



## Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 12:39 PM UTC

PDB ID : 9QTN / pdb\_00009qtn  
EMDB ID : EMD-53355  
Title : Human alpha7 nicotinic receptor in complex with the F1 nanobody  
Authors : Barilone, N.; Vangelatou, M.; Marouf, F.Z.; Dejean de la Batie, G.; Ayme, G.;  
Lafaye, P.; Corringer, P.-J.; Prevost, M.S.  
Deposited on : 2025-04-09  
Resolution : 2.28 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:

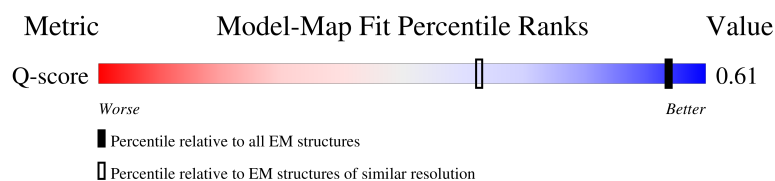
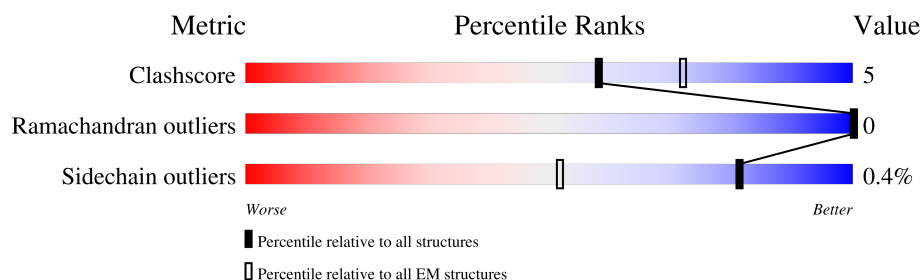
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 2.28 Å.

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




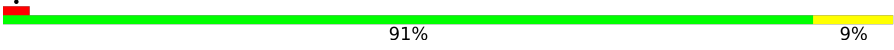
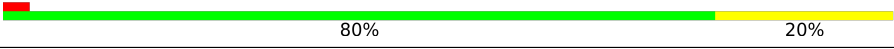

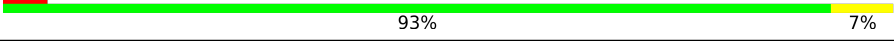

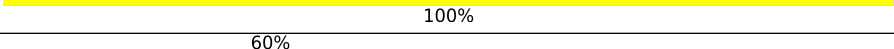
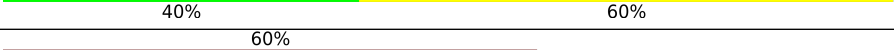

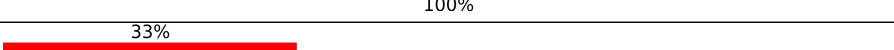
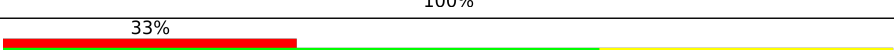
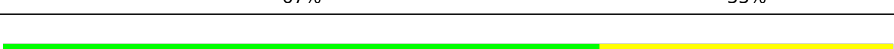


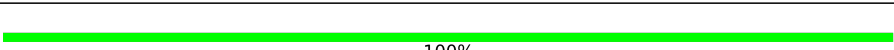




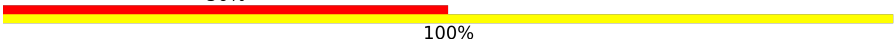

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3643 ( 1.78 - 2.78 )

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	479	
1	B	479	
1	C	479	
1	D	479	

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Mol	Chain	Length	Quality of chain
1	E	479	
2	F	131	
2	G	131	
2	H	131	
2	I	131	
2	J	131	
3	K	5	
3	Q	5	
3	T	5	
3	W	5	
4	L	3	
4	M	3	
4	N	3	
4	R	3	
4	U	3	
4	X	3	
5	O	5	
6	P	5	
7	S	3	
7	Y	3	
8	V	4	

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 14522 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.

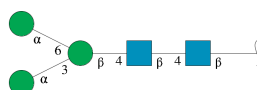
- Molecule 1 is a protein called Neuronal acetylcholine receptor subunit alpha-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	208	Total	C	N	O	S	0	0
			1729	1117	286	317	9		
1	B	208	Total	C	N	O	S	0	0
			1729	1117	286	317	9		
1	C	208	Total	C	N	O	S	0	0
			1729	1117	286	317	9		
1	D	208	Total	C	N	O	S	0	0
			1729	1117	286	317	9		
1	E	208	Total	C	N	O	S	0	0
			1729	1117	286	317	9		

- Molecule 2 is a protein called Nanobody F1.

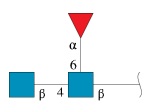
Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	131	Total	C	N	O	S	0	0
			1010	639	172	194	5		
2	G	131	Total	C	N	O	S	0	0
			1010	639	172	194	5		
2	H	131	Total	C	N	O	S	0	0
			1010	639	172	194	5		
2	I	131	Total	C	N	O	S	0	0
			1010	639	172	194	5		
2	J	131	Total	C	N	O	S	0	0
			1010	639	172	194	5		

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



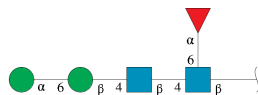
Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	5	Total	C	N	O	0	0
			61	34	2	25		
3	Q	5	Total	C	N	O	0	0
			61	34	2	25		
3	T	5	Total	C	N	O	0	0
			61	34	2	25		
3	W	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 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
4	L	3	Total	C	N	O	0	0
			38	22	2	14		
4	M	3	Total	C	N	O	0	0
			38	22	2	14		
4	N	3	Total	C	N	O	0	0
			38	22	2	14		
4	R	3	Total	C	N	O	0	0
			38	22	2	14		
4	U	3	Total	C	N	O	0	0
			38	22	2	14		
4	X	3	Total	C	N	O	0	0
			38	22	2	14		

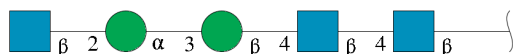
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	O	5	Total	C	N	O	0	0
			60	34	2	24		

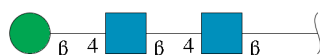
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alp

ha-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.



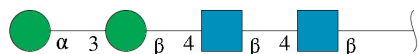
Mol	Chain	Residues	Atoms				AltConf	Trace
6	P	5	Total	C	N	O	0	0
			64	36	3	25		

- Molecule 7 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
7	S	3	Total	C	N	O	0	0
			39	22	2	15		
7	Y	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 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
8	V	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	19	Total	O	0
			19	19	
9	B	6	Total	O	0
			6	6	

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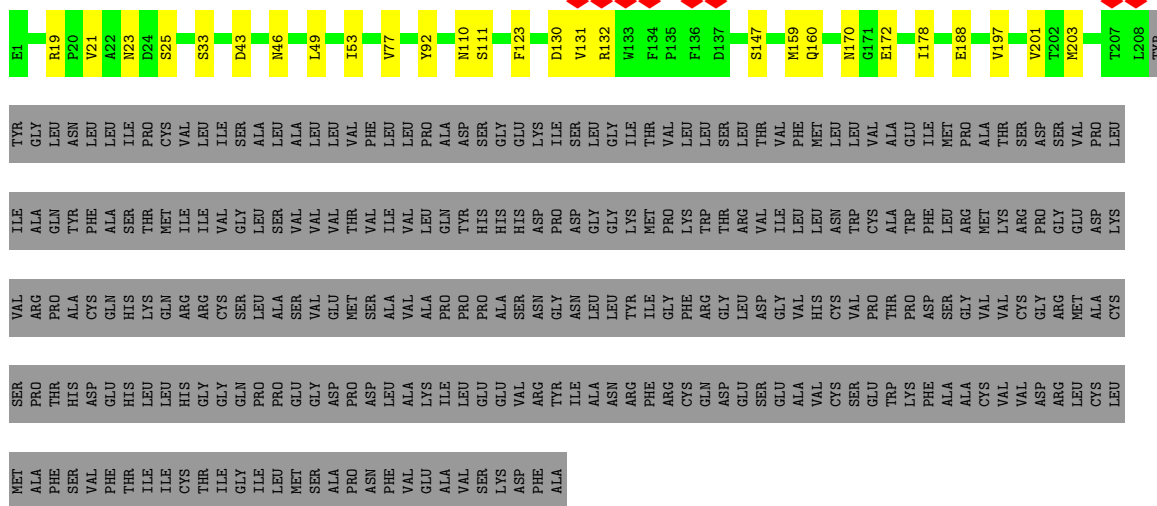
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Mol	Chain	Residues	Atoms		AltConf
9	C	21	Total 21	O 21	0
9	D	20	Total 20	O 20	0
9	E	15	Total 15	O 15	0
9	F	6	Total 6	O 6	0
9	G	4	Total 4	O 4	0
9	H	4	Total 4	O 4	0
9	I	6	Total 6	O 6	0
9	J	2	Total 2	O 2	0

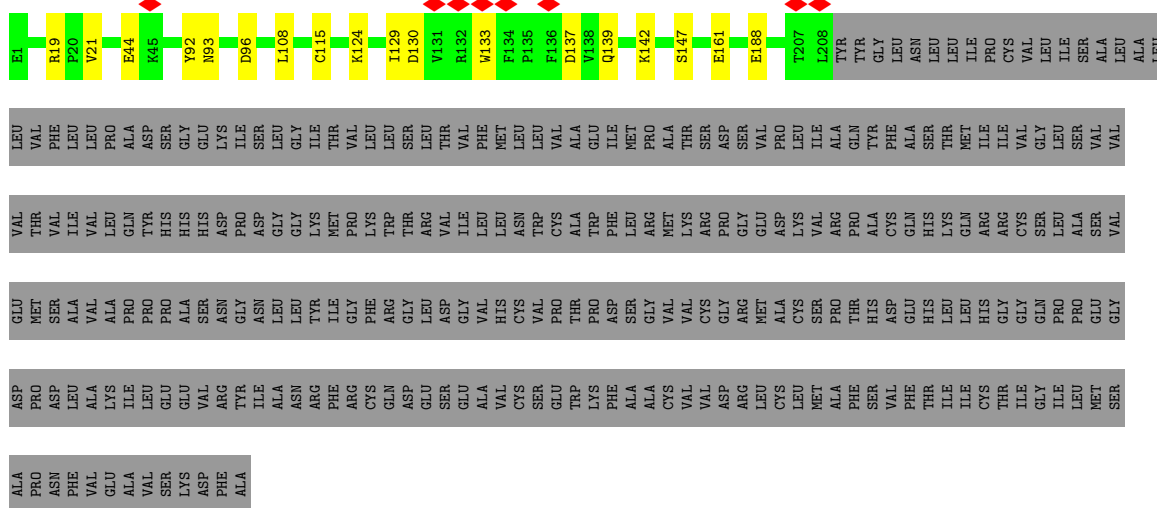




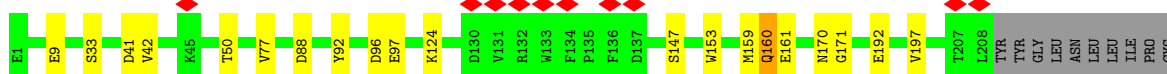
## Chain C:



Chain D:

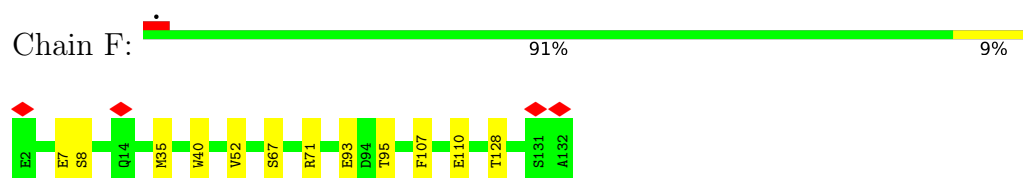


Chain E:

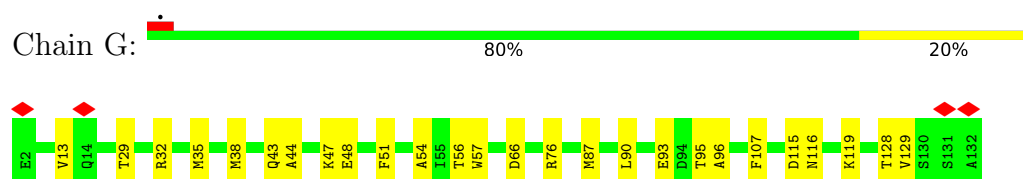


VAL	ILE	ARG	HIS	CYS
ILE	VAL	ARG	GLY	THR
GLY	VAL	CYS	GLN	ILE
LEU	LEU	SER	PRO	ILE
ALA	SER	ALA	PRO	LEU
ALA	VAL	SER	GLU	MET
LEU	VAL	VAL	GLY	SER
LEU	VAL	VAL	ASP	ALA
VAL	THR	MET	PRO	PRO
PHE	VAL	SER	ASP	ASN
LEU	ILE	ALA	LEU	PHE
LEU	VAL	VAL	ALA	VAL
PRO	LEU	ALA	ILE	GLU
ALA	GLN	PRO	ILE	ALA
ASP	TYR	PRO	LEU	VAL
SER	HIS	PRO	GLU	SER
GLY	HIS	ALA	GLU	LYS
GLU	HIS	SER	VAL	ASP
LYS	ASP	ASN	ARG	PHE
ILE	PRO	GLY	TYR	ALA
GLY	GLY	LEU	ALA	
GLY	GLY	LEU	ASN	
ILE	LYS	TYR	ARG	
THR	MET	ILE	PHE	
VAL	PRO	GLY	ARG	
LEU	LYS	PHE	CYS	
SER	TRP	ARG	GLN	
LEU	THR	GLY	ASP	
LEU	ARG	LEU	GLU	
THR	VAL	ASP	SER	
PHE	ILE	VAL	ALA	
MET	LEU	HIS	VAL	
LEU	ASN	CYS	CYS	
LEU	TRP	VAL	SER	
VAL	CYS	PRO	GLU	
ALA	ALA	THR	TRP	
GLU	TRP	PRO	LYS	
ILE	PHE	ASP	PHE	
MET	LEU	SER	ALA	
LEU	ARG	GLY	ALA	
VAL	THR	VAL	CYS	
ALA	LYS	CYS	VAL	
SER	ARG	GLY	ASP	
ASP	PRO	ARG	ARG	
VAL	GLY	MET	LEU	
LEU	ASP	ALA	CYS	
PHE	LYS	CYS	LEU	
ALA	VAL	SER	MET	
	ARG	PRO	ALA	
	THR	THR	PHE	
	GLN	HIS	SER	
	TYR	ALA	VAL	
	GLN	CYS	THR	
	ILE	GLU	PHE	
	THR	HIS	THR	
	LYS	LYS	ILE	
	GLN	LEU	THR	

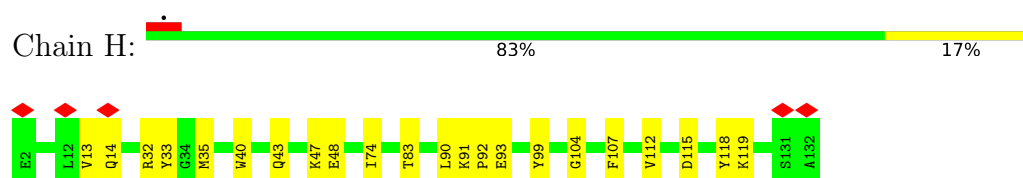
- Molecule 2: Nanobody F1



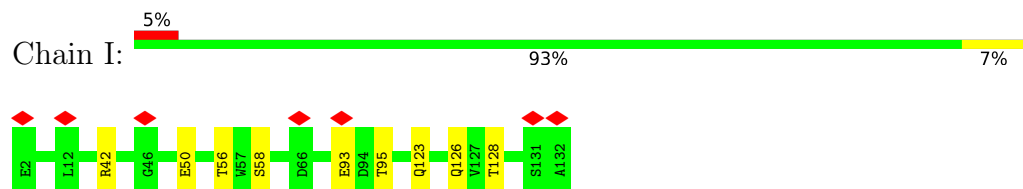
- Molecule 2: Nanobody F1



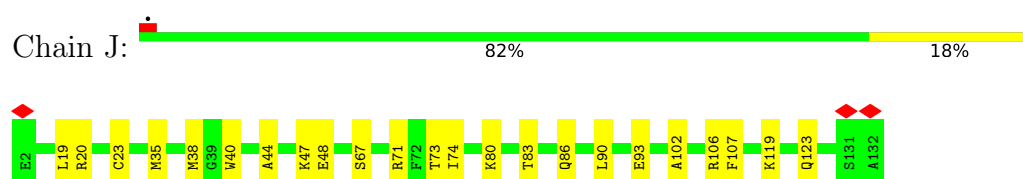
- Molecule 2: Nanobody F1



- Molecule 2: Nanobody F1



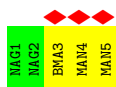
- Molecule 2: Nanobody F1



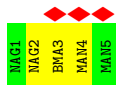
- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



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



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



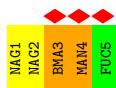
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



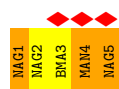
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	325670	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TITAN THEMIS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	47.155	Depositor
Minimum map value	-19.314	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	7	Depositor
Map size ( $\text{\AA}$ )	322.5, 322.5, 322.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.645, 0.645, 0.645	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, BMA, FUC

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	0.17	0/1784	0.31	0/2429
1	B	0.17	0/1784	0.34	0/2429
1	C	0.17	0/1784	0.34	0/2429
1	D	0.17	0/1784	0.31	0/2429
1	E	0.17	0/1784	0.33	0/2429
2	F	0.15	0/1034	0.32	0/1399
2	G	0.15	0/1034	0.35	0/1399
2	H	0.15	0/1034	0.32	0/1399
2	I	0.15	0/1034	0.34	0/1399
2	J	0.16	0/1034	0.38	0/1399
All	All	0.16	0/14090	0.33	0/19140

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

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	1729	0	1655	15	0
1	B	1729	0	1655	17	0
1	C	1729	0	1655	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1729	0	1655	10	0
1	E	1729	0	1655	13	0
2	F	1010	0	965	7	0
2	G	1010	0	965	16	0
2	H	1010	0	965	18	0
2	I	1010	0	965	6	0
2	J	1010	0	965	17	0
3	K	61	0	52	0	0
3	Q	61	0	52	0	0
3	T	61	0	52	0	0
3	W	61	0	52	0	0
4	L	38	0	34	0	0
4	M	38	0	34	0	0
4	N	38	0	34	0	0
4	R	38	0	34	0	0
4	U	38	0	34	0	0
4	X	38	0	34	0	0
5	O	60	0	52	1	0
6	P	64	0	55	3	0
7	S	39	0	34	1	0
7	Y	39	0	34	0	0
8	V	50	0	43	0	0
9	A	19	0	0	0	0
9	B	6	0	0	0	0
9	C	21	0	0	0	0
9	D	20	0	0	0	0
9	E	15	0	0	0	0
9	F	6	0	0	0	0
9	G	4	0	0	0	0
9	H	4	0	0	0	0
9	I	6	0	0	0	0
9	J	2	0	0	0	0
All	All	14522	0	13730	133	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 5.

