d	2	8	-	0/6/23/26	0/1/1/1
8	NAG	e	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	e	2	8	-	0/6/23/26	0/1/1/1
9	NAG	f	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	f	2	9	-	0/6/23/26	0/1/1/1
9	BMA	f	3	9	-	0/2/19/22	0/1/1/1
9	MAN	f	4	9	-	0/2/19/22	0/1/1/1
8	NAG	g	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	g	2	8	-	0/6/23/26	0/1/1/1
10	NAG	h	1	2,10	-	0/6/23/26	0/1/1/1
10	FUC	h	2	10	-	-	0/1/1/1
10	NAG	i	1	2,10	-	2/6/23/26	0/1/1/1
10	FUC	i	2	10	1/1/4/5	-	0/1/1/1

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	W	1	NAG	C1-C2	5.61	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	e	1	NAG	C1-C2	5.55	1.60	1.52
8	Q	1	NAG	C1-C2	5.49	1.60	1.52
9	f	1	NAG	C1-C2	5.25	1.60	1.52
9	R	1	NAG	C1-C2	5.24	1.60	1.52
10	h	1	NAG	C1-C2	5.23	1.60	1.52
8	P	1	NAG	C1-C2	5.10	1.60	1.52
8	d	1	NAG	C1-C2	4.92	1.59	1.52
10	U	1	NAG	C1-C2	4.85	1.59	1.52
9	Y	1	NAG	C1-C2	4.82	1.59	1.52
10	i	1	NAG	C1-C2	4.76	1.59	1.52
10	T	1	NAG	C1-C2	4.67	1.59	1.52
8	X	1	NAG	C1-C2	4.58	1.59	1.52
8	d	2	NAG	C1-C2	4.58	1.59	1.52
8	g	1	NAG	C1-C2	4.54	1.59	1.52
10	a	1	NAG	C1-C2	4.52	1.59	1.52
8	Z	1	NAG	C1-C2	4.50	1.59	1.52
9	Y	2	NAG	C1-C2	4.38	1.58	1.52
9	S	1	NAG	C1-C2	4.28	1.58	1.52
10	b	1	NAG	C1-C2	4.24	1.58	1.52
8	Q	2	NAG	C1-C2	4.23	1.58	1.52
8	W	2	NAG	C1-C2	4.18	1.58	1.52
8	e	2	NAG	C1-C2	4.17	1.58	1.52
8	Z	2	NAG	C1-C2	4.14	1.58	1.52
8	P	2	NAG	C1-C2	4.04	1.58	1.52
9	f	2	NAG	C1-C2	3.98	1.58	1.52
8	g	2	NAG	C1-C2	3.94	1.58	1.52
8	X	2	NAG	C1-C2	3.85	1.58	1.52
9	R	2	NAG	C1-C2	3.85	1.58	1.52
9	S	2	NAG	C1-C2	3.58	1.57	1.52
9	S	4	MAN	O5-C5	3.36	1.50	1.43
10	b	1	NAG	O5-C5	3.35	1.50	1.43
10	h	2	FUC	C2-C3	3.33	1.57	1.52
9	S	4	MAN	C2-C3	3.29	1.57	1.52
10	a	2	FUC	C2-C3	3.29	1.57	1.52
10	T	2	FUC	C2-C3	3.28	1.57	1.52
9	f	4	MAN	C2-C3	3.27	1.57	1.52
10	a	1	NAG	O5-C5	3.26	1.50	1.43
8	Z	2	NAG	O5-C5	3.25	1.50	1.43
9	f	4	MAN	O5-C5	3.23	1.50	1.43
9	R	4	MAN	O5-C5	3.21	1.49	1.43
10	U	1	NAG	O5-C5	3.18	1.49	1.43
10	i	1	NAG	O5-C5	3.16	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	h	2	FUC	C1-C2	3.16	1.59	1.52
9	R	4	MAN	C2-C3	3.14	1.57	1.52
10	h	1	NAG	O5-C5	3.11	1.49	1.43
9	Y	4	MAN	O5-C5	3.08	1.49	1.43
8	P	2	NAG	O5-C5	3.08	1.49	1.43
8	W	2	NAG	O5-C5	3.07	1.49	1.43
9	f	2	NAG	O5-C5	3.05	1.49	1.43
8	e	2	NAG	O5-C5	3.03	1.49	1.43
9	Y	4	MAN	C2-C3	3.00	1.56	1.52
8	g	2	NAG	O5-C5	2.99	1.49	1.43
10	i	2	FUC	C2-C3	2.99	1.56	1.52
8	Q	2	NAG	O5-C5	2.93	1.49	1.43
10	T	2	FUC	O5-C5	2.92	1.49	1.43
10	T	1	NAG	O5-C5	2.90	1.49	1.43
8	d	2	NAG	O5-C5	2.90	1.49	1.43
10	a	2	FUC	C1-C2	2.88	1.58	1.52
10	h	2	FUC	O5-C5	2.88	1.49	1.43
8	X	2	NAG	O5-C5	2.88	1.49	1.43
10	b	2	FUC	C2-C3	2.87	1.56	1.52
10	a	2	FUC	O5-C5	2.86	1.49	1.43
9	S	2	NAG	O5-C5	2.85	1.49	1.43
10	U	2	FUC	C2-C3	2.84	1.56	1.52
9	R	2	NAG	O5-C5	2.81	1.49	1.43
8	d	1	NAG	O5-C5	2.81	1.49	1.43
10	b	2	FUC	C1-C2	2.81	1.58	1.52
10	b	2	FUC	O5-C5	2.80	1.49	1.43
8	g	1	NAG	O5-C5	2.80	1.49	1.43
8	X	1	NAG	O5-C5	2.76	1.49	1.43
8	P	1	NAG	O5-C5	2.76	1.49	1.43
10	T	2	FUC	C1-C2	2.74	1.58	1.52
10	i	2	FUC	O5-C5	2.73	1.49	1.43
9	Y	2	NAG	O5-C5	2.72	1.49	1.43
10	i	2	FUC	C1-C2	2.72	1.58	1.52
8	e	1	NAG	O5-C5	2.70	1.48	1.43
8	Z	1	NAG	O5-C5	2.69	1.48	1.43
9	Y	4	MAN	C1-C2	2.66	1.58	1.52
10	U	2	FUC	C1-C2	2.64	1.58	1.52
10	i	1	NAG	O5-C1	2.63	1.47	1.43
10	U	2	FUC	O5-C5	2.62	1.49	1.43
10	h	2	FUC	C4-C5	2.59	1.58	1.52
10	b	2	FUC	C4-C5	2.59	1.58	1.52
8	e	1	NAG	O5-C1	2.58	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Y	4	MAN	C4-C5	2.56	1.58	1.53
9	S	1	NAG	O5-C5	2.55	1.48	1.43
9	f	2	NAG	C4-C5	2.55	1.58	1.53
9	S	4	MAN	C1-C2	2.54	1.58	1.52
9	R	4	MAN	C1-C2	2.53	1.58	1.52
8	W	1	NAG	O5-C5	2.48	1.48	1.43
8	g	1	NAG	O5-C1	2.48	1.47	1.43
9	f	4	MAN	C1-C2	2.48	1.57	1.52
8	Q	2	NAG	C3-C2	2.48	1.57	1.52
10	U	1	NAG	O5-C1	2.47	1.47	1.43
8	Q	1	NAG	C4-C5	2.47	1.58	1.53
8	X	1	NAG	O5-C1	2.46	1.47	1.43
9	S	4	MAN	C4-C5	2.45	1.58	1.53
10	b	1	NAG	O5-C1	2.45	1.47	1.43
9	Y	1	NAG	O5-C5	2.45	1.48	1.43
8	P	2	NAG	C4-C5	2.44	1.58	1.53
9	Y	2	NAG	C3-C2	2.42	1.57	1.52
8	Q	2	NAG	C4-C5	2.42	1.58	1.53
10	a	2	FUC	C4-C5	2.42	1.58	1.52
8	X	2	NAG	C3-C2	2.40	1.57	1.52
8	e	2	NAG	C3-C2	2.39	1.57	1.52
8	g	2	NAG	C4-C5	2.39	1.58	1.53
8	Q	1	NAG	C4-C3	2.39	1.58	1.52
10	T	1	NAG	C3-C2	2.38	1.57	1.52
8	Z	2	NAG	C3-C2	2.38	1.57	1.52
10	T	2	FUC	C4-C5	2.37	1.58	1.52
8	d	1	NAG	C4-C5	2.37	1.58	1.53
8	d	2	NAG	C3-C2	2.36	1.57	1.52
8	Z	1	NAG	C4-C5	2.36	1.58	1.53
9	S	1	NAG	O5-C1	2.36	1.47	1.43
8	W	2	NAG	C3-C2	2.35	1.57	1.52
9	Y	1	NAG	C3-C2	2.35	1.57	1.52
10	b	1	NAG	C3-C2	2.33	1.57	1.52
9	f	1	NAG	O5-C5	2.32	1.48	1.43
8	W	1	NAG	C3-C2	2.32	1.57	1.52
9	f	1	NAG	C3-C2	2.31	1.57	1.52
8	Q	1	NAG	O5-C5	2.31	1.48	1.43
8	Z	1	NAG	O5-C1	2.31	1.47	1.43
8	X	2	NAG	C4-C5	2.31	1.57	1.53
9	R	2	NAG	C3-C2	2.31	1.57	1.52
10	b	1	NAG	C4-C5	2.30	1.57	1.53
9	f	4	MAN	C4-C5	2.29	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	1	NAG	O5-C1	2.29	1.47	1.43
8	e	1	NAG	C4-C5	2.29	1.57	1.53
8	e	2	NAG	C4-C5	2.29	1.57	1.53
9	R	2	NAG	C4-C5	2.28	1.57	1.53
8	W	2	NAG	C4-C5	2.27	1.57	1.53
9	S	4	MAN	O5-C1	2.27	1.47	1.43
10	h	1	NAG	O5-C1	2.27	1.47	1.43
8	P	2	NAG	C3-C2	2.26	1.57	1.52
9	R	1	NAG	C3-C2	2.26	1.57	1.52
8	Z	2	NAG	C4-C5	2.26	1.57	1.53
9	R	4	MAN	C4-C5	2.23	1.57	1.53
8	d	2	NAG	C4-C5	2.23	1.57	1.53
10	U	2	FUC	C4-C5	2.22	1.57	1.52
10	i	1	NAG	C3-C2	2.21	1.57	1.52
10	i	1	NAG	C4-C5	2.21	1.57	1.53
9	R	1	NAG	O5-C5	2.21	1.47	1.43
8	g	1	NAG	C4-C5	2.20	1.57	1.53
10	T	1	NAG	O5-C1	2.20	1.47	1.43
9	f	2	NAG	C3-C2	2.20	1.57	1.52
8	g	2	NAG	C3-C2	2.18	1.57	1.52
8	X	1	NAG	C4-C3	2.18	1.57	1.52
8	P	2	NAG	C4-C3	2.18	1.57	1.52
9	S	2	NAG	C4-C5	2.18	1.57	1.53
10	i	2	FUC	C4-C5	2.17	1.57	1.52
9	R	4	MAN	O5-C1	2.15	1.47	1.43
8	W	1	NAG	O5-C1	2.15	1.47	1.43
9	f	4	MAN	O5-C1	2.15	1.47	1.43
8	P	1	NAG	O5-C1	2.14	1.47	1.43
8	P	1	NAG	C4-C5	2.13	1.57	1.53
9	R	2	NAG	C4-C3	2.13	1.57	1.52
10	U	1	NAG	C4-C5	2.12	1.57	1.53
10	a	1	NAG	C3-C2	2.12	1.57	1.52
10	b	2	FUC	O5-C1	2.11	1.47	1.43
8	Q	1	NAG	C3-C2	2.11	1.57	1.52
9	S	2	NAG	C4-C3	2.11	1.57	1.52
8	Q	1	NAG	O5-C1	2.10	1.47	1.43
10	a	2	FUC	O5-C1	2.09	1.47	1.43
10	T	2	FUC	O5-C1	2.09	1.47	1.43
8	X	1	NAG	C4-C5	2.09	1.57	1.53
9	R	1	NAG	O5-C1	2.09	1.47	1.43
10	h	1	NAG	C3-C2	2.08	1.56	1.52
9	Y	4	MAN	O5-C1	2.08	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Y	1	NAG	O5-C1	2.08	1.47	1.43
10	T	2	FUC	C4-C3	2.08	1.57	1.52
9	Y	4	MAN	C4-C3	2.07	1.57	1.52
9	S	1	NAG	C4-C5	2.07	1.57	1.53
8	P	1	NAG	C3-C2	2.07	1.56	1.52
8	e	2	NAG	C4-C3	2.07	1.57	1.52
8	X	2	NAG	C4-C3	2.07	1.57	1.52
10	U	1	NAG	C4-C3	2.07	1.57	1.52
9	f	1	NAG	O5-C1	2.07	1.47	1.43
10	a	2	FUC	C4-C3	2.06	1.57	1.52
10	U	1	NAG	C3-C2	2.06	1.56	1.52
9	Y	2	NAG	C4-C3	2.06	1.57	1.52
10	b	2	FUC	C4-C3	2.05	1.57	1.52
8	d	2	NAG	C2-N2	2.04	1.49	1.46
10	i	2	FUC	C4-C3	2.04	1.57	1.52
8	g	2	NAG	C4-C3	2.04	1.57	1.52
8	Z	2	NAG	C4-C3	2.04	1.57	1.52
8	Q	2	NAG	C4-C3	2.01	1.57	1.52
10	b	1	NAG	C4-C3	2.01	1.57	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	e	1	NAG	C2-N2-C7	28.08	162.89	122.90
10	b	1	NAG	C2-N2-C7	27.88	162.59	122.90
8	Q	1	NAG	C2-N2-C7	26.99	161.34	122.90
8	e	1	NAG	C8-C7-N2	5.23	124.96	116.10
8	Q	1	NAG	C8-C7-N2	5.09	124.71	116.10
8	c	2	NAG	C1-O5-C5	4.56	118.38	112.19
7	O	1	NAG	C1-O5-C5	3.38	116.77	112.19
8	e	1	NAG	O7-C7-N2	-3.24	116.00	121.95
11	V	1	NAG	C1-O5-C5	2.91	116.13	112.19
9	R	1	NAG	C8-C7-N2	2.83	120.89	116.10
8	X	1	NAG	C8-C7-N2	2.82	120.88	116.10
10	b	1	NAG	C1-C2-N2	-2.79	105.72	110.49
9	f	1	NAG	C8-C7-N2	2.74	120.74	116.10
7	O	4	MAN	O3-C3-C4	2.72	116.63	110.35
11	V	1	NAG	C1-C2-N2	-2.59	106.06	110.49
9	Y	1	NAG	C8-C7-N2	2.45	120.24	116.10
8	d	1	NAG	O4-C4-C3	-2.44	104.72	110.35
9	Y	2	NAG	C8-C7-N2	2.40	120.17	116.10
8	Q	1	NAG	O7-C7-N2	-2.39	117.56	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Q	1	NAG	O7-C7-C8	-2.33	117.72	122.06
9	S	3	BMA	C2-C3-C4	-2.33	106.86	110.89
8	c	1	NAG	C1-O5-C5	2.33	115.35	112.19
8	c	1	NAG	O5-C1-C2	-2.29	107.67	111.29
10	h	1	NAG	C8-C7-N2	2.27	119.95	116.10
9	f	3	BMA	C2-C3-C4	-2.27	106.97	110.89
8	P	2	NAG	C8-C7-N2	2.27	119.94	116.10
11	V	3	BMA	C1-O5-C5	2.26	115.26	112.19
8	Z	1	NAG	C8-C7-N2	2.25	119.91	116.10
9	R	1	NAG	C1-O5-C5	2.22	115.20	112.19
9	R	1	NAG	O7-C7-C8	-2.22	117.94	122.06
10	U	1	NAG	C8-C7-N2	2.21	119.83	116.10
8	d	2	NAG	C8-C7-N2	2.20	119.83	116.10
8	g	1	NAG	C8-C7-N2	2.18	119.80	116.10
9	f	1	NAG	O7-C7-C8	-2.18	118.00	122.06
8	W	2	NAG	C8-C7-N2	2.18	119.79	116.10
8	Z	2	NAG	C8-C7-N2	2.17	119.77	116.10
9	Y	1	NAG	O7-C7-C8	-2.15	118.06	122.06
9	R	3	BMA	C2-C3-C4	-2.14	107.19	110.89
9	f	1	NAG	C1-O5-C5	2.14	115.09	112.19
10	T	1	NAG	C8-C7-N2	2.13	119.71	116.10
9	Y	2	NAG	O7-C7-C8	-2.13	118.10	122.06
8	X	1	NAG	O7-C7-C8	-2.13	118.11	122.06
8	g	2	NAG	C8-C7-N2	2.12	119.70	116.10
8	X	2	NAG	C8-C7-N2	2.12	119.69	116.10
8	e	2	NAG	C8-C7-N2	2.12	119.69	116.10
7	O	4	MAN	C3-C4-C5	-2.12	106.46	110.24
10	b	1	NAG	C8-C7-N2	2.11	119.67	116.10
10	i	1	NAG	C8-C7-N2	2.11	119.67	116.10
9	Y	3	BMA	C2-C3-C4	-2.10	107.26	110.89
8	Q	2	NAG	C1-O5-C5	2.10	115.03	112.19
9	R	2	NAG	C8-C7-N2	2.10	119.65	116.10
7	O	1	NAG	O5-C1-C2	-2.09	107.98	111.29
7	O	3	BMA	O5-C1-C2	-2.09	107.55	110.77
8	W	2	NAG	O7-C7-C8	-2.08	118.20	122.06
9	f	2	NAG	C8-C7-N2	2.05	119.58	116.10
7	O	4	MAN	C1-C2-C3	-2.04	107.16	109.67
8	Q	2	NAG	C8-C7-N2	2.01	119.49	116.10
10	U	1	NAG	C1-C2-N2	-2.00	107.07	110.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	i	2	FUC	C4

