



## Full wwPDB EM Validation Report ⓘ

Aug 18, 2024 – 01:22 AM JST

PDB ID : 8Y89  
EMDB ID : EMD-39038  
Title : Structure of HCoV-HKU1C spike in the functionally anchored-3up conformation with 2TMPRSS2  
Authors : Lu, Y.C.; Wang, H.F.; Zhang, X.; Liu, X.C.; Sun, L.; Yang, H.T.  
Deposited on : 2024-02-06  
Resolution : 3.32 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.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

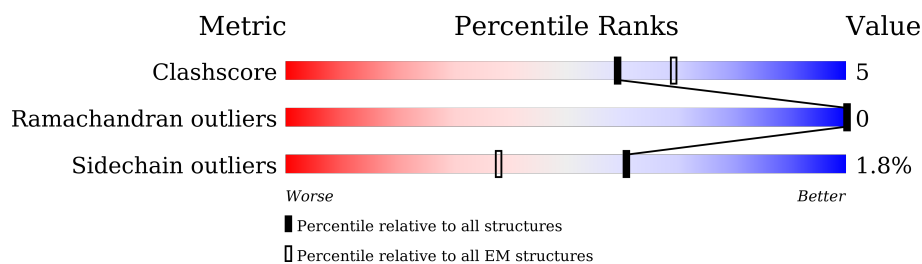
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.32 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	1263	 75% 12% 13%
1	B	1263	 82% 12% 5%
1	C	1263	 80% 14% 5%
2	G	383	 41% 53% 9% 38%
2	T	383	 30% 55% 7% 38%
3	D	2	 100%
3	E	2	 100%
3	F	2	 100%

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Mol	Chain	Length	Quality of chain
3	H	2	 100%
3	I	2	 100%
3	J	2	 100%
3	K	2	 100%
3	L	2	 100%
3	M	2	 100%
3	N	2	 100%
4	O	3	 100%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30645 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1094	Total	C	N	O	S	0	0
			8482	5425	1395	1619	43		
1	C	1194	Total	C	N	O	S	0	0
			9126	5816	1503	1753	54		
1	B	1194	Total	C	N	O	S	0	0
			9116	5807	1500	1755	54		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	752	GLY	ARG	engineered mutation	UNP Q0ZME7
A	753	GLY	ARG	engineered mutation	UNP Q0ZME7
A	754	SER	LYS	engineered mutation	UNP Q0ZME7
A	755	GLY	ARG	engineered mutation	UNP Q0ZME7
A	756	SER	ARG	engineered mutation	UNP Q0ZME7
A	902	PRO	LEU	engineered mutation	UNP Q0ZME7
A	980	PRO	SER	engineered mutation	UNP Q0ZME7
A	1023	PRO	ASN	engineered mutation	UNP Q0ZME7
A	1067	PRO	ASN	engineered mutation	UNP Q0ZME7
A	1068	PRO	LEU	engineered mutation	UNP Q0ZME7
C	752	GLY	ARG	engineered mutation	UNP Q0ZME7
C	753	GLY	ARG	engineered mutation	UNP Q0ZME7
C	754	SER	LYS	engineered mutation	UNP Q0ZME7
C	755	GLY	ARG	engineered mutation	UNP Q0ZME7
C	756	SER	ARG	engineered mutation	UNP Q0ZME7
C	902	PRO	LEU	engineered mutation	UNP Q0ZME7
C	980	PRO	SER	engineered mutation	UNP Q0ZME7
C	1023	PRO	ASN	engineered mutation	UNP Q0ZME7
C	1067	PRO	ASN	engineered mutation	UNP Q0ZME7
C	1068	PRO	LEU	engineered mutation	UNP Q0ZME7
B	752	GLY	ARG	engineered mutation	UNP Q0ZME7
B	753	GLY	ARG	engineered mutation	UNP Q0ZME7
B	754	SER	LYS	engineered mutation	UNP Q0ZME7
B	755	GLY	ARG	engineered mutation	UNP Q0ZME7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	756	SER	ARG	engineered mutation	UNP Q0ZME7
B	902	PRO	LEU	engineered mutation	UNP Q0ZME7
B	980	PRO	SER	engineered mutation	UNP Q0ZME7
B	1023	PRO	ASN	engineered mutation	UNP Q0ZME7
B	1067	PRO	ASN	engineered mutation	UNP Q0ZME7
B	1068	PRO	LEU	engineered mutation	UNP Q0ZME7

- Molecule 2 is a protein called Transmembrane protease serine 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	237	Total	C	N	O	S	0	0
			1702	1087	291	313	11		
2	G	237	Total	C	N	O	S	0	0
			1718	1100	291	314	13		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	251	ASP	SER	engineered mutation	UNP O15393
T	252	ASP	SER	engineered mutation	UNP O15393
T	?	-	ARG	deletion	UNP O15393
T	253	ASP	GLN	engineered mutation	UNP O15393
T	254	ASP	SER	engineered mutation	UNP O15393
T	255	LYS	ARG	engineered mutation	UNP O15393
G	251	ASP	SER	engineered mutation	UNP O15393
G	252	ASP	SER	engineered mutation	UNP O15393
G	?	-	ARG	deletion	UNP O15393
G	253	ASP	GLN	engineered mutation	UNP O15393
G	254	ASP	SER	engineered mutation	UNP O15393
G	255	LYS	ARG	engineered mutation	UNP O15393

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



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

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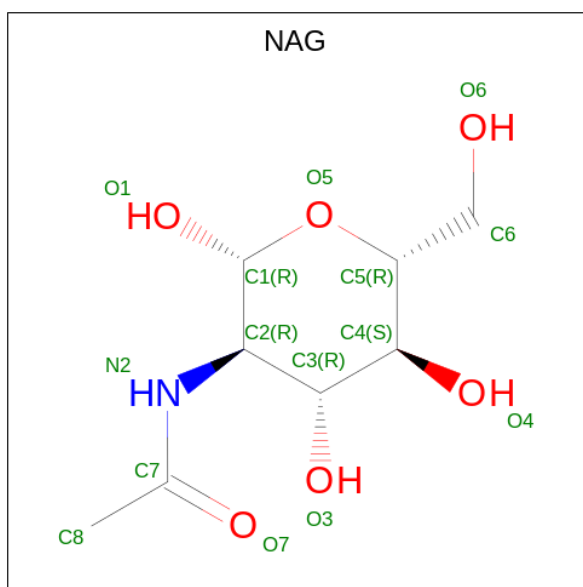
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		

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




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

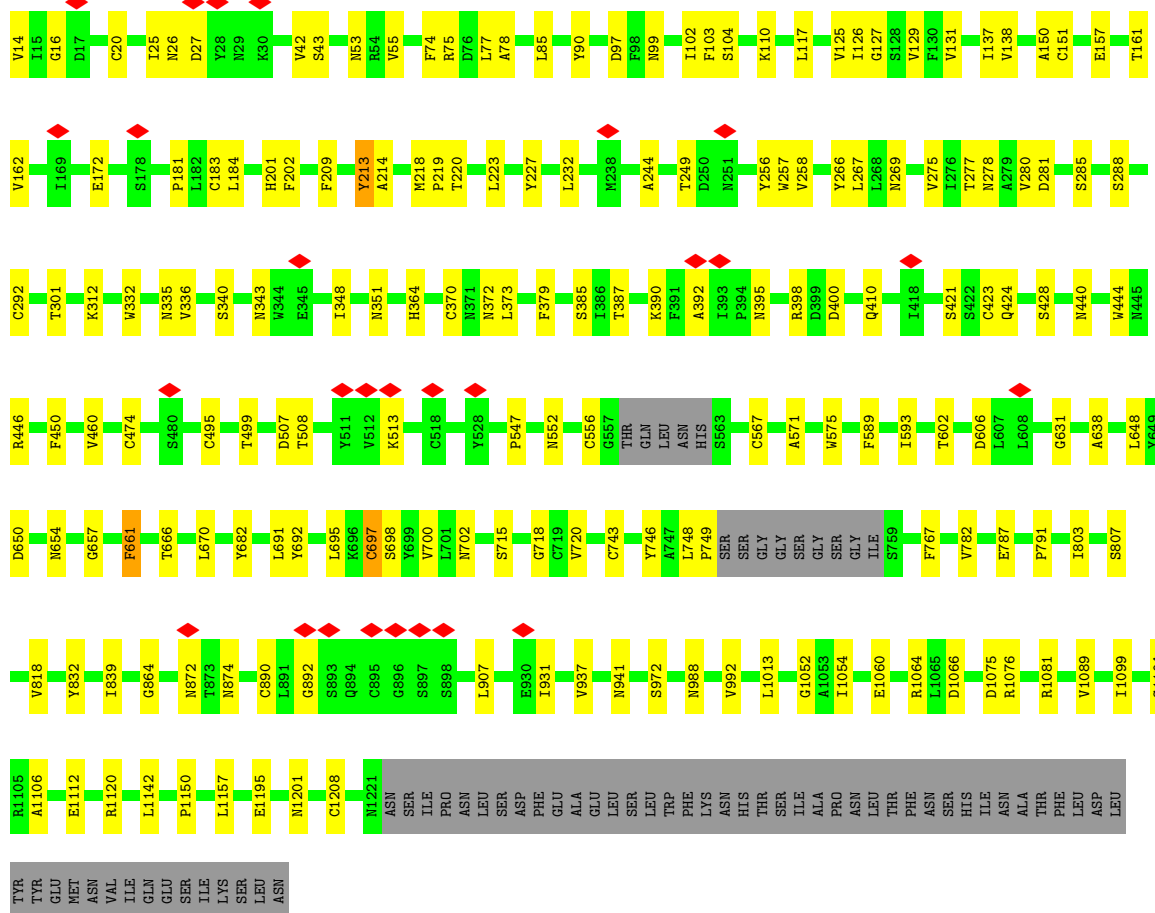
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).




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

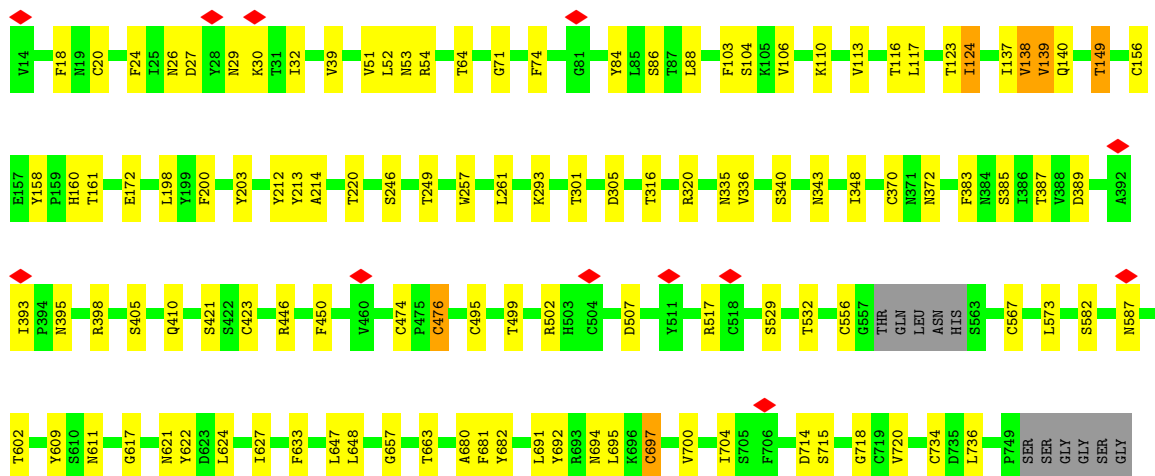


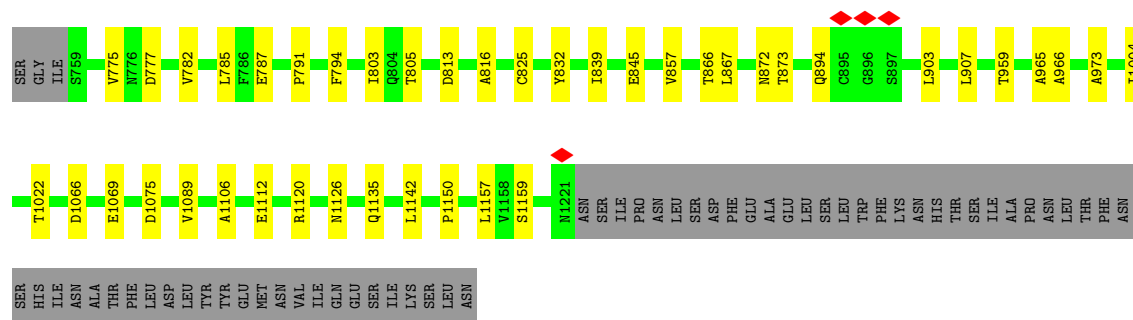
Chain C: 