All (133) 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)
2:J:48:GLU:N	2:J:48:GLU:OE2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:93:GLU:N	2:F:93:GLU:OE2	2.19	0.73
2:I:93:GLU:OE2	2:I:93:GLU:N	2.19	0.73
1:A:23:ASN:HB3	1:A:26:GLN:HG2	1.70	0.73
2:H:93:GLU:OE1	2:H:93:GLU:N	2.21	0.70
2:H:14:GLN:OE1	2:H:14:GLN:N	2.22	0.68
2:G:48:GLU:OE1	2:G:48:GLU:N	2.24	0.68
2:J:19:LEU:O	2:J:86:GLN:NE2	2.28	0.67
2:J:93:GLU:OE2	2:J:93:GLU:N	2.22	0.66
1:D:188:GLU:OE2	1:D:188:GLU:N	2.23	0.65
2:H:48:GLU:OE1	2:H:48:GLU:N	2.20	0.65
2:H:13:VAL:HG11	2:H:90:LEU:HD13	1.79	0.64
2:G:93:GLU:OE2	2:G:93:GLU:N	2.21	0.64
1:C:49:LEU:HD13	1:C:203:MET:HE1	1.80	0.63
1:A:81:ASP:OD2	1:A:104:HIS:ND1	2.30	0.63
1:D:130:ASP:H	1:D:139:GLN:HE22	1.47	0.60
2:F:7:GLU:OE1	2:F:7:GLU:N	2.36	0.58
2:H:43:GLN:NE2	2:H:47:LYS:O	2.35	0.58
1:D:44:GLU:HG2	1:D:129:ILE:HG21	1.85	0.58
2:H:35:MET:HG2	2:H:107:PHE:CZ	2.39	0.58
1:B:41:ASP:OD1	1:B:42:VAL:N	2.37	0.58
2:G:95:THR:HG23	2:G:128:THR:HA	1.86	0.58
2:G:87:MET:HE2	2:G:90:LEU:HD11	1.87	0.57
1:E:33:SER:HB2	1:E:160:GLN:HB2	1.87	0.56
2:J:35:MET:HG2	2:J:107:PHE:CZ	2.41	0.56
1:E:9:GLU:OE2	2:J:106:ARG:NE	2.32	0.56
2:I:95:THR:HG23	2:I:128:THR:HA	1.87	0.56
2:I:56:THR:HG22	2:I:58:SER:H	1.70	0.55
1:A:134:PHE:HB3	1:A:135:PRO:HD3	1.89	0.55
1:B:92:TYR:OH	1:B:147:SER:O	2.24	0.54
2:J:67:SER:O	2:J:71:ARG:NH1	2.40	0.54
2:H:32:ARG:HH11	2:H:35:MET:HE1	1.73	0.54
2:G:35:MET:HG2	2:G:107:PHE:CZ	2.43	0.54
1:E:41:ASP:OD1	1:E:42:VAL:N	2.41	0.53
1:A:7:TYR:CE1	1:A:77:VAL:HG13	2.44	0.53
1:C:25:SER:OG	7:S:1:NAG:H2	2.09	0.53
2:G:119:LYS:HB3	2:G:119:LYS:NZ	2.25	0.52
2:H:33:TYR:HH	2:H:83:THR:HG1	1.55	0.52
2:J:20:ARG:HH11	2:J:20:ARG:HG3	1.74	0.51
1:C:130:ASP:OD1	1:C:131:VAL:N	2.44	0.51
1:E:159:MET:HG3	1:E:197:VAL:HG13	1.93	0.51
1:C:178:ILE:HD12	1:C:201:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:GLU:H	1:E:161:GLU:CD	2.19	0.50
1:E:92:TYR:OH	1:E:147:SER:O	2.30	0.50
2:G:115:ASP:OD1	2:G:116:ASN:N	2.45	0.50
2:I:123:GLN:HA	2:I:123:GLN:OE1	2.12	0.50
1:B:114:HIS:CE1	6:P:1:NAG:H62	2.47	0.49
1:D:92:TYR:OH	1:D:147:SER:O	2.29	0.49
1:C:159:MET:HG3	1:C:197:VAL:HG13	1.93	0.49
2:G:51:PHE:HE1	2:G:54:ALA:HB2	1.77	0.49
2:I:42:ARG:NE	2:I:50:GLU:OE1	2.46	0.48
1:B:185:ARG:HH12	1:B:187:TYR:HE1	1.60	0.48
1:E:153:TRP:CD2	1:E:192:GLU:HG3	2.49	0.48
1:E:88:ASP:OD1	1:E:147:SER:OG	2.26	0.48
2:J:119:LYS:HB3	2:J:119:LYS:NZ	2.29	0.48
2:J:40:TRP:HD1	2:J:74:ILE:HD12	1.78	0.47
1:A:92:TYR:OH	1:A:147:SER:O	2.30	0.47
1:C:53:ILE:HB	1:C:123:PHE:CE1	2.50	0.47
1:E:50:THR:HG23	1:E:124:LYS:HG3	1.95	0.47
2:H:104:GLY:HA3	2:H:119:LYS:HD3	1.96	0.47
1:B:159:MET:HG3	1:B:197:VAL:HG13	1.97	0.47
2:F:35:MET:HG2	2:F:107:PHE:CZ	2.50	0.47
1:A:152:GLY:C	1:A:154:SER:H	2.23	0.46
1:A:188:GLU:CD	1:A:188:GLU:H	2.22	0.46
1:C:92:TYR:OH	1:C:147:SER:O	2.32	0.46
2:H:40:TRP:HD1	2:H:74:ILE:HD12	1.80	0.46
1:A:80:PRO:HG2	1:A:83:GLN:HG3	1.97	0.46
2:H:115:ASP:N	2:H:115:ASP:OD1	2.45	0.46
1:D:133:TRP:O	1:D:137:ASP:HB3	2.15	0.46
1:A:33:SER:HB2	1:A:160:GLN:HB2	1.97	0.46
1:C:170:ASN:OD1	1:C:172:GLU:N	2.46	0.46
1:C:130:ASP:OD1	1:C:132:ARG:HG3	2.16	0.46
2:J:123:GLN:HA	2:J:123:GLN:OE1	2.16	0.46
1:C:19:ARG:NH1	1:C:21:VAL:HG11	2.31	0.46
1:D:161:GLU:HA	1:D:161:GLU:OE1	2.16	0.45
2:G:44:ALA:HB3	2:G:47:LYS:HB2	1.98	0.45
1:A:159:MET:HE2	1:A:180:GLY:C	2.42	0.45
2:G:48:GLU:H	2:G:48:GLU:CD	2.21	0.45
2:F:95:THR:HG23	2:F:128:THR:HA	1.99	0.45
2:G:13:VAL:HG13	2:G:129:VAL:HG23	1.98	0.45
1:C:43:ASP:OD2	1:C:46:ASN:ND2	2.49	0.45
2:H:43:GLN:HB3	2:H:99:TYR:HE1	1.82	0.45
1:E:161:GLU:CD	1:E:161:GLU:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:TYR:CE1	1:B:77:VAL:HG13	2.53	0.44
2:H:119:LYS:HB3	2:H:119:LYS:HE3	1.71	0.44
5:O:3:BMA:H62	5:O:4:MAN:H2	1.77	0.44
1:E:159:MET:HE2	1:E:159:MET:HB3	1.92	0.44
1:B:178:ILE:HD12	1:B:201:VAL:HG22	2.00	0.44
2:F:40:TRP:O	2:F:52:VAL:HB	2.18	0.44
2:H:91:LYS:HB3	2:H:92:PRO:HD2	2.00	0.43
1:B:92:TYR:CD2	1:B:144:LYS:HE2	2.53	0.43
1:B:80:PRO:HG2	1:B:83:GLN:HG3	1.99	0.43
1:B:207:THR:OG1	1:B:208:LEU:N	2.50	0.43
1:D:108:LEU:O	1:D:115:CYS:HA	2.18	0.43
1:B:114:HIS:ND1	6:P:1:NAG:H62	2.33	0.43
1:E:170:ASN:OD1	1:E:171:GLY:N	2.52	0.43
2:G:66:ASP:OD1	2:G:66:ASP:N	2.50	0.43
2:J:44:ALA:HB3	2:J:47:LYS:HD3	2.00	0.43
6:P:4:MAN:H2	6:P:5:NAG:H2	1.72	0.43
1:A:131:VAL:HG12	1:A:131:VAL:O	2.19	0.43
2:I:126:GLN:OE1	2:I:128:THR:HG23	2.19	0.43
2:F:67:SER:O	2:F:71:ARG:NH2	2.45	0.42
1:E:96:ASP:OD1	1:E:97:GLU:N	2.53	0.42
2:H:47:LYS:N	2:H:47:LYS:HD2	2.34	0.42
2:J:38:MET:HE1	2:J:102:ALA:HB2	2.00	0.42
1:C:110:ASN:O	1:C:111:SER:OG	2.26	0.42
2:J:38:MET:HG3	2:J:83:THR:OG1	2.19	0.42
1:B:147:SER:OG	1:B:150:TYR:HB2	2.19	0.42
1:D:19:ARG:NH1	1:D:21:VAL:HG11	2.35	0.42
2:J:23:CYS:HB3	2:J:83:THR:HB	2.01	0.42
1:B:92:TYR:HD2	1:B:144:LYS:HE2	1.84	0.42
1:D:93:ASN:ND2	1:D:142:LYS:O	2.51	0.42
1:B:109:VAL:HA	1:B:114:HIS:O	2.20	0.41
1:B:33:SER:HB2	1:B:160:GLN:HB2	2.02	0.41
1:C:33:SER:HB2	1:C:160:GLN:HB2	2.02	0.41
2:G:38:MET:HG2	2:G:76:ARG:NH1	2.35	0.41
2:H:32:ARG:NH1	2:H:35:MET:HE1	2.34	0.41
1:A:185:ARG:HH22	1:A:187:TYR:HE1	1.68	0.41
2:J:90:LEU:HD12	2:J:90:LEU:H	1.86	0.41
2:G:43:GLN:O	2:G:96:ALA:HB1	2.21	0.41
1:A:44:GLU:HG3	1:A:129:ILE:HG21	2.03	0.41
1:B:5:LYS:HE2	2:F:110:GLU:HG3	2.02	0.41
2:G:56:THR:HG22	2:G:57:TRP:N	2.36	0.41
2:H:112:VAL:HG13	2:H:118:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:HD11	1:A:53:ILE:HD13	2.02	0.41
1:A:39:ILE:HD13	1:A:203:MET:HE3	2.02	0.40
2:H:14:GLN:H	2:H:14:GLN:CD	2.19	0.40
2:J:73:THR:CG2	2:J:86:GLN:HB3	2.51	0.40
1:B:161:GLU:OE2	1:B:161:GLU:HA	2.21	0.40
1:C:188:GLU:N	1:C:188:GLU:CD	2.78	0.40
1:D:96:ASP:HB2	1:D:124:LYS:HB2	2.04	0.40
2:G:29:THR:HB	2:G:32:ARG:HB2	2.03	0.40
2:J:80:LYS:NZ	2:J:80:LYS:HB3	2.35	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	206/479 (43%)	195 (95%)	11 (5%)	0	100	100
1	B	206/479 (43%)	198 (96%)	8 (4%)	0	100	100
1	C	206/479 (43%)	198 (96%)	8 (4%)	0	100	100
1	D	206/479 (43%)	198 (96%)	8 (4%)	0	100	100
1	E	206/479 (43%)	202 (98%)	4 (2%)	0	100	100
2	F	129/131 (98%)	129 (100%)	0	0	100	100
2	G	129/131 (98%)	129 (100%)	0	0	100	100
2	H	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
2	I	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
2	J	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
All	All	1675/3050 (55%)	1628 (97%)	47 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/424 (46%)	193 (100%)	0	100	100
1	B	193/424 (46%)	192 (100%)	1 (0%)	81	89
1	C	193/424 (46%)	191 (99%)	2 (1%)	68	81
1	D	193/424 (46%)	193 (100%)	0	100	100
1	E	193/424 (46%)	191 (99%)	2 (1%)	68	81
2	F	103/103 (100%)	102 (99%)	1 (1%)	68	81
2	G	103/103 (100%)	103 (100%)	0	100	100
2	H	103/103 (100%)	103 (100%)	0	100	100
2	I	103/103 (100%)	103 (100%)	0	100	100
2	J	103/103 (100%)	103 (100%)	0	100	100
All	All	1480/2635 (56%)	1474 (100%)	6 (0%)	81	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	75	LYS
1	C	23	ASN
1	C	77	VAL
1	E	77	VAL
1	E	160	GLN
2	F	8	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	B	3	GLN
1	B	47	GLN
1	B	104	HIS
1	C	158	GLN

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Mol	Chain	Res	Type
1	D	139	GLN
1	E	3	GLN
1	E	26	GLN
1	E	104	HIS
2	F	123	GLN
2	F	126	GLN
2	G	126	GLN
2	H	43	GLN
2	I	86	GLN
2	J	86	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

58 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	K	1	1,3	14,14,15	0.80	0	17,19,21	0.92	1 (5%)
3	NAG	K	2	3	14,14,15	0.75	0	17,19,21	1.02	1 (5%)
3	BMA	K	3	3	11,11,12	0.85	0	15,15,17	2.18	3 (20%)
3	MAN	K	4	3	11,11,12	0.74	0	15,15,17	0.96	1 (6%)
3	MAN	K	5	3	11,11,12	0.74	0	15,15,17	1.00	1 (6%)
4	NAG	L	1	1,4	14,14,15	0.83	0	17,19,21	0.86	0
4	NAG	L	2	4	14,14,15	0.72	0	17,19,21	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FUC	L	3	4	10,10,11	0.77	0	14,14,16	0.99	0
4	NAG	M	1	1,4	14,14,15	0.64	0	17,19,21	1.14	0
4	NAG	M	2	4	14,14,15	0.75	0	17,19,21	0.80	0
4	FUC	M	3	4	10,10,11	0.75	0	14,14,16	1.24	2 (14%)
4	NAG	N	1	1,4	14,14,15	0.72	0	17,19,21	1.26	2 (11%)
4	NAG	N	2	4	14,14,15	0.78	0	17,19,21	0.85	0
4	FUC	N	3	4	10,10,11	0.77	0	14,14,16	0.94	0
5	NAG	O	1	1,5	14,14,15	0.67	0	17,19,21	1.03	1 (5%)
5	NAG	O	2	5	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
5	BMA	O	3	5	11,11,12	0.93	0	15,15,17	2.38	4 (26%)
5	MAN	O	4	5	11,11,12	0.66	0	15,15,17	1.38	1 (6%)
5	FUC	O	5	5	10,10,11	0.74	0	14,14,16	0.98	0
6	NAG	P	1	6,1	14,14,15	0.84	1 (7%)	17,19,21	1.37	3 (17%)
6	NAG	P	2	6	14,14,15	0.72	0	17,19,21	1.17	2 (11%)
6	BMA	P	3	6	11,11,12	0.82	0	15,15,17	1.91	2 (13%)
6	MAN	P	4	6	11,11,12	0.64	0	15,15,17	1.55	1 (6%)
6	NAG	P	5	6	14,14,15	0.89	1 (7%)	17,19,21	1.77	3 (17%)
3	NAG	Q	1	1,3	14,14,15	0.79	0	17,19,21	0.93	0
3	NAG	Q	2	3	14,14,15	0.75	0	17,19,21	0.96	0
3	BMA	Q	3	3	11,11,12	0.80	0	15,15,17	2.63	5 (33%)
3	MAN	Q	4	3	11,11,12	0.69	0	15,15,17	1.23	1 (6%)
3	MAN	Q	5	3	11,11,12	0.80	1 (9%)	15,15,17	0.84	0
4	NAG	R	1	1,4	14,14,15	0.88	0	17,19,21	1.09	1 (5%)
4	NAG	R	2	4	14,14,15	0.70	0	17,19,21	0.90	0
4	FUC	R	3	4	10,10,11	0.76	0	14,14,16	0.99	0
7	NAG	S	1	1,7	14,14,15	0.85	0	17,19,21	1.96	5 (29%)
7	NAG	S	2	7	14,14,15	0.79	1 (7%)	17,19,21	1.79	4 (23%)
7	BMA	S	3	7	11,11,12	0.80	0	15,15,17	3.24	5 (33%)
3	NAG	T	1	1,3	14,14,15	0.80	0	17,19,21	0.88	0
3	NAG	T	2	3	14,14,15	0.77	0	17,19,21	1.02	1 (5%)
3	BMA	T	3	3	11,11,12	0.73	0	15,15,17	2.77	4 (26%)
3	MAN	T	4	3	11,11,12	0.67	0	15,15,17	1.28	1 (6%)
3	MAN	T	5	3	11,11,12	0.79	0	15,15,17	0.93	0
4	NAG	U	1	1,4	14,14,15	0.80	0	17,19,21	0.83	1 (5%)
4	NAG	U	2	4	14,14,15	0.70	0	17,19,21	0.90	0
4	FUC	U	3	4	10,10,11	0.79	0	14,14,16	0.96	0
8	NAG	V	1	8,1	14,14,15	0.78	0	17,19,21	1.26	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	V	2	8	14,14,15	0.78	0	17,19,21	1.80	5 (29%)
8	BMA	V	3	8	11,11,12	0.75	0	15,15,17	2.43	7 (46%)
8	MAN	V	4	8	11,11,12	0.70	0	15,15,17	1.11	1 (6%)
3	NAG	W	1	1,3	14,14,15	0.82	0	17,19,21	1.24	3 (17%)
3	NAG	W	2	3	14,14,15	0.69	0	17,19,21	0.97	1 (5%)
3	BMA	W	3	3	11,11,12	0.81	0	15,15,17	2.50	5 (33%)
3	MAN	W	4	3	11,11,12	0.66	0	15,15,17	1.34	1 (6%)
3	MAN	W	5	3	11,11,12	0.78	0	15,15,17	0.88	1 (6%)
4	NAG	X	1	1,4	14,14,15	0.82	0	17,19,21	0.89	0
4	NAG	X	2	4	14,14,15	0.70	0	17,19,21	0.92	0
4	FUC	X	3	4	10,10,11	0.76	0	14,14,16	0.98	0
7	NAG	Y	1	1,7	14,14,15	0.73	0	17,19,21	1.09	2 (11%)
7	NAG	Y	2	7	14,14,15	0.72	0	17,19,21	0.96	0
7	BMA	Y	3	7	11,11,12	0.86	0	15,15,17	2.19	5 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	1/2/19/22	0/1/1/1
3	MAN	K	4	3	-	1/2/19/22	0/1/1/1
3	MAN	K	5	3	-	0/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	FUC	L	3	4	-	-	0/1/1/1
4	NAG	M	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	FUC	M	3	4	-	-	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	FUC	N	3	4	-	-	0/1/1/1
5	NAG	O	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	1/2/19/22	0/1/1/1
5	MAN	O	4	5	-	0/2/19/22	0/1/1/1
5	FUC	O	5	5	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	P	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	BMA	P	3	6	-	0/2/19/22	0/1/1/1
6	MAN	P	4	6	-	2/2/19/22	0/1/1/1
6	NAG	P	5	6	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	1/2/19/22	0/1/1/1
3	MAN	Q	4	3	-	0/2/19/22	0/1/1/1
3	MAN	Q	5	3	-	0/2/19/22	0/1/1/1
4	NAG	R	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	FUC	R	3	4	-	-	0/1/1/1
7	NAG	S	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
7	BMA	S	3	7	-	1/2/19/22	0/1/1/1
3	NAG	T	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	BMA	T	3	3	-	0/2/19/22	0/1/1/1
3	MAN	T	4	3	-	1/2/19/22	1/1/1/1
3	MAN	T	5	3	-	0/2/19/22	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1
4	FUC	U	3	4	-	-	0/1/1/1
8	NAG	V	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	V	2	8	-	2/6/23/26	0/1/1/1
8	BMA	V	3	8	-	1/2/19/22	0/1/1/1
8	MAN	V	4	8	-	1/2/19/22	0/1/1/1
3	NAG	W	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	2/6/23/26	0/1/1/1
3	BMA	W	3	3	-	1/2/19/22	0/1/1/1
3	MAN	W	4	3	-	0/2/19/22	0/1/1/1
3	MAN	W	5	3	-	0/2/19/22	0/1/1/1
4	NAG	X	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	FUC	X	3	4	-	-	0/1/1/1
7	NAG	Y	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	2/6/23/26	0/1/1/1
7	BMA	Y	3	7	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	5	NAG	C1-C2	2.50	1.55	1.52
7	S	2	NAG	C1-C2	2.10	1.55	1.52
6	P	1	NAG	C1-C2	2.09	1.55	1.52
3	Q	5	MAN	O5-C1	-2.05	1.40	1.43