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	Q	1	NAG	C1-C2-N2-C7
8	e	1	NAG	C1-C2-N2-C7
8	c	2	NAG	C8-C7-N2-C2
8	c	2	NAG	O7-C7-N2-C2
8	c	2	NAG	C4-C5-C6-O6
8	c	2	NAG	O5-C5-C6-O6
10	b	1	NAG	C1-C2-N2-C7
11	V	2	NAG	O5-C5-C6-O6
8	Q	1	NAG	C8-C7-N2-C2
8	Q	1	NAG	O7-C7-N2-C2
8	c	1	NAG	C8-C7-N2-C2
8	e	1	NAG	C8-C7-N2-C2
8	e	1	NAG	O7-C7-N2-C2
10	i	1	NAG	O5-C5-C6-O6
7	O	7	MAN	O5-C5-C6-O6
10	i	1	NAG	C4-C5-C6-O6
7	O	7	MAN	C4-C5-C6-O6
8	c	1	NAG	O7-C7-N2-C2
7	O	2	NAG	C8-C7-N2-C2
11	V	2	NAG	C4-C5-C6-O6
9	Y	3	BMA	O5-C5-C6-O6
9	R	3	BMA	O5-C5-C6-O6
11	V	1	NAG	O5-C5-C6-O6
7	O	3	BMA	O5-C5-C6-O6
7	O	2	NAG	O7-C7-N2-C2
9	Y	4	MAN	O5-C5-C6-O6
8	c	1	NAG	C4-C5-C6-O6
8	c	1	NAG	O5-C5-C6-O6
11	V	3	BMA	O5-C5-C6-O6
7	O	3	BMA	C4-C5-C6-O6
10	U	1	NAG	O5-C5-C6-O6
10	b	1	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

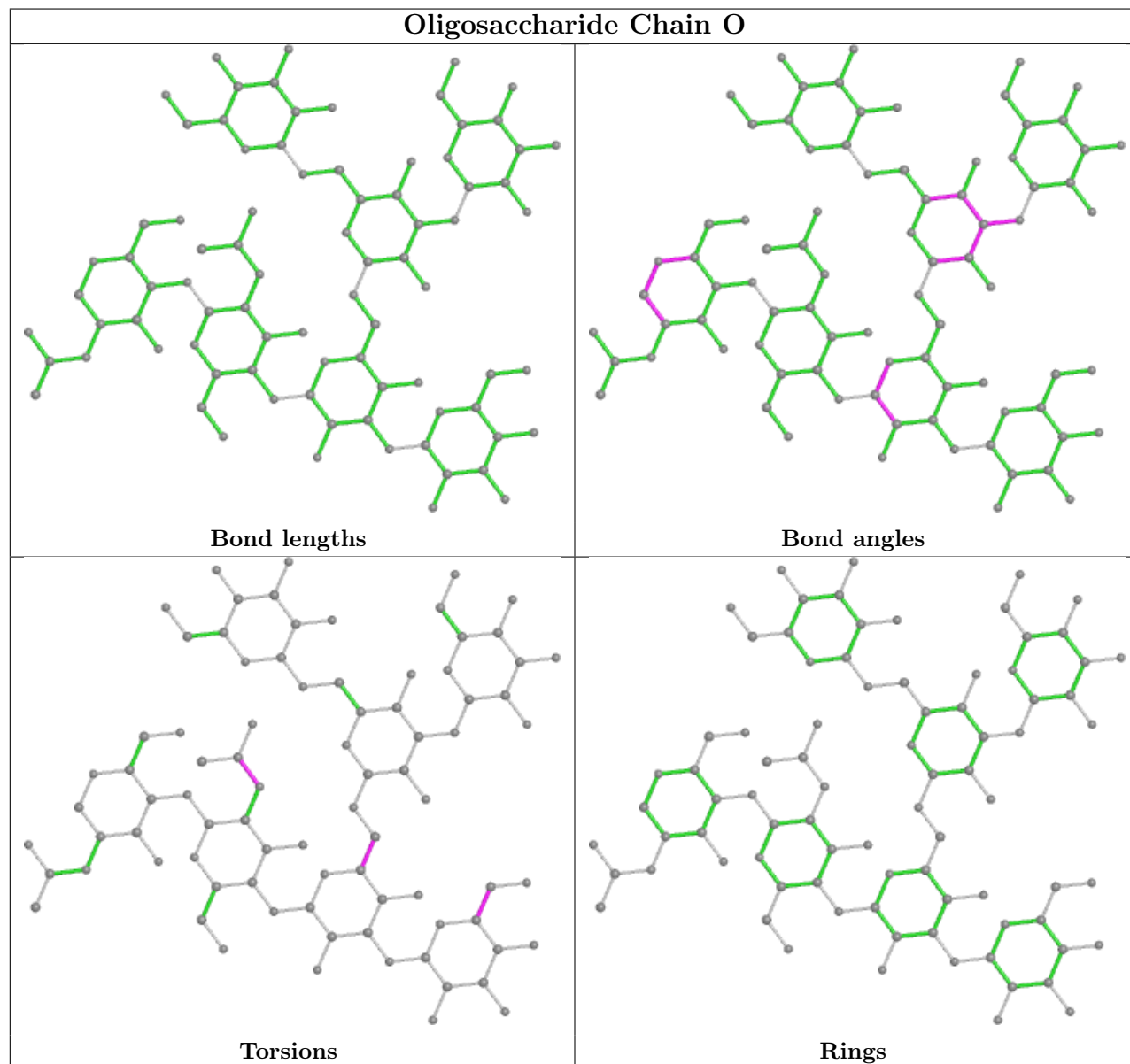
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	Z	1	NAG	1	0

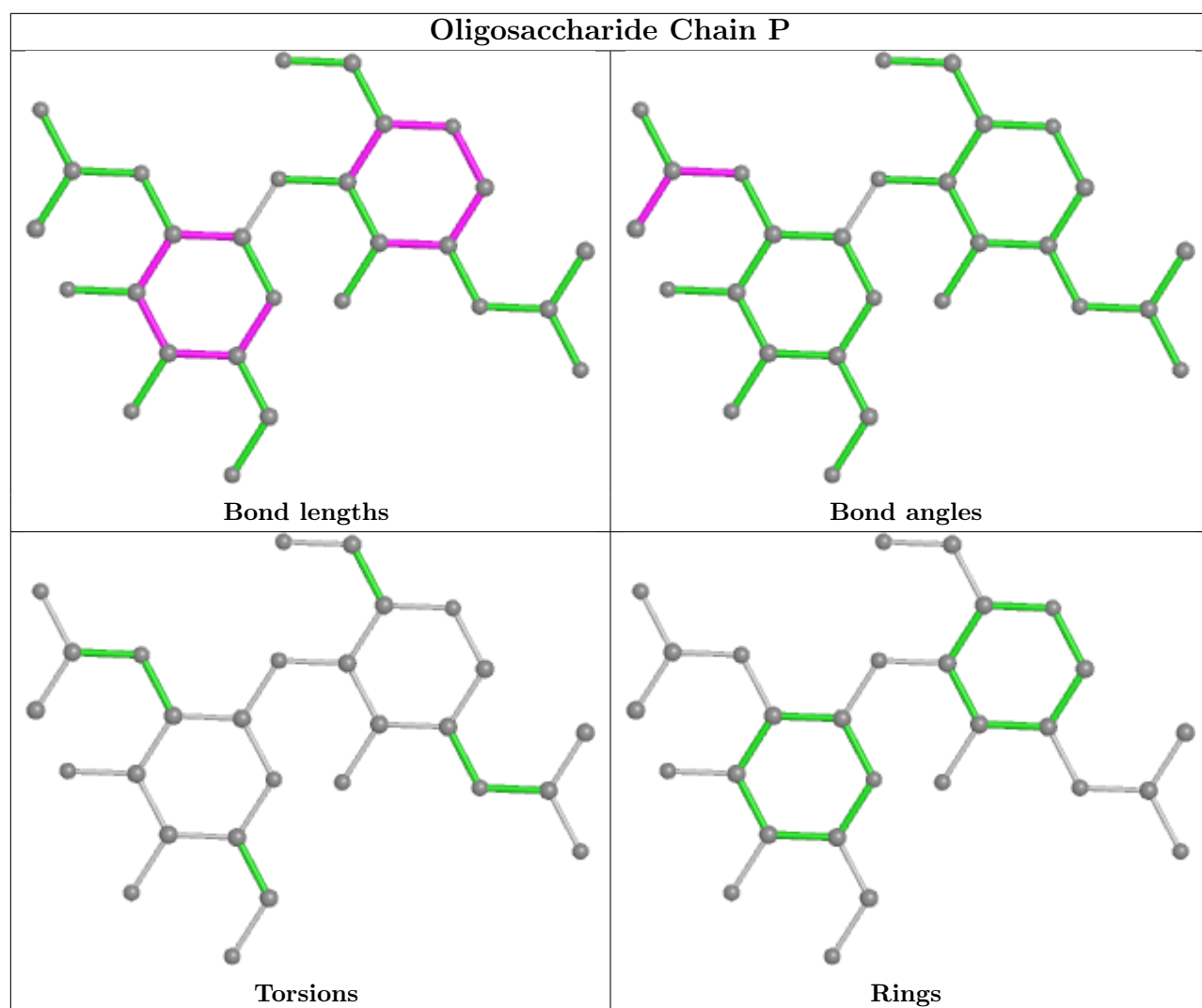
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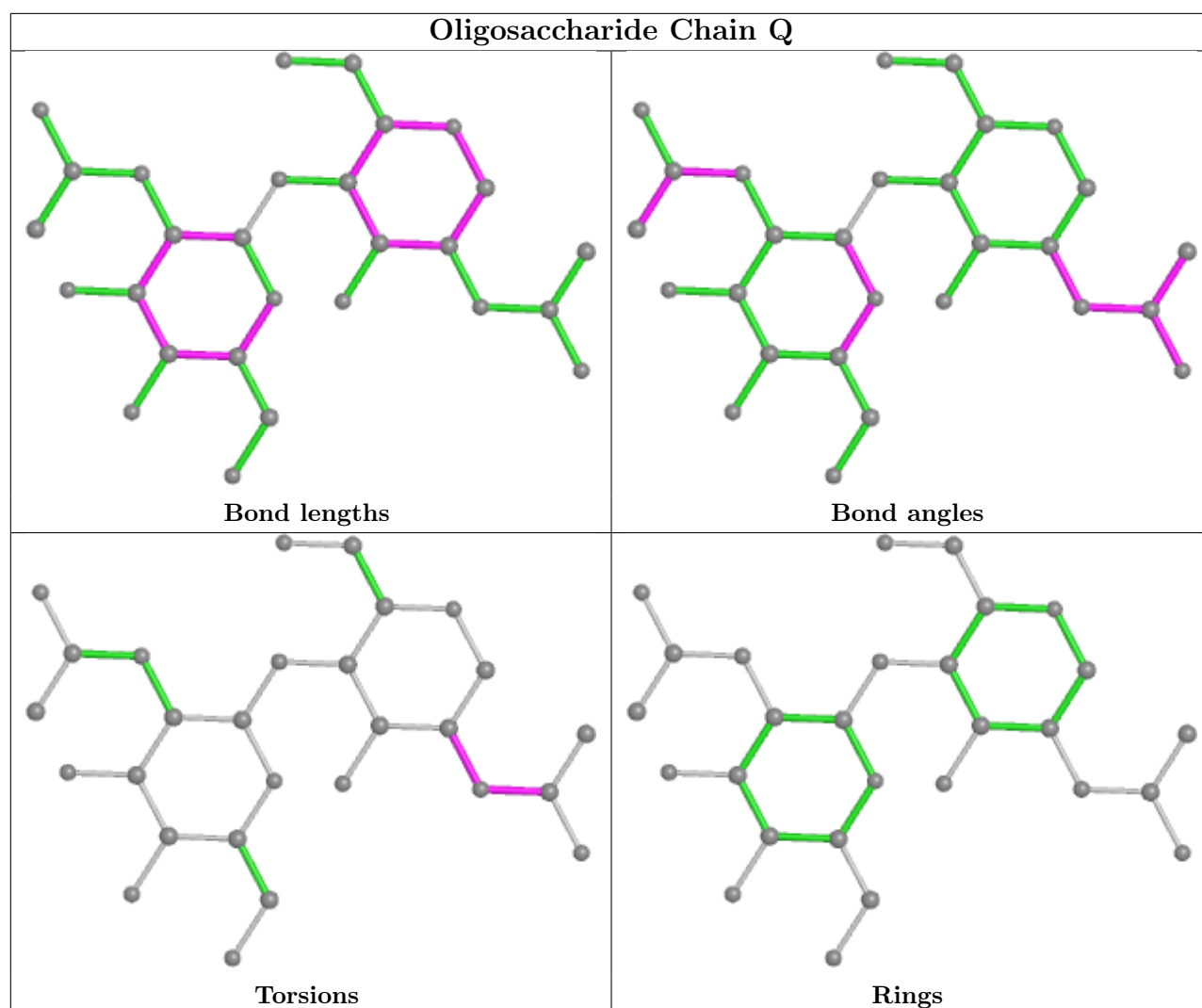
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	S	1	NAG	1	0
7	O	1	NAG	1	0

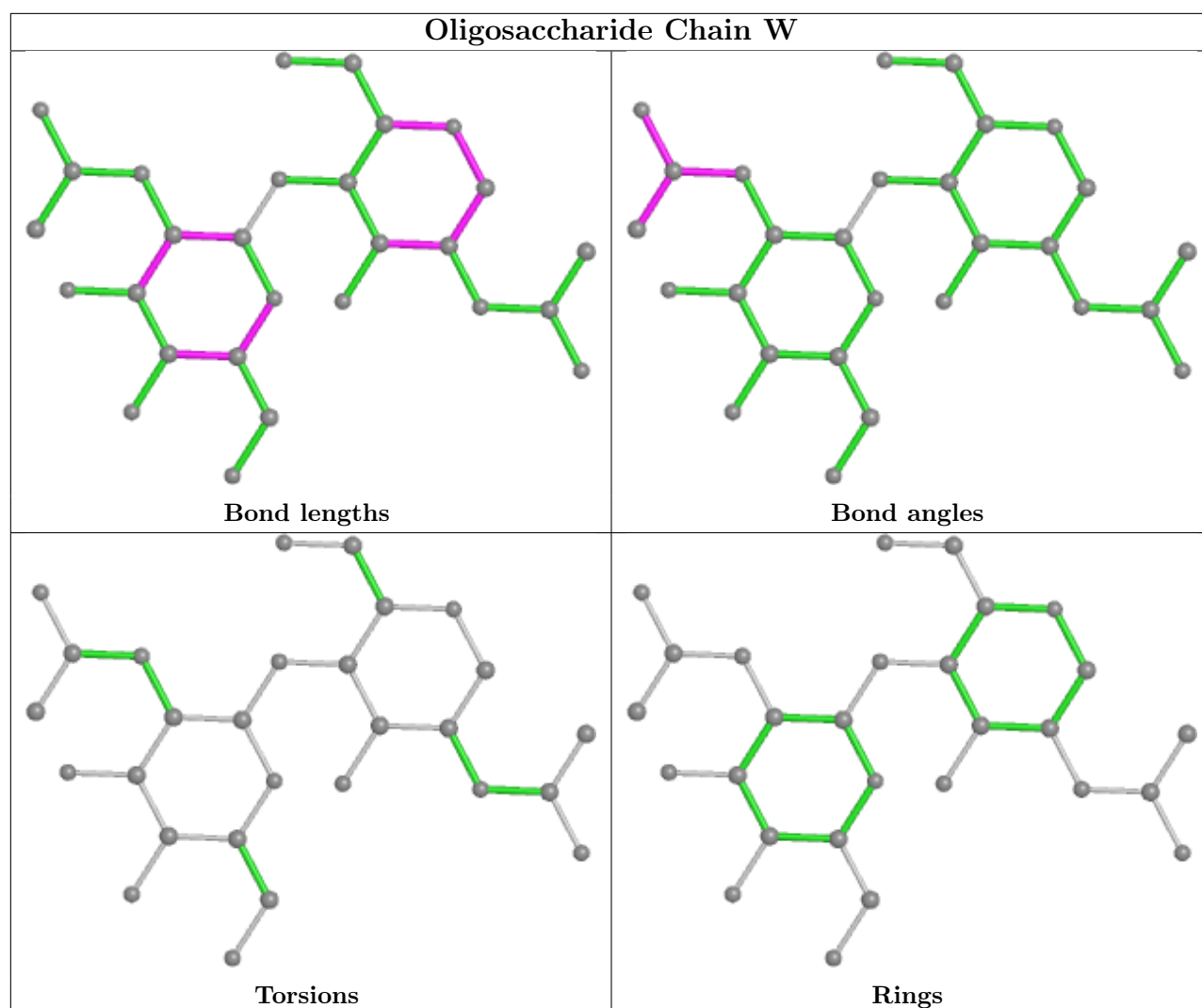
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