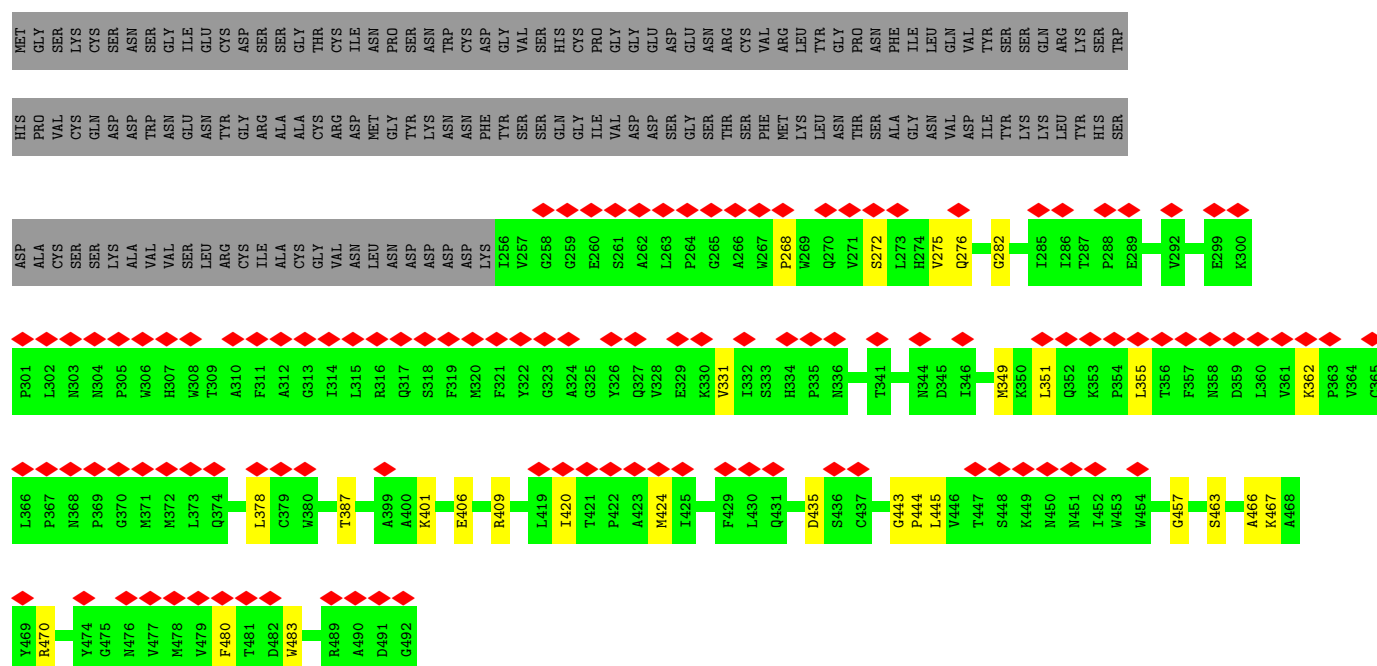
### • Molecule 1: Spike glycoprotein

Chain B: 

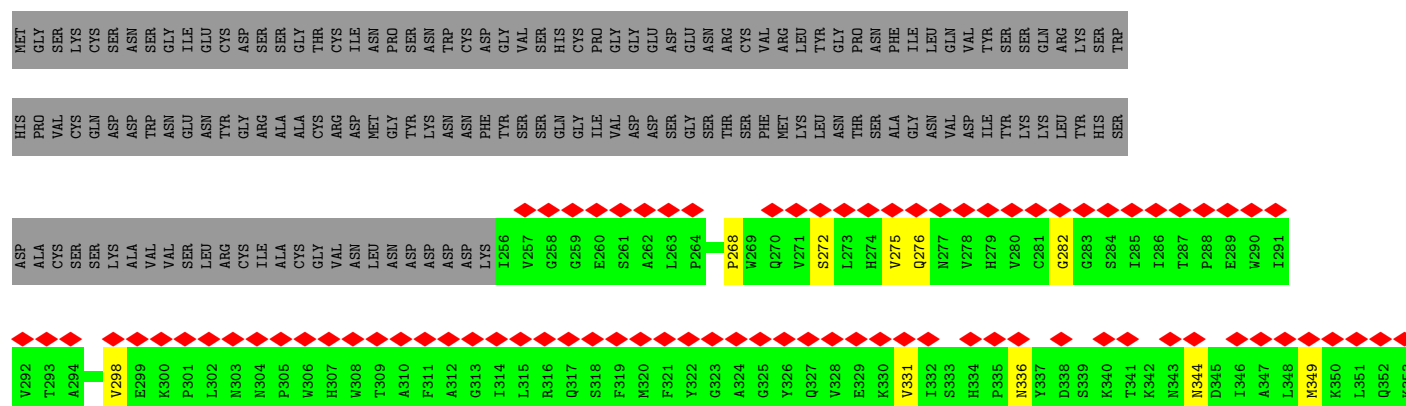
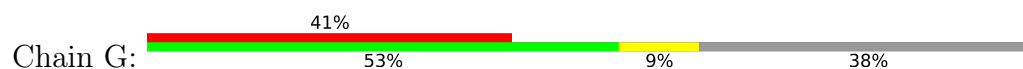


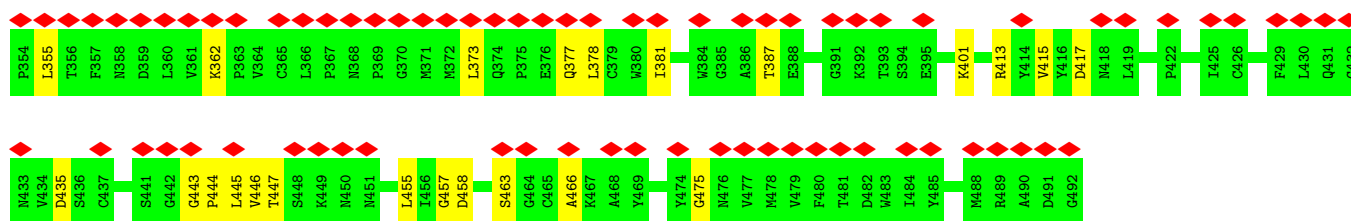


• Molecule 2: Transmembrane protease serine 2



• Molecule 2: Transmembrane protease serine 2





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

Chain D: 100%



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

Chain E: 100%



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

Chain F: 100%



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

Chain H: 100%



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

Chain I: 100%



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

Chain J: 100%



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

Chain K:  100%



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

Chain L:  100%



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

Chain M:  100%



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

Chain N:  100%



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

Chain O:  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116931	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.900	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	328.0, 328.0, 328.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.24	0/8682	0.41	0/11819
1	B	0.24	0/9335	0.42	0/12736
1	C	0.24	0/9342	0.41	0/12743
2	G	0.24	0/1765	0.43	0/2425
2	T	0.23	0/1750	0.43	0/2408
All	All	0.24	0/30874	0.41	0/42131