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	3	BMA	C1-O5-C5	10.11	125.74	112.19
3	T	3	BMA	C1-O5-C5	8.86	124.07	112.19
3	Q	3	BMA	C1-O5-C5	7.92	122.80	112.19
3	W	3	BMA	C1-O5-C5	7.45	122.17	112.19
3	K	3	BMA	C1-O5-C5	6.77	121.26	112.19
5	O	3	BMA	C1-O5-C5	6.42	120.79	112.19
7	Y	3	BMA	C1-O5-C5	6.32	120.65	112.19
7	S	2	NAG	O5-C1-C2	-5.21	103.24	111.29
6	P	3	BMA	C1-O5-C5	5.02	118.91	112.19
8	V	3	BMA	C1-O5-C5	4.94	118.81	112.19
6	P	4	MAN	C1-O5-C5	4.79	118.61	112.19
7	S	1	NAG	C4-C3-C2	4.70	117.91	111.02
6	P	5	NAG	C2-N2-C7	4.43	128.84	122.90
5	O	4	MAN	C1-O5-C5	4.42	118.11	112.19
8	V	2	NAG	C4-C3-C2	4.38	117.44	111.02
3	W	4	MAN	C1-O5-C5	4.30	117.95	112.19
3	T	4	MAN	C1-O5-C5	4.02	117.57	112.19
8	V	3	BMA	C1-C2-C3	-3.86	104.02	109.64
7	S	3	BMA	C3-C4-C5	3.80	117.12	110.23
3	Q	4	MAN	C1-O5-C5	3.77	117.24	112.19
7	S	3	BMA	C2-C3-C4	3.58	117.15	110.86
7	S	1	NAG	C1-O5-C5	-3.55	107.43	112.19
5	O	3	BMA	C2-C3-C4	3.46	116.94	110.86
8	V	3	BMA	O3-C3-C4	3.43	118.46	110.38
5	O	2	NAG	O5-C1-C2	-3.28	106.21	111.29
3	Q	3	BMA	C3-C4-C5	3.27	116.16	110.23
3	W	3	BMA	C3-C4-C5	3.26	116.14	110.23
5	O	3	BMA	C3-C4-C5	3.25	116.13	110.23
8	V	1	NAG	O4-C4-C3	-3.16	102.92	110.38
8	V	3	BMA	C3-C4-C5	3.16	115.96	110.23
8	V	2	NAG	C1-O5-C5	-3.09	108.04	112.19
7	S	1	NAG	C2-N2-C7	2.91	126.80	122.90
7	S	2	NAG	C1-C2-N2	2.86	114.94	110.43
7	S	1	NAG	O5-C1-C2	-2.83	106.91	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	3	BMA	O5-C5-C4	2.82	117.69	110.83
7	Y	3	BMA	C3-C4-C5	2.78	115.27	110.23
8	V	2	NAG	C2-N2-C7	2.73	126.56	122.90
7	Y	3	BMA	C2-C3-C4	2.67	115.56	110.86
7	S	1	NAG	O4-C4-C3	-2.61	104.22	110.38
6	P	1	NAG	C1-C2-N2	2.61	114.54	110.43
8	V	2	NAG	C3-C4-C5	2.60	114.95	110.23
4	R	1	NAG	C2-N2-C7	2.60	126.38	122.90
6	P	5	NAG	C4-C3-C2	2.57	114.79	111.02
7	Y	1	NAG	O5-C1-C2	-2.55	107.34	111.29
7	S	3	BMA	O4-C4-C3	-2.55	104.37	110.38
6	P	1	NAG	O5-C1-C2	-2.54	107.36	111.29
3	K	3	BMA	C3-C4-C5	2.49	114.75	110.23
3	K	5	MAN	C1-O5-C5	2.48	115.51	112.19
4	N	1	NAG	C1-O5-C5	2.47	115.49	112.19
7	S	2	NAG	O4-C4-C3	-2.47	104.56	110.38
3	K	4	MAN	C1-O5-C5	2.46	115.48	112.19
3	T	3	BMA	C3-C4-C5	2.46	114.69	110.23
3	Q	3	BMA	O4-C4-C3	-2.43	104.65	110.38
8	V	2	NAG	O5-C1-C2	-2.42	107.55	111.29
3	W	3	BMA	O4-C4-C3	-2.42	104.67	110.38
3	W	1	NAG	O5-C1-C2	-2.42	107.55	111.29
6	P	3	BMA	C2-C3-C4	2.41	115.10	110.86
8	V	3	BMA	O4-C4-C3	-2.41	104.70	110.38
6	P	2	NAG	O4-C4-C3	-2.39	104.74	110.38
3	K	2	NAG	C2-N2-C7	2.37	126.08	122.90
4	M	3	FUC	C1-O5-C5	2.33	118.47	112.97
6	P	2	NAG	C2-N2-C7	2.33	126.02	122.90
6	P	1	NAG	C2-N2-C7	2.30	125.98	122.90
3	W	1	NAG	C1-O5-C5	2.30	115.26	112.19
3	T	3	BMA	O4-C4-C3	-2.28	105.00	110.38
8	V	3	BMA	O5-C5-C4	2.28	116.37	110.83
8	V	4	MAN	C1-O5-C5	2.23	115.17	112.19
3	T	3	BMA	O3-C3-C2	-2.22	105.52	110.05
3	Q	3	BMA	C2-C3-C4	2.19	114.72	110.86
8	V	3	BMA	O2-C2-C3	2.19	114.69	110.15
5	O	3	BMA	O4-C4-C3	-2.19	105.22	110.38
6	P	5	NAG	O5-C5-C4	-2.18	105.53	110.83
3	Q	3	BMA	O5-C5-C4	2.17	116.12	110.83
3	T	2	NAG	O4-C4-C3	-2.14	105.34	110.38
3	W	2	NAG	C2-N2-C7	2.10	125.71	122.90
4	N	1	NAG	C2-N2-C7	2.07	125.68	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	2	NAG	C2-N2-C7	2.07	125.68	122.90
3	W	1	NAG	C1-C2-N2	2.07	113.69	110.43
3	K	3	BMA	O4-C4-C3	-2.06	105.52	110.38
4	M	3	FUC	C1-C2-C3	2.06	112.64	109.64
3	W	5	MAN	C1-O5-C5	2.05	114.93	112.19
3	K	1	NAG	O4-C4-C3	-2.05	105.55	110.38
7	Y	3	BMA	O3-C3-C2	-2.04	105.88	110.05
3	W	3	BMA	C2-C3-C4	2.03	114.44	110.86
5	O	1	NAG	O5-C1-C2	-2.03	108.15	111.29
4	U	1	NAG	O5-C1-C2	-2.02	108.16	111.29
7	Y	3	BMA	O4-C4-C3	-2.02	105.61	110.38
3	W	3	BMA	O5-C5-C4	2.02	115.73	110.83
8	V	1	NAG	O5-C1-C2	-2.01	108.18	111.29
7	Y	1	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	P	4	MAN	O5-C5-C6-O6
7	S	3	BMA	O5-C5-C6-O6
8	V	3	BMA	O5-C5-C6-O6
6	P	4	MAN	C4-C5-C6-O6
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	Q	2	NAG	C8-C7-N2-C2
3	Q	2	NAG	O7-C7-N2-C2
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	W	2	NAG	C8-C7-N2-C2
3	W	2	NAG	O7-C7-N2-C2
4	M	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
4	X	1	NAG	C8-C7-N2-C2
4	X	1	NAG	O7-C7-N2-C2
5	O	1	NAG	C8-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2
6	P	1	NAG	C8-C7-N2-C2
6	P	1	NAG	O7-C7-N2-C2
6	P	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	P	2	NAG	O7-C7-N2-C2
7	S	1	NAG	C8-C7-N2-C2
7	S	1	NAG	O7-C7-N2-C2
7	S	2	NAG	C8-C7-N2-C2
7	S	2	NAG	O7-C7-N2-C2
7	Y	1	NAG	C8-C7-N2-C2
7	Y	1	NAG	O7-C7-N2-C2
7	Y	2	NAG	C8-C7-N2-C2
7	Y	2	NAG	O7-C7-N2-C2
8	V	1	NAG	C8-C7-N2-C2
8	V	1	NAG	O7-C7-N2-C2
8	V	2	NAG	C8-C7-N2-C2
8	V	2	NAG	O7-C7-N2-C2
3	K	3	BMA	O5-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
3	K	4	MAN	O5-C5-C6-O6
3	T	4	MAN	O5-C5-C6-O6
8	V	4	MAN	O5-C5-C6-O6
6	P	5	NAG	O5-C5-C6-O6
6	P	5	NAG	C3-C2-N2-C7
3	W	3	BMA	O5-C5-C6-O6
3	Q	3	BMA	O5-C5-C6-O6
7	Y	3	BMA	O5-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

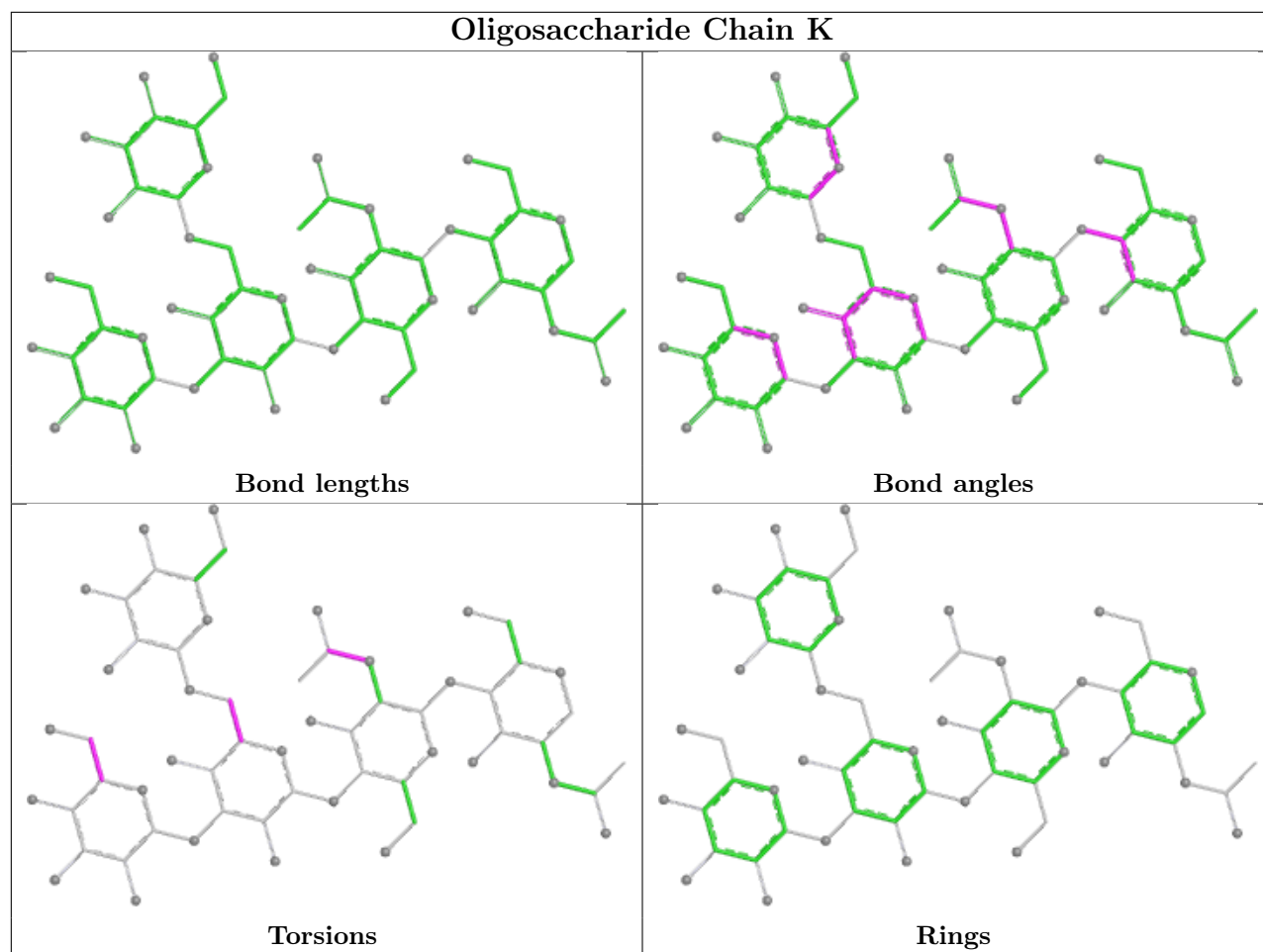
Mol	Chain	Res	Type	Atoms
3	T	4	MAN	C1-C2-C3-C4-C5-O5

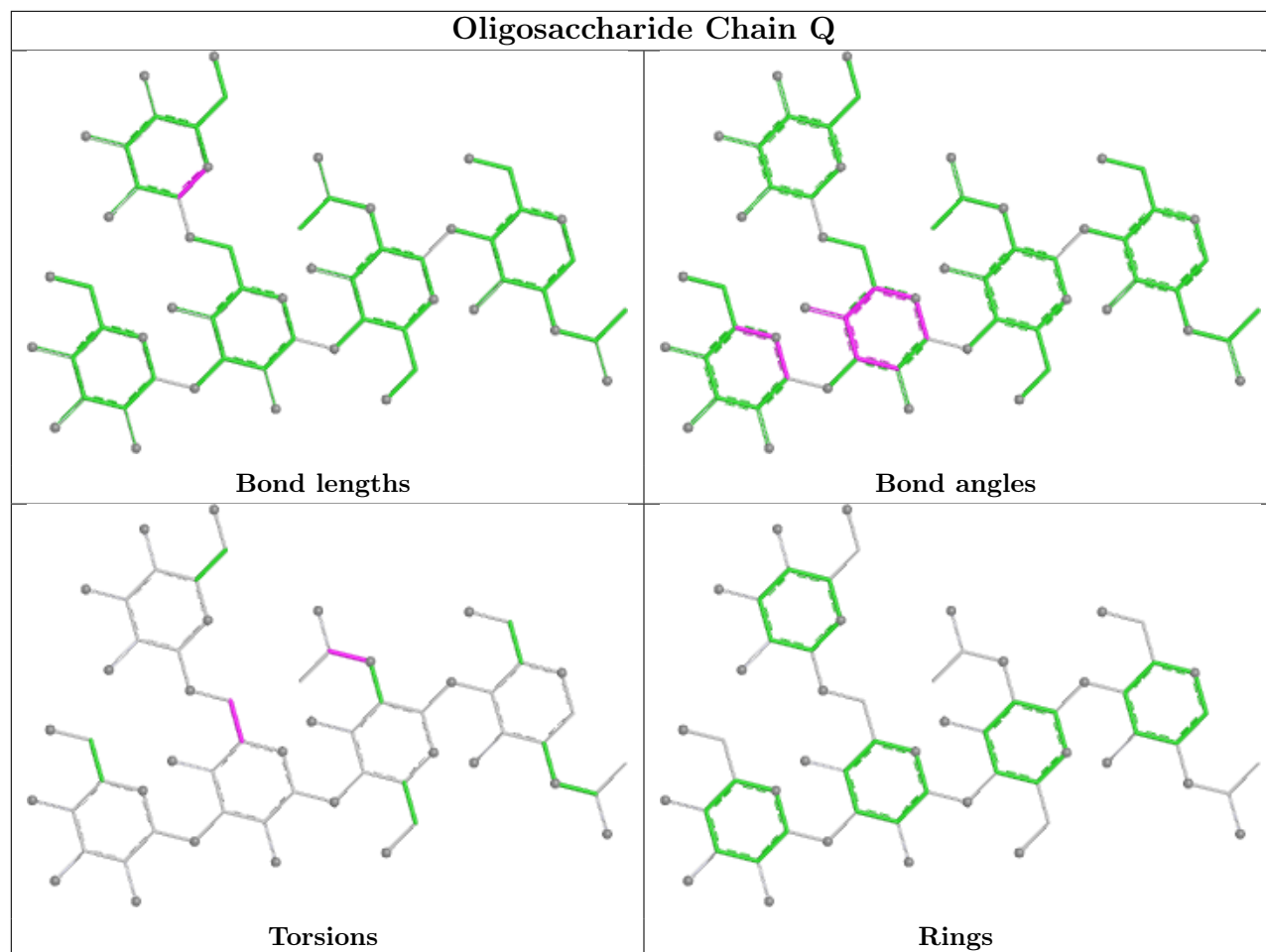
6 monomers are involved in 5 short contacts:

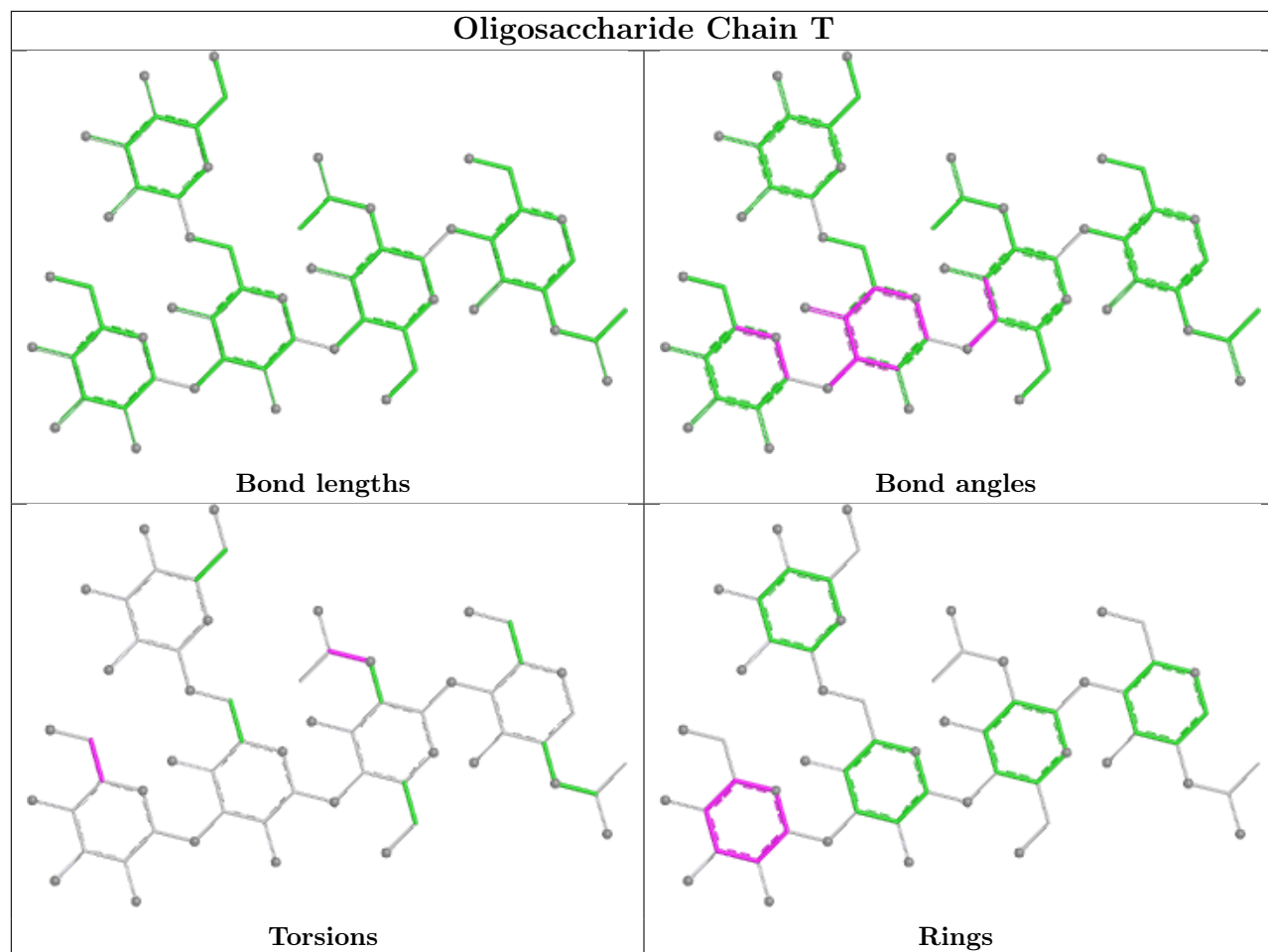
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	P	5	NAG	1	0
5	O	4	MAN	1	0
6	P	1	NAG	2	0
5	O	3	BMA	1	0
7	S	1	NAG	1	0
6	P	4	MAN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

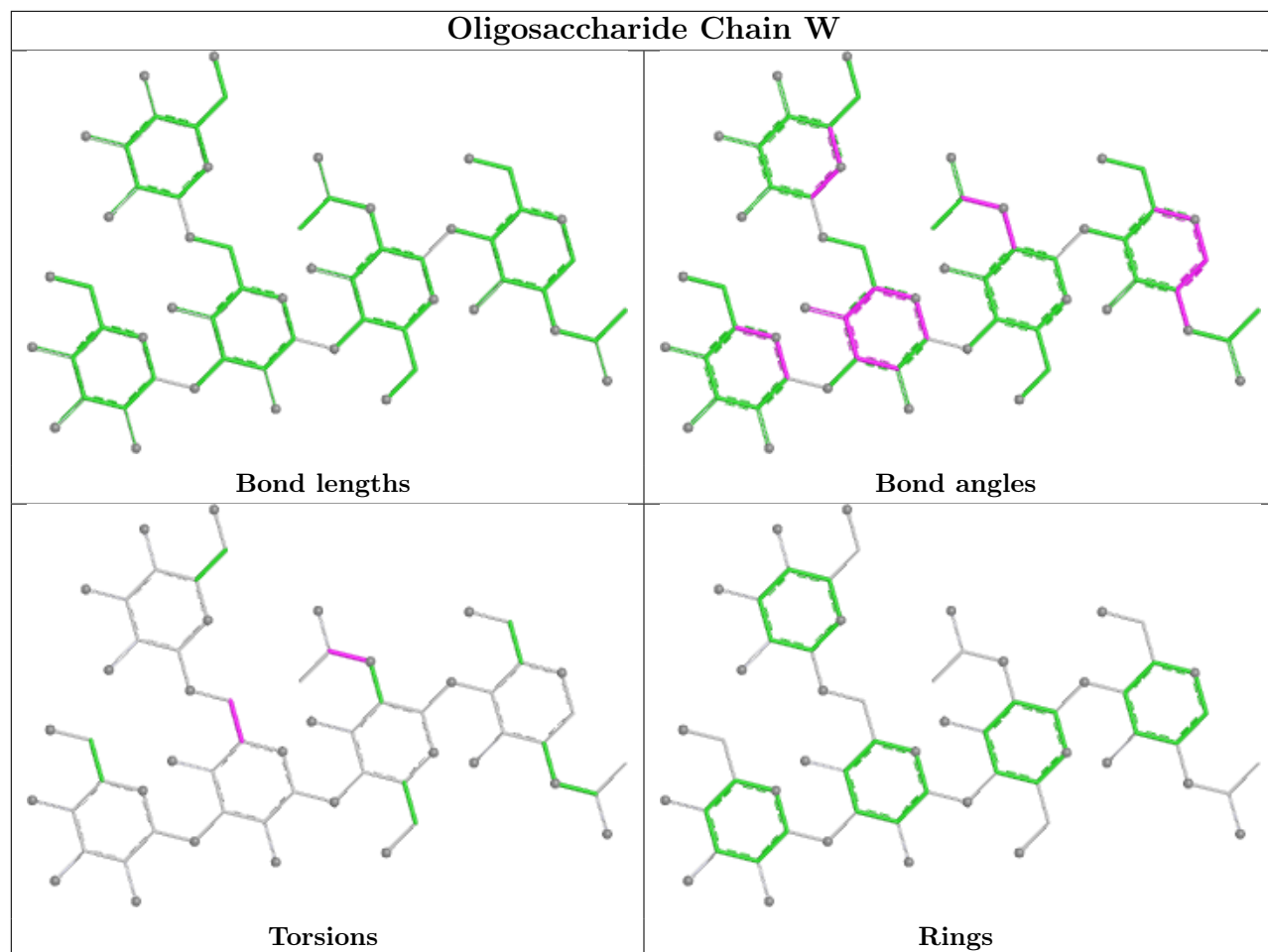
bond angles, torsion angles, and ring geometry for oligosaccharide.