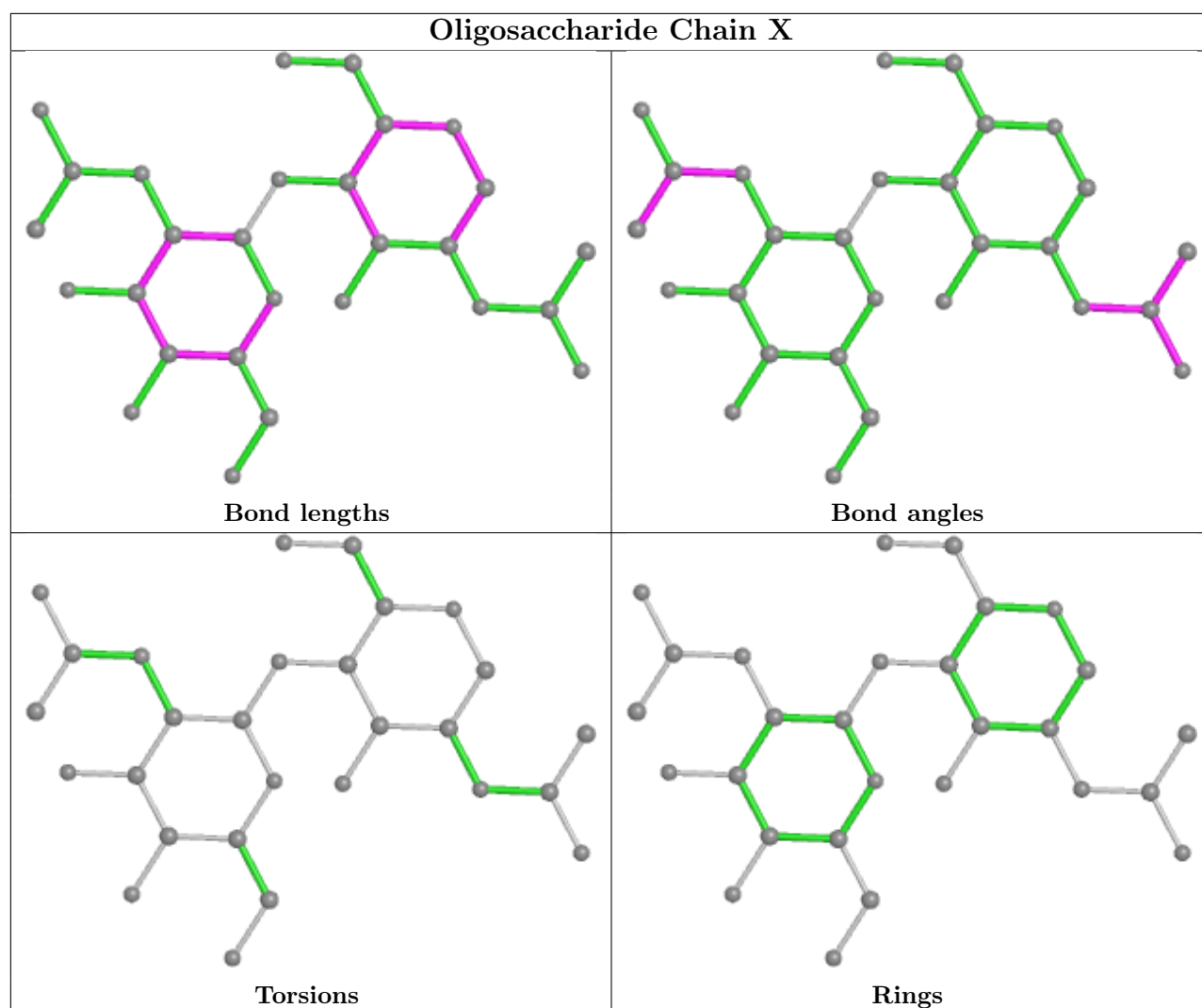


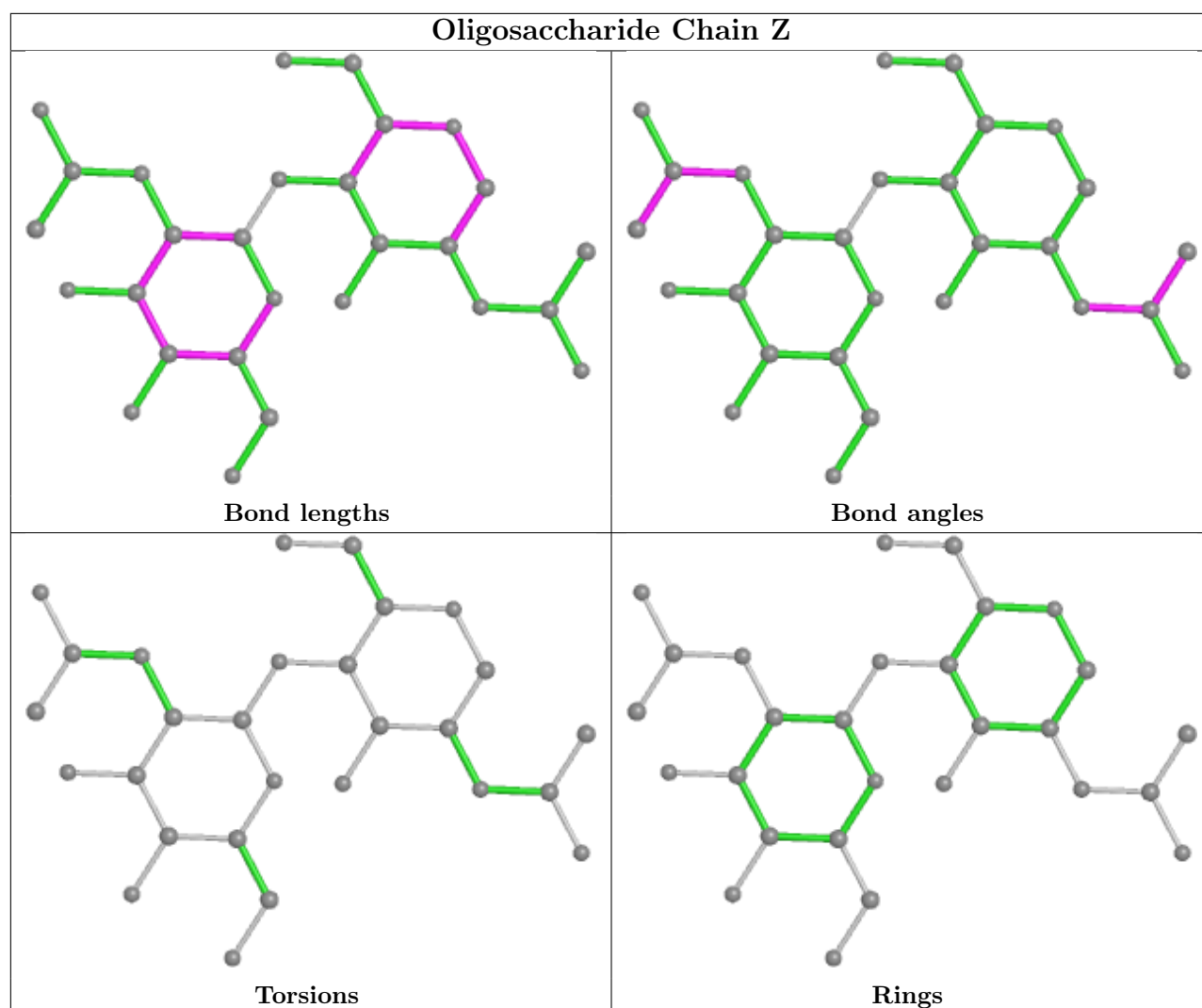


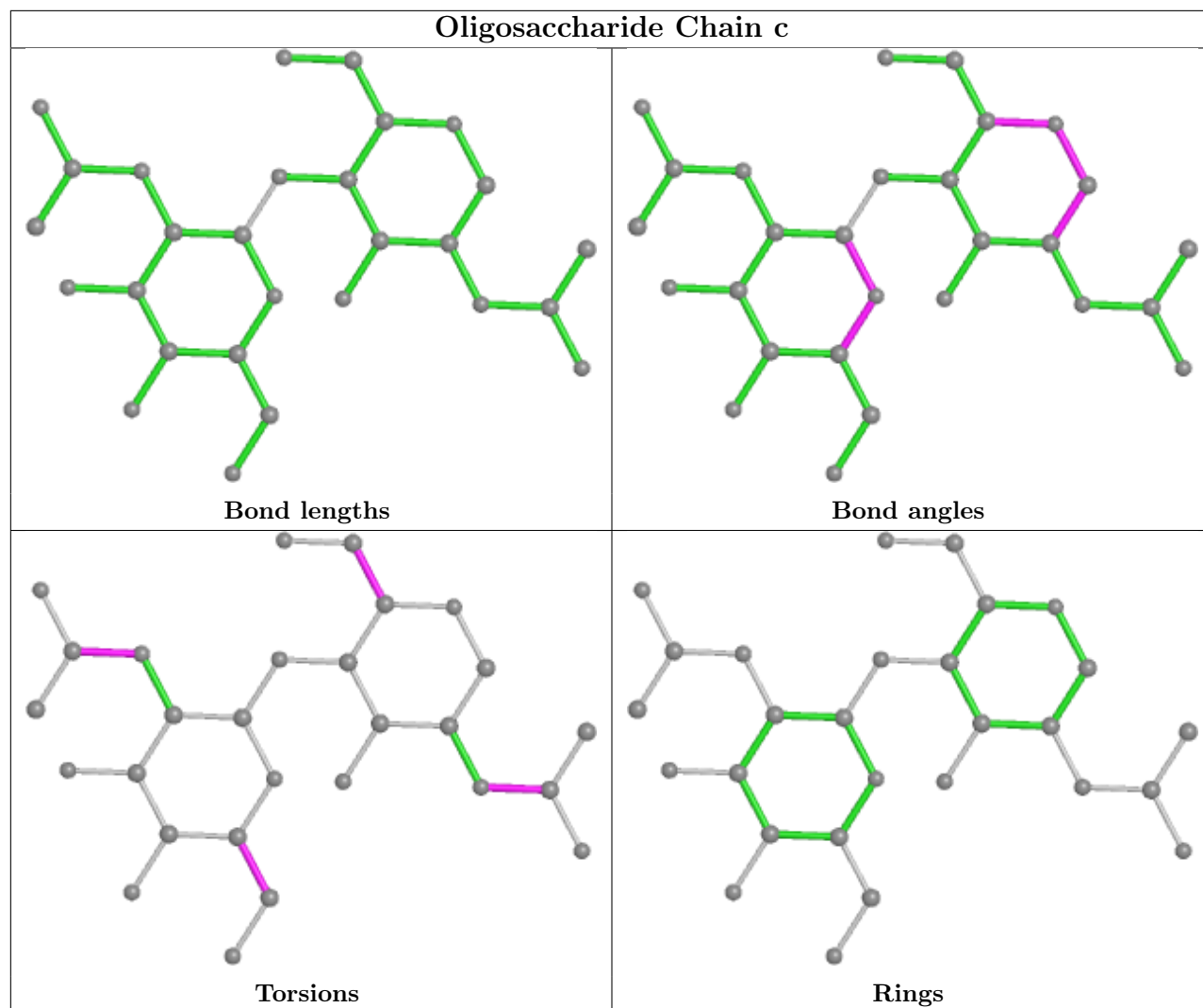


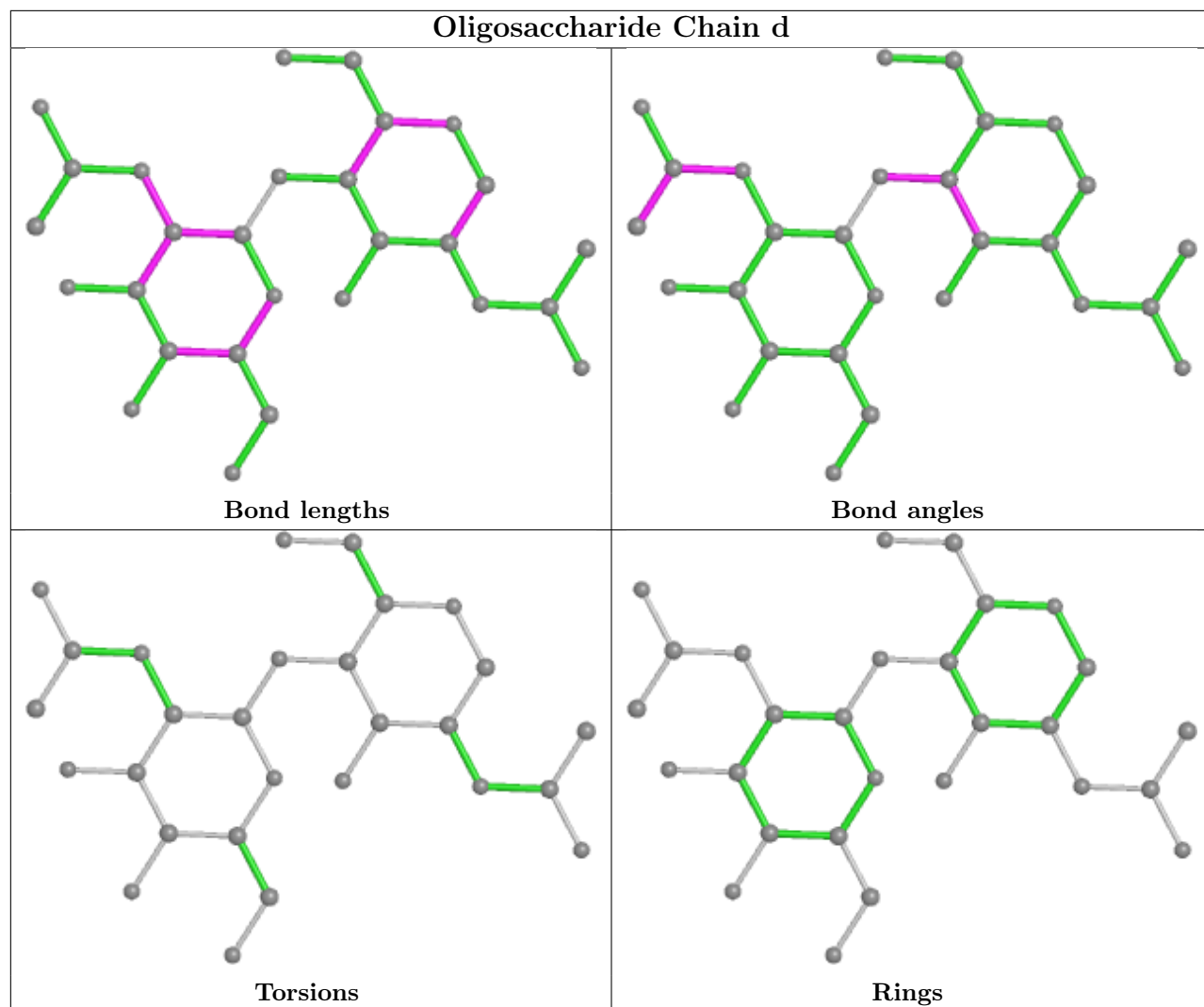


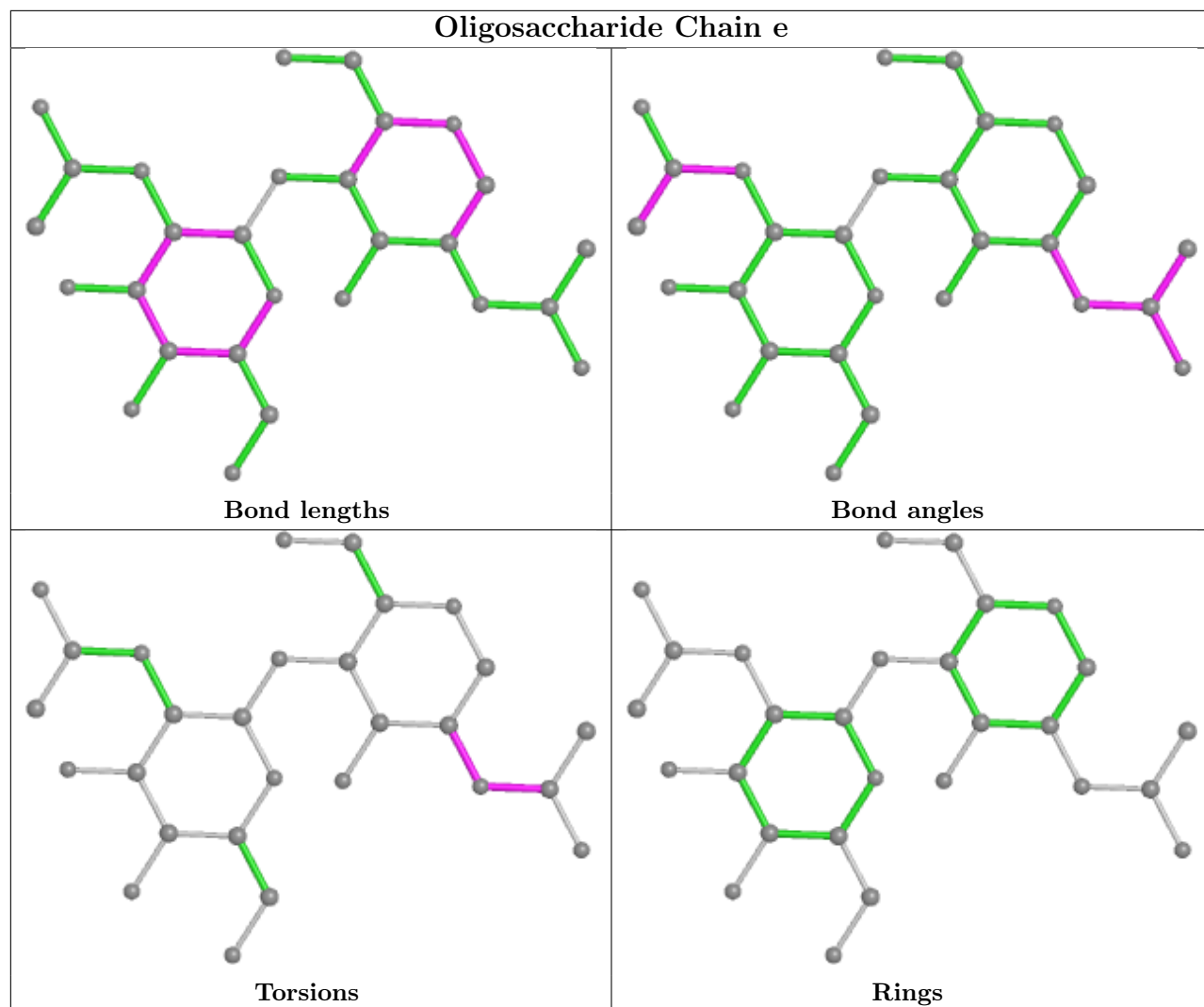


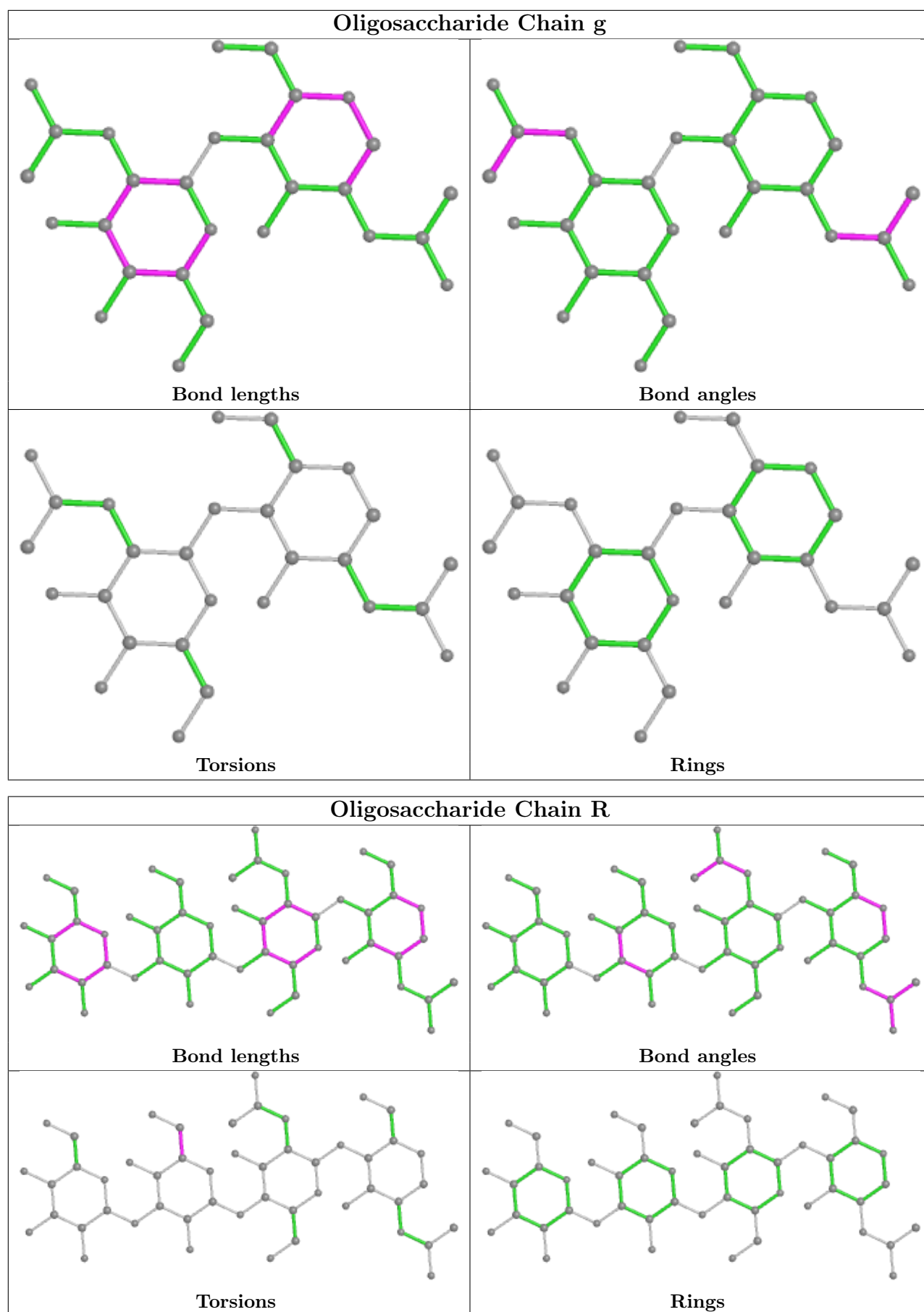