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8482	0	8095	85	0
1	B	9116	0	8610	81	0
1	C	9126	0	8678	95	0
2	G	1718	0	1597	18	0
2	T	1702	0	1548	15	0
3	D	28	0	25	0	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
4	O	39	0	34	0	0
5	A	56	0	52	1	0
5	B	70	0	65	0	0
5	C	56	0	52	0	0
All	All	30645	0	28981	285	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 (285) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:VAL:HG11	1:B:54:ARG:HB2	1.75	0.67
1:B:214:ALA:HB2	1:B:220:THR:HA	1.77	0.66
2:G:378:LEU:HD11	2:G:401:LYS:HD2	1.78	0.66
1:A:320:ARG:H	1:A:320:ARG:HD3	1.60	0.66
1:A:58:ASN:HA	1:A:270:PHE:O	1.94	0.66
1:C:1052:GLY:HA3	1:C:1076:ARG:HH21	1.60	0.66
1:C:214:ALA:HB2	1:C:220:THR:HA	1.76	0.65
1:C:26:ASN:ND2	1:C:85:LEU:O	2.29	0.65
1:B:138:VAL:HG13	1:B:149:THR:HG23	1.79	0.65
2:T:378:LEU:HD11	2:T:401:LYS:HD2	1.79	0.64
1:C:556:CYS:HA	1:C:567:CYS:HA	1.77	0.64
1:B:622:TYR:HB2	1:B:624:LEU:HD13	1.79	0.64
1:A:319:ARG:NH2	1:A:612:THR:O	2.30	0.64
1:B:556:CYS:HA	1:B:567:CYS:HA	1.80	0.63
1:C:440:ASN:H	1:C:446:ARG:HH21	1.44	0.63
1:B:124:ILE:HG23	1:B:139:VAL:HG13	1.81	0.63
1:B:966:ALA:HB2	1:B:973:ALA:HB3	1.80	0.63
1:B:74:PHE:HB3	1:B:257:TRP:HB3	1.82	0.62
2:G:445:LEU:HD23	2:G:457:GLY:HA3	1.81	0.62
1:A:168:SER:HB2	1:A:242:CYS:HA	1.82	0.61
1:A:1073:GLN:OE1	1:A:1076:ARG:NH2	2.34	0.61
1:C:74:PHE:HB3	1:C:257:TRP:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ILE:HD11	1:C:258:VAL:HB	1.82	0.60
1:B:1112:GLU:OE1	1:B:1120:ARG:NH2	2.34	0.60
1:A:691:LEU:HD13	1:A:720:VAL:HG22	1.82	0.60
1:C:213:TYR:HD1	1:C:223:LEU:HD21	1.66	0.60
1:B:348:ILE:HD11	1:B:385:SER:HB2	1.82	0.60
1:C:110:LYS:HB3	1:C:117:LEU:HD11	1.83	0.60
1:C:400:ASP:O	1:C:410:GLN:NE2	2.34	0.60
1:A:641:TYR:HB3	1:A:659:LYS:HD2	1.83	0.60
1:A:201:HIS:HB3	1:A:212:TYR:HB2	1.84	0.59
1:C:937:VAL:O	1:C:941:ASN:ND2	2.33	0.59
1:A:262:SER:OG	1:A:264:ARG:NH1	2.33	0.59
1:C:269:ASN:ND2	1:C:277:THR:OG1	2.31	0.59
1:C:691:LEU:HD13	1:C:720:VAL:HG22	1.84	0.59
1:C:697:CYS:HA	1:C:700:VAL:HG12	1.85	0.59
1:C:1060:GLU:O	1:C:1064:ARG:HB2	2.02	0.59
1:C:988:ASN:ND2	1:C:992:VAL:O	2.36	0.58
1:A:709:GLN:HG3	1:A:721:LEU:HD23	1.84	0.58
1:C:373:LEU:HB2	1:C:421:SER:HB2	1.85	0.58
1:C:25:ILE:HG13	1:C:85:LEU:HB2	1.85	0.58
1:A:646:ASN:H	1:C:53:ASN:HB3	1.67	0.58
1:C:1054:ILE:HD12	1:C:1064:ARG:HH21	1.69	0.58
1:C:161:THR:HA	1:C:172:GLU:HG3	1.85	0.58
1:A:582:SER:OG	1:A:587:ASN:ND2	2.35	0.57
1:A:1105:ARG:NH2	1:C:1104:SER:OG	2.37	0.57
1:B:700:VAL:HG23	1:B:704:ILE:HD11	1.85	0.57
2:T:351:LEU:HD12	2:T:355:LEU:HD11	1.85	0.57
2:T:272:SER:HA	2:T:282:GLY:HA2	1.86	0.57
1:A:281:ASP:OD1	1:A:282:CYS:N	2.36	0.57
1:C:14:VAL:N	1:C:90:TYR:O	2.37	0.57
1:B:582:SER:OG	1:B:587:ASN:ND2	2.36	0.57
1:C:97:ASP:O	1:C:99:ASN:ND2	2.37	0.57
1:C:1112:GLU:OE1	1:C:1120:ARG:NH2	2.37	0.57
1:B:405:SER:O	1:B:410:GLN:NE2	2.38	0.57
1:B:680:ALA:HB1	1:B:736:LEU:HD13	1.87	0.57
1:A:332:TRP:O	1:A:390:LYS:NZ	2.32	0.56
1:A:923:ASN:OD1	1:B:694:ASN:ND2	2.38	0.56
1:B:405:SER:H	1:B:410:GLN:HE22	1.52	0.56
1:C:103:PHE:HD1	1:C:201:HIS:HB3	1.69	0.56
1:C:495:CYS:SG	1:C:499:THR:OG1	2.63	0.56
2:G:272:SER:HA	2:G:282:GLY:HA2	1.88	0.56
1:B:517:ARG:NH2	2:G:415:VAL:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:ALA:O	1:A:1041:ASN:ND2	2.33	0.55
1:B:495:CYS:SG	1:B:499:THR:OG1	2.63	0.55
1:A:387:THR:HG23	1:A:593:ILE:HB	1.88	0.55
1:A:791:PRO:HB3	1:A:1150:PRO:HB3	1.89	0.55
1:C:218:MET:SD	1:C:218:MET:N	2.79	0.55
2:G:268:PRO:HB2	2:G:362:LYS:H	1.72	0.55
1:B:839:ILE:HG23	1:B:1089:VAL:HG11	1.88	0.54
1:C:364:HIS:ND1	1:C:428:SER:OG	2.40	0.54
1:B:832:TYR:OH	1:B:1075:ASP:OD1	2.25	0.54
2:T:268:PRO:HB2	2:T:362:LYS:H	1.72	0.54
1:C:446:ARG:HA	1:C:450:PHE:HB3	1.89	0.54
1:A:214:ALA:HB2	1:A:220:THR:HA	1.88	0.54
1:C:818:VAL:O	1:C:1081:ARG:NH1	2.41	0.54
1:B:785:LEU:HD22	1:B:1159:SER:HB2	1.90	0.53
1:C:638:ALA:HB3	1:C:666:THR:HG21	1.90	0.53
1:B:161:THR:HG23	1:B:172:GLU:HG3	1.91	0.53
1:C:631:GLY:CA	1:C:670:LEU:O	2.57	0.53
1:A:24:PHE:HB3	1:A:84:TYR:HA	1.91	0.53
1:B:301:THR:HA	1:B:681:PHE:O	2.08	0.53
1:C:16:GLY:H	1:C:157:GLU:HA	1.74	0.52
1:C:791:PRO:HB3	1:C:1150:PRO:HB3	1.91	0.52
1:C:907:LEU:HD11	1:C:1142:LEU:HD22	1.91	0.52
1:B:51:VAL:HG21	1:B:54:ARG:HD3	1.91	0.52
2:T:480:PHE:O	2:T:483:TRP:HB3	2.10	0.52
1:A:51:VAL:HG21	1:A:56:TYR:HE1	1.75	0.52
2:G:435:ASP:HB3	2:G:466:ALA:H	1.75	0.52
1:A:839:ILE:HG23	1:A:1089:VAL:HG11	1.92	0.52
1:C:267:LEU:HB3	1:C:280:VAL:HG23	1.92	0.52
1:B:446:ARG:NH1	1:B:450:PHE:O	2.43	0.52
1:A:644:TRP:CD1	1:A:645:GLN:HG3	2.45	0.52
1:B:715:SER:OG	1:B:718:GLY:O	2.27	0.52
1:A:670:LEU:HD22	1:C:931:ILE:HB	1.92	0.51
1:C:370:CYS:HA	1:C:423:CYS:HA	1.93	0.51
1:B:775:VAL:HG12	1:B:777:ASP:H	1.75	0.51
1:C:162:VAL:HG22	1:C:172:GLU:HB2	1.92	0.51
1:C:692:TYR:HB3	1:C:695:LEU:HD12	1.91	0.51
1:C:125:VAL:HG12	1:C:138:VAL:HG22	1.92	0.51
1:B:389:ASP:OD1	1:B:389:ASP:N	2.43	0.51
1:B:648:LEU:HB3	1:B:657:GLY:H	1.75	0.51
1:A:746:TYR:HE1	1:A:761:PRO:HB2	1.74	0.51
1:C:715:SER:OG	1:C:718:GLY:O	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:VAL:HG21	1:C:266:TYR:HE2	1.74	0.51
1:B:395:ASN:OD1	1:B:398:ARG:NH2	2.44	0.51
1:A:818:VAL:HA	1:A:1081:ARG:HH11	1.75	0.51
1:A:1112:GLU:OE1	1:A:1120:ARG:NH1	2.39	0.51
1:B:959:THR:HG21	1:B:1135:GLN:HA	1.93	0.51
1:B:791:PRO:HB3	1:B:1150:PRO:HB3	1.92	0.51
1:C:832:TYR:OH	1:C:1075:ASP:OD1	2.29	0.51
1:B:316:THR:HG22	1:B:621:ASN:HB2	1.93	0.51
1:B:692:TYR:HB3	1:B:695:LEU:HD12	1.93	0.51
1:A:692:TYR:HB3	1:A:695:LEU:HD12	1.93	0.50
1:C:444:TRP:NE1	1:C:547:PRO:O	2.44	0.50
1:C:748:LEU:HD12	1:C:749:PRO:HD2	1.92	0.50
1:C:872:ASN:HB2	1:C:892:GLY:HA2	1.93	0.50
1:B:27:ASP:OD1	1:B:27:ASP:N	2.44	0.50
1:B:52:LEU:HD12	1:B:52:LEU:H	1.76	0.50
1:A:74:PHE:HB3	1:A:257:TRP:HB3	1.94	0.50
1:B:18:PHE:HB3	1:B:156:CYS:HA	1.92	0.50
2:T:445:LEU:HD23	2:T:457:GLY:HA3	1.92	0.50
1:C:807:SER:HB2	1:C:1099:ILE:HD13	1.94	0.50
2:G:458:ASP:O	2:G:475:GLY:N	2.42	0.49
1:C:698:SER:O	1:C:702:ASN:ND2	2.44	0.49
1:B:872:ASN:O	1:B:894:GLN:NE2	2.45	0.49
1:A:301:THR:HA	1:A:681:PHE:O	2.12	0.49
1:A:1023:PRO:HD2	1:A:1026:LEU:HB3	1.94	0.49
1:C:332:TRP:O	1:C:390:LYS:NZ	2.44	0.49
1:B:691:LEU:HD13	1:B:720:VAL:HG12	1.94	0.49
2:G:446:VAL:HG12	2:G:455:LEU:HA	1.95	0.49
1:C:244:ALA:HA	1:C:249:THR:HG21	1.94	0.49
1:B:370:CYS:HA	1:B:423:CYS:HA	1.95	0.49
1:A:1066:ASP:HB2	1:A:1068:PRO:HD2	1.95	0.49
1:C:1060:GLU:O	1:C:1064:ARG:CB	2.61	0.49
1:C:301:THR:HG23	1:C:682:TYR:HA	1.95	0.49
1:A:126:ILE:HG23	1:A:235:TYR:HB3	1.94	0.48
1:C:372:ASN:HB2	1:C:421:SER:HA	1.94	0.48
1:A:812:ILE:HG23	1:A:943:ILE:HG12	1.96	0.48
1:A:102:ILE:HG23	1:A:258:VAL:HG13	1.95	0.48
1:B:246:SER:N	1:B:249:THR:OG1	2.46	0.48
1:A:121:PHE:HZ	1:A:146:LEU:HD21	1.79	0.48
1:A:440:ASN:H	1:A:446:ARG:HH21	1.61	0.48
1:B:53:ASN:OD1	1:B:53:ASN:N	2.45	0.48
2:T:435:ASP:HB3	2:T:466:ALA:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:867:LEU:HD11	1:B:965:ALA:HA	1.95	0.48