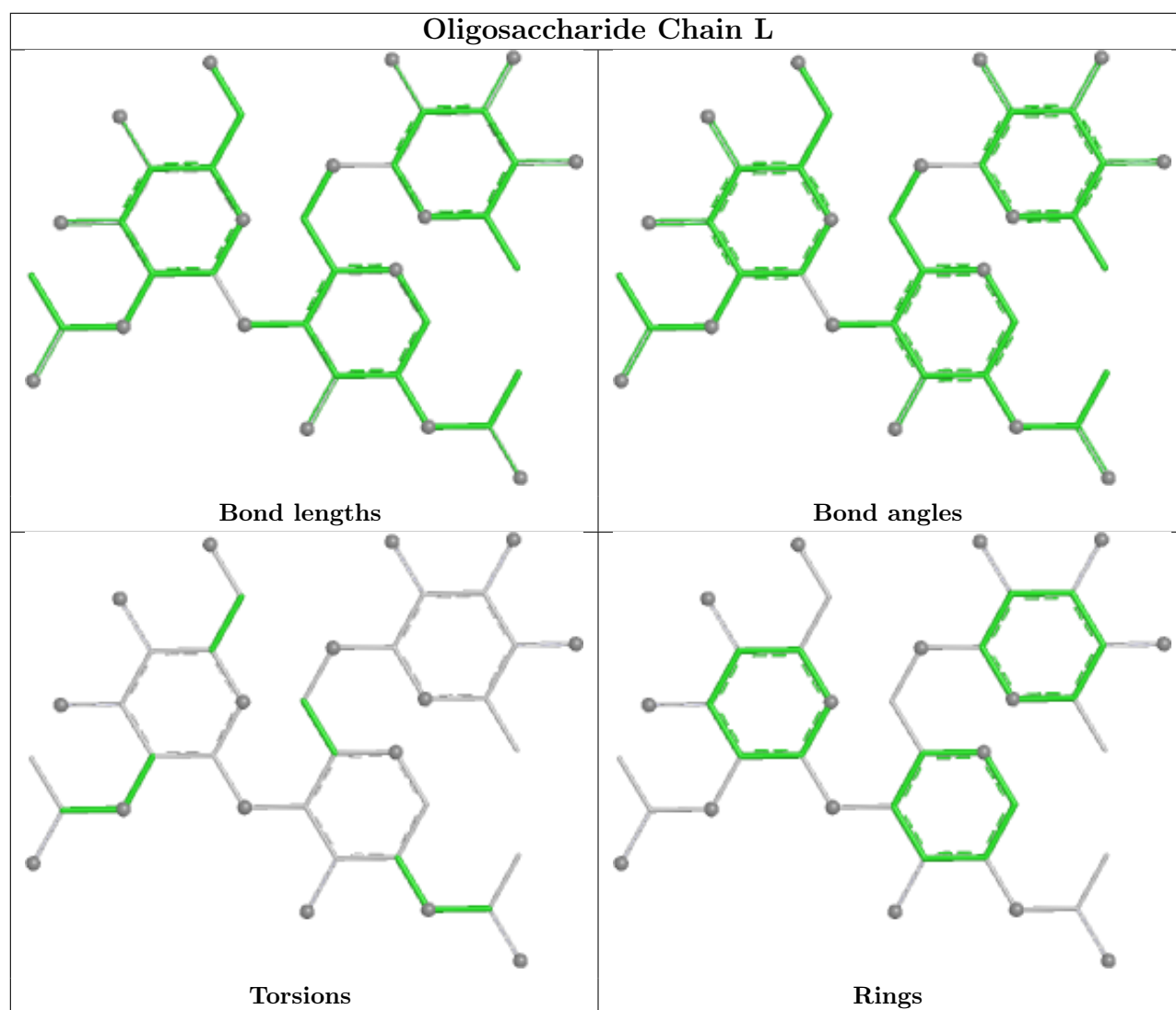


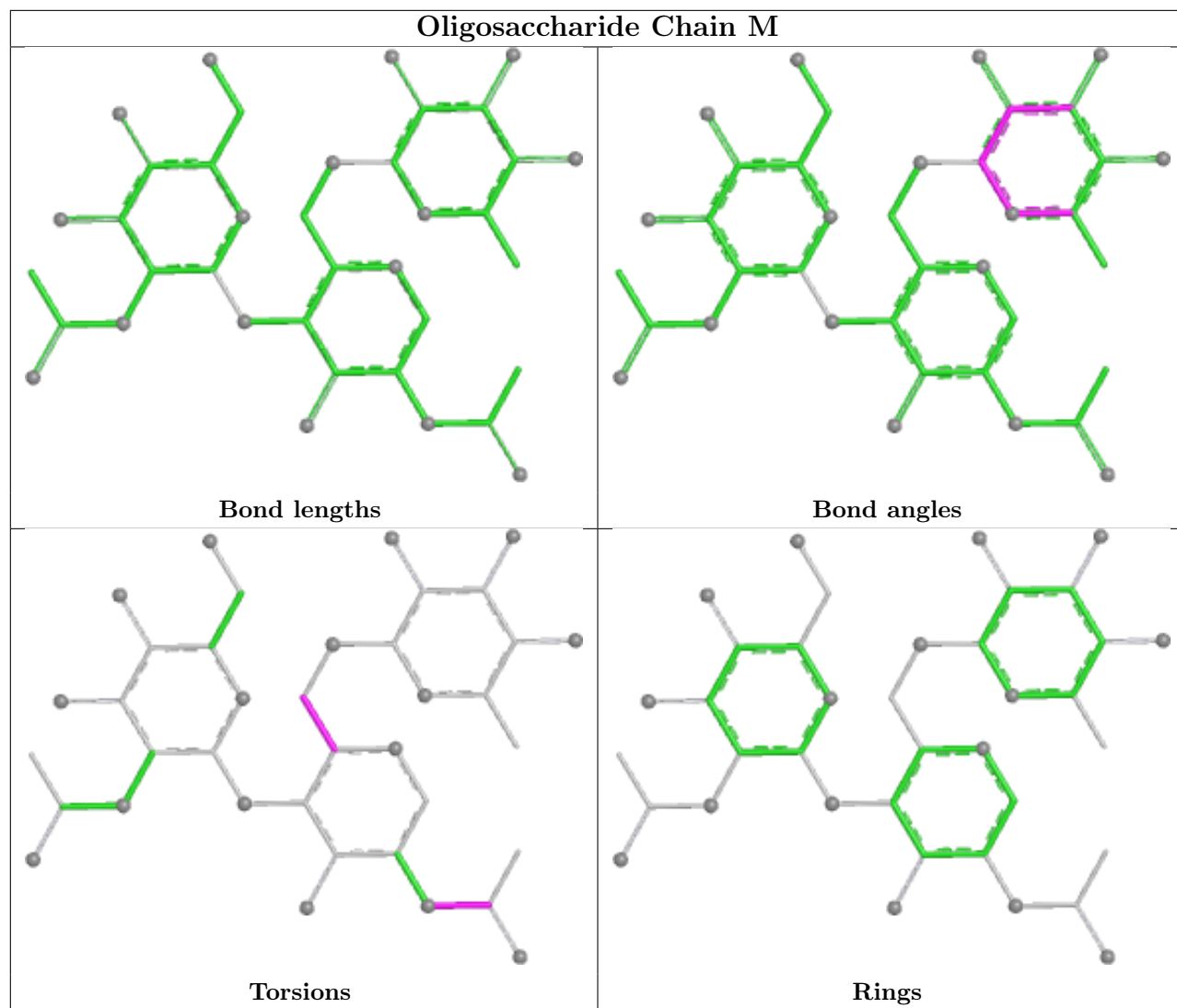


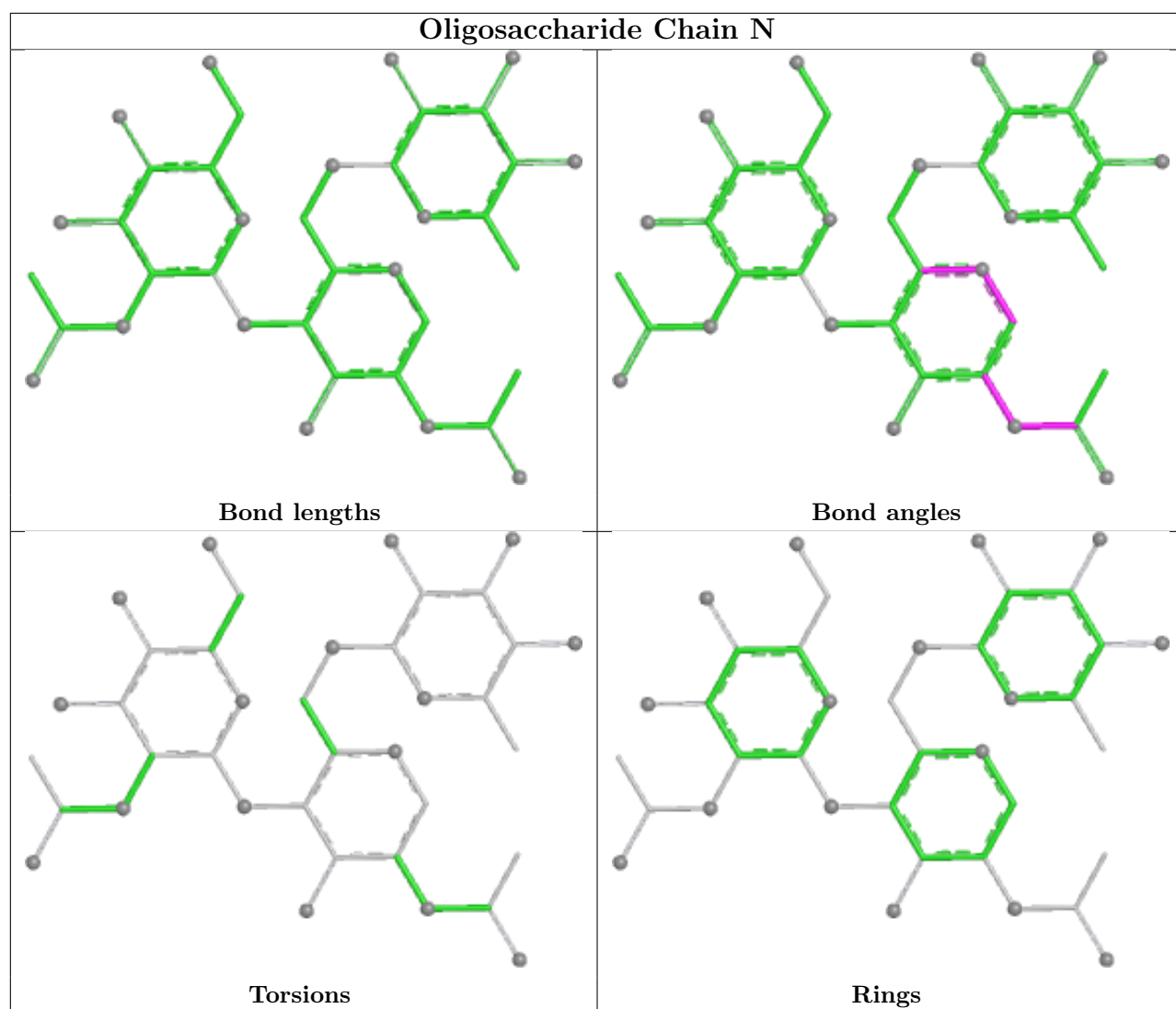


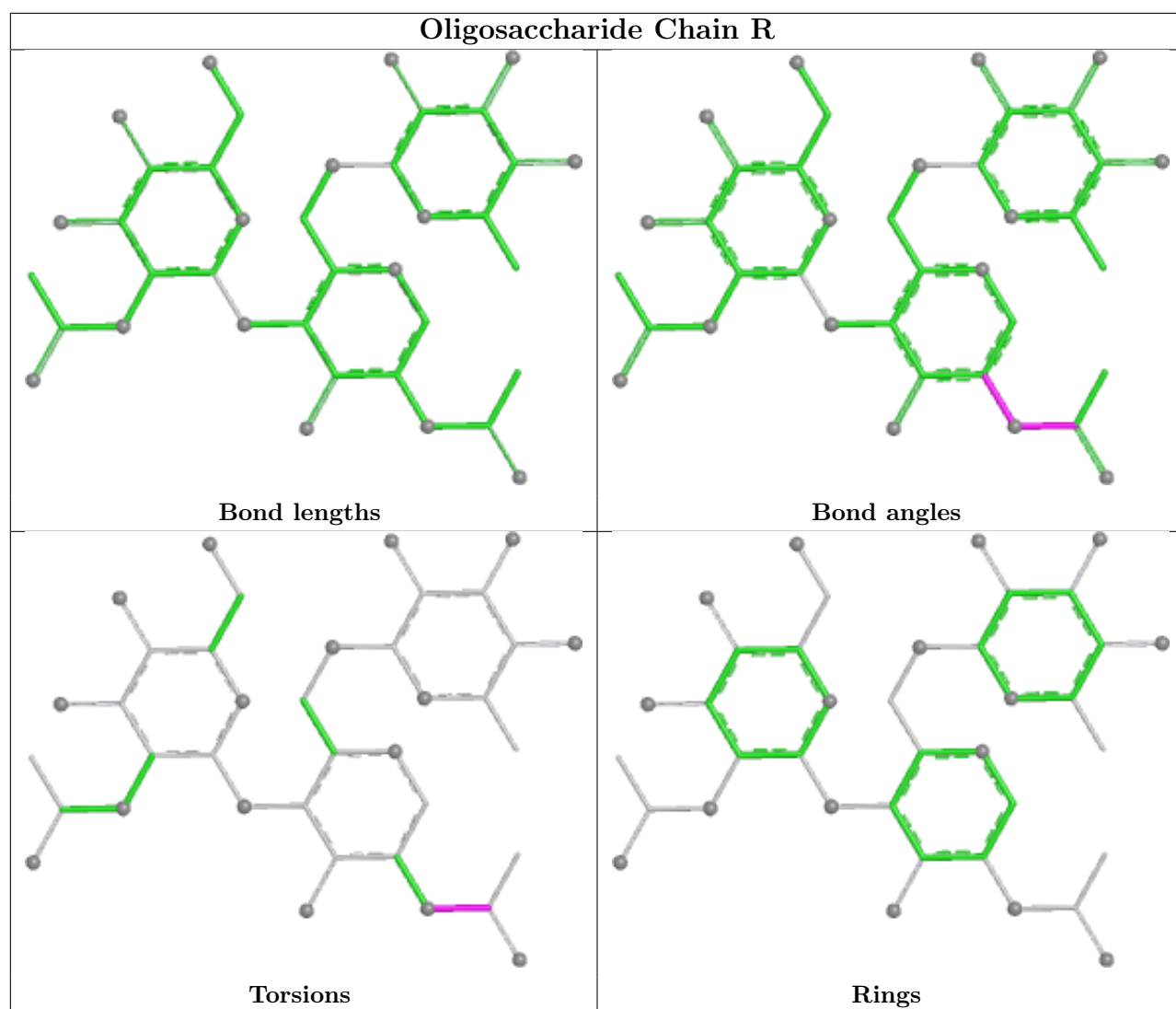


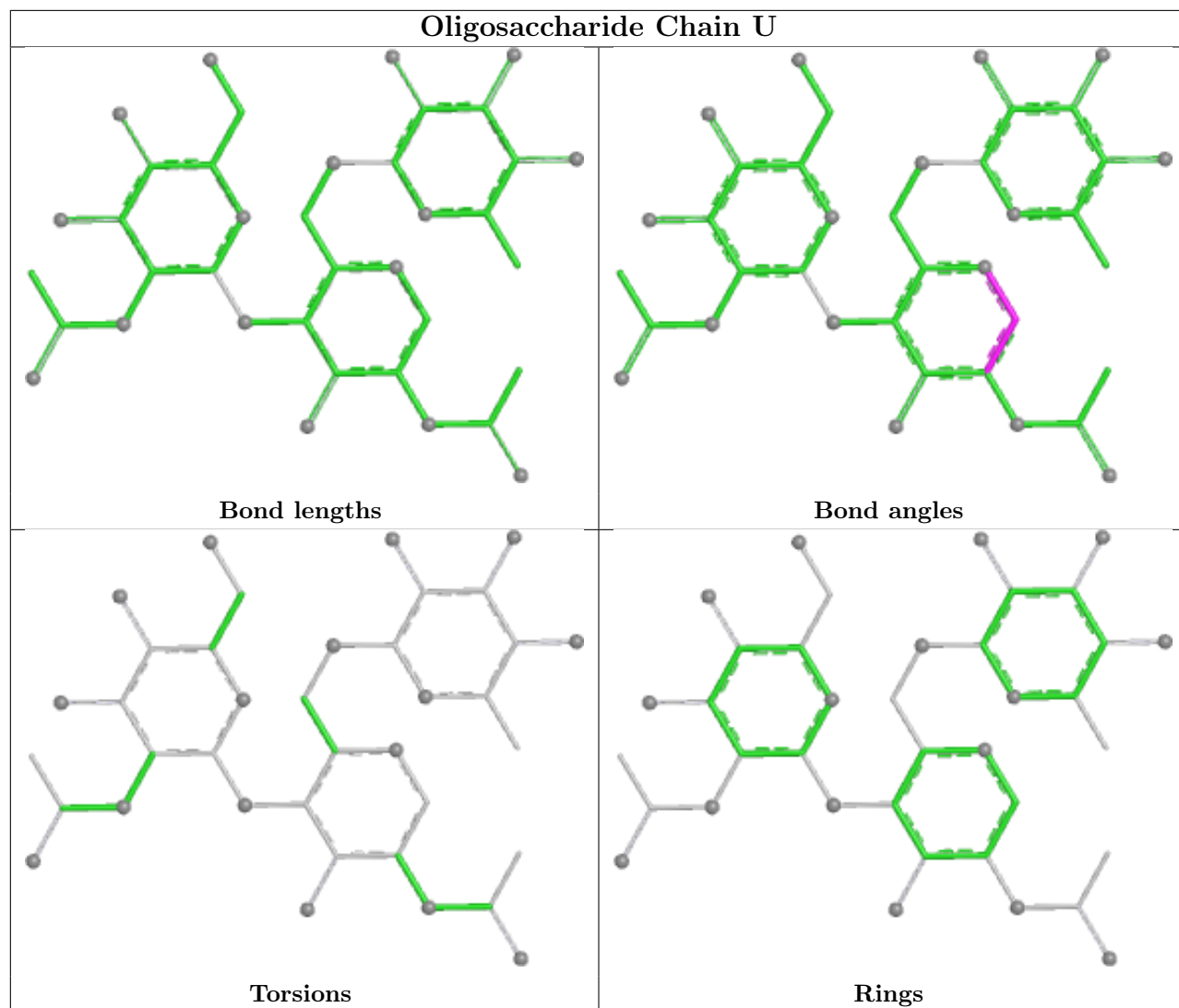


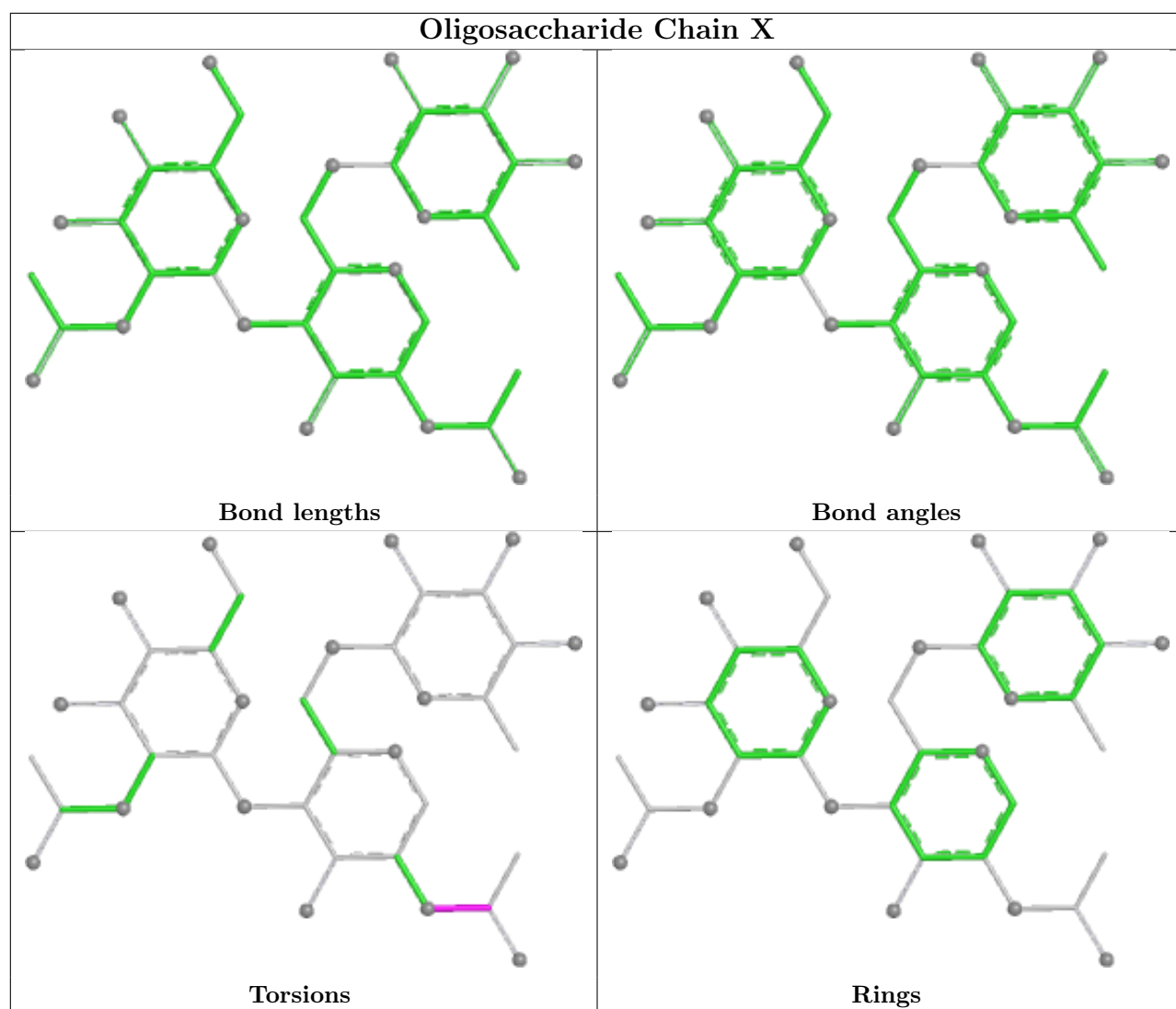


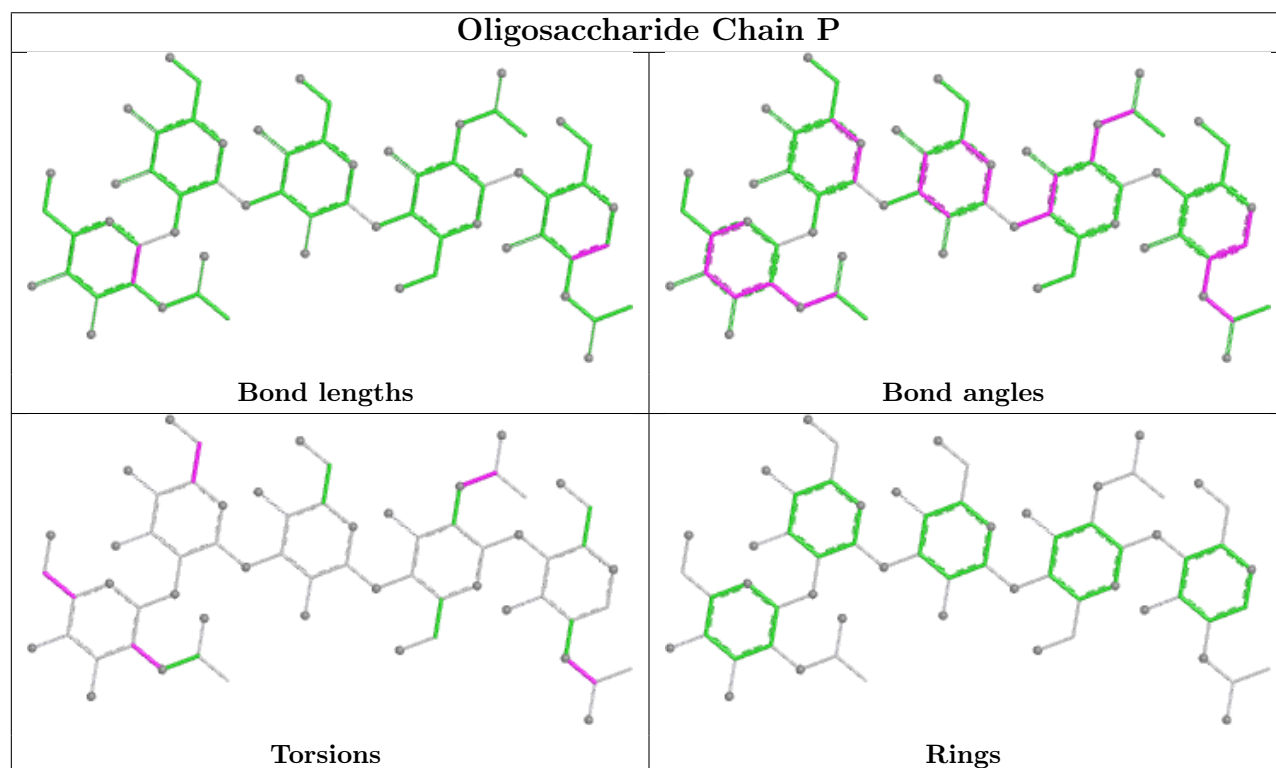
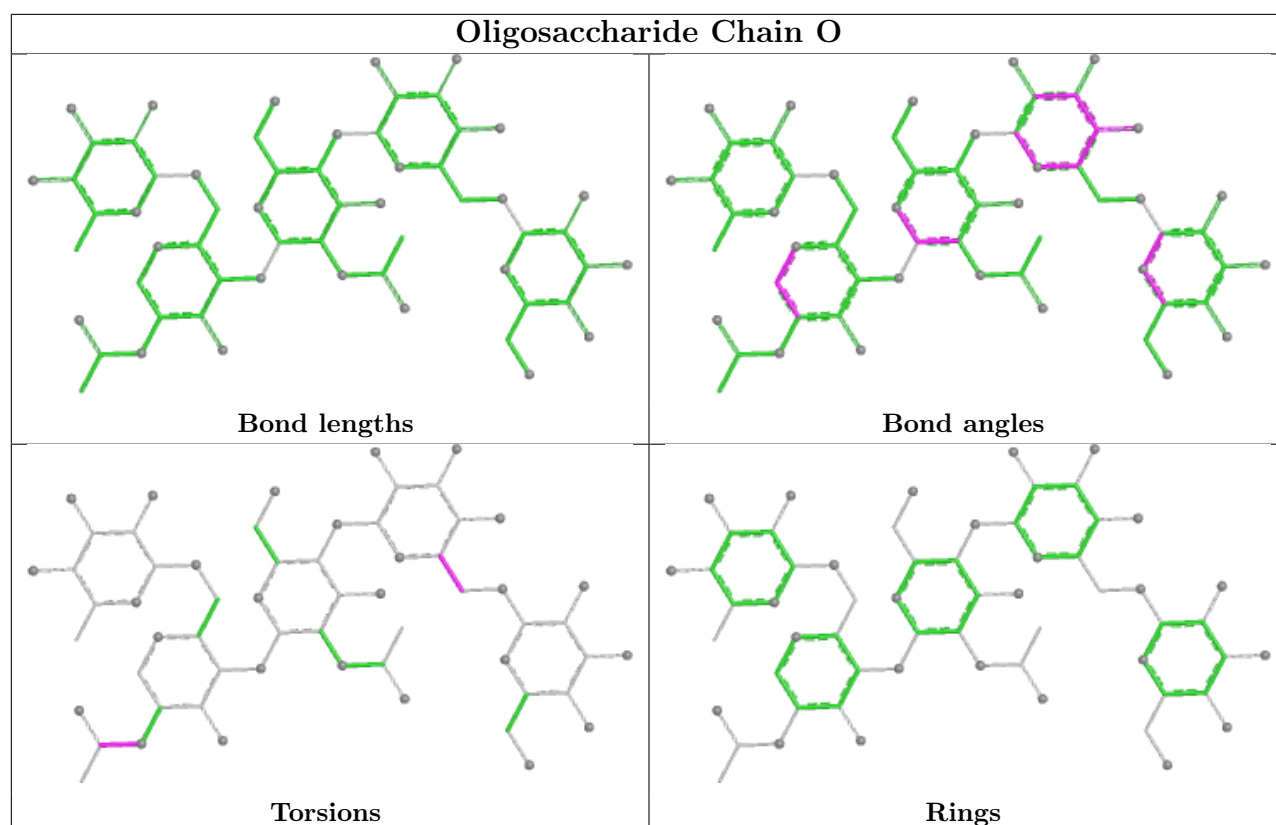