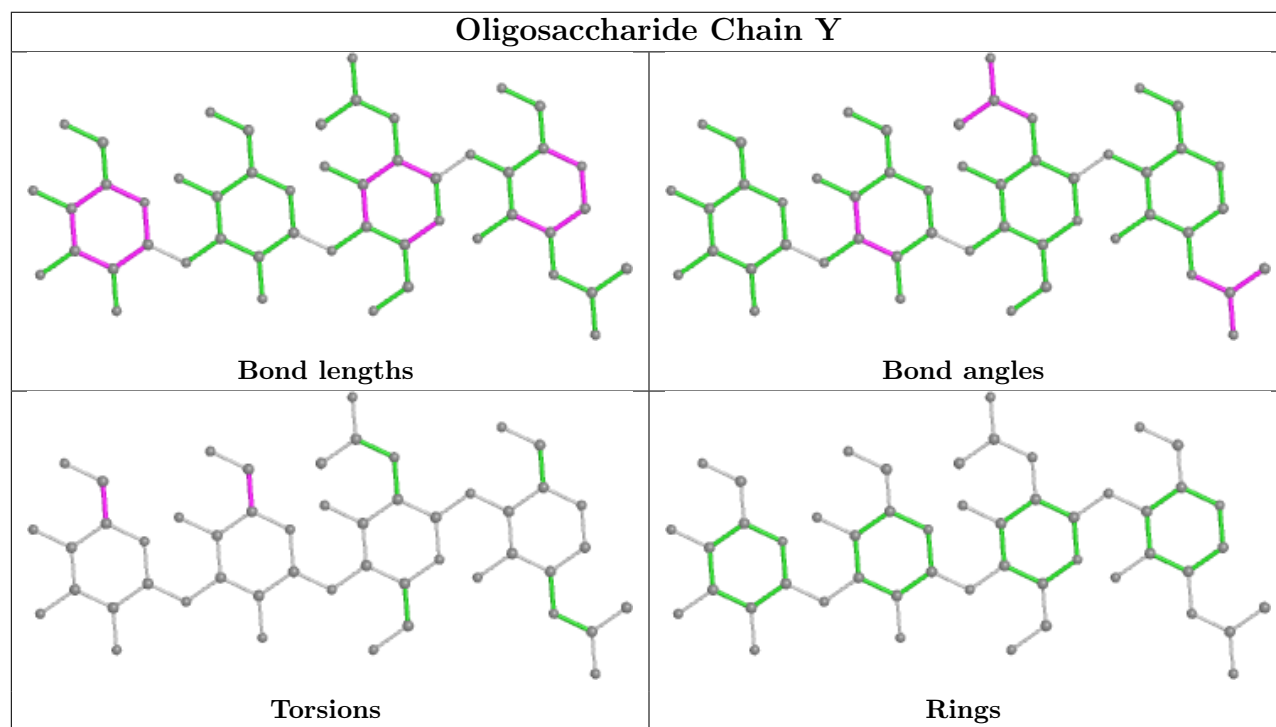
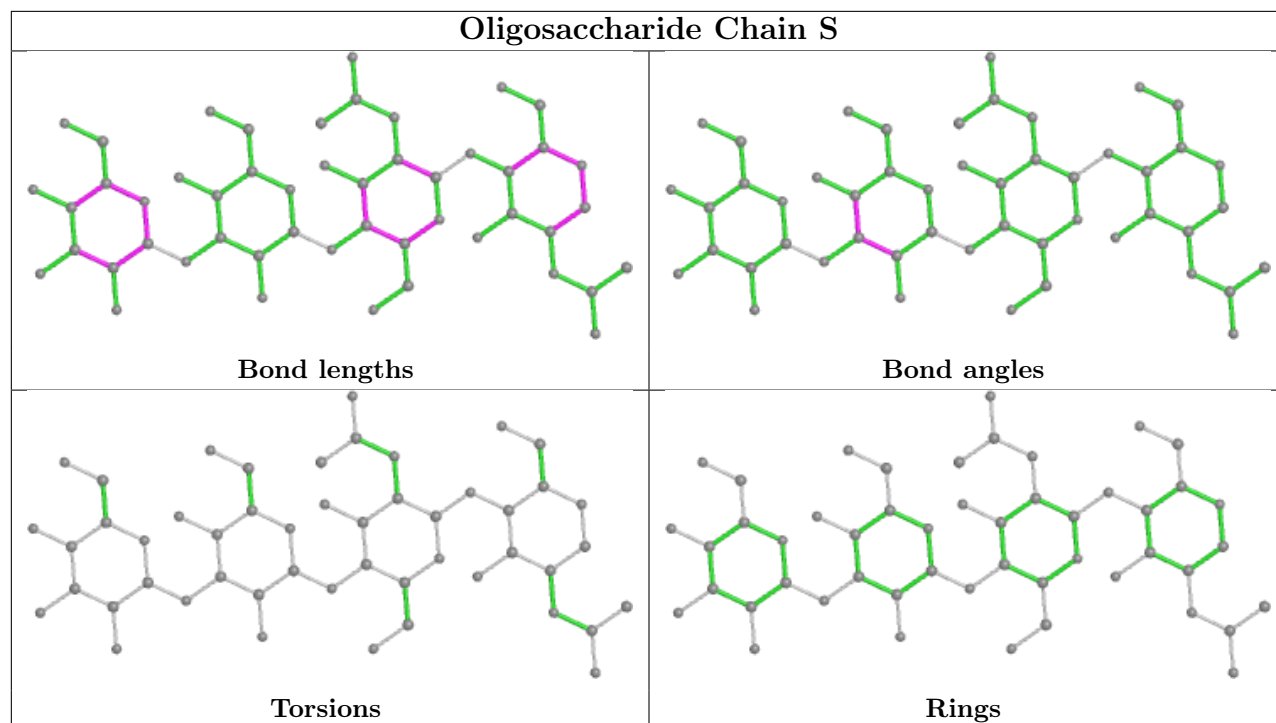




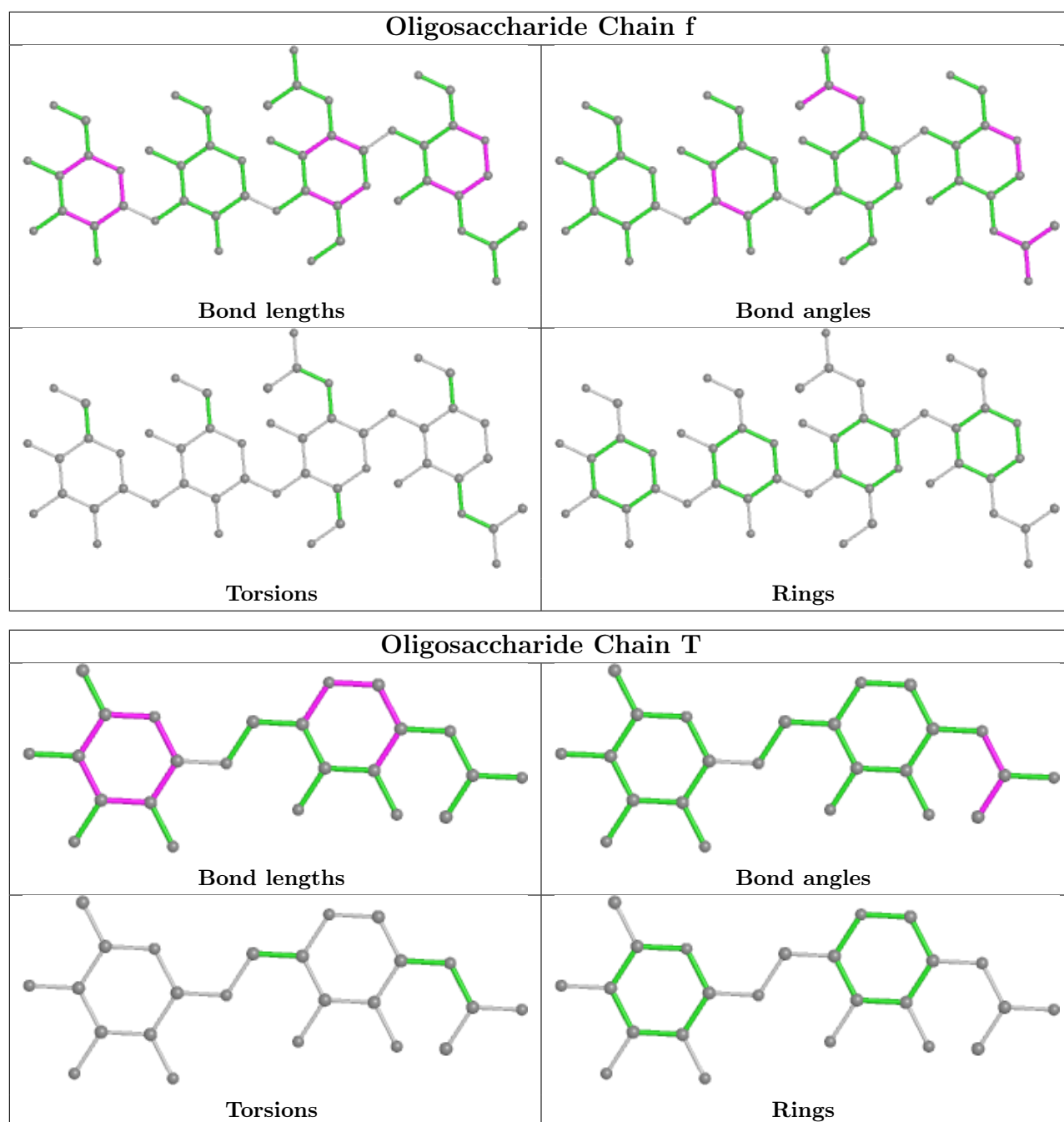


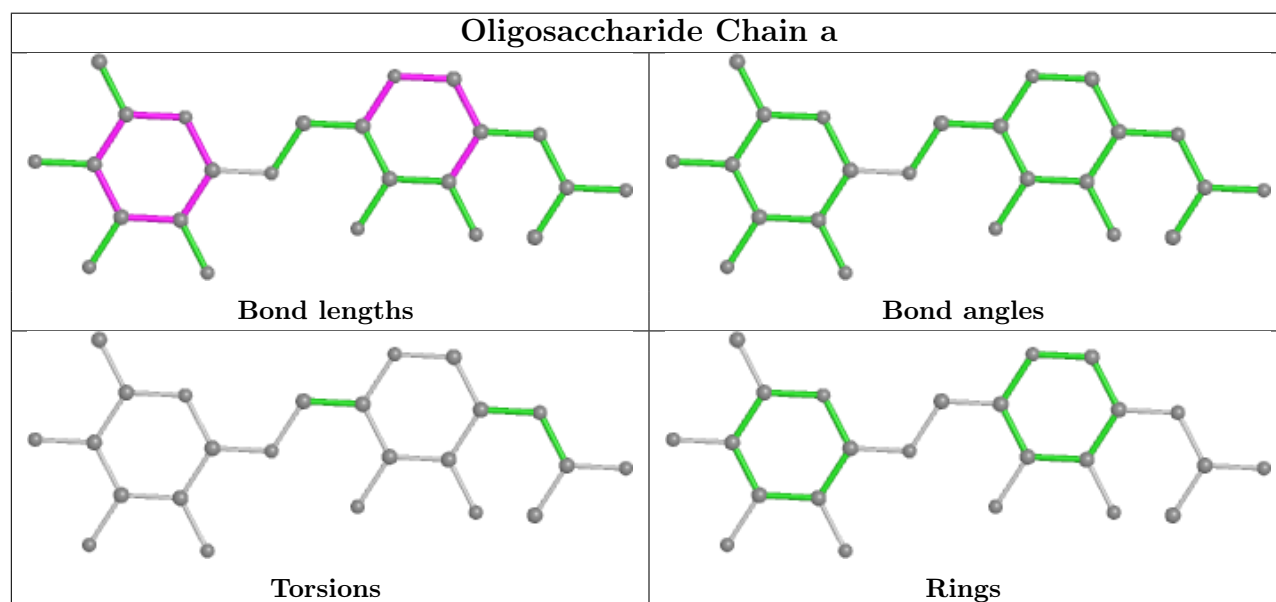
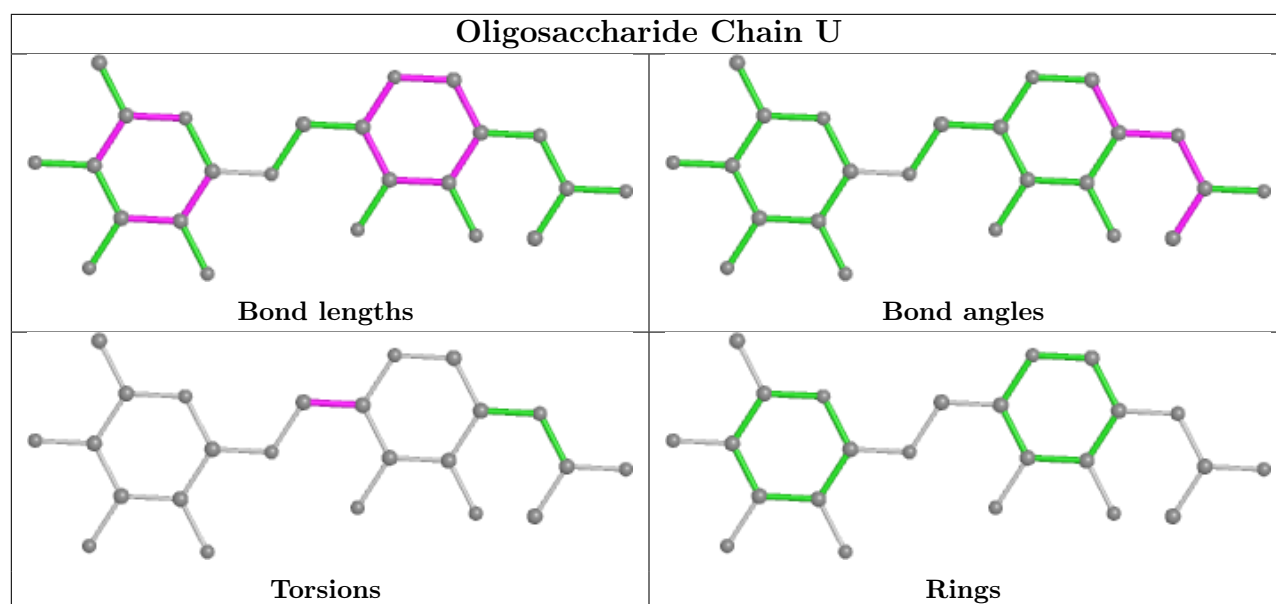


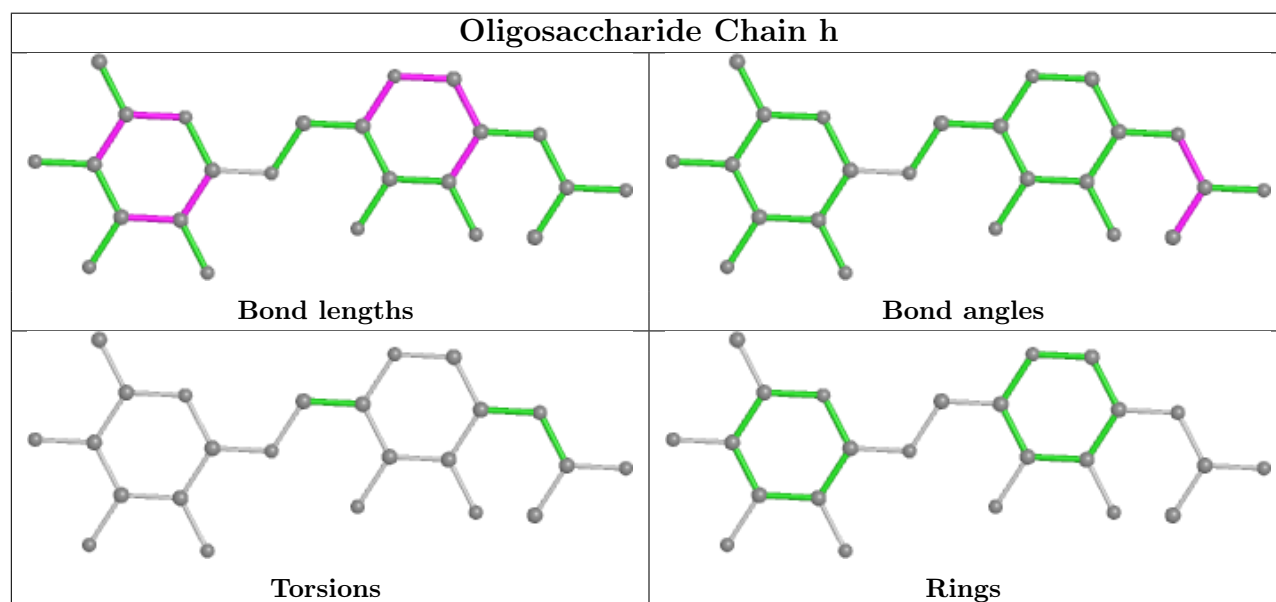
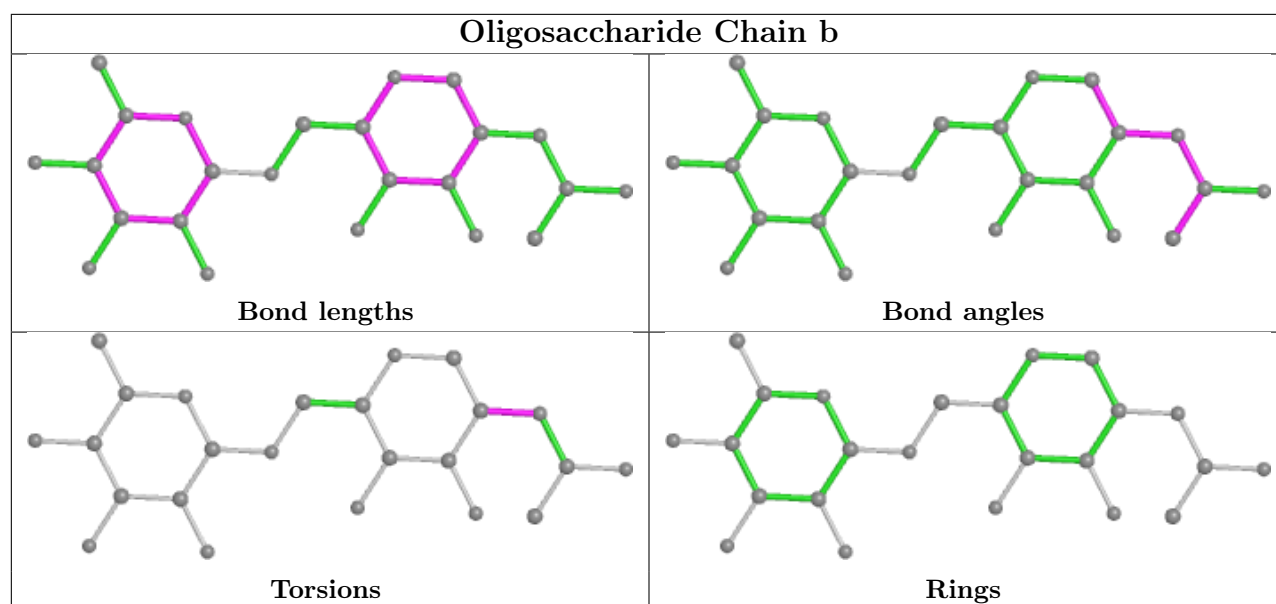