1:B:110:LYS:HB3	1:B:117:LEU:HD11	1.96	0.48
2:G:336:ASN:O	2:G:344:ASN:ND2	2.41	0.48
1:B:203:TYR:HE1	1:B:212:TYR:HE1	1.62	0.48
1:B:335:ASN:OD1	1:B:336:VAL:N	2.46	0.48
1:A:319:ARG:NH1	1:A:660:ASP:OD2	2.46	0.48
1:A:1120:ARG:NH2	1:C:1112:GLU:OE2	2.42	0.47
1:C:348:ILE:HD11	1:C:385:SER:HB2	1.96	0.47
1:A:110:LYS:HB3	1:A:117:LEU:HD11	1.96	0.47
1:C:661:PHE:H	1:C:661:PHE:HD1	1.62	0.47
1:B:907:LEU:HD11	1:B:1142:LEU:HD22	1.96	0.47
1:C:552:ASN:HB3	1:C:571:ALA:HB1	1.97	0.47
1:C:650:ASP:OD1	1:C:654:ASN:N	2.47	0.47
1:B:106:VAL:HG22	1:B:198:LEU:HB2	1.95	0.47
1:A:100:ASN:HD21	1:A:262:SER:HA	1.78	0.47
1:A:816:ALA:HA	1:A:820:SER:HA	1.96	0.47
1:C:874:ASN:HD21	1:C:890:CYS:HA	1.79	0.47
1:B:20:CYS:SG	1:B:158:TYR:N	2.77	0.47
1:B:507:ASP:OD2	2:G:463:SER:OG	2.33	0.47
1:C:335:ASN:OD1	1:C:336:VAL:N	2.47	0.47
1:A:353:ASN:HB3	1:A:605:ASN:HD21	1.79	0.47
1:A:66:TYR:HB3	1:A:261:LEU:HD23	1.97	0.47
1:A:245:ILE:HG13	1:A:254:LEU:HB2	1.97	0.47
1:A:364:HIS:ND1	1:A:428:SER:OG	2.48	0.47
1:C:129:VAL:HB	1:C:131:VAL:HG22	1.96	0.47
1:B:805:THR:HG21	1:B:857:VAL:HG21	1.95	0.46
1:B:24:PHE:HB3	1:B:84:TYR:HA	1.96	0.46
1:A:673:TYR:CZ	1:A:695:LEU:HD11	2.50	0.46
1:A:135:TYR:HA	1:A:151:CYS:O	2.15	0.46
1:A:218:MET:HB2	1:A:219:PRO:HD3	1.96	0.46
2:T:331:VAL:HG22	2:T:349:MET:HG2	1.96	0.46
1:A:1199:ASP:HA	1:A:1202:VAL:HG12	1.98	0.46
1:A:648:LEU:HD13	1:C:55:VAL:HG23	1.98	0.46
1:C:218:MET:HB2	1:C:219:PRO:HD3	1.98	0.46
1:A:38:ASP:OD1	1:A:39:VAL:N	2.46	0.46
1:A:747:ALA:HB2	1:A:763:ARG:HE	1.81	0.45
1:A:301:THR:HG23	1:A:682:TYR:HA	1.98	0.45
1:C:395:ASN:OD1	1:C:398:ARG:NH2	2.50	0.45
1:B:39:VAL:HB	1:B:71:GLY:HA2	1.98	0.45
1:B:372:ASN:HB2	1:B:421:SER:HA	1.98	0.45
2:G:298:VAL:HG11	2:G:331:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:377:GLN:NE2	2:G:447:THR:OG1	2.50	0.45
1:A:132:ASN:OD1	1:A:132:ASN:N	2.48	0.45
1:C:508:THR:HG22	1:C:513:LYS:HA	1.98	0.45
1:B:529:SER:HG	1:B:532:THR:HG1	1.62	0.45
1:A:680:ALA:HB1	1:A:736:LEU:HD13	1.99	0.45
1:B:476:CYS:O	1:B:502:ARG:N	2.50	0.45
1:A:89:TRP:HA	1:A:94:PHE:HD2	1.81	0.45
1:A:103:PHE:HB3	1:A:259:THR:HG23	1.99	0.45
1:C:340:SER:OG	1:C:343:ASN:OD1	2.31	0.45
1:C:507:ASP:OD2	2:T:463:SER:OG	2.35	0.45
1:B:113:VAL:O	1:B:116:THR:OG1	2.21	0.45
1:A:182:LEU:HD23	1:A:182:LEU:H	1.83	0.44
1:B:26:ASN:HB2	1:B:86:SER:HA	1.97	0.44
2:T:406:GLU:HG3	2:T:409:ARG:H	1.82	0.44
1:B:30:LYS:HG2	1:B:32:ILE:HG23	2.00	0.44
1:A:144:GLY:HA2	1:A:191:TYR:CZ	2.53	0.44
1:A:627:ILE:HG21	1:A:655:ILE:HG13	1.98	0.44
1:B:787:GLU:HB3	1:B:1157:LEU:HD23	1.98	0.44
1:C:864:GLY:O	1:C:972:SER:OG	2.34	0.44
1:C:1066:ASP:N	1:C:1066:ASP:OD1	2.48	0.44
2:G:275:VAL:HG22	2:G:276:GLN:HG2	2.00	0.44
1:A:446:ARG:HA	1:A:450:PHE:HB3	1.99	0.43
1:B:393:ILE:HD12	1:B:587:ASN:HB3	2.00	0.43
1:B:903:LEU:HD23	1:B:1135:GLN:HG3	2.00	0.43
1:B:1126:ASN:OD1	1:B:1126:ASN:N	2.50	0.43
2:T:275:VAL:HG22	2:T:276:GLN:HG2	1.99	0.43
1:C:27:ASP:OD1	1:C:27:ASP:N	2.46	0.43
1:B:617:GLY:HA2	1:B:633:PHE:H	1.84	0.43
1:B:611:ASN:OD1	1:B:611:ASN:N	2.51	0.43
2:T:443:GLY:HA2	2:T:444:PRO:HD3	1.88	0.43
1:B:103:PHE:HB2	1:B:261:LEU:HD21	1.99	0.43
1:C:126:ILE:HB	1:C:137:ILE:HG13	2.00	0.43
1:C:351:ASN:ND2	1:C:351:ASN:O	2.52	0.43
1:B:697:CYS:HA	1:B:700:VAL:HG12	2.00	0.43
2:T:420:ILE:HG23	2:T:424:MET:HB3	2.00	0.43
2:T:467:LYS:HB3	2:T:470:ARG:HH11	1.83	0.43
1:A:335:ASN:OD1	1:A:336:VAL:N	2.52	0.43
1:A:967:MET:HB2	1:A:967:MET:HE3	1.86	0.43
1:C:150:ALA:HB3	1:C:184:LEU:HB3	2.01	0.43
1:C:202:PHE:HB3	1:C:209:PHE:CZ	2.54	0.43
1:B:320:ARG:O	1:B:609:TYR:OH	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:THR:OG1	1:C:593:ILE:HB	2.19	0.42
1:B:340:SER:OG	1:B:343:ASN:OD1	2.35	0.42
1:B:813:ASP:HB3	1:B:816:ALA:HB3	2.01	0.42
2:G:331:VAL:HG22	2:G:349:MET:HG2	2.00	0.42
1:A:139:VAL:HG13	1:A:148:ILE:HG12	2.01	0.42
2:G:381:ILE:HG22	2:G:445:LEU:HD13	2.02	0.42
1:A:109:THR:OG1	1:A:120:GLU:O	2.38	0.42
1:C:392:ALA:HB3	1:C:460:VAL:HG11	2.01	0.42
1:A:166:LYS:HB3	1:A:243:ASN:HD22	1.84	0.42
1:A:393:ILE:HD12	1:A:587:ASN:HB3	2.00	0.42
1:B:1066:ASP:N	1:B:1069:GLU:OE2	2.52	0.42
1:B:301:THR:HG23	1:B:682:TYR:HA	2.02	0.42
1:C:78:ALA:HB2	1:C:256:TYR:HB2	2.01	0.42
1:A:52:LEU:HD21	1:A:210:TYR:CE2	2.55	0.41
1:A:317:VAL:HB	1:A:622:TYR:HA	2.02	0.41
1:C:151:CYS:SG	1:C:181:PRO:HG2	2.60	0.41
1:C:43:SER:O	1:C:278:ASN:ND2	2.53	0.41
1:B:627:ILE:HD11	1:B:647:LEU:HD13	2.02	0.41
1:B:714:ASP:OD1	1:B:715:SER:N	2.49	0.41
1:A:648:LEU:HG	1:A:656:ILE:HB	2.03	0.41
1:C:266:TYR:CZ	1:C:281:ASP:HB3	2.55	0.41
1:C:803:ILE:HG21	1:C:1106:ALA:HB2	2.02	0.41
1:A:139:VAL:HG22	1:A:148:ILE:HG23	2.02	0.41
1:C:127:GLY:HA2	1:C:232:LEU:HD22	2.01	0.41
2:G:443:GLY:HA2	2:G:444:PRO:HD3	1.90	0.41
1:A:201:HIS:CE1	1:A:261:LEU:HD21	2.55	0.41
1:C:351:ASN:N	1:C:602:THR:OG1	2.45	0.41
1:C:379:PHE:HA	1:C:606:ASP:HB2	2.03	0.41
1:C:631:GLY:HA3	1:C:670:LEU:O	2.19	0.41
1:B:123:THR:HG23	1:B:140:GLN:HB3	2.03	0.41
1:B:293:LYS:NZ	1:B:305:ASP:O	2.53	0.41
2:G:373:LEU:HD22	2:G:377:GLN:HE22	1.85	0.41
1:A:622:TYR:HE1	1:A:627:ILE:HG22	1.85	0.41
1:A:803:ILE:HG21	1:A:1106:ALA:HB2	2.03	0.41
1:A:58:ASN:CA	1:A:270:PHE:O	2.67	0.41
1:B:383:PHE:N	1:B:602:THR:O	2.46	0.41
1:B:803:ILE:HG21	1:B:1106:ALA:HB2	2.02	0.41
1:A:875:LEU:HG	1:A:876:HIS:CD2	2.56	0.41
1:C:787:GLU:HG2	1:C:1157:LEU:HG	2.03	0.41
2:T:445:LEU:HB3	2:T:457:GLY:HA3	2.02	0.41
1:A:255:GLU:HB3	1:A:257:TRP:NE1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:GLN:HB3	1:C:589:PHE:HE1	1.86	0.41
1:B:29:ASN:H	1:B:88:LEU:HD12	1.86	0.41
1:A:40:VAL:HB	1:A:71:GLY:HA2	2.03	0.41
1:A:351:ASN:ND2	1:A:601:THR:OG1	2.41	0.41
1:A:702:ASN:HD22	5:A:1302:NAG:HN2	1.69	0.40
1:C:839:ILE:HG23	1:C:1089:VAL:HG21	2.03	0.40
1:A:1129:HIS:NE2	1:A:1132:SER:OG	2.39	0.40
1:C:285:SER:O	1:C:288:SER:OG	2.33	0.40
1:B:104:SER:OG	1:B:200:PHE:HB2	2.21	0.40
1:B:794:PHE:HE2	1:B:1004:ILE:HD11	1.86	0.40
1:C:104:SER:HB3	1:C:258:VAL:HG12	2.04	0.40
1:C:1195:GLU:OE2	1:C:1201:ASN:ND2	2.54	0.40
1:A:52:LEU:HD21	1:A:210:TYR:HE2	1.86	0.40
1:A:372:ASN:HB2	1:A:421:SER:HA	2.03	0.40
1:C:151:CYS:HA	1:C:183:CYS:HA	2.03	0.40
1:C:648:LEU:HB3	1:C:657:GLY:HA3	2.04	0.40
2:G:413:ARG:HA	2:G:417:ASP:HA	2.02	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	1076/1263 (85%)	1029 (96%)	47 (4%)	0	100	100
1	B	1188/1263 (94%)	1141 (96%)	47 (4%)	0	100	100
1	C	1188/1263 (94%)	1145 (96%)	43 (4%)	0	100	100
2	G	235/383 (61%)	219 (93%)	16 (7%)	0	100	100
2	T	235/383 (61%)	216 (92%)	19 (8%)	0	100	100
All	All	3922/4555 (86%)	3750 (96%)	172 (4%)	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	947/1132 (84%)	931 (98%)	16 (2%)	60	79
1	B	1009/1132 (89%)	988 (98%)	21 (2%)	53	76
1	C	1018/1132 (90%)	1000 (98%)	18 (2%)	59	79
2	G	170/325 (52%)	168 (99%)	2 (1%)	71	84
2	T	163/325 (50%)	162 (99%)	1 (1%)	86	92
All	All	3307/4046 (82%)	3249 (98%)	58 (2%)	61	79