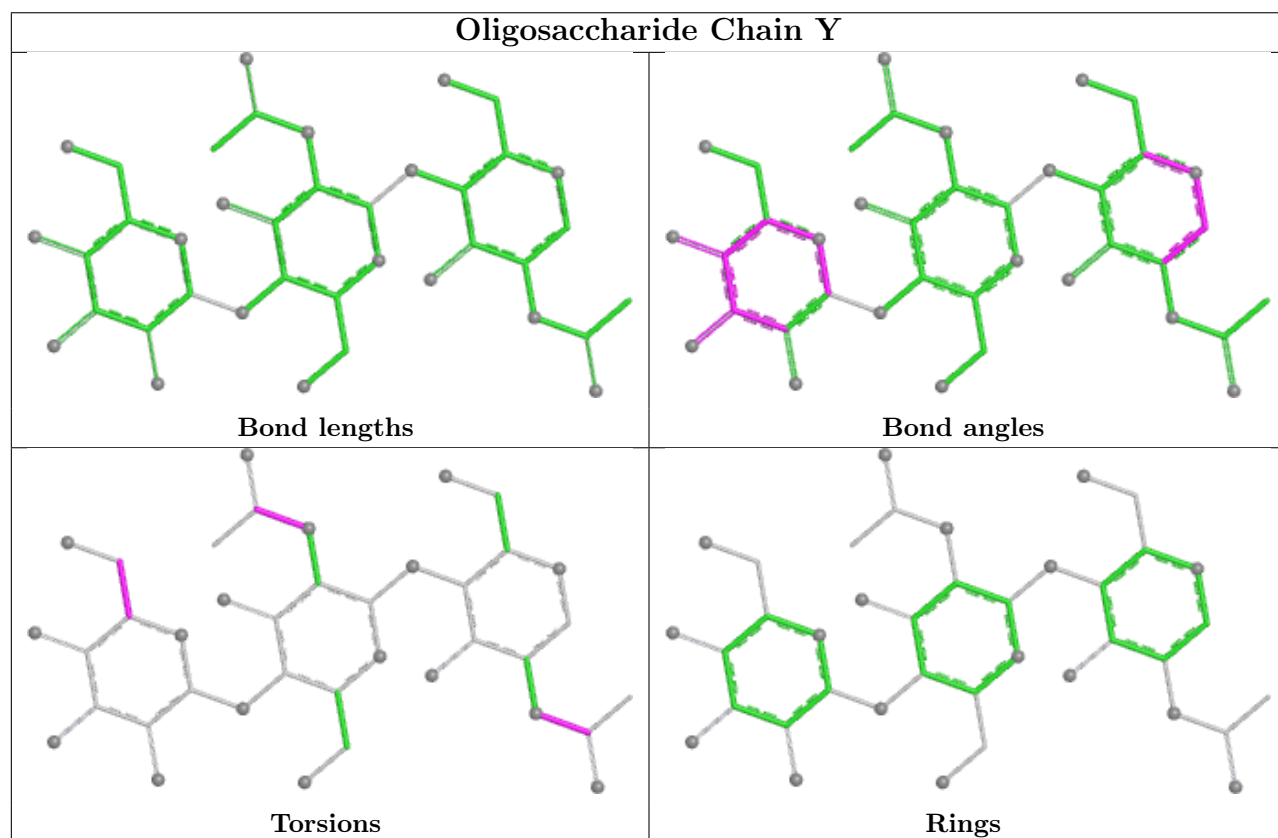
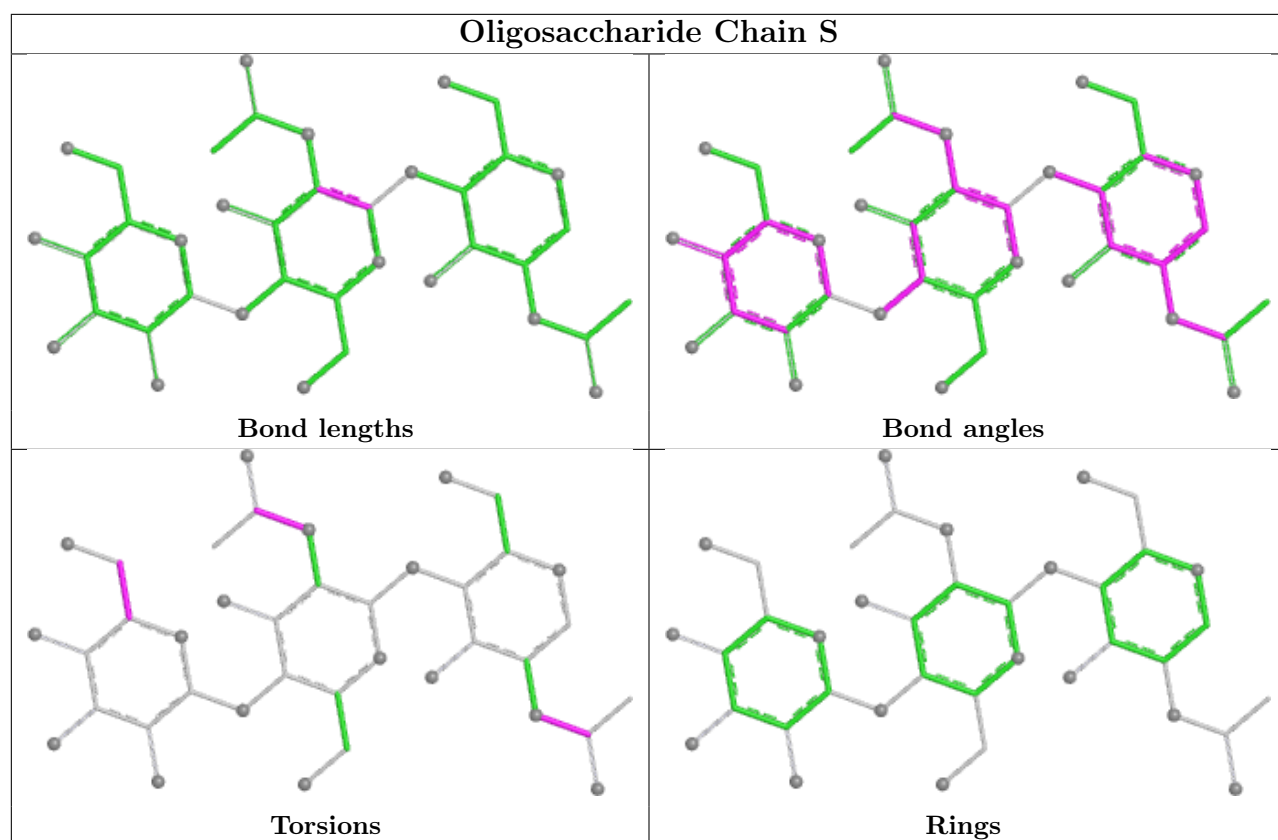


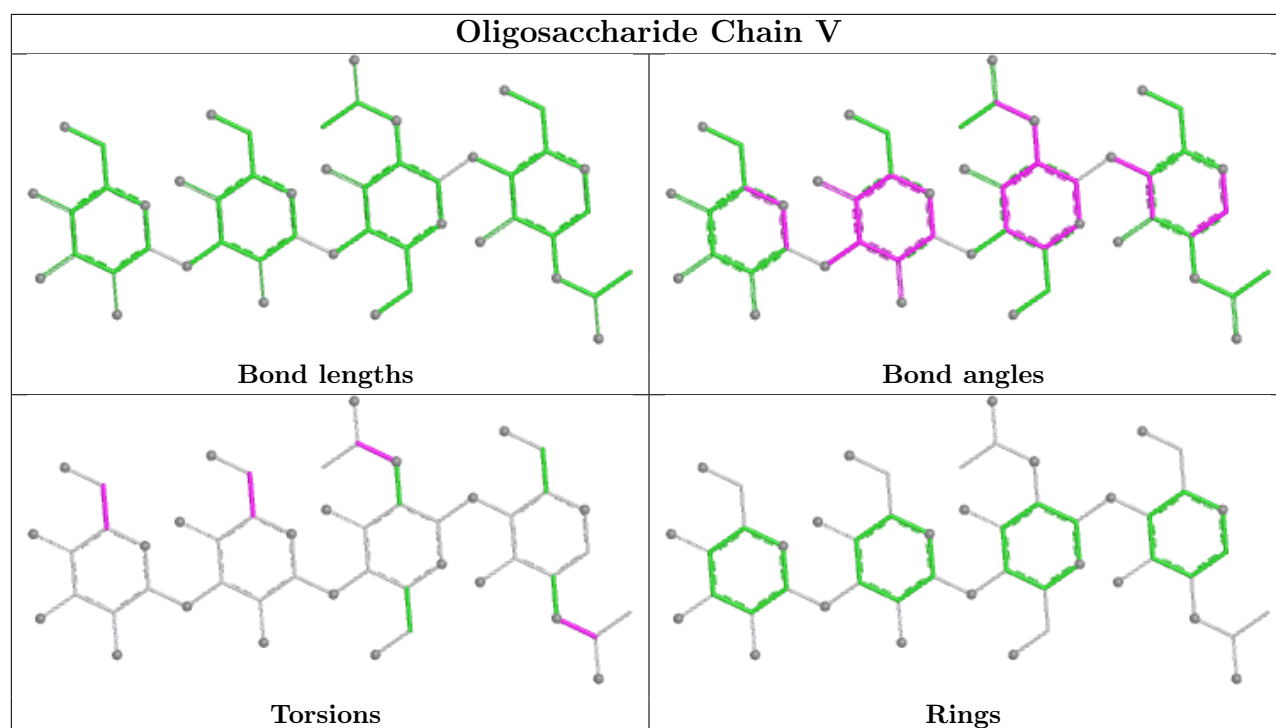












## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

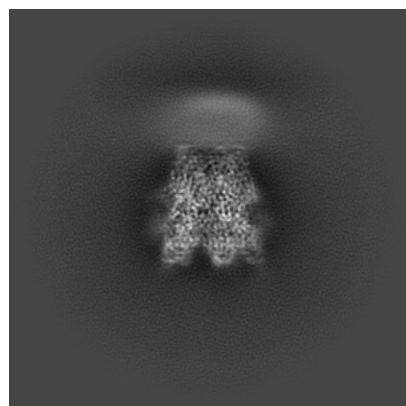
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53355. These allow visual inspection of the internal detail of the map and identification of artifacts.

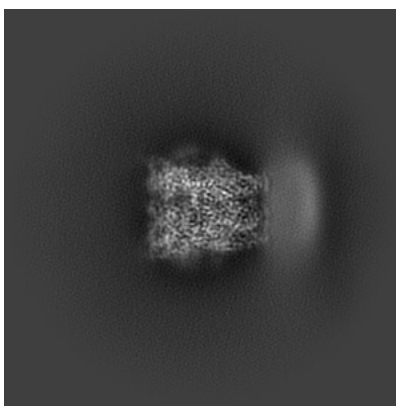
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

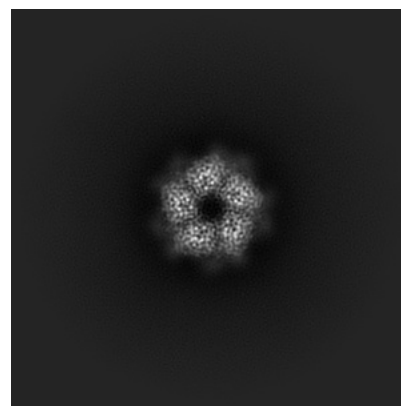
#### 6.1.1 Primary map



X

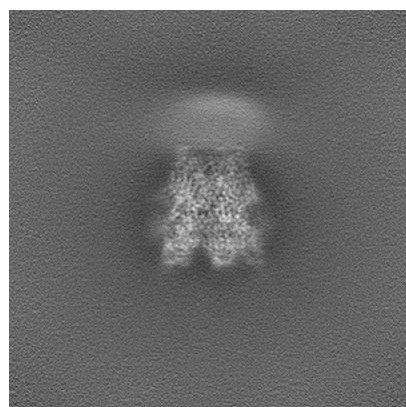


Y

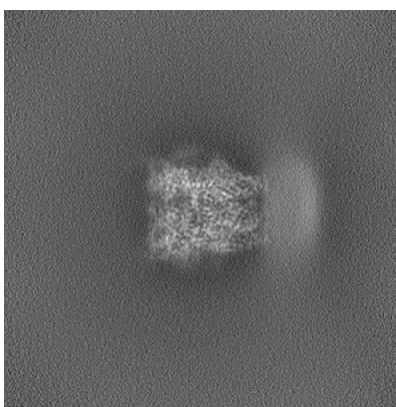


Z

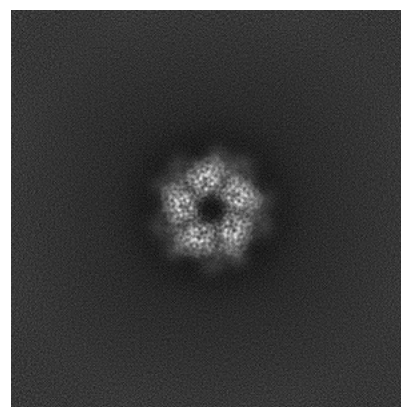
#### 6.1.2 Raw map



X



Y

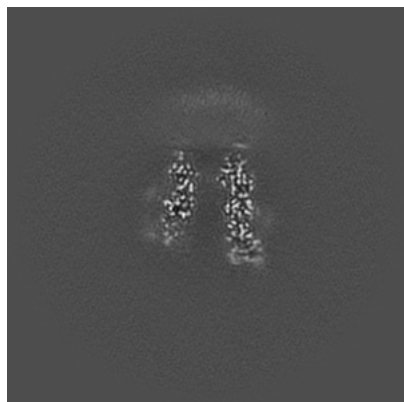


Z

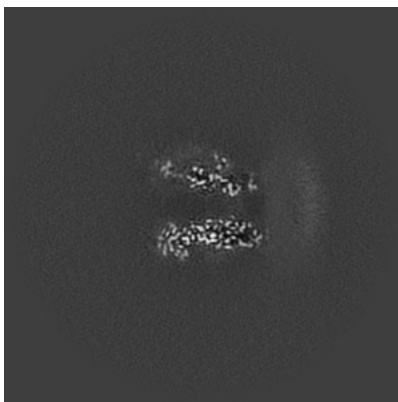
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

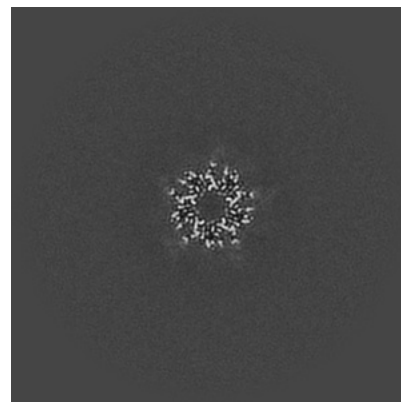
### 6.2.1 Primary map



X Index: 250

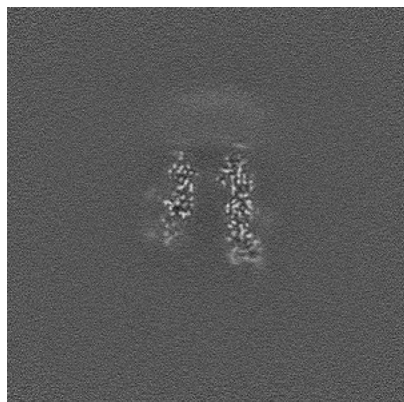


Y Index: 250

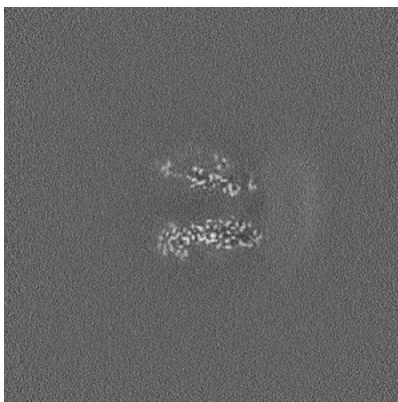


Z Index: 250

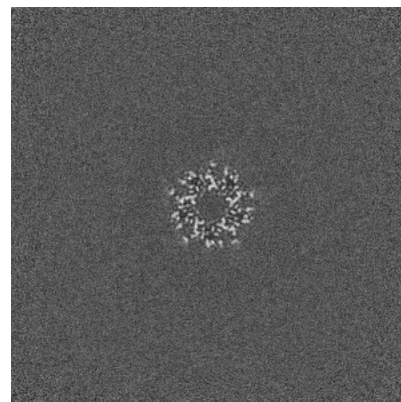
### 6.2.2 Raw map



X Index: 250



Y Index: 250

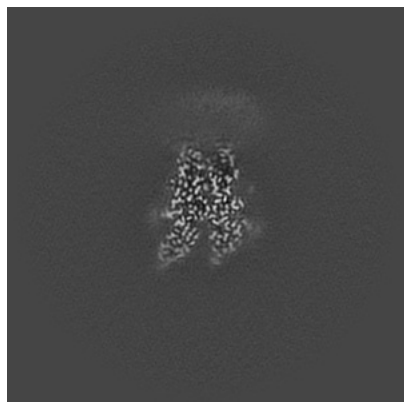


Z Index: 250

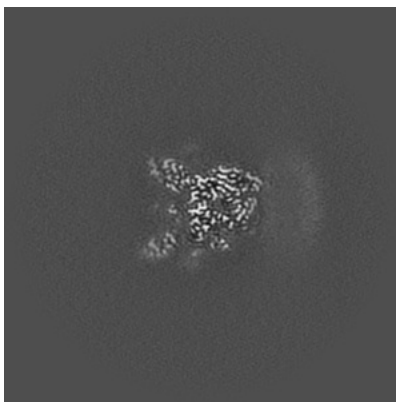
The images above show central slices of the map in three orthogonal directions.