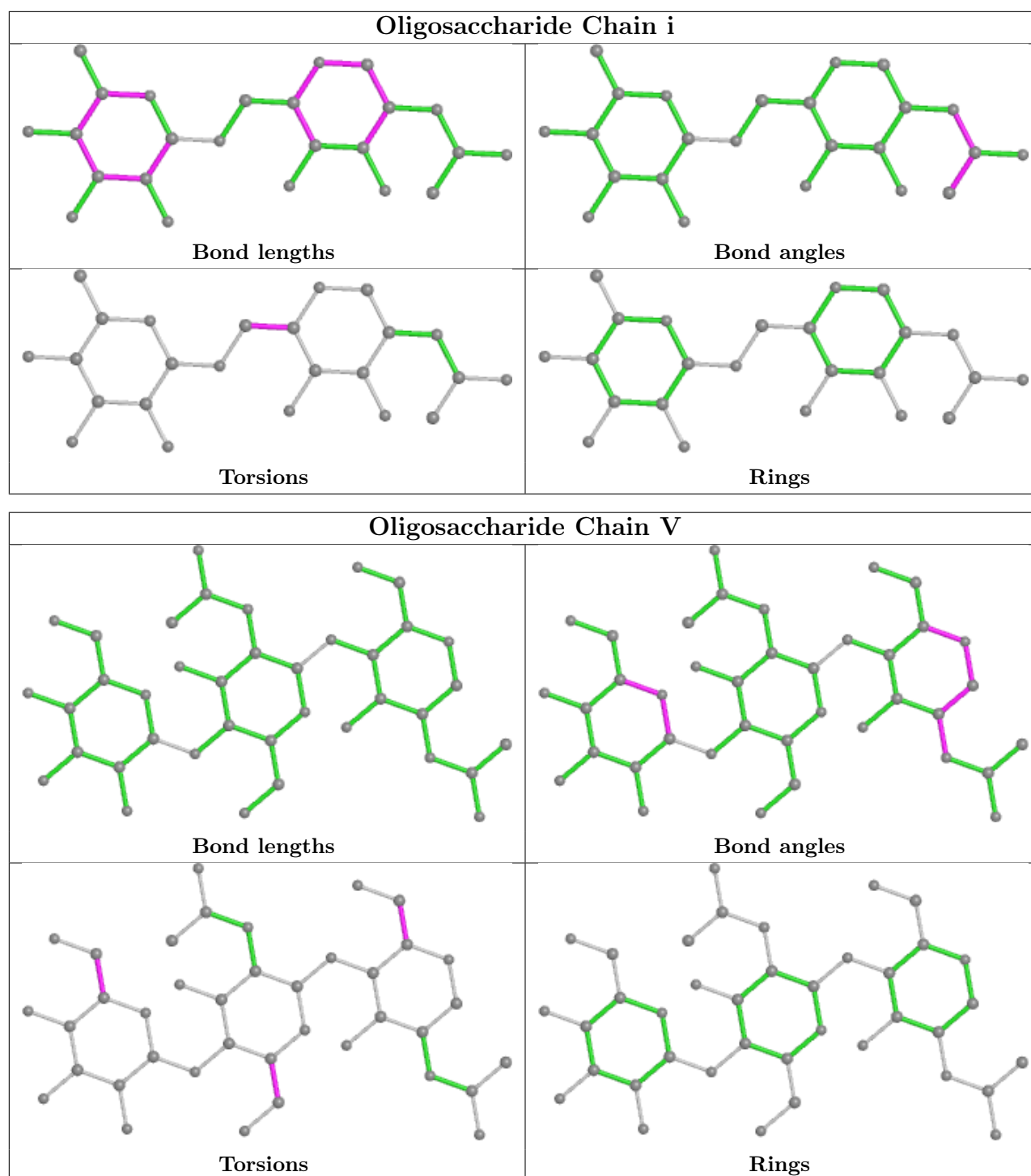












## 5.6 Ligand geometry [i](#)

42 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
12	NAG	D	701	2	14,14,15	2.06	5 (35%)	17,19,21	6.54	2 (11%)
12	NAG	A	602	1	14,14,15	2.01	5 (35%)	17,19,21	1.00	1 (5%)
12	NAG	A	601	1	14,14,15	1.92	5 (35%)	17,19,21	1.25	2 (11%)
12	NAG	A	603	1	14,14,15	2.08	6 (42%)	17,19,21	1.03	1 (5%)
12	NAG	B	701	2	14,14,15	2.11	5 (35%)	17,19,21	6.58	4 (23%)
12	NAG	F	702	2	14,14,15	0.29	0	17,19,21	0.75	0
12	NAG	D	702	2	14,14,15	1.97	5 (35%)	17,19,21	1.07	1 (5%)
12	NAG	C	611	1	14,14,15	1.96	5 (35%)	17,19,21	1.18	2 (11%)
12	NAG	E	604	1	14,14,15	2.14	5 (35%)	17,19,21	0.95	1 (5%)
12	NAG	C	603	1	14,14,15	2.10	5 (35%)	17,19,21	1.02	1 (5%)
12	NAG	C	610	1	14,14,15	2.12	5 (35%)	17,19,21	0.93	0
12	NAG	A	605	1	14,14,15	1.95	5 (35%)	17,19,21	1.09	2 (11%)
12	NAG	A	611	1	14,14,15	1.89	5 (35%)	17,19,21	1.12	1 (5%)
12	NAG	C	602	1	14,14,15	1.99	6 (42%)	17,19,21	1.05	1 (5%)
12	NAG	E	605	1	14,14,15	1.96	6 (42%)	17,19,21	1.10	2 (11%)
12	NAG	E	606	1	14,14,15	1.99	5 (35%)	17,19,21	1.07	1 (5%)
12	NAG	C	605	1	14,14,15	1.92	5 (35%)	17,19,21	1.01	1 (5%)
12	NAG	C	609	1	14,14,15	2.01	5 (35%)	17,19,21	1.06	1 (5%)
12	NAG	F	701	2	14,14,15	2.19	6 (42%)	17,19,21	1.08	2 (11%)
12	NAG	A	609	1	14,14,15	1.99	5 (35%)	17,19,21	1.08	1 (5%)
12	NAG	A	604	1	14,14,15	2.13	5 (35%)	17,19,21	0.97	1 (5%)
12	NAG	E	611	1	14,14,15	2.01	5 (35%)	17,19,21	1.18	2 (11%)
12	NAG	E	602	1	14,14,15	2.02	6 (42%)	17,19,21	1.00	1 (5%)
12	NAG	C	607	1	14,14,15	2.12	6 (42%)	17,19,21	1.00	1 (5%)
12	NAG	C	612	1	14,14,15	2.09	4 (28%)	17,19,21	0.95	1 (5%)
12	NAG	A	608	1	14,14,15	1.99	5 (35%)	17,19,21	0.99	1 (5%)
12	NAG	C	601	1	14,14,15	1.96	6 (42%)	17,19,21	1.03	1 (5%)
12	NAG	A	612	1	14,14,15	2.07	5 (35%)	17,19,21	0.98	1 (5%)
12	NAG	E	609	1	14,14,15	1.92	4 (28%)	17,19,21	1.01	0
12	NAG	E	612	1	14,14,15	2.07	5 (35%)	17,19,21	0.95	1 (5%)
12	NAG	E	608	1	14,14,15	1.90	7 (50%)	17,19,21	1.00	1 (5%)
12	NAG	E	603	1	14,14,15	2.13	5 (35%)	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	NAG	C	604	1	14,14,15	2.17	5 (35%)	17,19,21	0.97	1 (5%)
12	NAG	B	702	2	14,14,15	2.00	5 (35%)	17,19,21	0.98	1 (5%)
12	NAG	A	606	1	14,14,15	2.11	6 (42%)	17,19,21	1.07	1 (5%)
12	NAG	A	610	1	14,14,15	2.05	5 (35%)	17,19,21	0.96	1 (5%)
12	NAG	C	608	1	14,14,15	1.95	7 (50%)	17,19,21	0.98	1 (5%)
12	NAG	C	606	1	14,14,15	2.19	7 (50%)	17,19,21	1.09	1 (5%)
12	NAG	E	607	1	14,14,15	2.14	7 (50%)	17,19,21	1.11	2 (11%)
12	NAG	E	610	1	14,14,15	2.03	5 (35%)	17,19,21	0.86	0
12	NAG	A	607	1	14,14,15	2.08	5 (35%)	17,19,21	1.04	2 (11%)
12	NAG	E	601	1	14,14,15	1.96	6 (42%)	17,19,21	1.09	3 (17%)

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
12	NAG	D	701	2	-	1/6/23/26	0/1/1/1
12	NAG	A	602	1	-	1/6/23/26	0/1/1/1
12	NAG	A	601	1	-	0/6/23/26	0/1/1/1
12	NAG	A	603	1	-	0/6/23/26	0/1/1/1
12	NAG	B	701	2	-	2/6/23/26	0/1/1/1
12	NAG	F	702	2	-	3/6/23/26	0/1/1/1
12	NAG	D	702	2	-	0/6/23/26	0/1/1/1
12	NAG	C	611	1	-	0/6/23/26	0/1/1/1
12	NAG	E	604	1	-	0/6/23/26	0/1/1/1
12	NAG	C	603	1	-	0/6/23/26	0/1/1/1
12	NAG	C	610	1	-	0/6/23/26	0/1/1/1
12	NAG	A	605	1	-	2/6/23/26	0/1/1/1
12	NAG	A	611	1	-	0/6/23/26	0/1/1/1
12	NAG	C	602	1	-	1/6/23/26	0/1/1/1
12	NAG	E	605	1	-	2/6/23/26	0/1/1/1
12	NAG	E	606	1	-	0/6/23/26	0/1/1/1
12	NAG	C	605	1	-	0/6/23/26	0/1/1/1
12	NAG	C	609	1	-	1/6/23/26	0/1/1/1
12	NAG	F	701	2	-	1/6/23/26	0/1/1/1
12	NAG	A	609	1	-	1/6/23/26	0/1/1/1
12	NAG	A	604	1	-	0/6/23/26	0/1/1/1
12	NAG	E	611	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	E	602	1	-	1/6/23/26	0/1/1/1
12	NAG	C	607	1	-	2/6/23/26	0/1/1/1
12	NAG	C	612	1	-	0/6/23/26	0/1/1/1
12	NAG	A	608	1	-	1/6/23/26	0/1/1/1
12	NAG	C	601	1	-	0/6/23/26	0/1/1/1
12	NAG	A	612	1	-	1/6/23/26	0/1/1/1
12	NAG	E	609	1	-	1/6/23/26	0/1/1/1
12	NAG	E	612	1	-	0/6/23/26	0/1/1/1
12	NAG	E	608	1	-	0/6/23/26	0/1/1/1
12	NAG	E	603	1	-	0/6/23/26	0/1/1/1
12	NAG	C	604	1	-	0/6/23/26	0/1/1/1
12	NAG	B	702	2	-	0/6/23/26	0/1/1/1
12	NAG	A	606	1	-	0/6/23/26	0/1/1/1
12	NAG	A	610	1	-	1/6/23/26	0/1/1/1
12	NAG	C	608	1	-	0/6/23/26	0/1/1/1
12	NAG	C	606	1	-	1/6/23/26	0/1/1/1
12	NAG	E	607	1	-	1/6/23/26	0/1/1/1
12	NAG	E	610	1	-	1/6/23/26	0/1/1/1
12	NAG	A	607	1	-	1/6/23/26	0/1/1/1
12	NAG	E	601	1	-	0/6/23/26	0/1/1/1