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	138	VAL
1	A	175	HIS
1	A	213	TYR
1	A	215	ASP
1	A	227	TYR
1	A	237	VAL
1	A	240	LEU
1	A	318	TYR
1	A	320	ARG
1	A	387	THR
1	A	697	CYS
1	A	734	CYS
1	A	812	ILE
1	A	1019	PHE
1	A	1022	THR
1	C	20	CYS
1	C	75	ARG
1	C	77	LEU
1	C	213	TYR
1	C	227	TYR

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Mol	Chain	Res	Type
1	C	275	VAL
1	C	292	CYS
1	C	312	LYS
1	C	474	CYS
1	C	575	TRP
1	C	661	PHE
1	C	697	CYS
1	C	743	CYS
1	C	746	TYR
1	C	767	PHE
1	C	782	VAL
1	C	1013	LEU
1	C	1208	CYS
1	B	64	THR
1	B	124	ILE
1	B	137	ILE
1	B	138	VAL
1	B	139	VAL
1	B	149	THR
1	B	160	HIS
1	B	213	TYR
1	B	387	THR
1	B	474	CYS
1	B	476	CYS
1	B	573	LEU
1	B	663	THR
1	B	697	CYS
1	B	734	CYS
1	B	782	VAL
1	B	825	CYS
1	B	845	GLU
1	B	866	THR
1	B	873	THR
1	B	1022	THR
2	T	387	THR
2	G	355	LEU
2	G	387	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN

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Mol	Chain	Res	Type
1	A	243	ASN
1	A	587	ASN
1	A	591	ASN
1	A	605	ASN
1	A	621	ASN
1	A	630	GLN
1	A	709	GLN
1	A	847	ASN
1	A	1046	GLN
1	C	26	ASN
1	C	99	ASN
1	C	140	GLN
1	C	591	ASN
1	C	605	ASN
1	C	654	ASN
1	C	1038	GLN
1	B	410	GLN
1	B	587	ASN
1	B	863	GLN
1	B	1079	ASN
2	T	276	GLN
2	T	377	GLN
2	G	276	GLN
2	G	377	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

23 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	D	1	1,3	14,14,15	0.26	0	17,19,21	0.53	0
3	NAG	D	2	3	14,14,15	0.23	0	17,19,21	0.38	0
3	NAG	E	1	1,3	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	E	2	3	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	F	1	1,3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	F	2	3	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	H	1	1,3	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	H	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	I	1	1,3	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	I	2	3	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	J	1	1,3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	J	2	3	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	K	1	1,3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	K	2	3	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	L	1	1,3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	L	2	3	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	M	1	1,3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	M	2	3	14,14,15	0.22	0	17,19,21	0.40	0
3	NAG	N	1	1,3	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	N	2	3	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	O	1	1,4	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	O	2	4	14,14,15	0.21	0	17,19,21	0.41	0
4	BMA	O	3	4	11,11,12	0.60	0	15,15,17	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

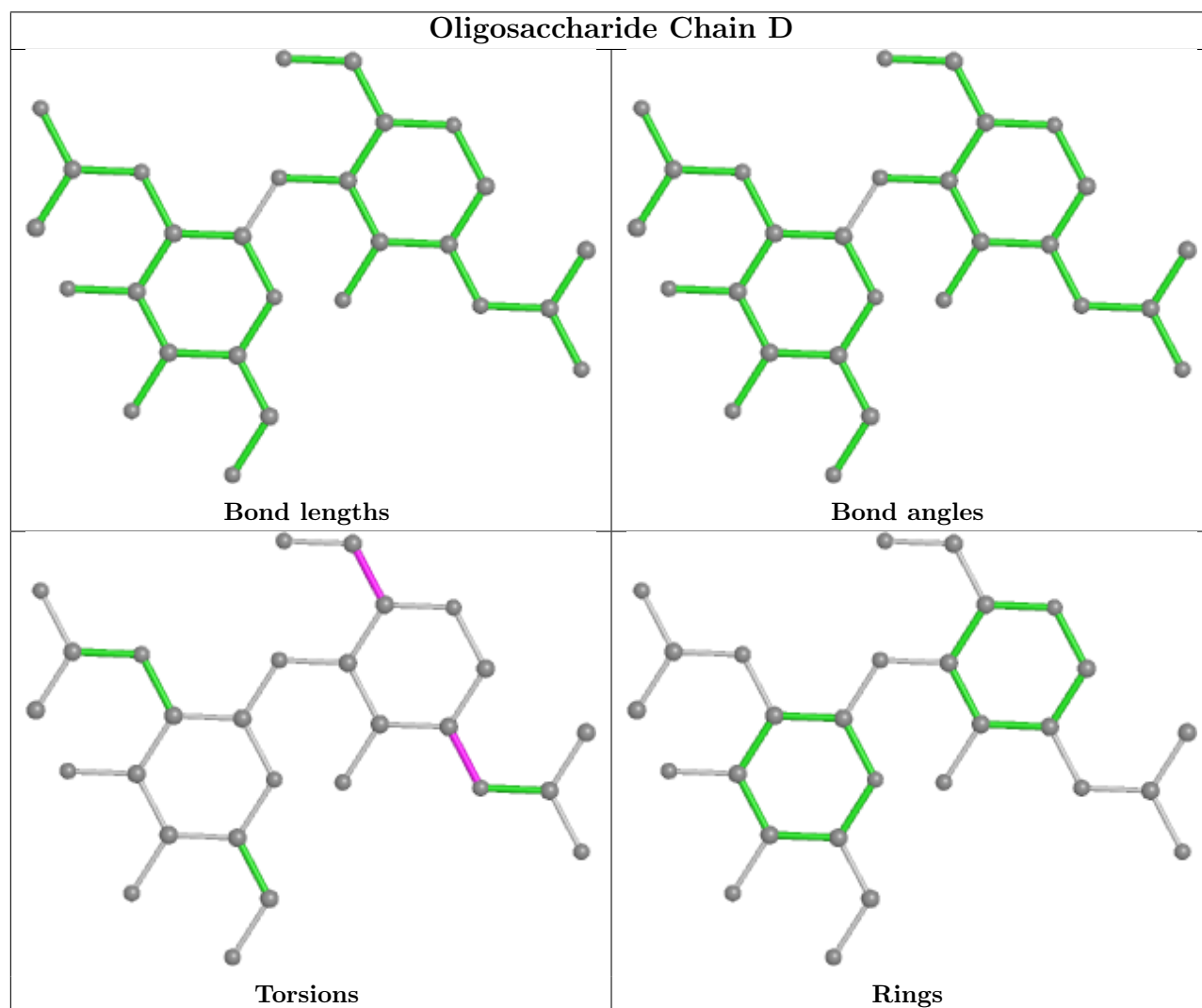
All (15) torsion outliers are listed below:

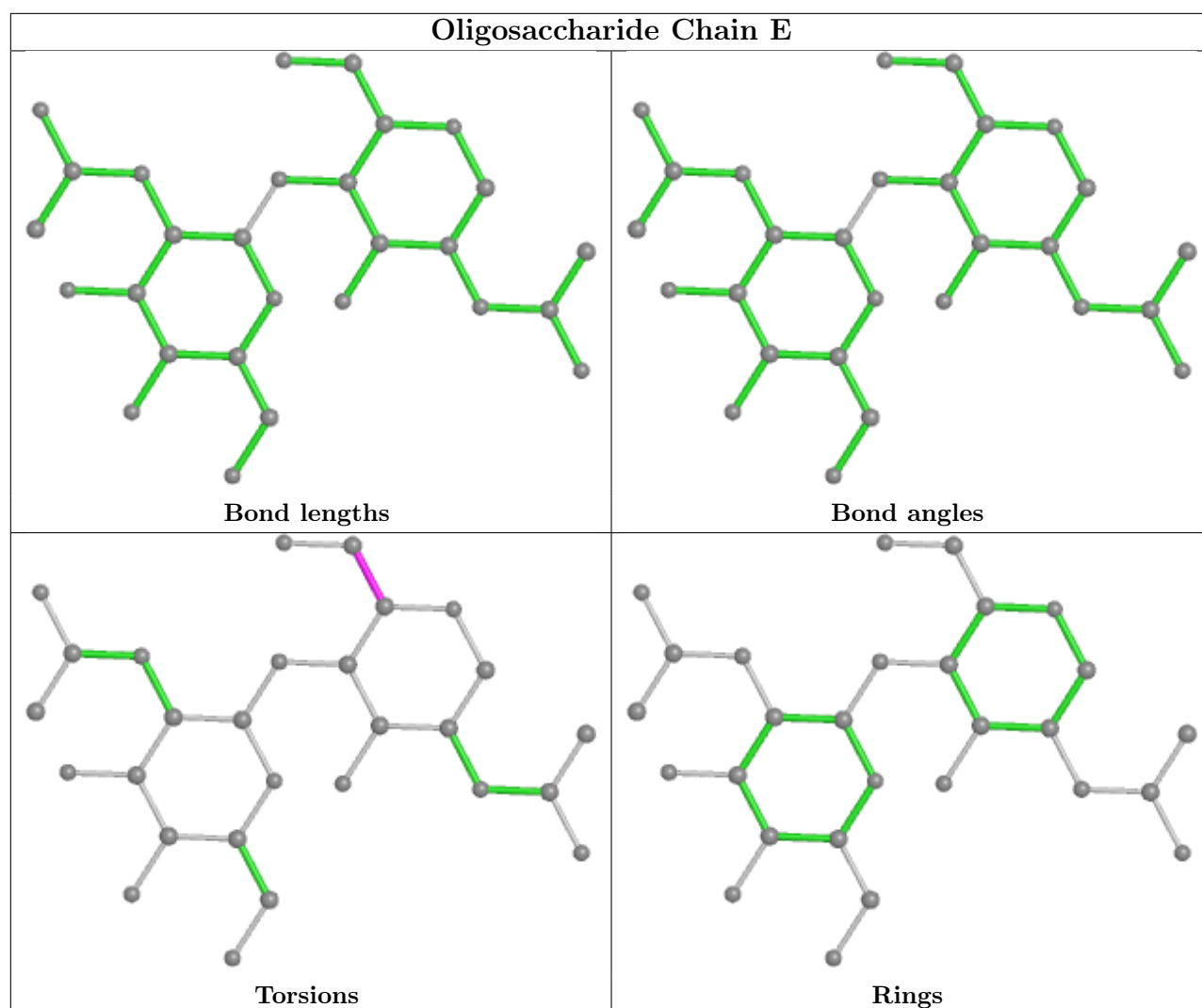
Mol	Chain	Res	Type	Atoms
3	K	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	K	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
4	O	3	BMA	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C3-C2-N2-C7
4	O	2	NAG	O5-C5-C6-O6

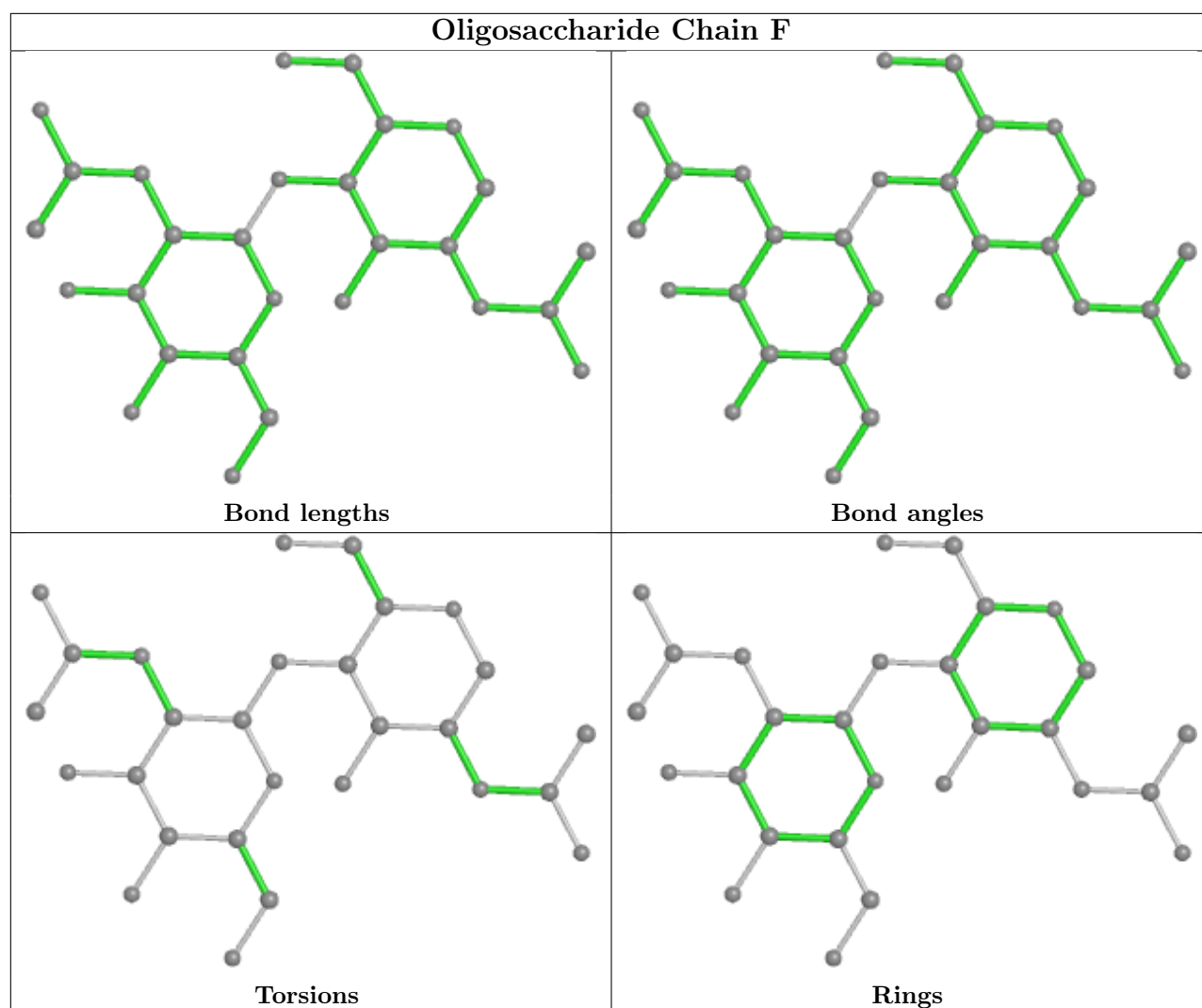
There are no ring outliers.

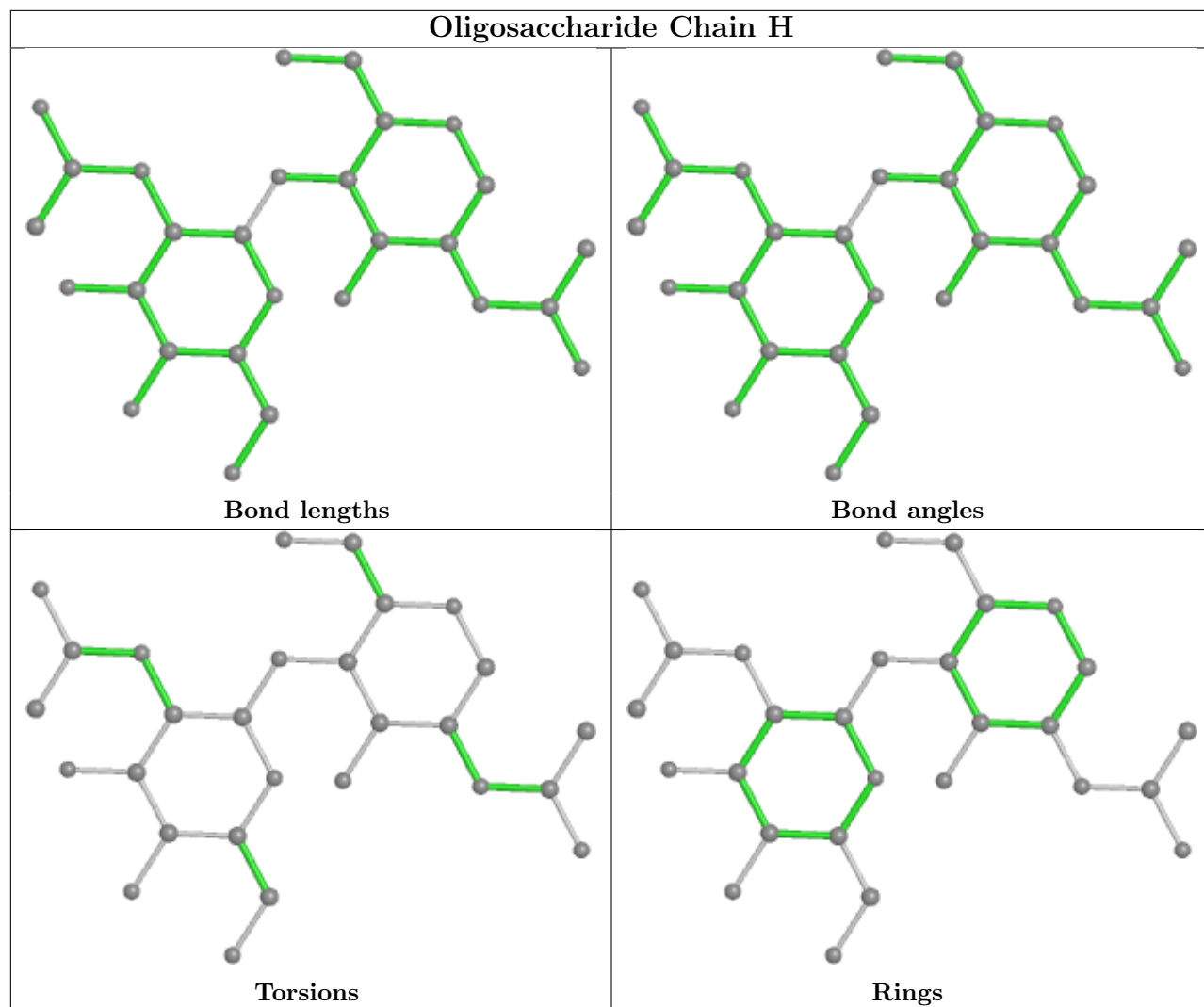
No monomer is involved in short contacts.

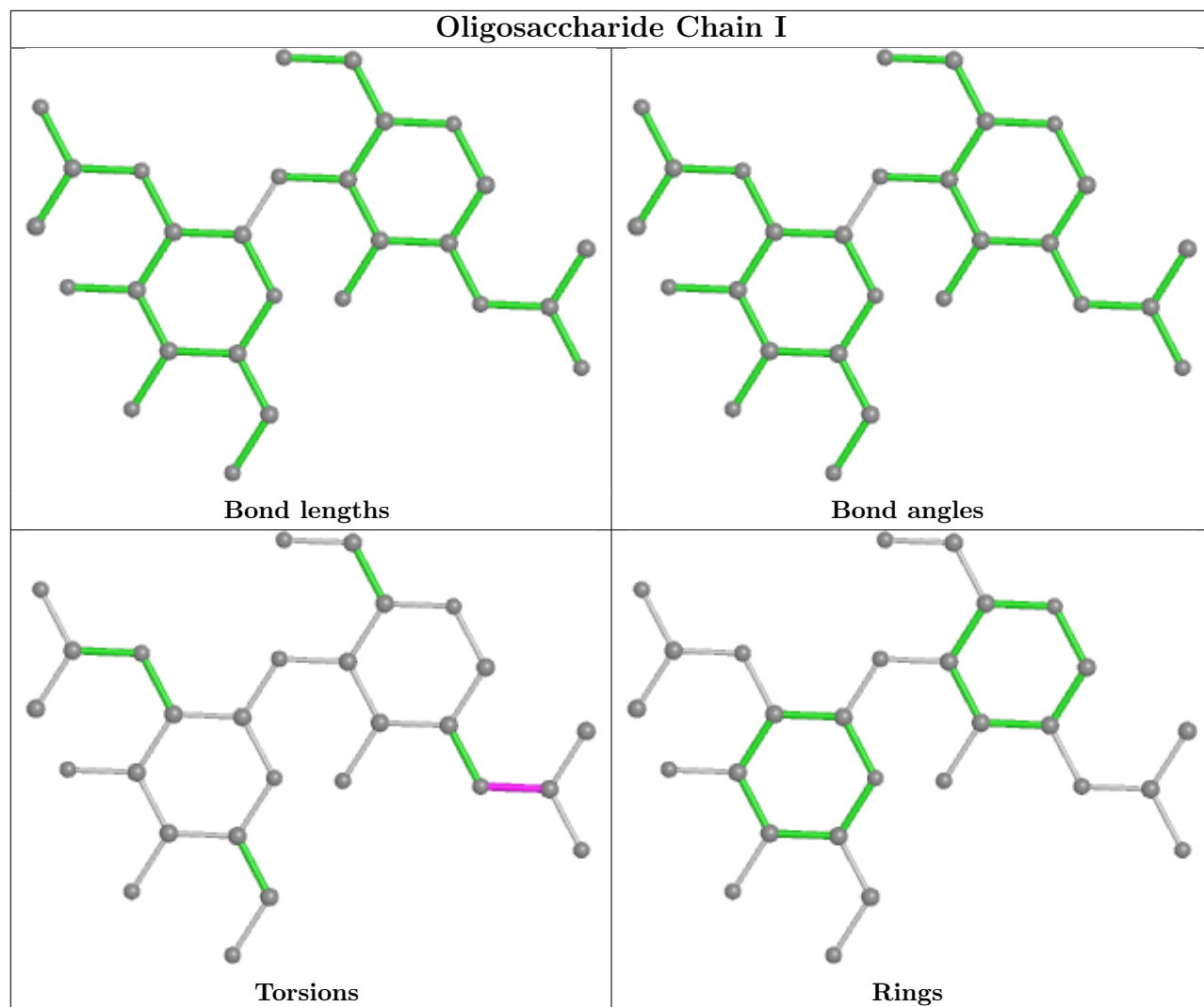
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