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

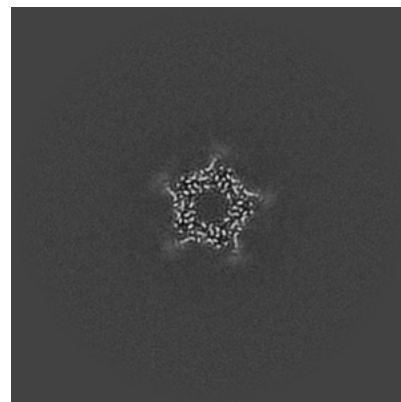
### 6.3.1 Primary map



X Index: 281

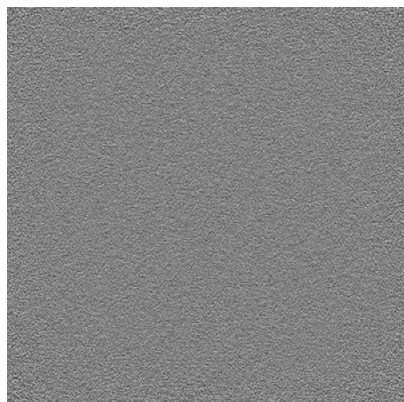


Y Index: 275

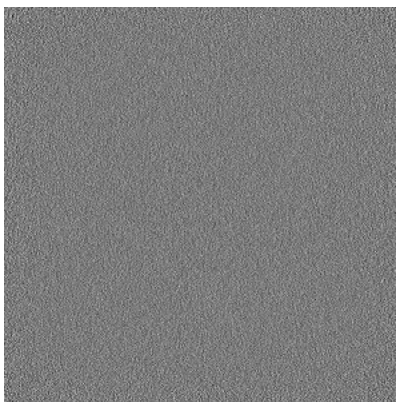


Z Index: 242

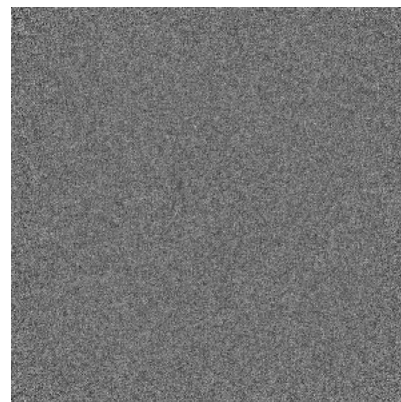
### 6.3.2 Raw map



X Index: 0



Y Index: 0



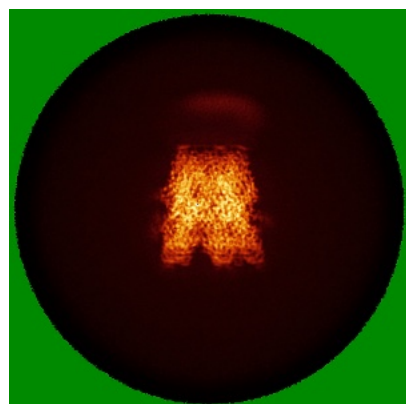
Z Index: 499

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

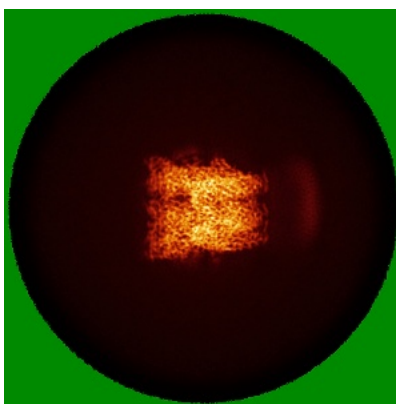


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

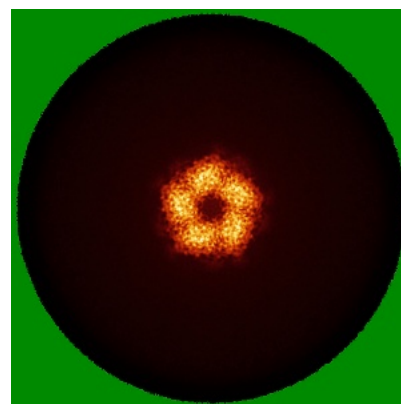
### 6.4.1 Primary map



X

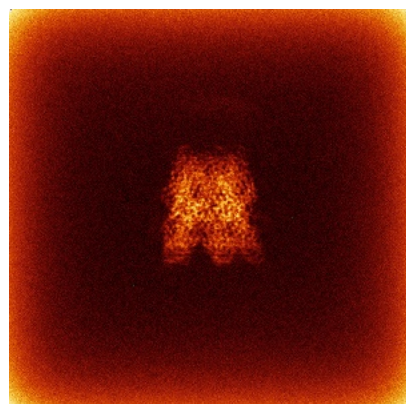


Y

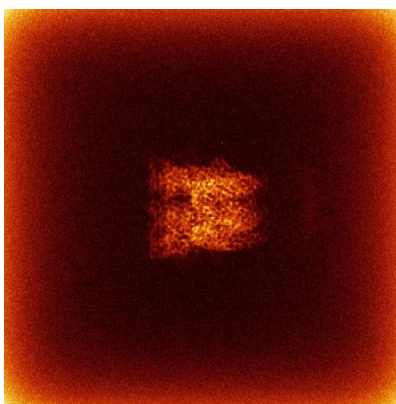


Z

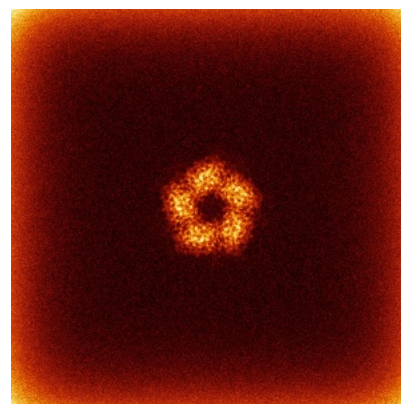
### 6.4.2 Raw map



X



Y

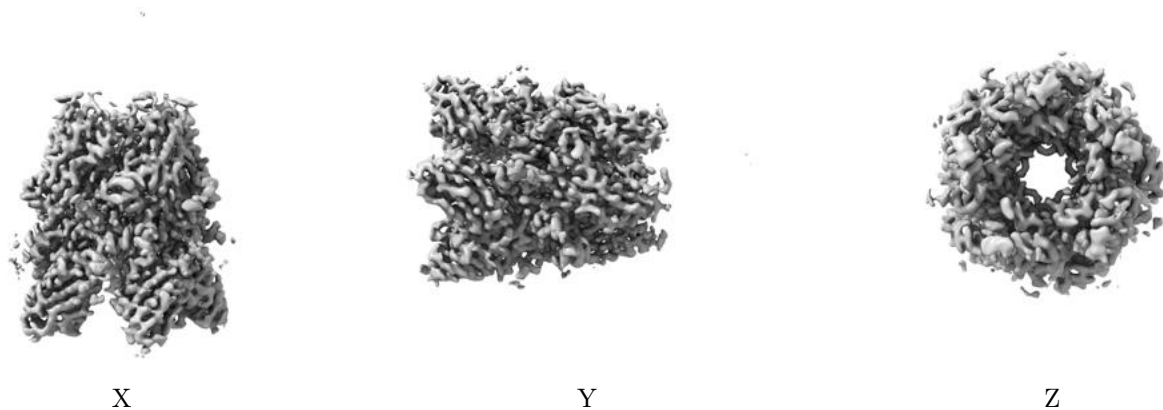


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

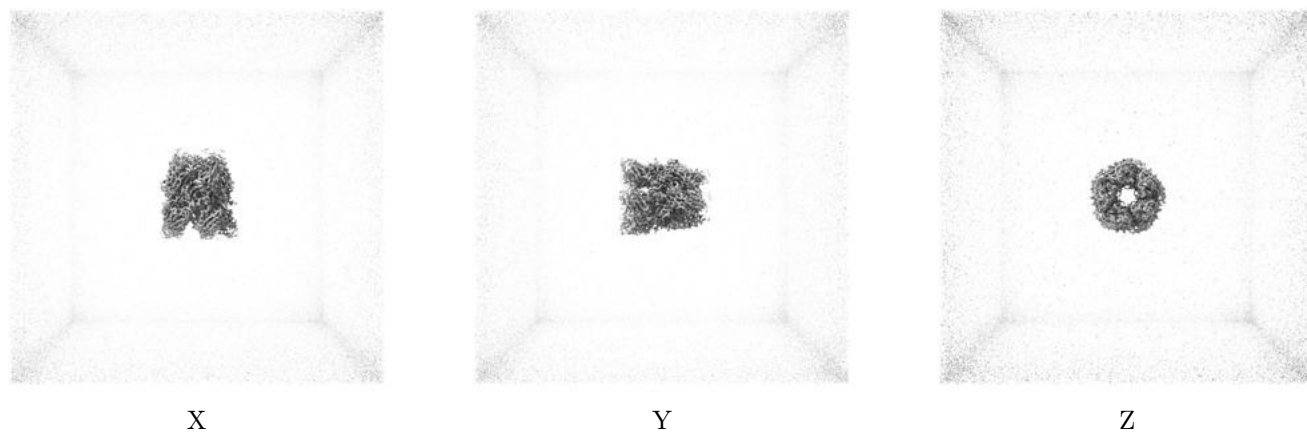
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

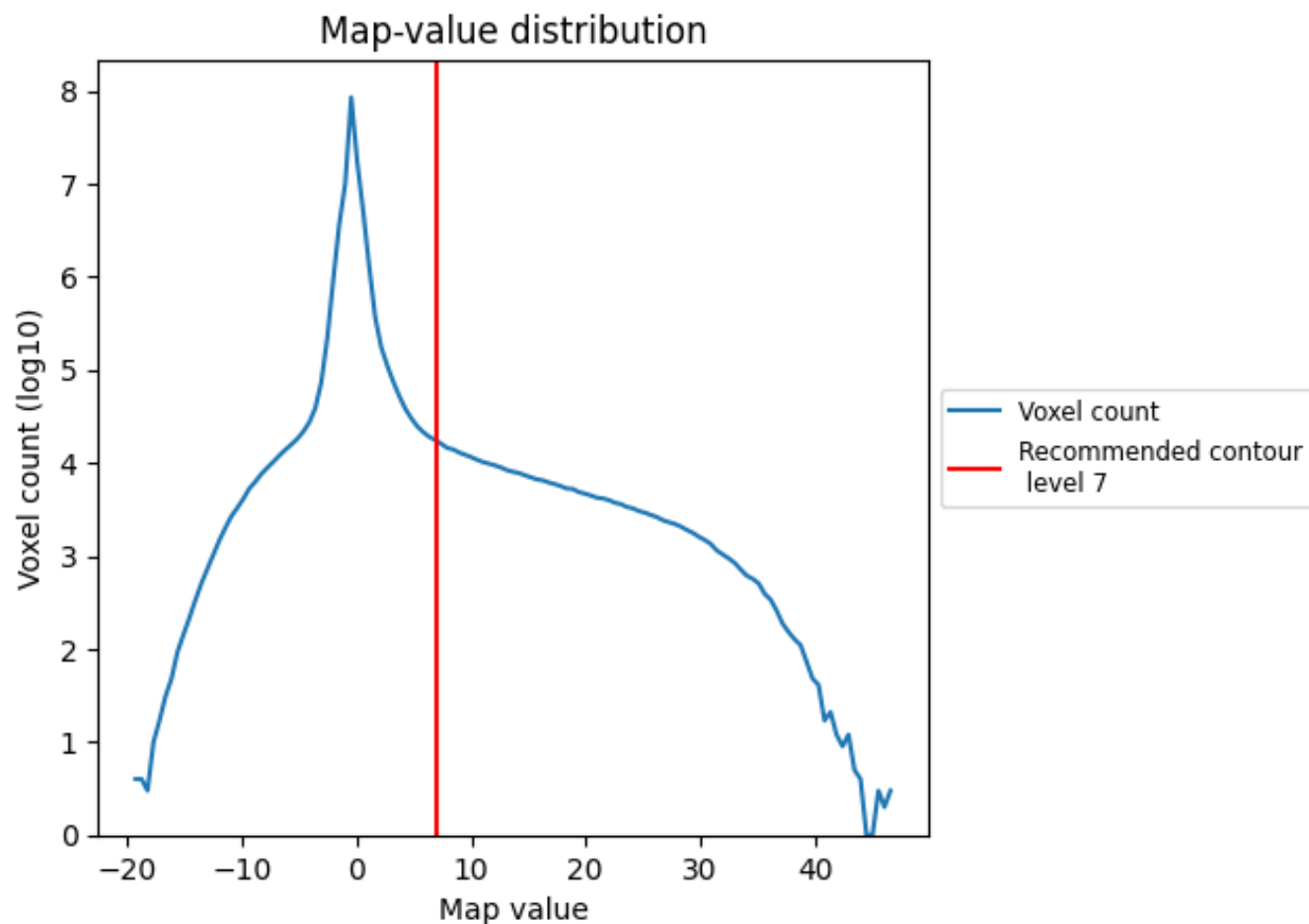
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

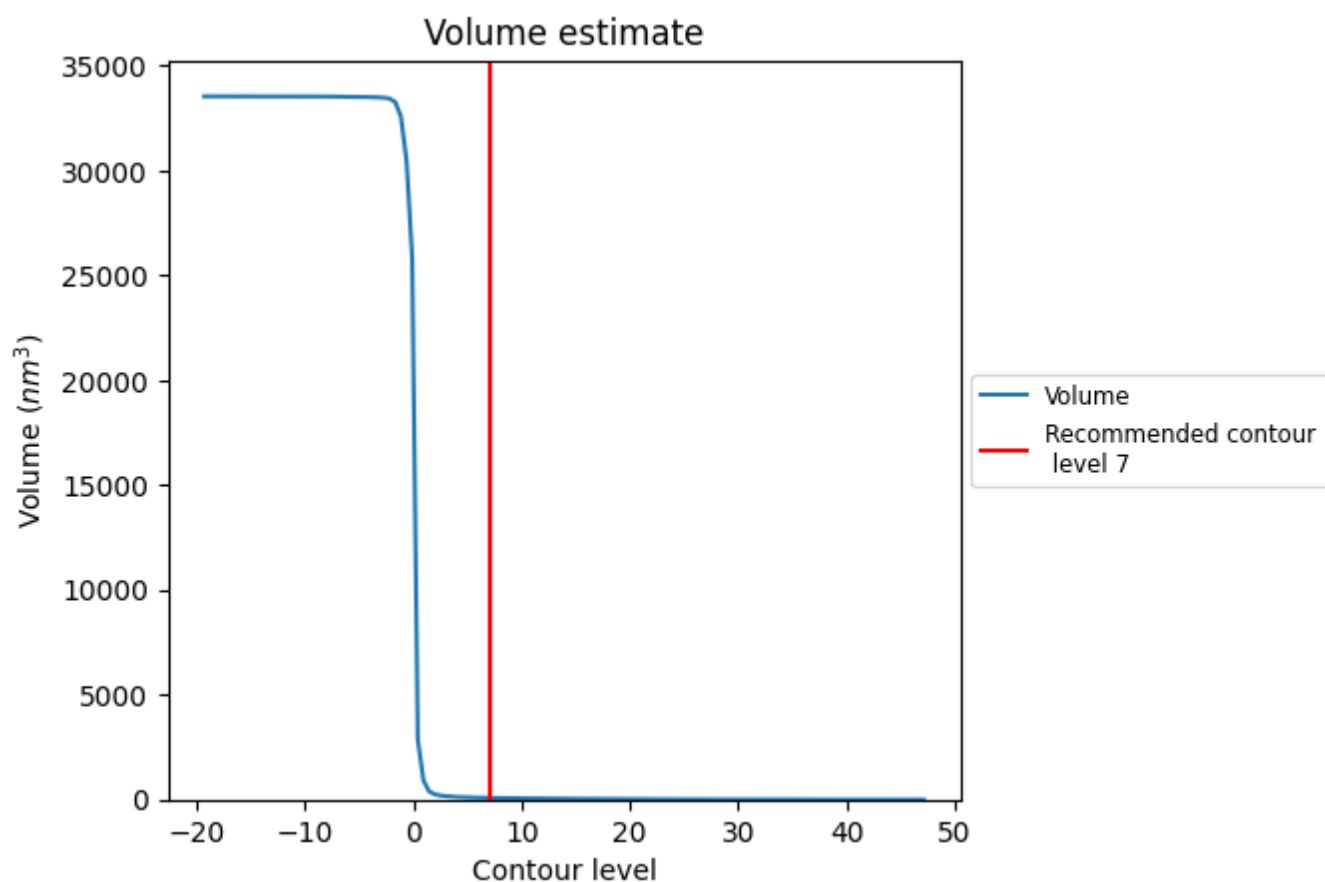
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