All (220) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	604	NAG	C1-C2	5.57	1.60	1.52
12	E	604	NAG	C1-C2	5.53	1.60	1.52
12	F	701	NAG	C1-C2	5.38	1.60	1.52
12	C	606	NAG	C1-C2	5.37	1.60	1.52
12	B	701	NAG	C1-C2	5.36	1.60	1.52
12	C	612	NAG	C1-C2	5.35	1.60	1.52
12	C	610	NAG	C1-C2	5.26	1.60	1.52
12	A	606	NAG	C1-C2	5.14	1.60	1.52
12	E	610	NAG	C1-C2	5.08	1.59	1.52
12	A	602	NAG	C1-C2	5.08	1.59	1.52
12	E	612	NAG	C1-C2	5.08	1.59	1.52
12	E	603	NAG	C1-C2	5.07	1.59	1.52
12	C	603	NAG	C1-C2	5.06	1.59	1.52
12	A	610	NAG	C1-C2	5.01	1.59	1.52
12	D	701	NAG	C1-C2	5.00	1.59	1.52
12	A	612	NAG	C1-C2	5.00	1.59	1.52
12	E	605	NAG	C1-C2	4.99	1.59	1.52
12	A	604	NAG	C1-C2	4.97	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	609	NAG	C1-C2	4.94	1.59	1.52
12	E	602	NAG	C1-C2	4.93	1.59	1.52
12	C	608	NAG	C1-C2	4.90	1.59	1.52
12	A	609	NAG	C1-C2	4.90	1.59	1.52
12	A	603	NAG	C1-C2	4.87	1.59	1.52
12	A	605	NAG	C1-C2	4.86	1.59	1.52
12	E	611	NAG	C1-C2	4.83	1.59	1.52
12	B	702	NAG	C1-C2	4.80	1.59	1.52
12	C	607	NAG	C1-C2	4.79	1.59	1.52
12	A	607	NAG	C1-C2	4.78	1.59	1.52
12	E	606	NAG	C1-C2	4.75	1.59	1.52
12	D	702	NAG	C1-C2	4.73	1.59	1.52
12	A	608	NAG	C1-C2	4.72	1.59	1.52
12	C	611	NAG	C1-C2	4.71	1.59	1.52
12	E	607	NAG	C1-C2	4.67	1.59	1.52
12	E	609	NAG	C1-C2	4.66	1.59	1.52
12	A	611	NAG	C1-C2	4.56	1.59	1.52
12	C	605	NAG	C1-C2	4.52	1.59	1.52
12	C	602	NAG	C1-C2	4.50	1.59	1.52
12	E	608	NAG	C1-C2	4.47	1.59	1.52
12	C	601	NAG	C1-C2	4.43	1.59	1.52
12	E	601	NAG	C1-C2	4.40	1.58	1.52
12	A	601	NAG	C1-C2	4.31	1.58	1.52
12	E	607	NAG	O5-C5	3.34	1.50	1.43
12	C	607	NAG	O5-C5	3.33	1.50	1.43
12	C	610	NAG	O5-C5	3.28	1.50	1.43
12	A	604	NAG	O5-C5	3.28	1.50	1.43
12	A	607	NAG	O5-C5	3.27	1.50	1.43
12	B	701	NAG	O5-C5	3.24	1.50	1.43
12	E	603	NAG	O5-C5	3.23	1.50	1.43
12	E	601	NAG	O5-C5	3.22	1.50	1.43
12	D	701	NAG	O5-C5	3.21	1.49	1.43
12	A	612	NAG	O5-C5	3.19	1.49	1.43
12	E	612	NAG	O5-C5	3.15	1.49	1.43
12	C	609	NAG	O5-C5	3.13	1.49	1.43
12	A	603	NAG	O5-C5	3.12	1.49	1.43
12	A	601	NAG	O5-C5	3.12	1.49	1.43
12	C	603	NAG	O5-C5	3.11	1.49	1.43
12	A	606	NAG	O5-C5	3.11	1.49	1.43
12	A	608	NAG	O5-C5	3.08	1.49	1.43
12	C	601	NAG	O5-C5	3.07	1.49	1.43
12	C	606	NAG	O5-C5	3.06	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	609	NAG	O5-C5	3.06	1.49	1.43
12	F	701	NAG	O5-C5	3.05	1.49	1.43
12	A	610	NAG	O5-C5	3.05	1.49	1.43
12	E	611	NAG	O5-C5	3.04	1.49	1.43
12	C	607	NAG	O5-C1	3.04	1.48	1.43
12	C	612	NAG	O5-C5	3.03	1.49	1.43
12	E	610	NAG	O5-C5	3.03	1.49	1.43
12	C	604	NAG	O5-C5	3.03	1.49	1.43
12	E	606	NAG	O5-C5	3.02	1.49	1.43
12	E	604	NAG	O5-C5	2.99	1.49	1.43
12	A	609	NAG	O5-C5	2.98	1.49	1.43
12	A	604	NAG	O5-C1	2.98	1.48	1.43
12	C	611	NAG	O5-C5	2.96	1.49	1.43
12	E	607	NAG	O5-C1	2.94	1.48	1.43
12	C	605	NAG	O5-C5	2.91	1.49	1.43
12	F	701	NAG	O5-C1	2.90	1.48	1.43
12	B	701	NAG	O5-C1	2.90	1.48	1.43
12	C	606	NAG	O5-C1	2.87	1.48	1.43
12	C	602	NAG	O5-C5	2.87	1.49	1.43
12	D	702	NAG	O5-C5	2.86	1.49	1.43
12	B	702	NAG	O5-C5	2.85	1.49	1.43
12	E	602	NAG	O5-C5	2.78	1.49	1.43
12	A	605	NAG	O5-C5	2.78	1.49	1.43
12	D	701	NAG	O5-C1	2.77	1.48	1.43
12	A	607	NAG	O5-C1	2.76	1.48	1.43
12	A	606	NAG	O5-C1	2.75	1.48	1.43
12	A	602	NAG	O5-C5	2.75	1.49	1.43
12	A	611	NAG	O5-C5	2.75	1.49	1.43
12	A	608	NAG	O5-C1	2.74	1.48	1.43
12	C	609	NAG	O5-C1	2.74	1.48	1.43
12	A	601	NAG	O5-C1	2.74	1.48	1.43
12	C	604	NAG	O5-C1	2.73	1.48	1.43
12	E	603	NAG	O5-C1	2.72	1.48	1.43
12	C	601	NAG	O5-C1	2.71	1.48	1.43
12	C	603	NAG	O5-C1	2.68	1.48	1.43
12	E	604	NAG	O5-C1	2.68	1.48	1.43
12	A	603	NAG	O5-C1	2.68	1.48	1.43
12	A	610	NAG	O5-C1	2.64	1.47	1.43
12	C	610	NAG	O5-C1	2.64	1.47	1.43
12	E	601	NAG	O5-C1	2.63	1.47	1.43
12	E	608	NAG	O5-C5	2.63	1.48	1.43
12	E	611	NAG	O5-C1	2.61	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	609	NAG	O5-C1	2.60	1.47	1.43
12	A	609	NAG	O5-C1	2.59	1.47	1.43
12	E	610	NAG	O5-C1	2.58	1.47	1.43
12	B	702	NAG	O5-C1	2.57	1.47	1.43
12	A	612	NAG	O5-C1	2.57	1.47	1.43
12	E	612	NAG	O5-C1	2.55	1.47	1.43
12	C	605	NAG	O5-C1	2.54	1.47	1.43
12	C	608	NAG	O5-C5	2.51	1.48	1.43
12	E	606	NAG	O5-C1	2.51	1.47	1.43
12	C	602	NAG	O5-C1	2.50	1.47	1.43
12	E	603	NAG	C3-C2	2.50	1.57	1.52
12	C	612	NAG	O5-C1	2.50	1.47	1.43
12	C	611	NAG	O5-C1	2.50	1.47	1.43
12	C	602	NAG	C3-C2	2.49	1.57	1.52
12	E	605	NAG	O5-C5	2.45	1.48	1.43
12	D	702	NAG	O5-C1	2.45	1.47	1.43
12	E	607	NAG	C2-N2	2.44	1.50	1.46
12	E	602	NAG	O5-C1	2.44	1.47	1.43
12	C	603	NAG	C3-C2	2.41	1.57	1.52
12	A	603	NAG	C3-C2	2.41	1.57	1.52
12	F	701	NAG	C3-C2	2.40	1.57	1.52
12	C	610	NAG	C3-C2	2.40	1.57	1.52
12	D	701	NAG	C3-C2	2.40	1.57	1.52
12	E	607	NAG	C4-C5	2.37	1.58	1.53
12	E	612	NAG	C3-C2	2.35	1.57	1.52
12	A	611	NAG	O5-C1	2.34	1.47	1.43
12	C	607	NAG	C4-C5	2.34	1.58	1.53
12	A	605	NAG	C3-C2	2.33	1.57	1.52
12	C	612	NAG	C3-C2	2.33	1.57	1.52
12	C	602	NAG	C4-C5	2.32	1.57	1.53
12	E	610	NAG	C3-C2	2.32	1.57	1.52
12	A	602	NAG	O5-C1	2.32	1.47	1.43
12	C	606	NAG	C2-N2	2.32	1.50	1.46
12	A	607	NAG	C4-C5	2.32	1.57	1.53
12	E	602	NAG	C3-C2	2.30	1.57	1.52
12	A	602	NAG	C3-C2	2.30	1.57	1.52
12	F	701	NAG	C4-C5	2.30	1.57	1.53
12	C	601	NAG	C3-C2	2.29	1.57	1.52
12	A	604	NAG	C4-C5	2.28	1.57	1.53
12	C	604	NAG	C3-C2	2.26	1.57	1.52
12	A	612	NAG	C3-C2	2.26	1.57	1.52
12	B	701	NAG	C3-C2	2.26	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	608	NAG	C3-C2	2.26	1.57	1.52
12	C	605	NAG	C3-C2	2.26	1.57	1.52
12	C	604	NAG	C4-C5	2.23	1.57	1.53
12	D	702	NAG	C3-C2	2.23	1.57	1.52
12	D	701	NAG	C4-C5	2.22	1.57	1.53
12	B	702	NAG	C3-C2	2.21	1.57	1.52
12	E	604	NAG	C3-C2	2.21	1.57	1.52
12	A	603	NAG	C4-C5	2.21	1.57	1.53
12	C	606	NAG	C3-C2	2.19	1.57	1.52
12	C	606	NAG	C4-C5	2.19	1.57	1.53
12	E	607	NAG	C3-C2	2.19	1.57	1.52
12	E	606	NAG	C4-C5	2.19	1.57	1.53
12	E	605	NAG	C4-C5	2.19	1.57	1.53
12	E	601	NAG	C4-C5	2.18	1.57	1.53
12	A	609	NAG	C4-C5	2.18	1.57	1.53
12	A	610	NAG	C3-C2	2.18	1.57	1.52
12	E	605	NAG	C3-C2	2.18	1.57	1.52
12	E	608	NAG	O5-C1	2.17	1.47	1.43
12	E	608	NAG	C3-C2	2.17	1.57	1.52
12	A	604	NAG	C3-C2	2.17	1.57	1.52
12	E	607	NAG	C4-C3	2.17	1.57	1.52
12	E	603	NAG	C4-C5	2.17	1.57	1.53
12	C	603	NAG	C4-C5	2.17	1.57	1.53
12	A	606	NAG	C3-C2	2.16	1.57	1.52
12	A	605	NAG	O5-C1	2.16	1.47	1.43
12	A	606	NAG	C4-C5	2.16	1.57	1.53
12	E	611	NAG	C3-C2	2.15	1.57	1.52
12	A	610	NAG	C4-C5	2.15	1.57	1.53
12	C	601	NAG	C4-C5	2.15	1.57	1.53
12	B	701	NAG	C4-C5	2.15	1.57	1.53
12	A	612	NAG	C4-C5	2.15	1.57	1.53
12	C	609	NAG	C4-C5	2.14	1.57	1.53
12	B	702	NAG	C4-C5	2.14	1.57	1.53
12	C	607	NAG	C3-C2	2.14	1.57	1.52
12	E	602	NAG	C4-C5	2.13	1.57	1.53
12	A	607	NAG	C3-C2	2.13	1.57	1.52
12	E	612	NAG	C4-C5	2.12	1.57	1.53
12	A	611	NAG	C4-C5	2.12	1.57	1.53
12	E	605	NAG	O5-C1	2.12	1.47	1.43
12	C	610	NAG	C4-C5	2.11	1.57	1.53
12	E	602	NAG	C2-N2	2.11	1.49	1.46
12	E	608	NAG	C4-C3	2.10	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	609	NAG	C4-C5	2.10	1.57	1.53
12	E	606	NAG	C3-C2	2.10	1.57	1.52
12	E	608	NAG	C2-N2	2.10	1.49	1.46
12	E	601	NAG	C4-C3	2.09	1.57	1.52
12	E	610	NAG	C4-C5	2.09	1.57	1.53
12	A	611	NAG	C3-C2	2.09	1.56	1.52
12	C	609	NAG	C3-C2	2.09	1.56	1.52
12	C	601	NAG	C4-C3	2.08	1.57	1.52
12	E	608	NAG	C4-C5	2.08	1.57	1.53
12	A	605	NAG	C4-C5	2.08	1.57	1.53
12	E	601	NAG	C3-C2	2.08	1.56	1.52
12	A	602	NAG	C4-C5	2.08	1.57	1.53
12	A	601	NAG	C3-C2	2.08	1.56	1.52
12	E	611	NAG	C4-C5	2.07	1.57	1.53
12	A	601	NAG	C4-C5	2.07	1.57	1.53
12	C	608	NAG	C4-C5	2.06	1.57	1.53
12	C	611	NAG	C4-C5	2.06	1.57	1.53
12	C	608	NAG	C4-C3	2.06	1.57	1.52
12	F	701	NAG	C4-C3	2.06	1.57	1.52
12	E	604	NAG	C4-C5	2.05	1.57	1.53
12	C	602	NAG	C4-C3	2.05	1.57	1.52
12	C	607	NAG	C2-N2	2.04	1.49	1.46
12	A	606	NAG	C2-N2	2.04	1.49	1.46
12	C	608	NAG	O5-C1	2.04	1.47	1.43
12	A	609	NAG	C3-C2	2.04	1.56	1.52
12	A	608	NAG	C4-C5	2.03	1.57	1.53
12	A	603	NAG	C2-N2	2.03	1.49	1.46
12	A	608	NAG	C3-C2	2.03	1.56	1.52
12	D	702	NAG	C4-C5	2.03	1.57	1.53
12	E	605	NAG	C4-C3	2.02	1.57	1.52
12	C	608	NAG	C2-N2	2.01	1.49	1.46
12	C	605	NAG	C4-C5	2.01	1.57	1.53
12	C	606	NAG	C4-C3	2.00	1.57	1.52
12	C	611	NAG	C3-C2	2.00	1.56	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	701	NAG	C2-N2-C7	26.70	160.92	122.90
12	D	701	NAG	C2-N2-C7	26.63	160.82	122.90
12	A	601	NAG	C8-C7-N2	3.38	121.82	116.10
12	E	607	NAG	C8-C7-N2	2.99	121.16	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	611	NAG	C8-C7-N2	2.82	120.88	116.10
12	A	606	NAG	C8-C7-N2	2.71	120.69	116.10
12	D	701	NAG	C8-C7-N2	2.71	120.68	116.10
12	E	602	NAG	C8-C7-N2	2.65	120.59	116.10
12	C	606	NAG	C8-C7-N2	2.64	120.58	116.10
12	A	602	NAG	C8-C7-N2	2.63	120.55	116.10
12	C	611	NAG	C8-C7-N2	2.62	120.54	116.10
12	A	601	NAG	O7-C7-C8	-2.59	117.25	122.06
12	A	611	NAG	C8-C7-N2	2.56	120.43	116.10
12	C	602	NAG	C8-C7-N2	2.55	120.42	116.10
12	C	607	NAG	C8-C7-N2	2.52	120.37	116.10
12	E	601	NAG	C8-C7-N2	2.51	120.35	116.10
12	A	607	NAG	C8-C7-N2	2.50	120.33	116.10
12	B	701	NAG	C8-C7-N2	2.40	120.17	116.10
12	E	605	NAG	C1-O5-C5	2.39	115.43	112.19
12	E	606	NAG	C8-C7-N2	2.38	120.13	116.10
12	E	608	NAG	C8-C7-N2	2.34	120.06	116.10
12	C	601	NAG	C8-C7-N2	2.33	120.05	116.10
12	A	605	NAG	C1-O5-C5	2.32	115.33	112.19
12	A	604	NAG	C8-C7-N2	2.32	120.03	116.10
12	D	702	NAG	C8-C7-N2	2.30	120.00	116.10
12	C	608	NAG	C8-C7-N2	2.26	119.93	116.10
12	A	610	NAG	C8-C7-N2	2.25	119.92	116.10
12	E	601	NAG	O7-C7-C8	-2.23	117.92	122.06
12	A	608	NAG	C8-C7-N2	2.20	119.82	116.10
12	E	607	NAG	O7-C7-C8	-2.18	118.00	122.06
12	C	603	NAG	C8-C7-N2	2.18	119.80	116.10
12	C	611	NAG	C1-O5-C5	2.18	115.15	112.19
12	E	605	NAG	C8-C7-N2	2.14	119.73	116.10
12	B	701	NAG	C1-O5-C5	2.12	115.06	112.19
12	A	612	NAG	C8-C7-N2	2.10	119.65	116.10
12	A	603	NAG	C8-C7-N2	2.08	119.63	116.10
12	F	701	NAG	C1-O5-C5	2.08	115.01	112.19
12	E	604	NAG	C8-C7-N2	2.08	119.62	116.10
12	B	702	NAG	C8-C7-N2	2.08	119.62	116.10
12	F	701	NAG	C8-C7-N2	2.08	119.61	116.10
12	B	701	NAG	O5-C1-C2	-2.07	108.02	111.29
12	E	603	NAG	C8-C7-N2	2.07	119.61	116.10
12	C	609	NAG	O5-C1-C2	-2.07	108.02	111.29
12	A	605	NAG	C8-C7-N2	2.06	119.58	116.10
12	A	607	NAG	O7-C7-C8	-2.04	118.27	122.06
12	A	609	NAG	C8-C7-N2	2.03	119.54	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	612	NAG	C8-C7-N2	2.03	119.54	116.10
12	C	605	NAG	C8-C7-N2	2.03	119.53	116.10
12	E	601	NAG	C1-C2-N2	-2.02	107.04	110.49
12	C	604	NAG	C8-C7-N2	2.02	119.51	116.10
12	E	611	NAG	O7-C7-C8	-2.02	118.31	122.06
12	C	612	NAG	C8-C7-N2	2.01	119.49	116.10

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	F	702	NAG	C8-C7-N2-C2
12	F	702	NAG	O7-C7-N2-C2
12	B	701	NAG	C1-C2-N2-C7
12	C	607	NAG	O5-C5-C6-O6
12	E	607	NAG	O5-C5-C6-O6
12	E	610	NAG	O5-C5-C6-O6
12	A	607	NAG	O5-C5-C6-O6
12	A	605	NAG	C4-C5-C6-O6
12	C	609	NAG	O5-C5-C6-O6
12	A	608	NAG	O5-C5-C6-O6
12	E	602	NAG	O5-C5-C6-O6
12	C	602	NAG	O5-C5-C6-O6
12	E	605	NAG	C4-C5-C6-O6
12	A	610	NAG	O5-C5-C6-O6
12	A	602	NAG	O5-C5-C6-O6
12	E	609	NAG	O5-C5-C6-O6
12	F	702	NAG	O5-C5-C6-O6
12	C	606	NAG	O5-C5-C6-O6
12	A	609	NAG	O5-C5-C6-O6
12	F	701	NAG	O5-C5-C6-O6
12	A	605	NAG	O5-C5-C6-O6
12	E	605	NAG	O5-C5-C6-O6
12	C	607	NAG	C4-C5-C6-O6
12	A	612	NAG	C4-C5-C6-O6
12	B	701	NAG	C3-C2-N2-C7
12	D	701	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	601	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.



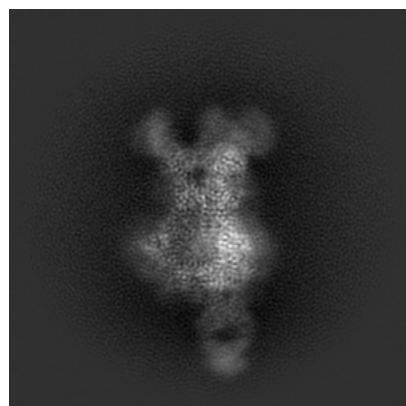
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25733. These allow visual inspection of the internal detail of the map and identification of artifacts.

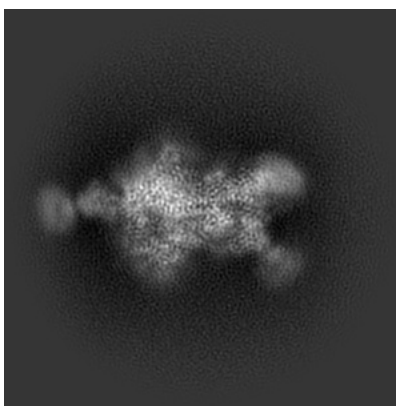
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