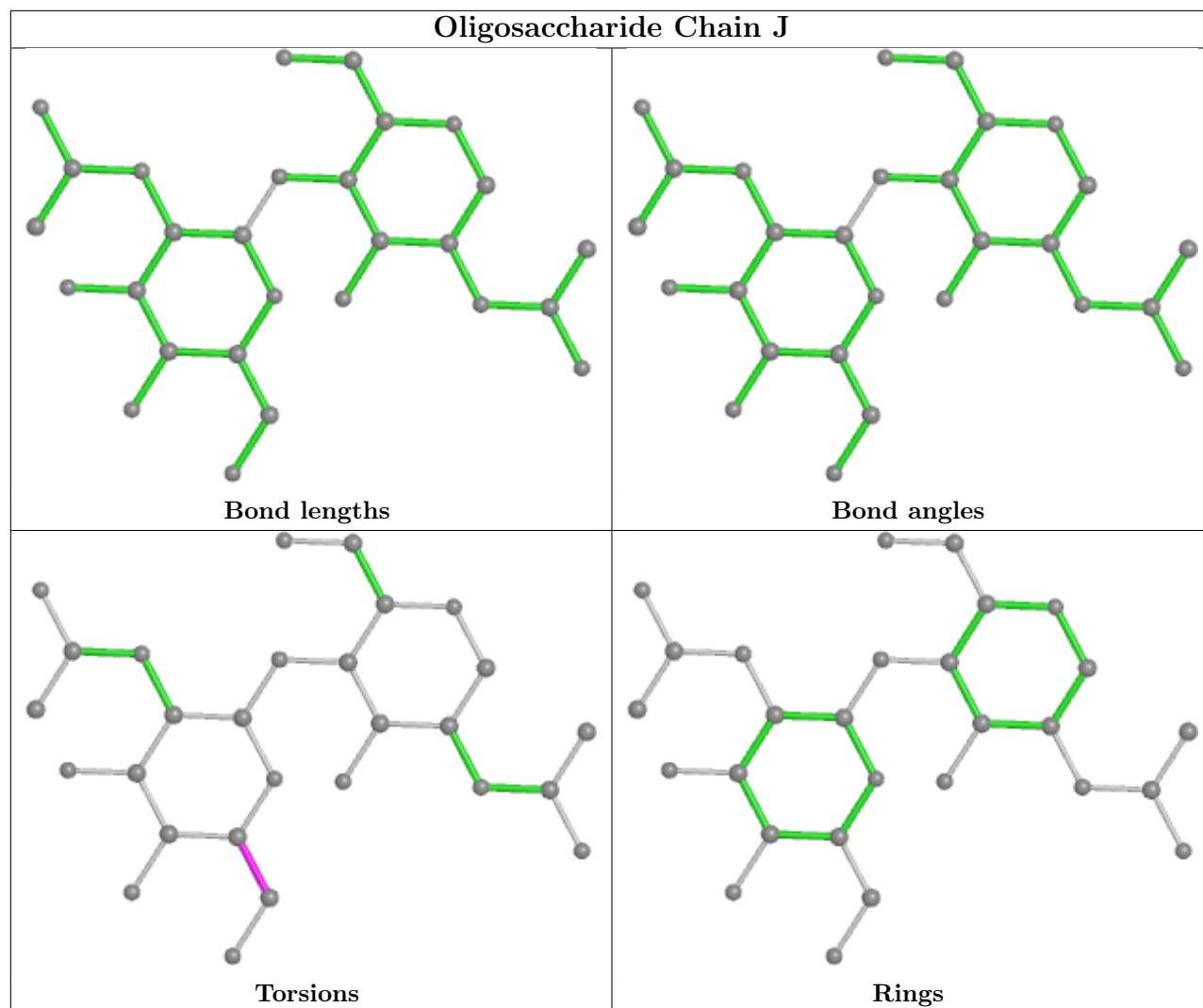


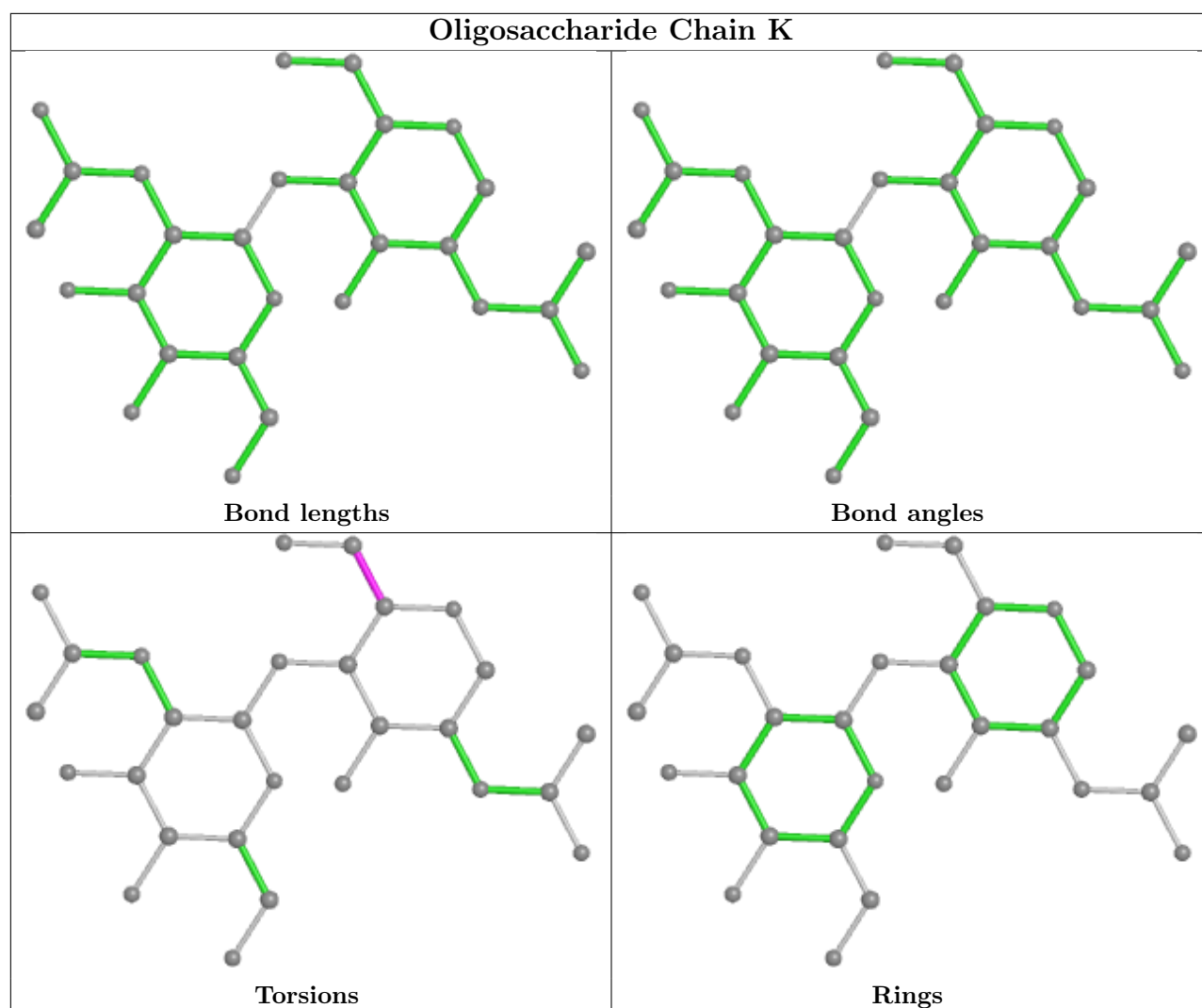


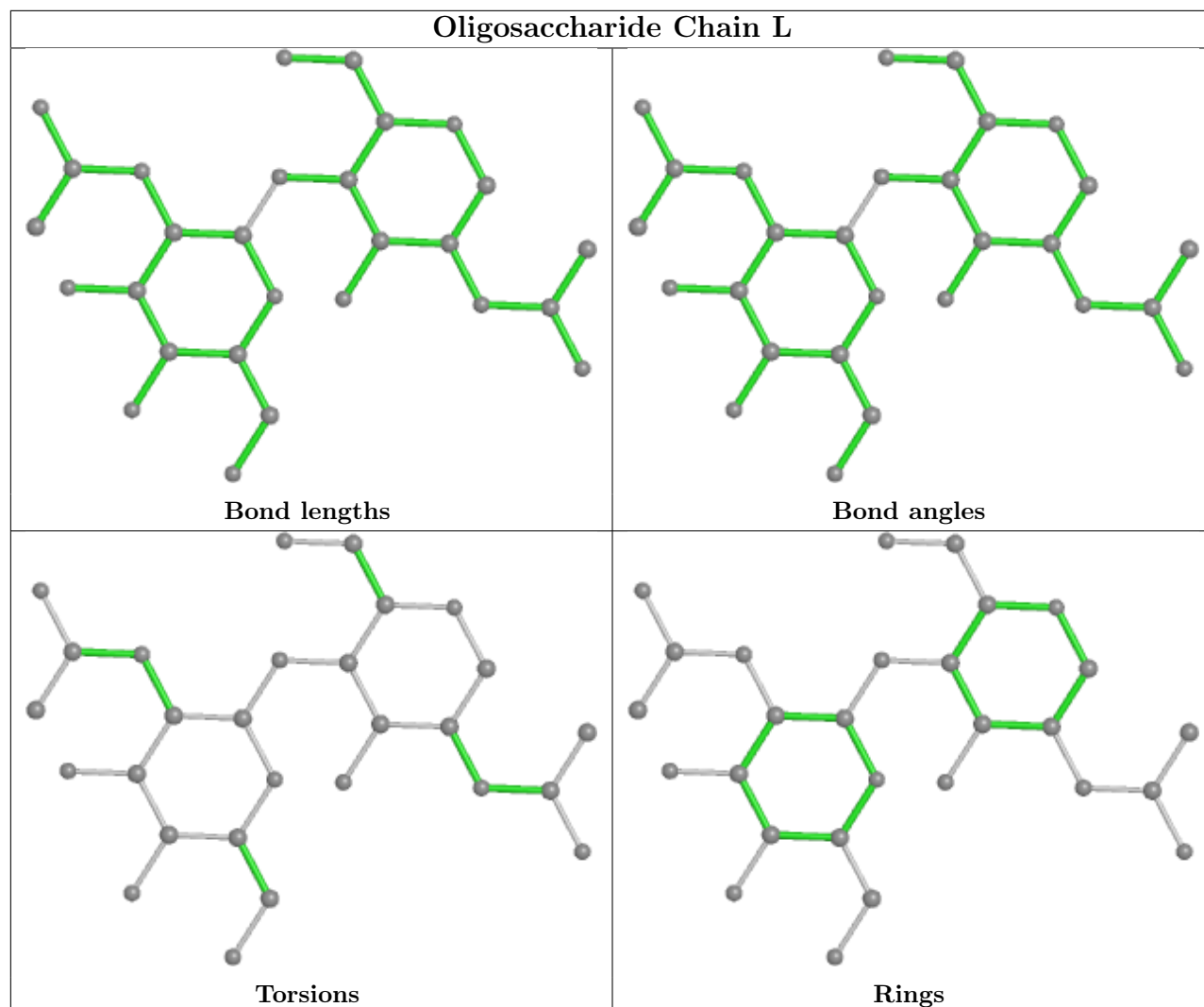


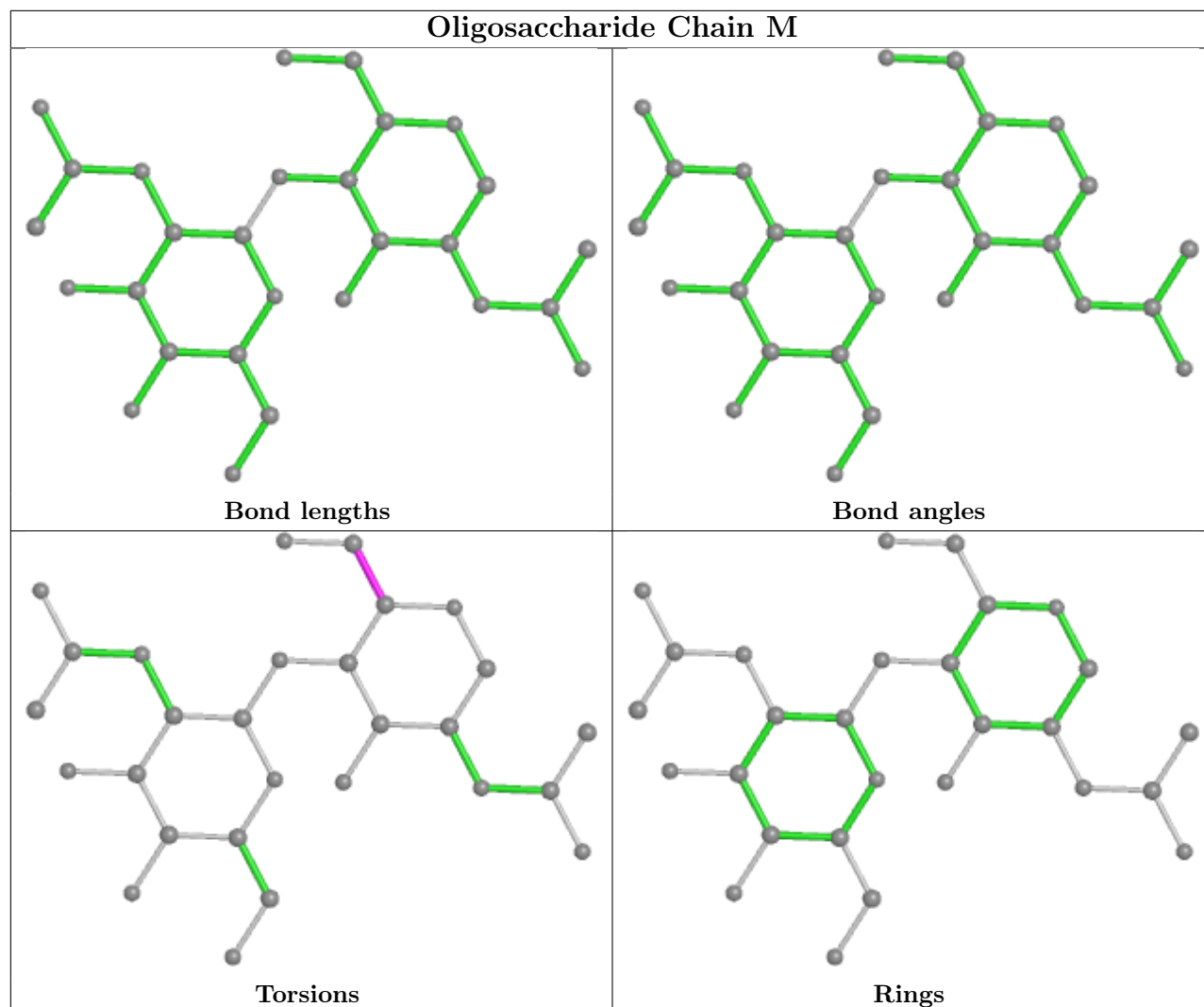


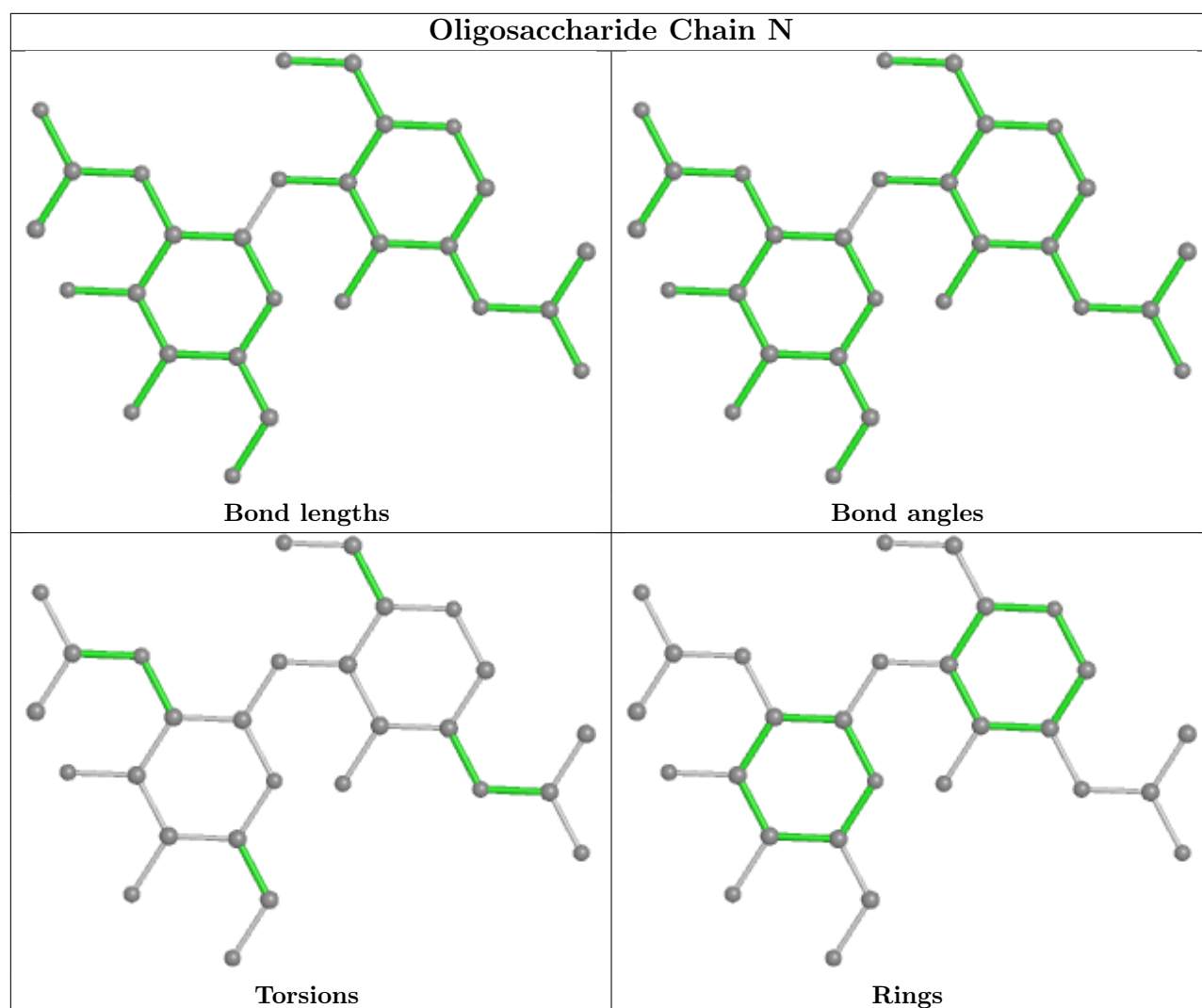


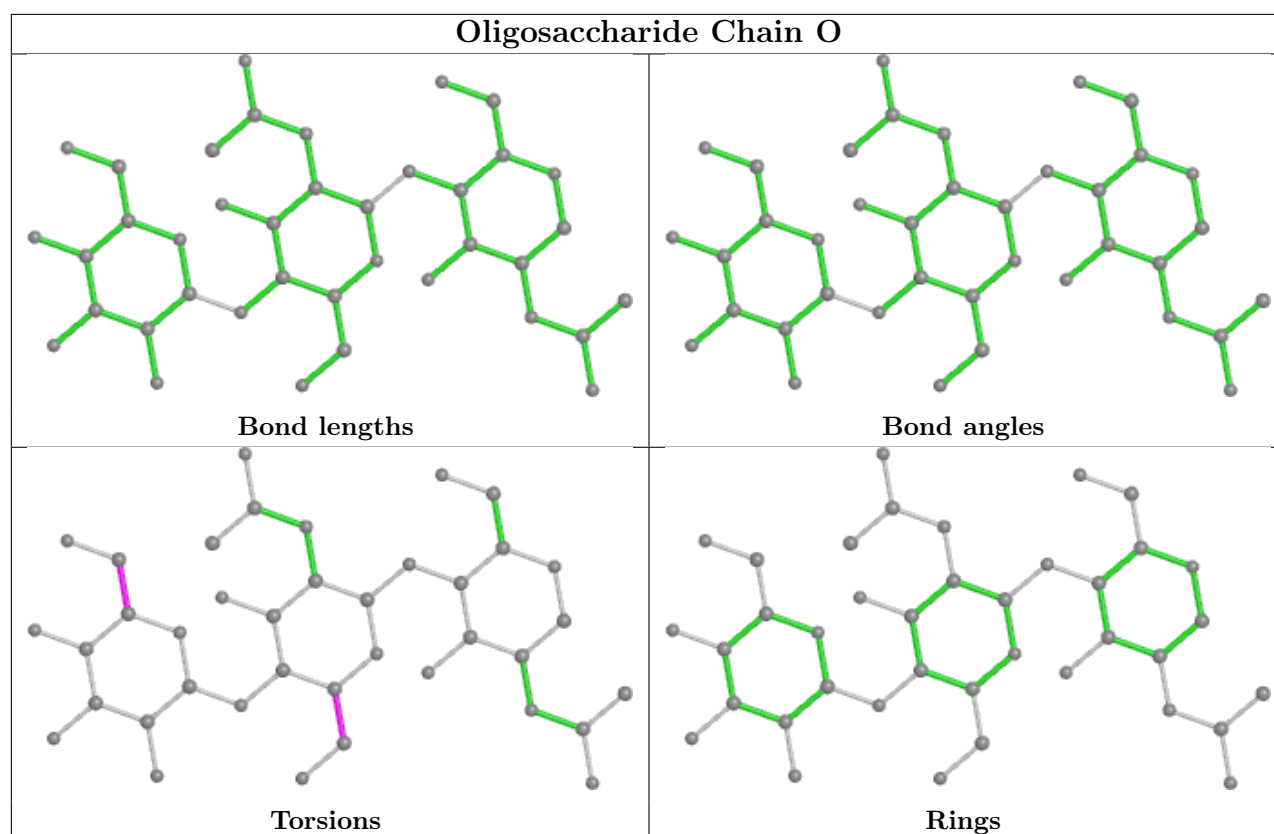












## 5.6 Ligand geometry [i](#)

13 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	$\# Z  > 2$
5	NAG	B	1305	1	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	B	1303	1	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	C	1301	1	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	A	1301	1	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	B	1301	1	14,14,15	0.22	0	17,19,21	0.40	0
5	NAG	B	1302	1	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	C	1302	1	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	A	1303	1	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	C	1303	1	14,14,15	0.21	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	A	1302	1	14,14,15	0.25	0	17,19,21	0.43	0
5	NAG	C	1304	1	14,14,15	0.22	0	17,19,21	0.42	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
5	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
5	B	1303	NAG	C4-C5-C6-O6
5	B	1305	NAG	C4-C5-C6-O6
5	C	1302	NAG	C4-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	B	1305	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1302	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-39038. These allow visual inspection of the internal detail of the map and identification of artifacts.

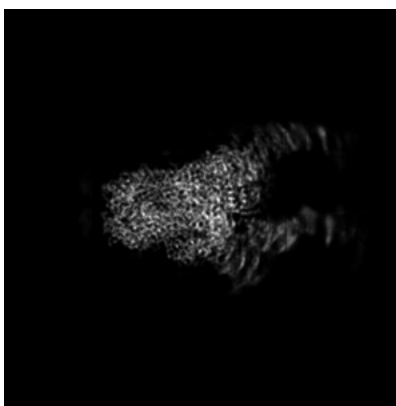
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