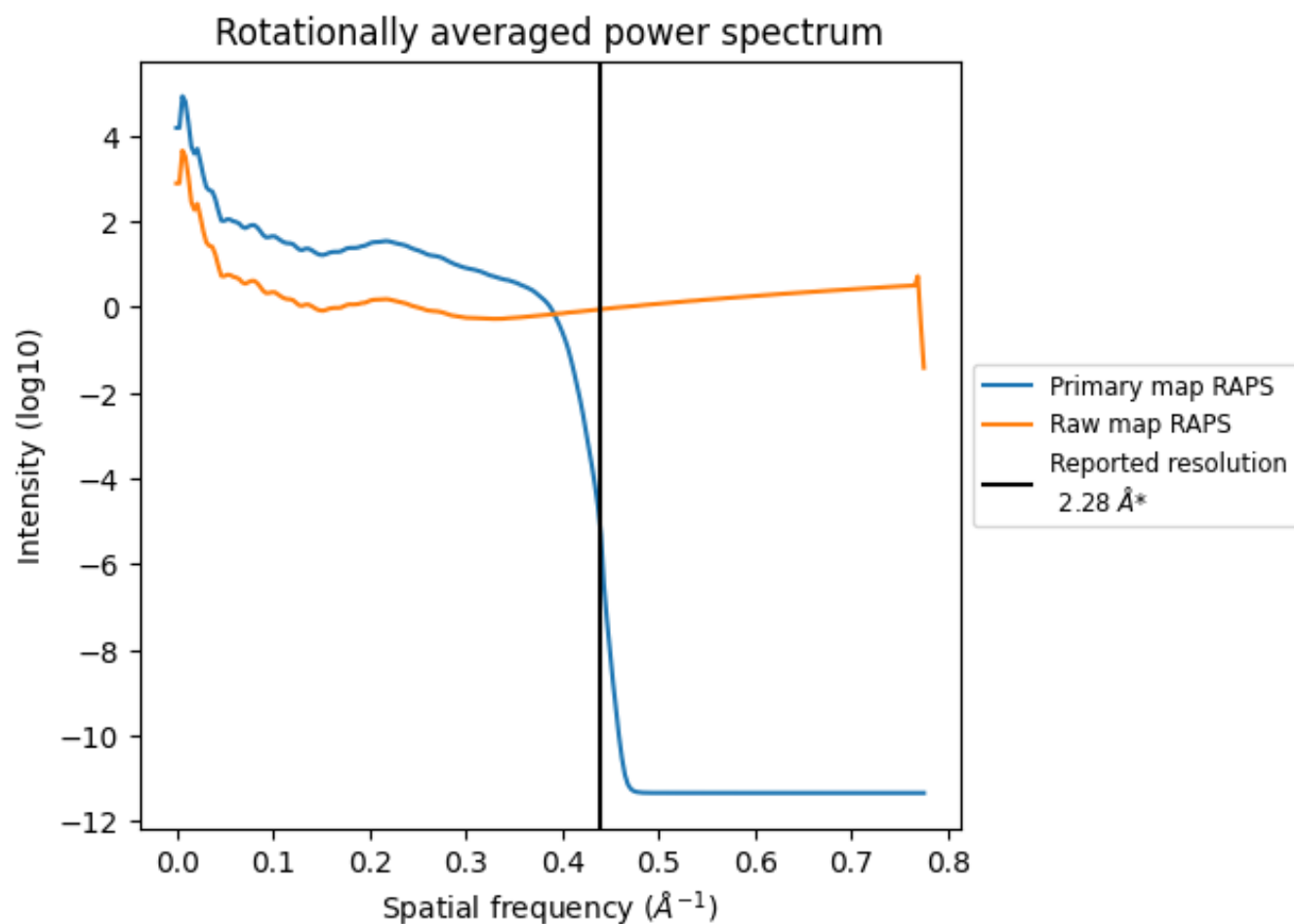
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm<sup>3</sup>; this corresponds to an approximate mass of 73 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 ⓘ

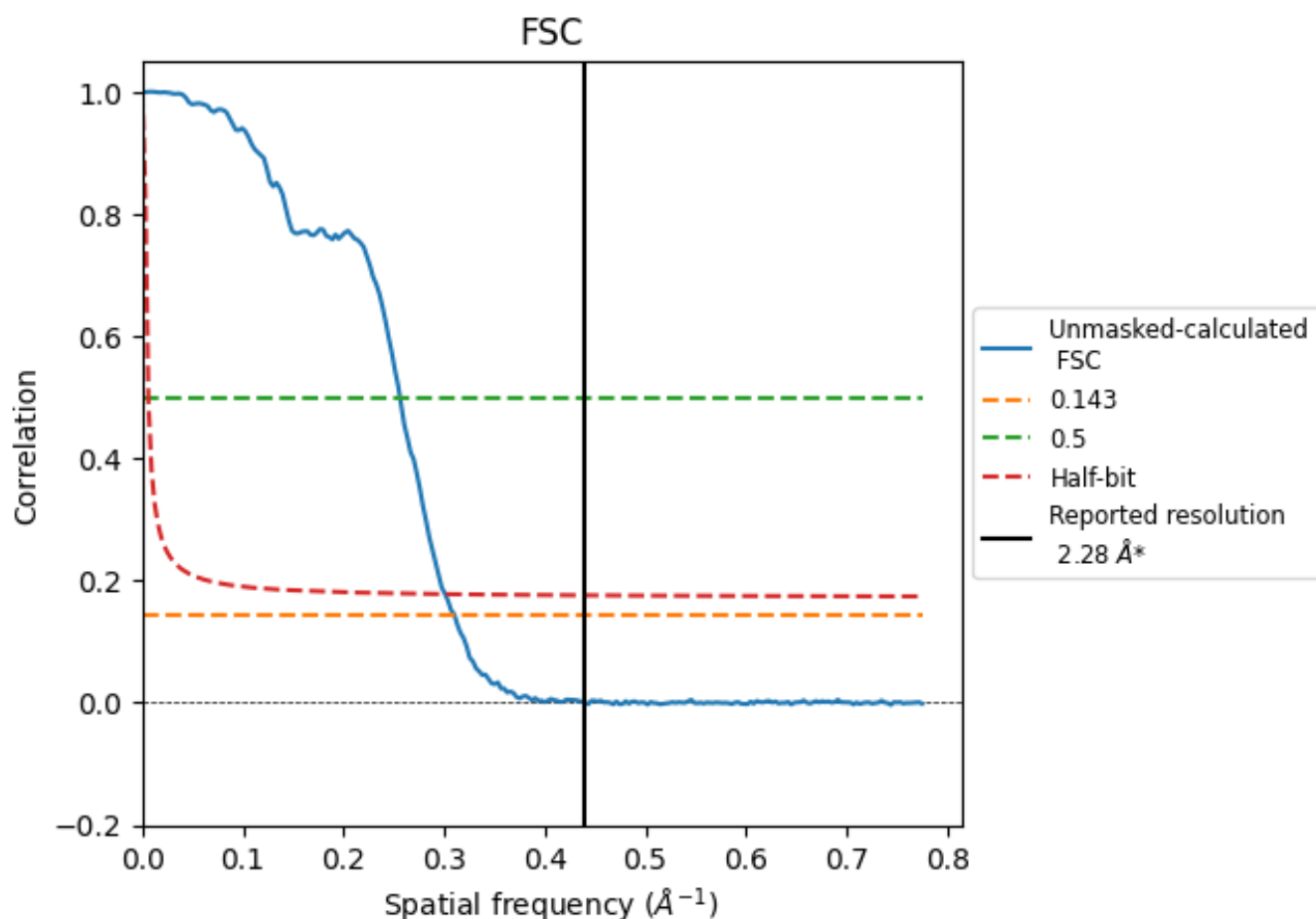


\*Reported resolution corresponds to spatial frequency of 0.439 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

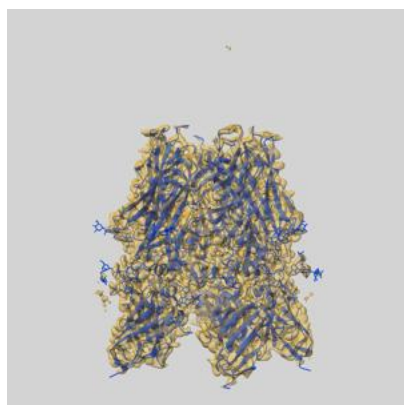
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.28	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.22	3.90	3.32

\*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 3.22 differs from the reported value 2.28 by more than 10 %

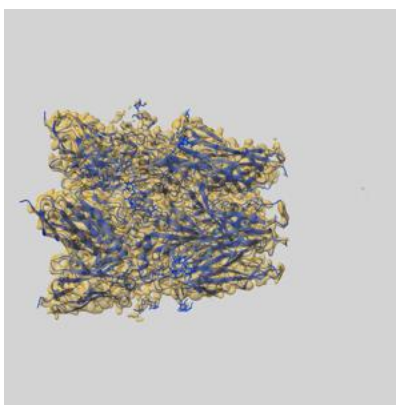
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53355 and PDB model 9QTN. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

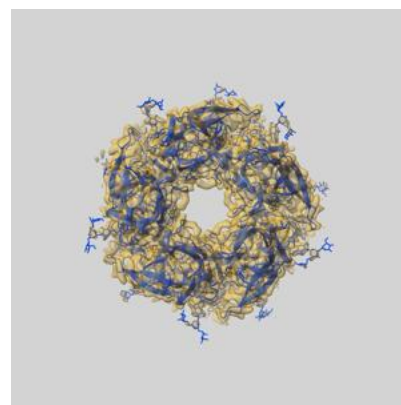
### 9.1 Map-model overlay [i](#)



X



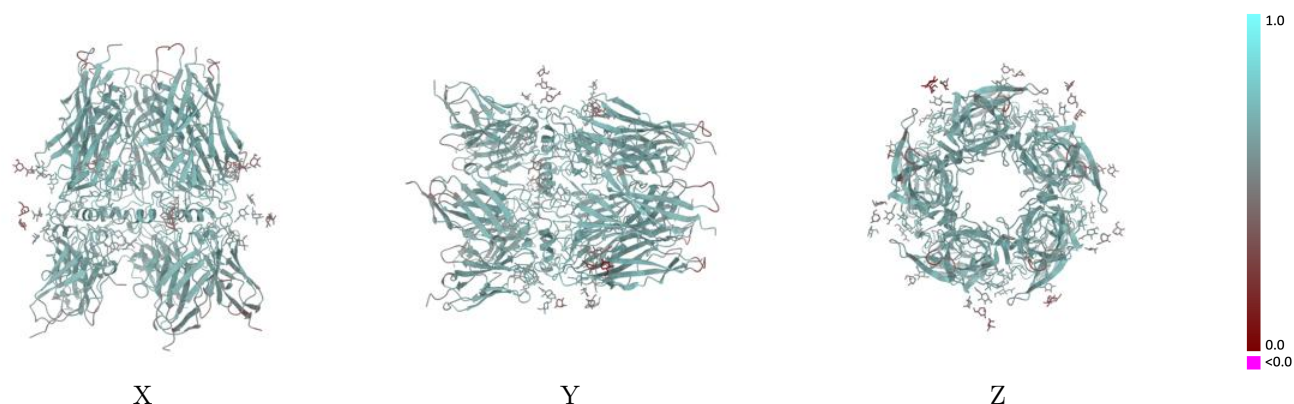
Y



Z

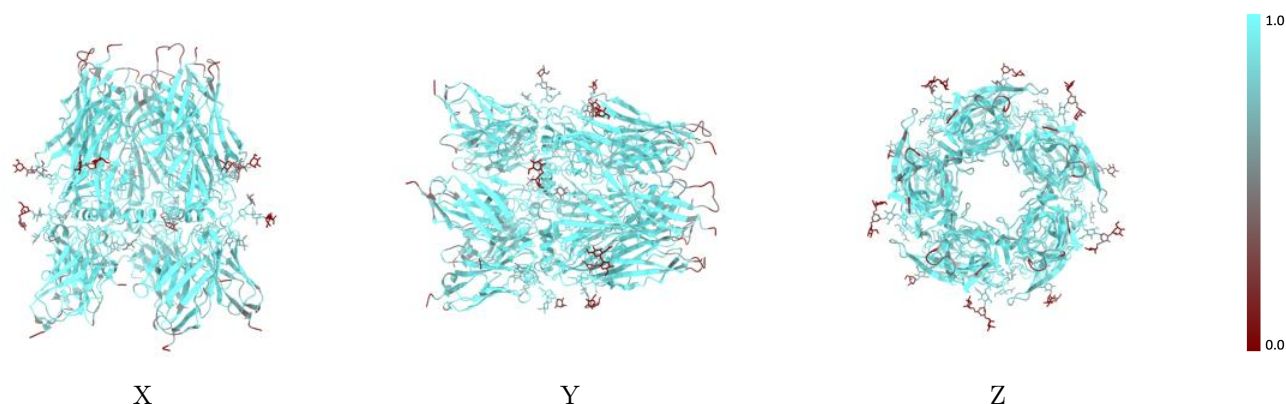
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



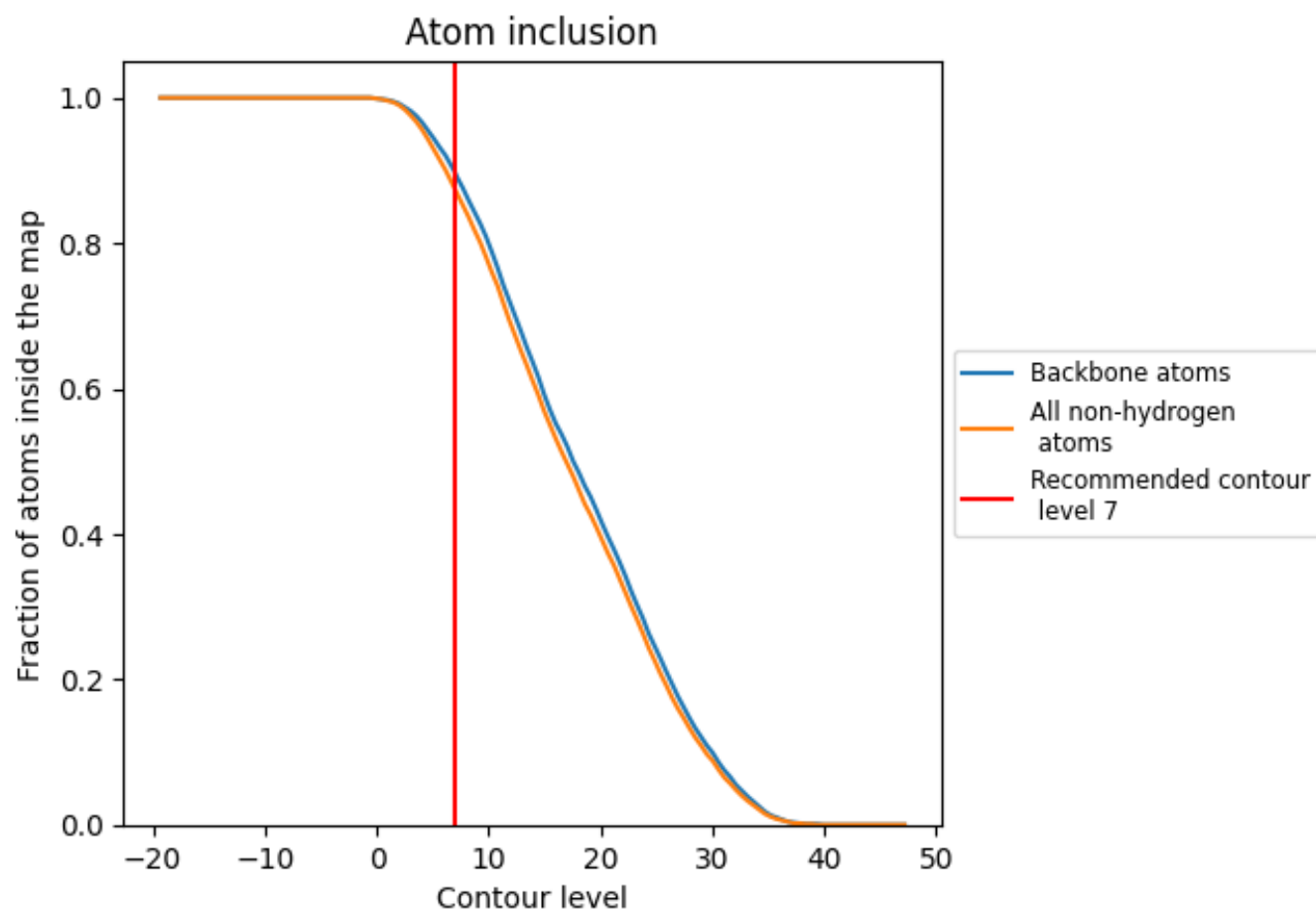
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7).





















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.6100
A	 0.8960	 0.6230
B	 0.8920	 0.6240
C	 0.9010	 0.6270
D	 0.9040	 0.6270
E	 0.8980	 0.6260
F	 0.8980	 0.6070
G	 0.8850	 0.5990
H	 0.8790	 0.6020
I	 0.8850	 0.6030
J	 0.8780	 0.5980
K	 0.4590	 0.5200
L	 0.7110	 0.5300
M	 0.6580	 0.4960
N	 0.7370	 0.5420
O	 0.4670	 0.4930
P	 0.4530	 0.3700
Q	 0.4920	 0.4810
R	 0.7370	 0.5190
S	 0.5640	 0.4000
T	 0.4750	 0.5280
U	 0.7370	 0.5370
V	 0.4600	 0.4270
W	 0.4750	 0.4750
X	 0.7630	 0.5510
Y	 0.5640	 0.5060