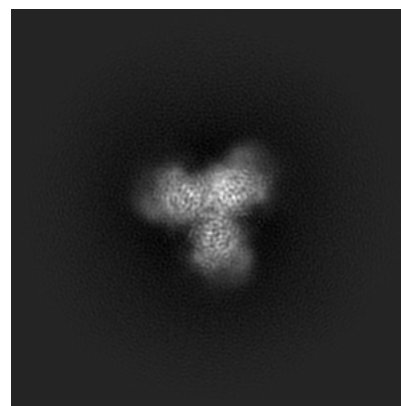
#### 6.1.1 Primary map



X

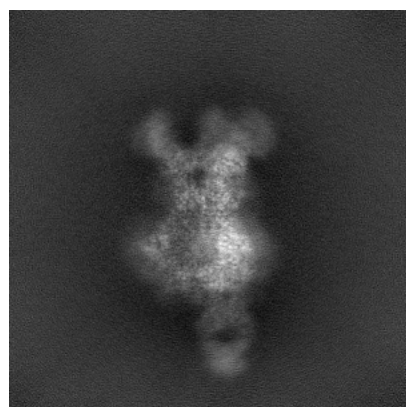


Y

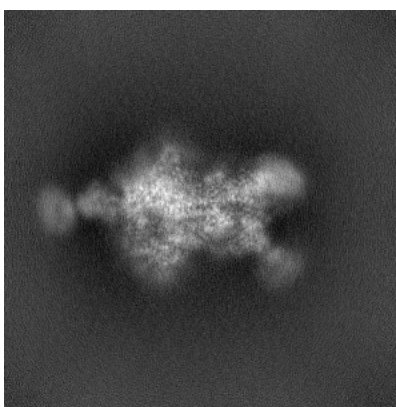


Z

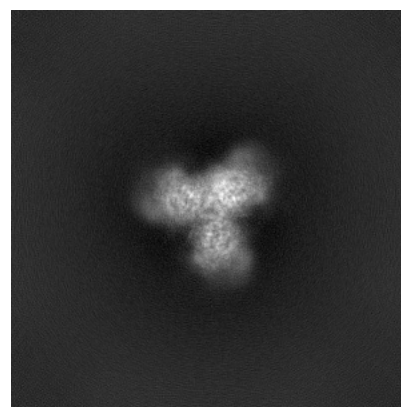
#### 6.1.2 Raw map



X



Y



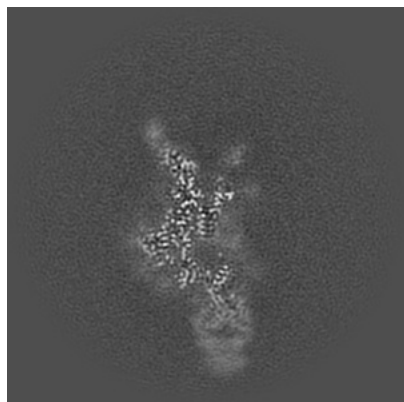
Z

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

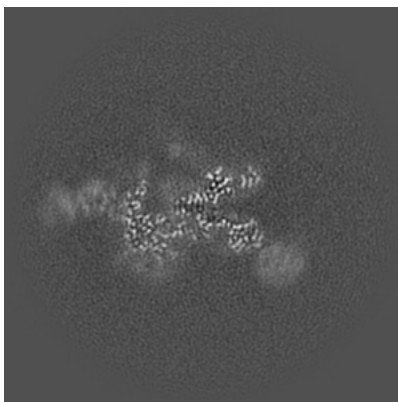


## 6.2 Central slices [i](#)

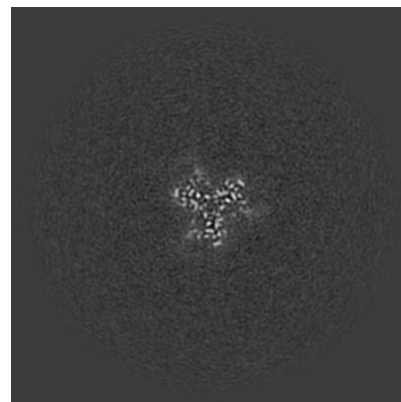
### 6.2.1 Primary map



X Index: 175

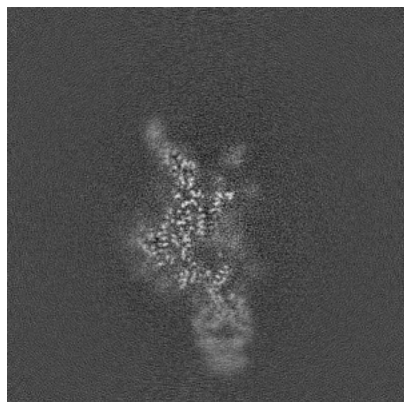


Y Index: 175

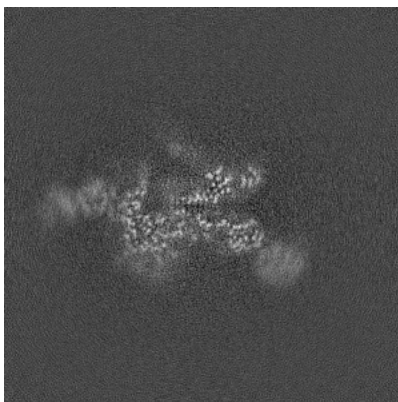


Z Index: 175

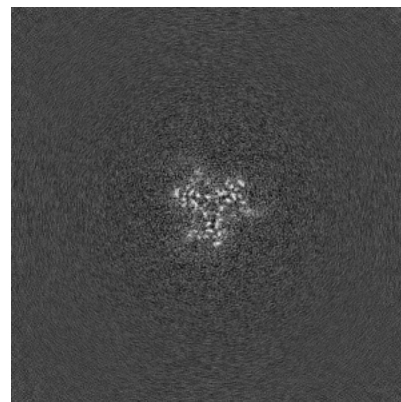
### 6.2.2 Raw map



X Index: 175



Y Index: 175

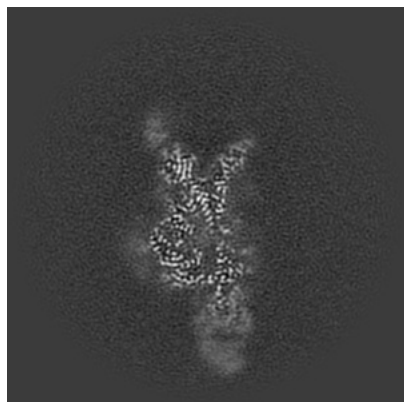


Z Index: 175

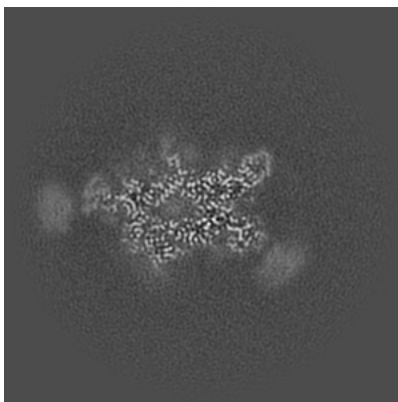
The images above show central slices of the map in three orthogonal directions.

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

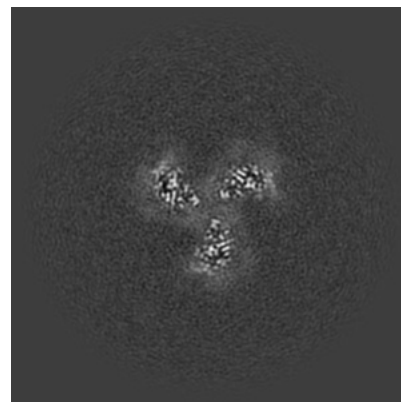
### 6.3.1 Primary map



X Index: 183

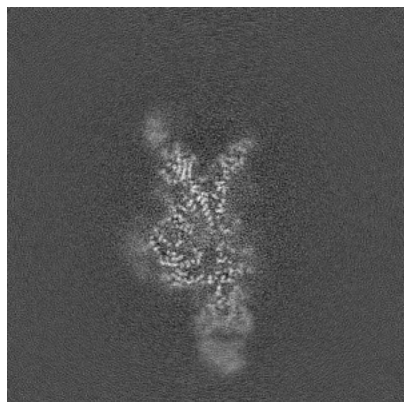


Y Index: 185

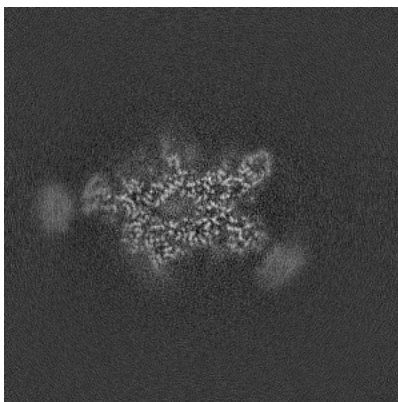


Z Index: 142

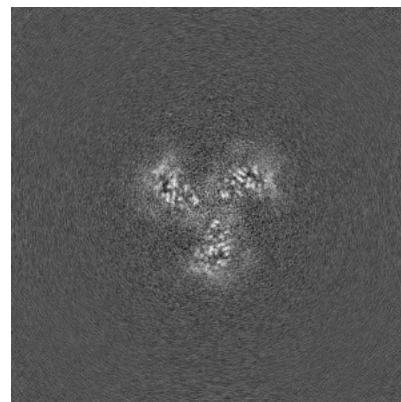
### 6.3.2 Raw map



X Index: 183



Y Index: 185

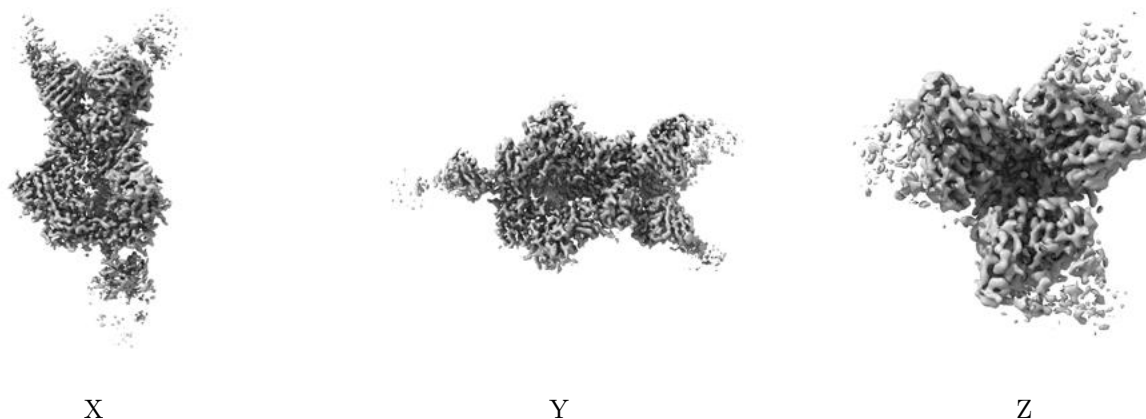


Z Index: 142

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

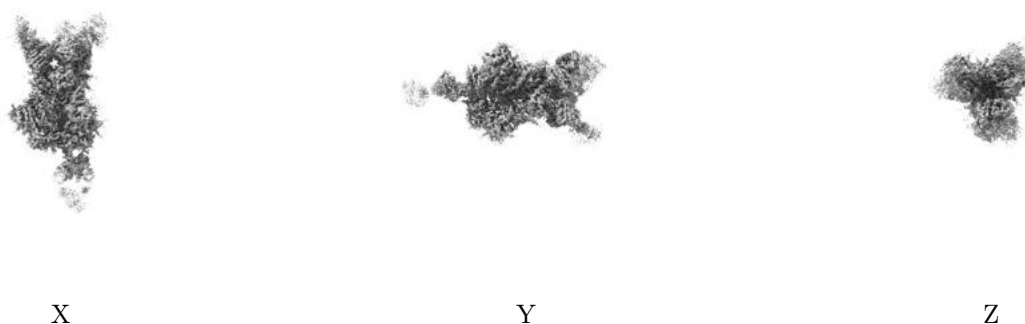
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

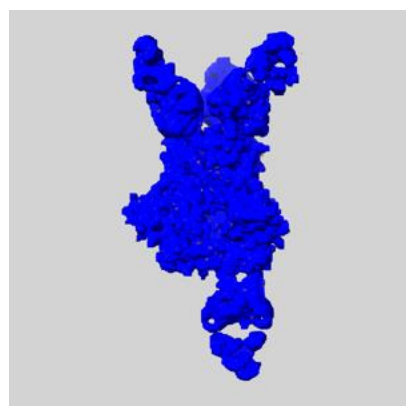
## 6.5 Mask visualisation [i](#)

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

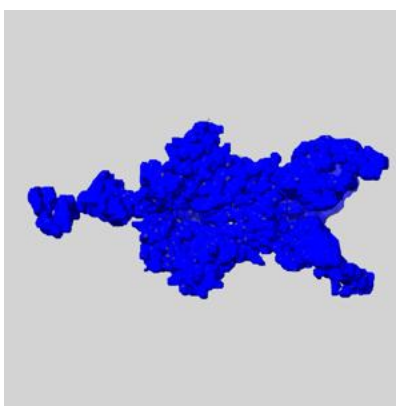
A mask typically either:

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

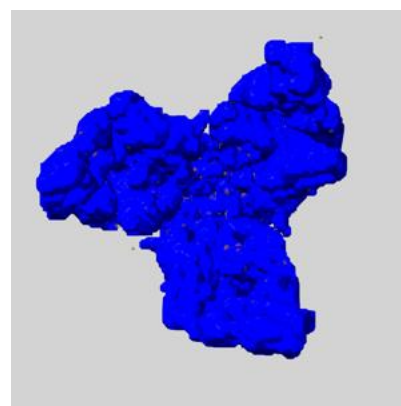
### 6.5.1 emd\_25733\_msk\_1.map [i](#)



X



Y

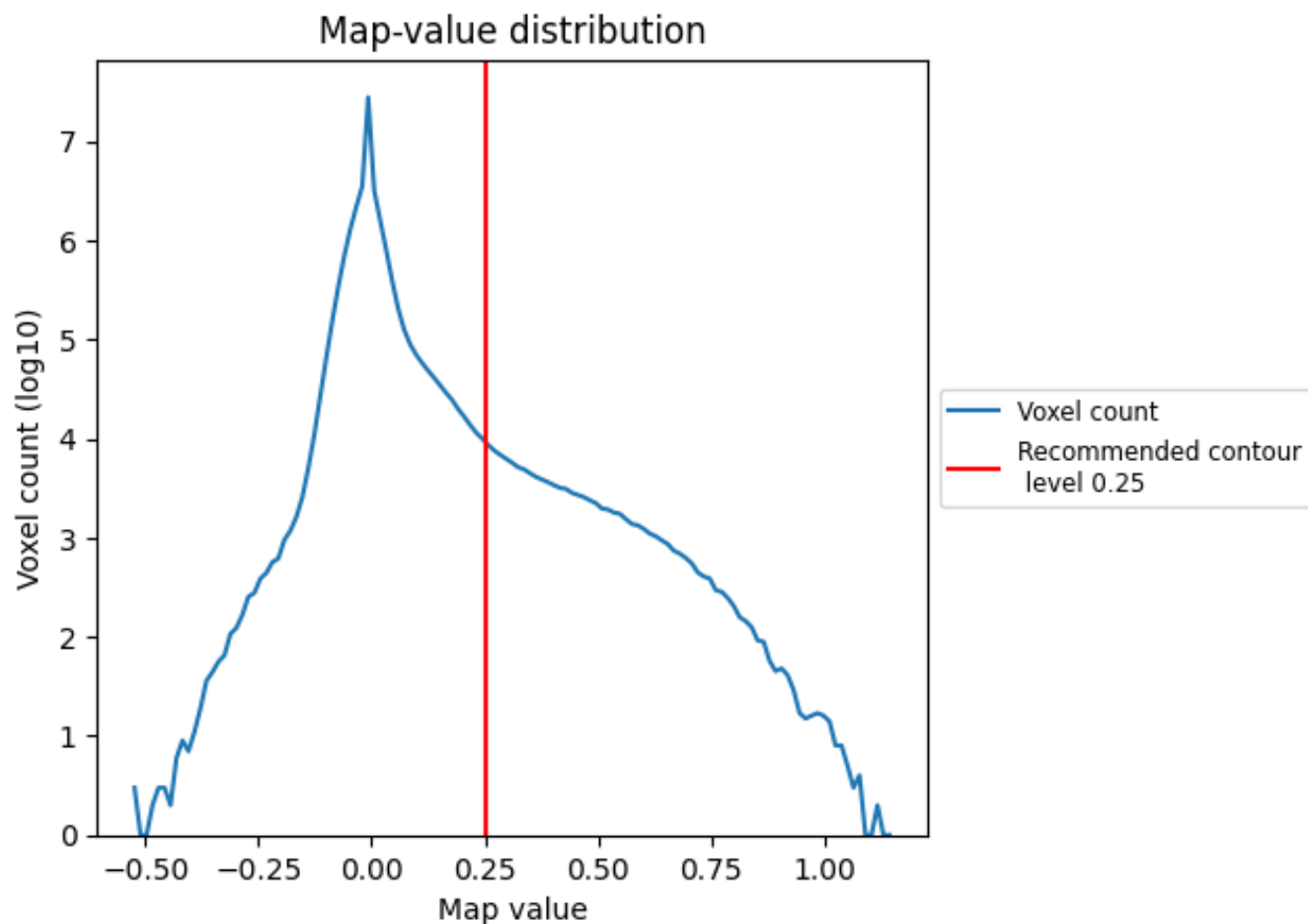


Z

## 7 Map analysis [i](#)

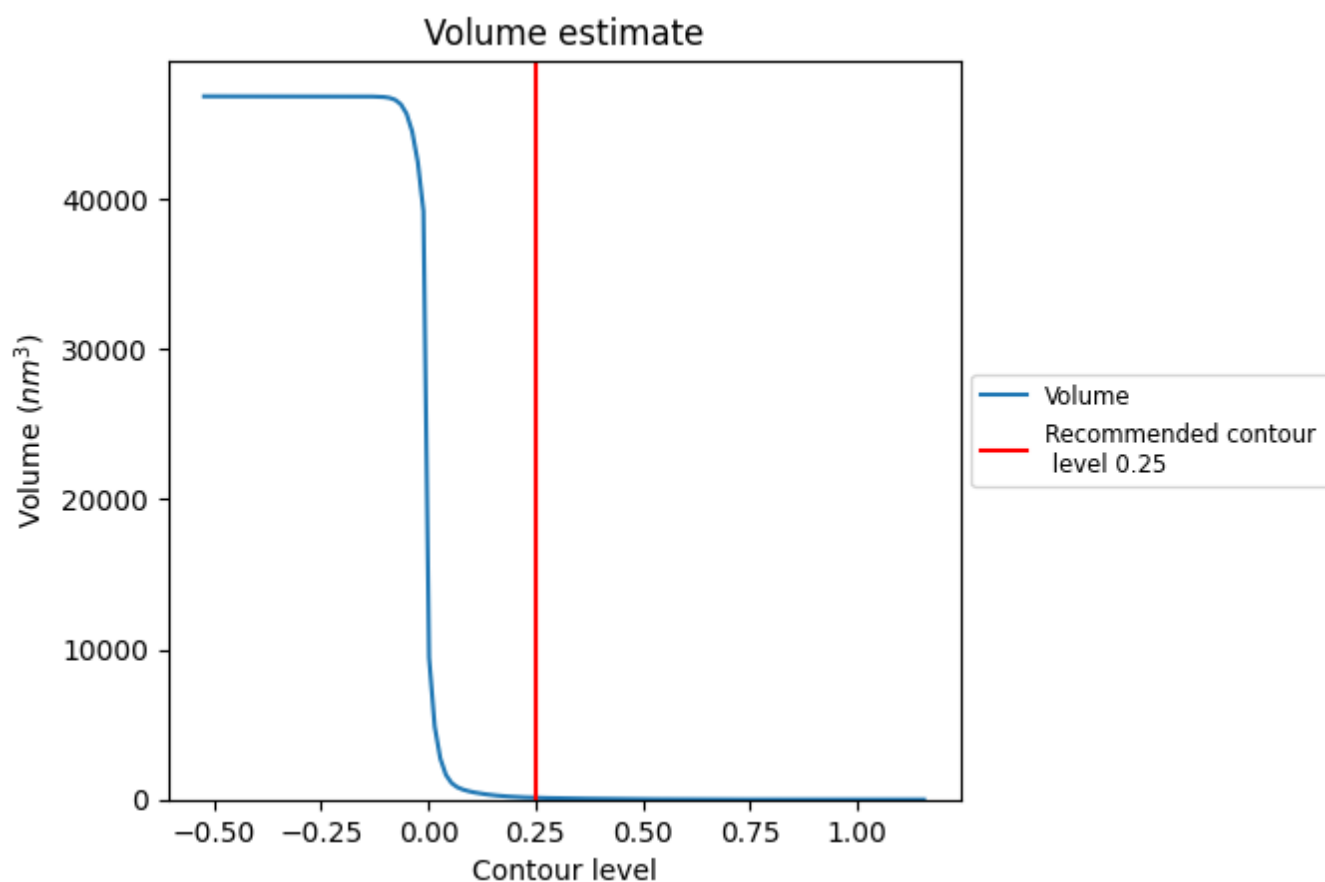
This section contains the results of statistical analysis of the map.

### 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.

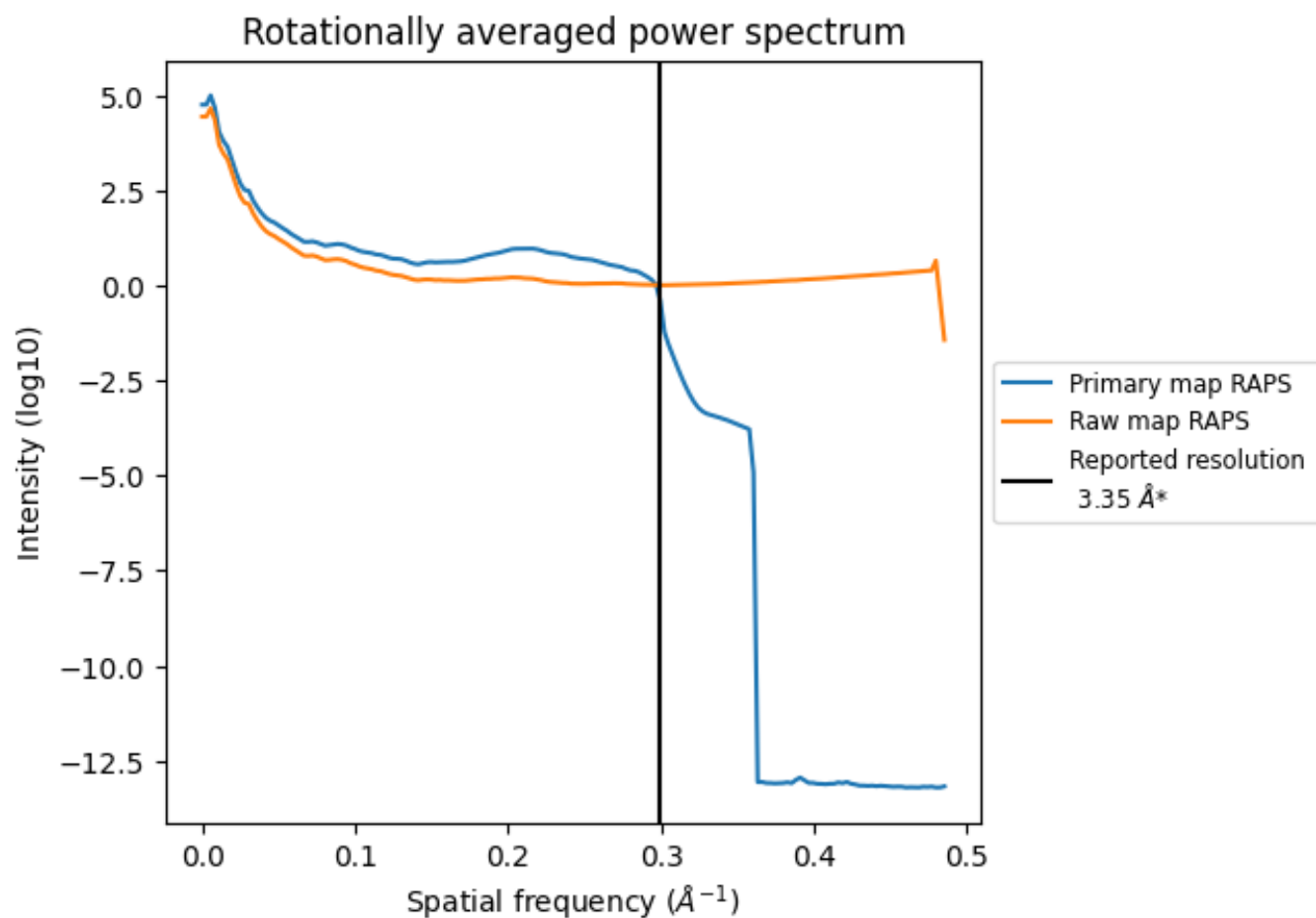
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 122 nm<sup>3</sup>; this corresponds to an approximate mass of 110 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

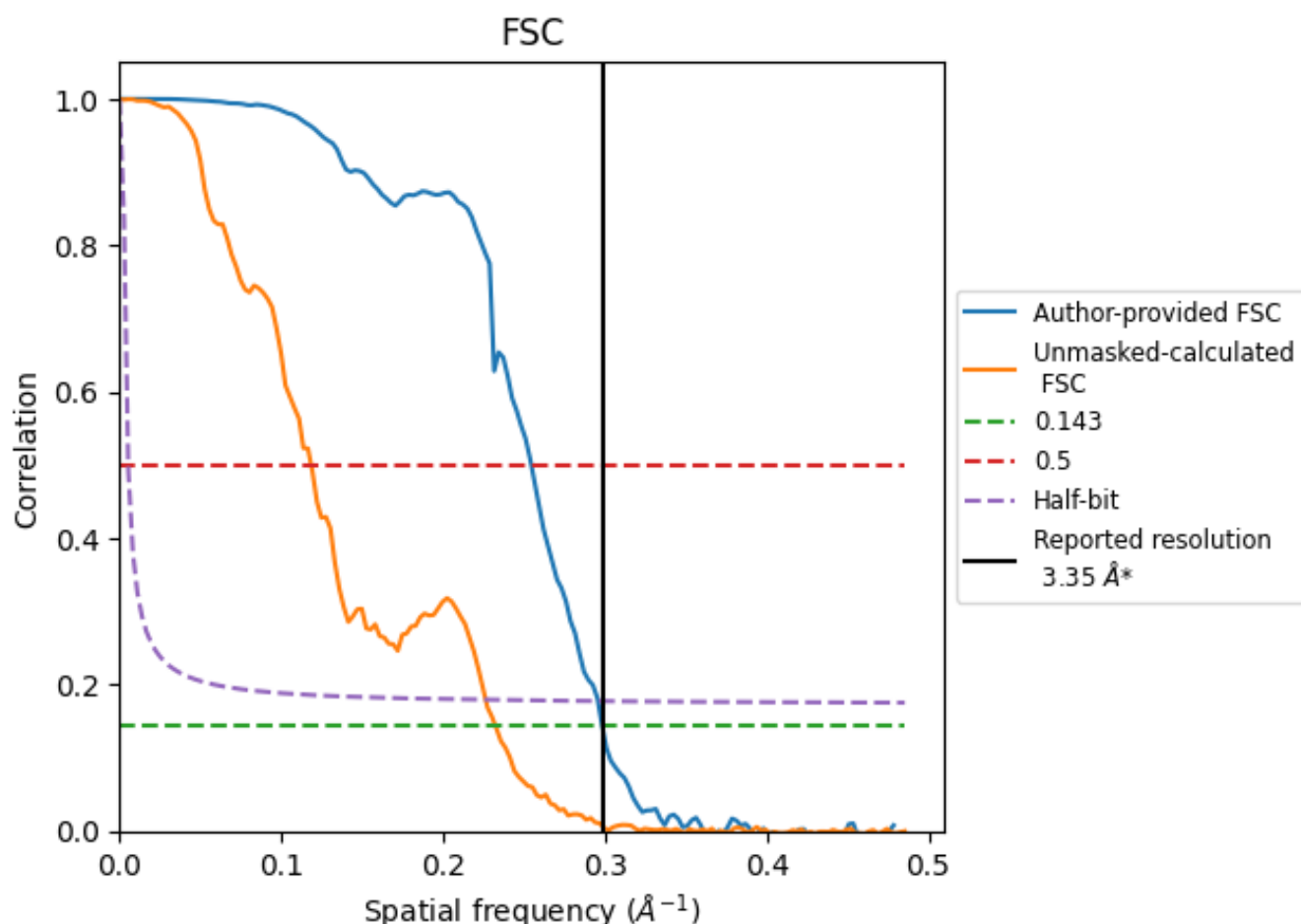


\*Reported resolution corresponds to spatial frequency of 0.299 Å<sup>-1</sup>

## 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 0.299 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

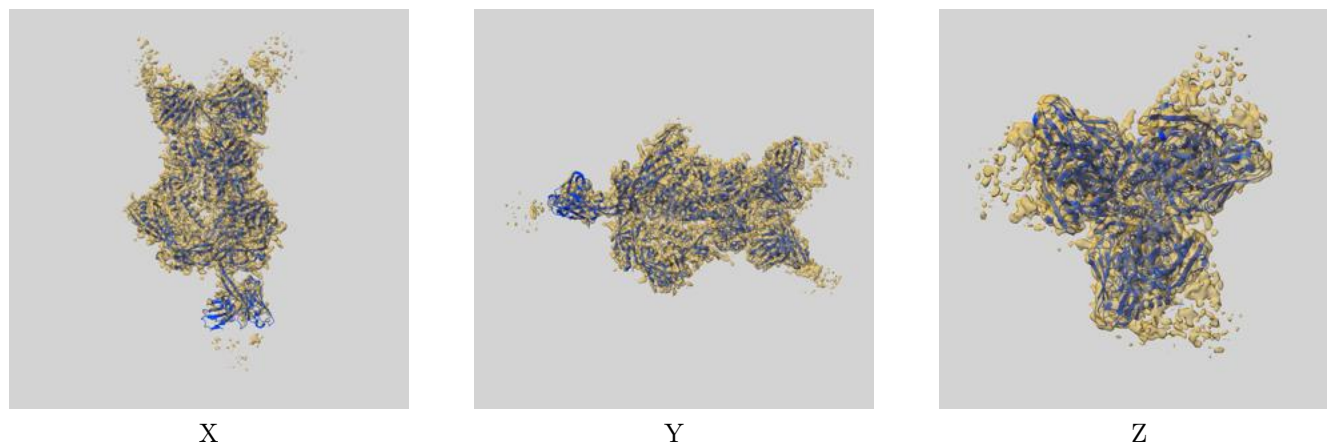
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.35	3.93	3.38
Unmasked-calculated*	4.30	8.45	4.42

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 3.35 by more than 10 %

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

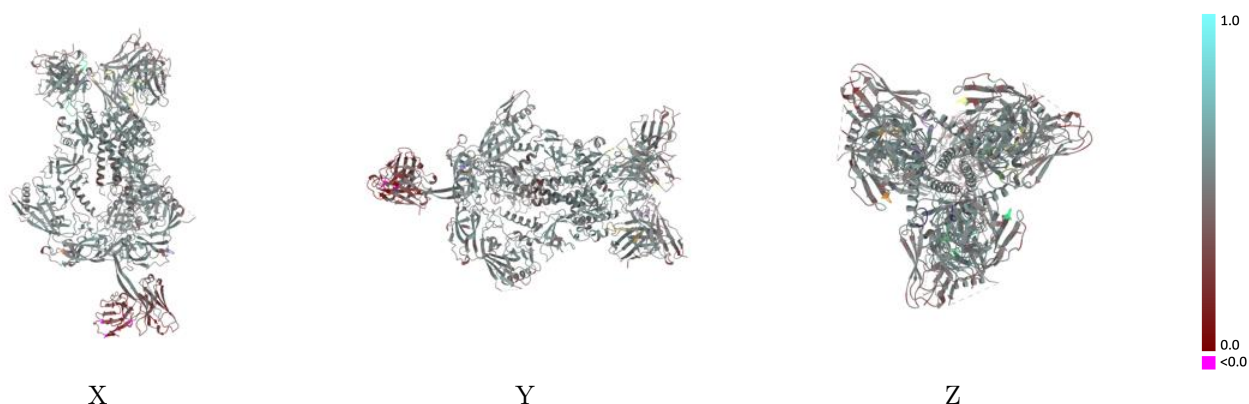
This section contains information regarding the fit between EMDB map EMD-25733 and PDB model 7T74. Per-residue inclusion information can be found in section [3](#) on page [11](#).

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



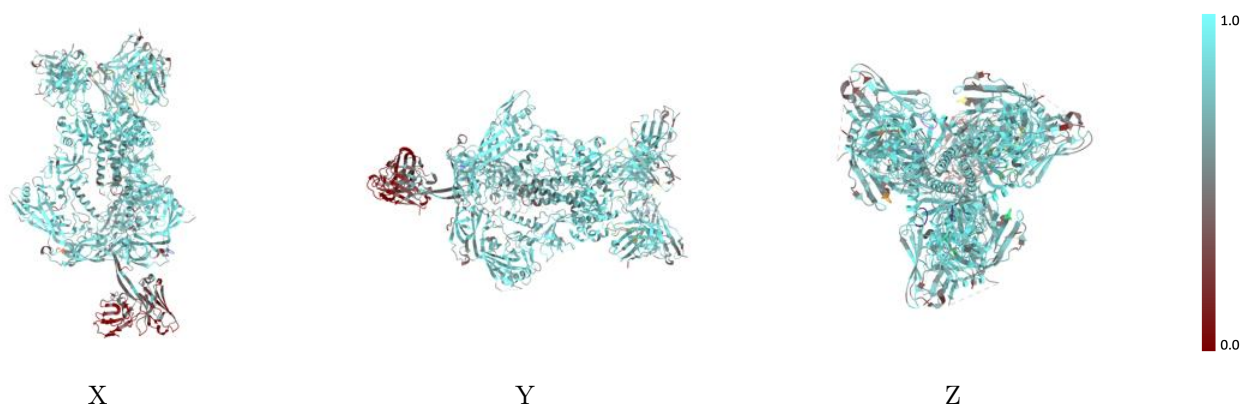
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



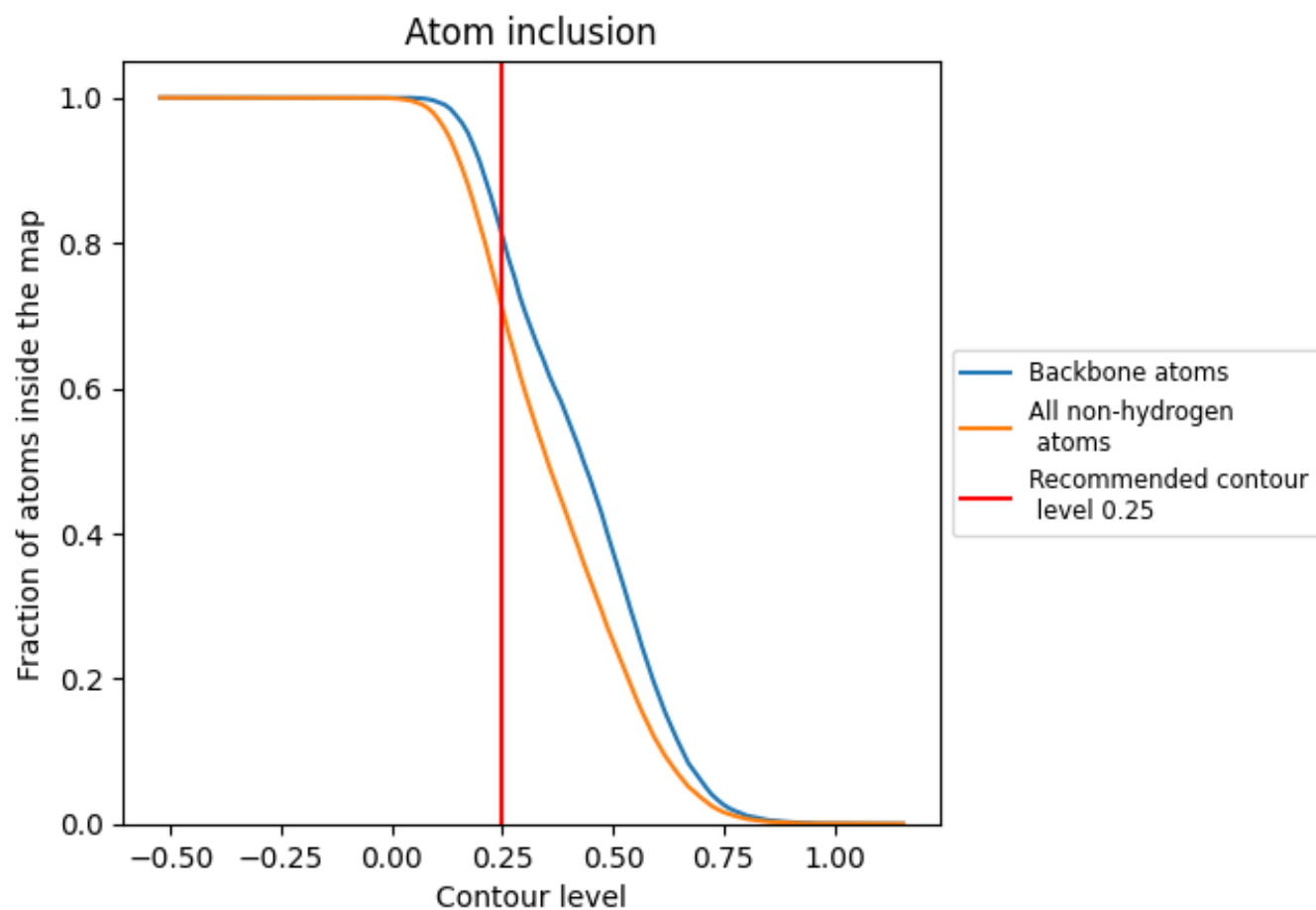
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).









































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 71% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7089	 0.4760
A	 0.7615	 0.5000
B	 0.7872	 0.5010
C	 0.7422	 0.4930
D	 0.7872	 0.5120
E	 0.7562	 0.4990
F	 0.8128	 0.5110
G	 0.7254	 0.4630
H	 0.3881	 0.3530
I	 0.7657	 0.4920
J	 0.7254	 0.4690
K	 0.7473	 0.4890
L	 0.2000	 0.2500
M	 0.7581	 0.4900
N	 0.7280	 0.4740
O	 0.6747	 0.4810
P	 0.5000	 0.4520
Q	 0.3929	 0.3830
R	 0.6600	 0.4530
S	 0.5200	 0.4460
T	 0.2083	 0.3840
U	 0.3750	 0.2920
V	 0.4103	 0.5050
W	 0.5000	 0.4030
X	 0.4643	 0.3870
Y	 0.6400	 0.4540
Z	 0.4286	 0.4340
a	 0.2917	 0.3000
b	 0.3333	 0.4290
c	 0.3214	 0.3990
d	 0.5357	 0.4040
e	 0.4643	 0.4550
f	 0.6200	 0.4810
g	 0.5357	 0.4040
h	 0.2083	 0.3620
i	 0.2917	 0.2890