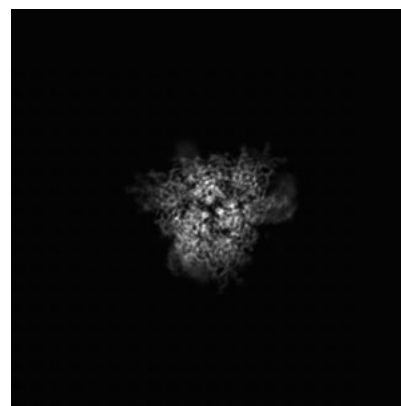
#### 6.1.1 Primary map



X

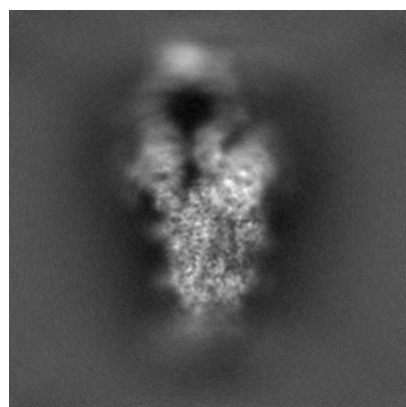


Y

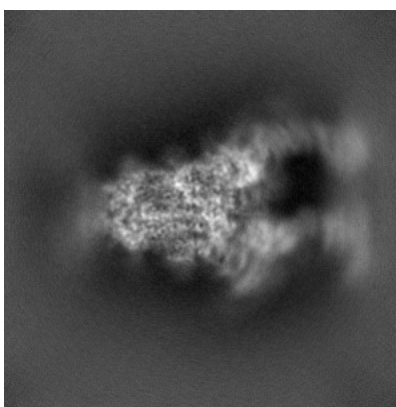


Z

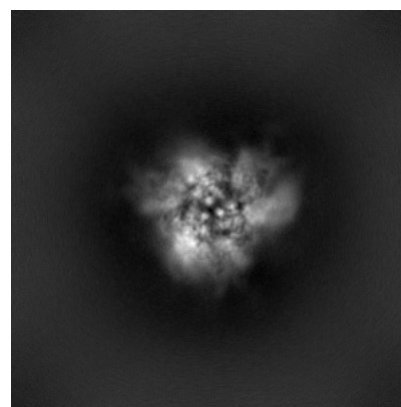
#### 6.1.2 Raw map



X



Y

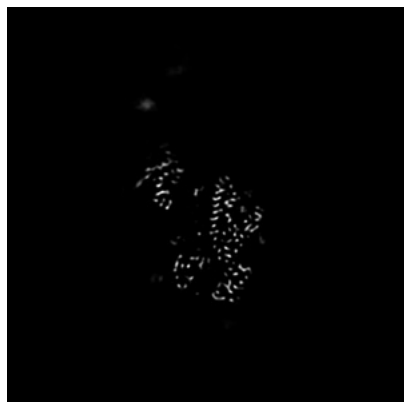


Z

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

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 200

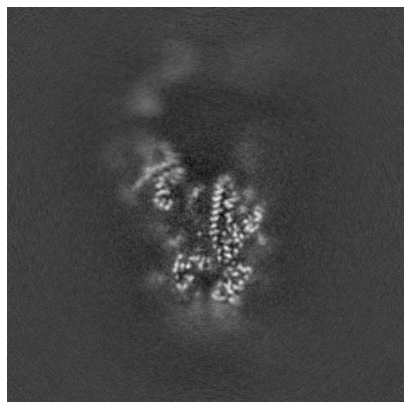


Y Index: 200

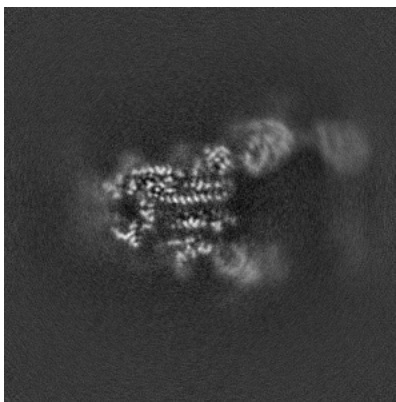


Z Index: 200

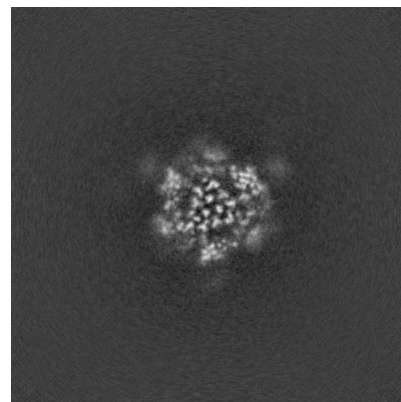
### 6.2.2 Raw map



X Index: 200



Y Index: 200

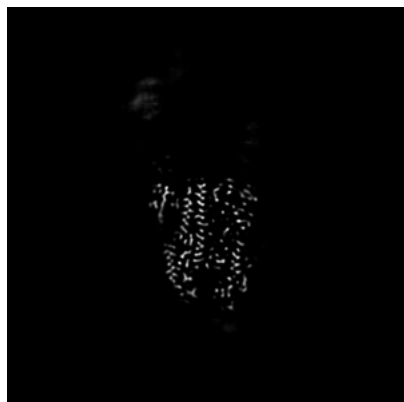


Z Index: 200

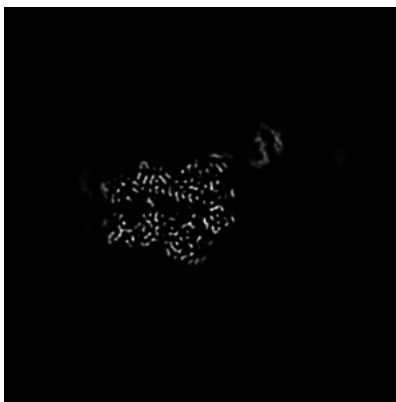
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 192

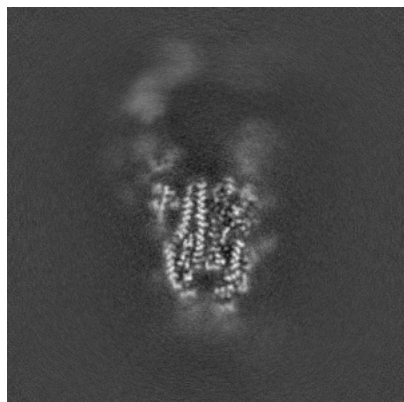


Y Index: 188

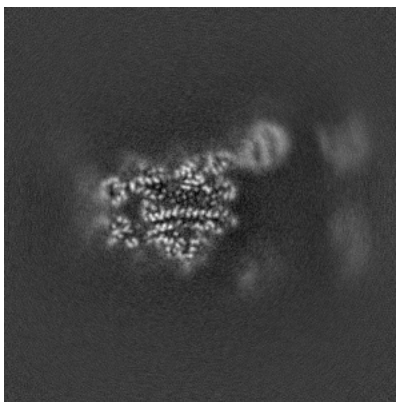


Z Index: 214

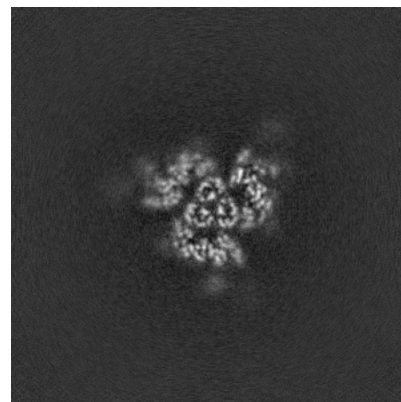
### 6.3.2 Raw map



X Index: 193



Y Index: 191

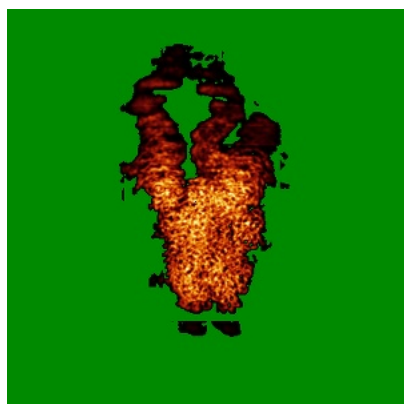


Z Index: 214

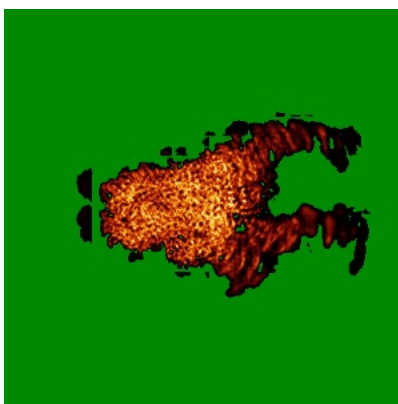
The images above show the largest variance slices of the map in three orthogonal directions.

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

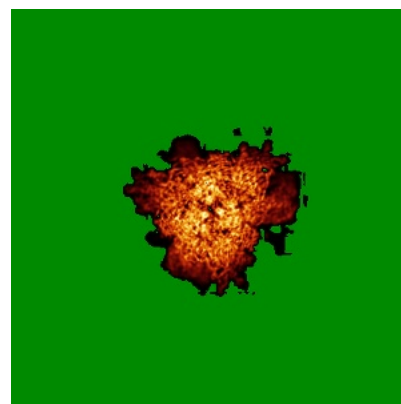
### 6.4.1 Primary map



X

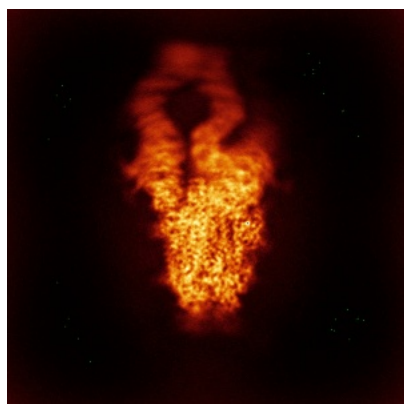


Y

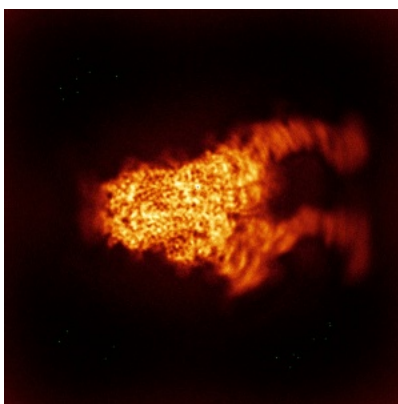


Z

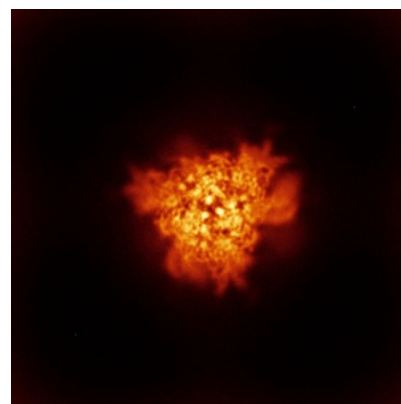
### 6.4.2 Raw map



X



Y



Z

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

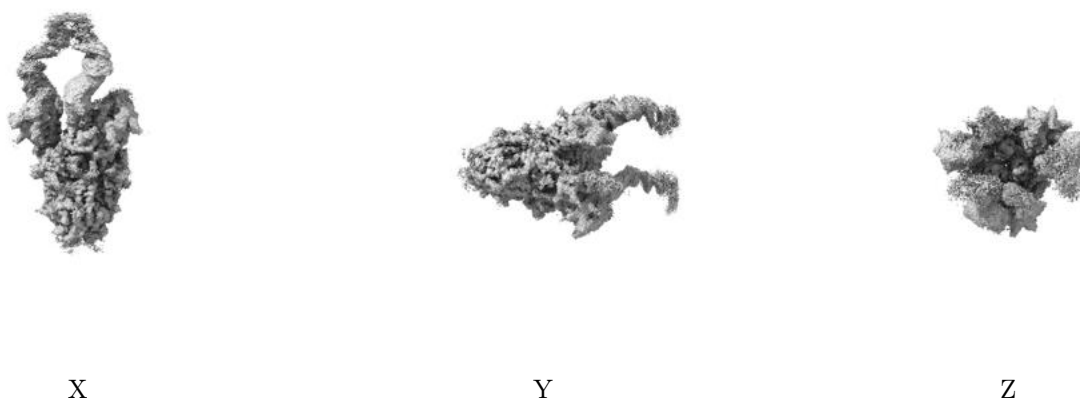
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

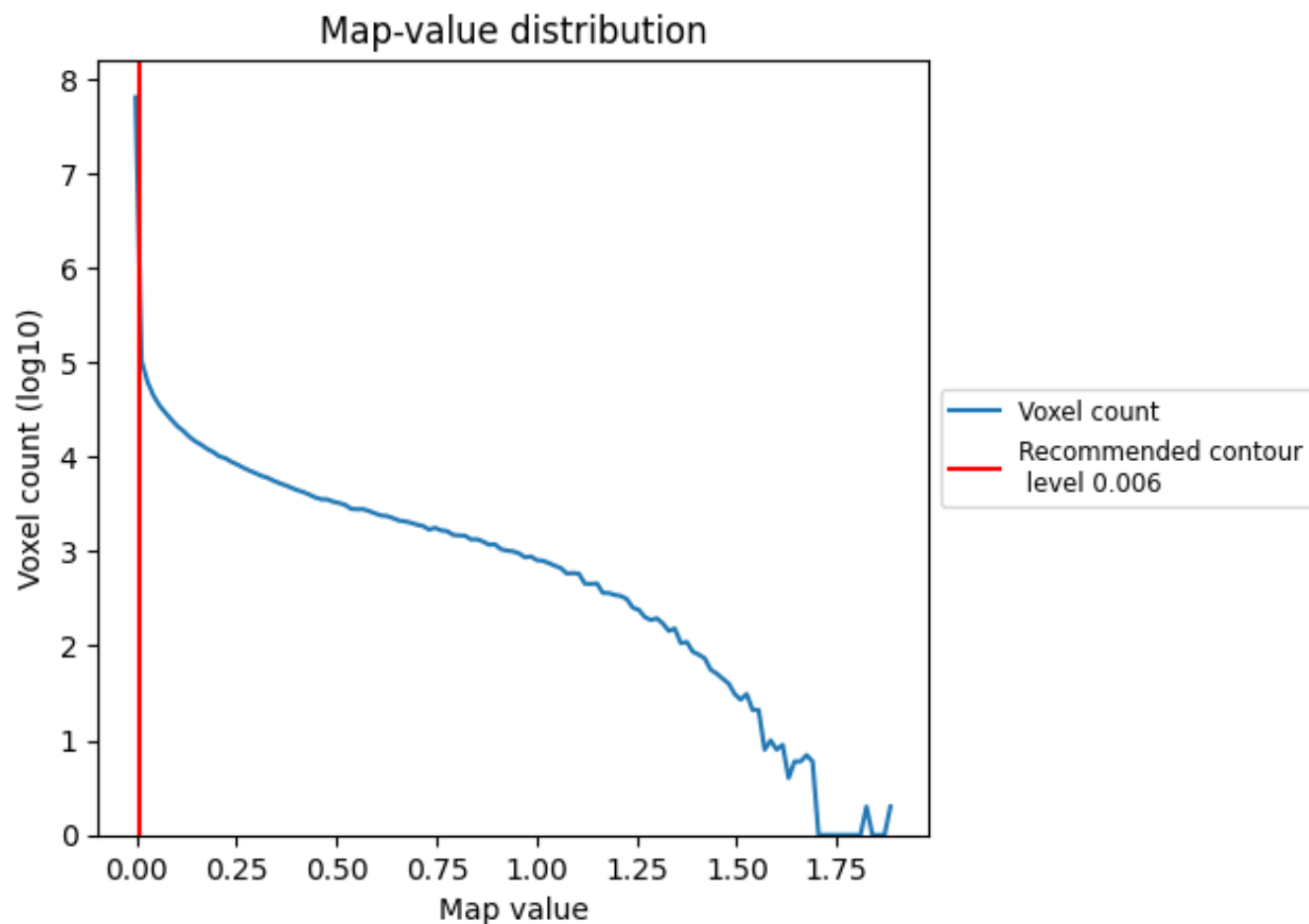
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

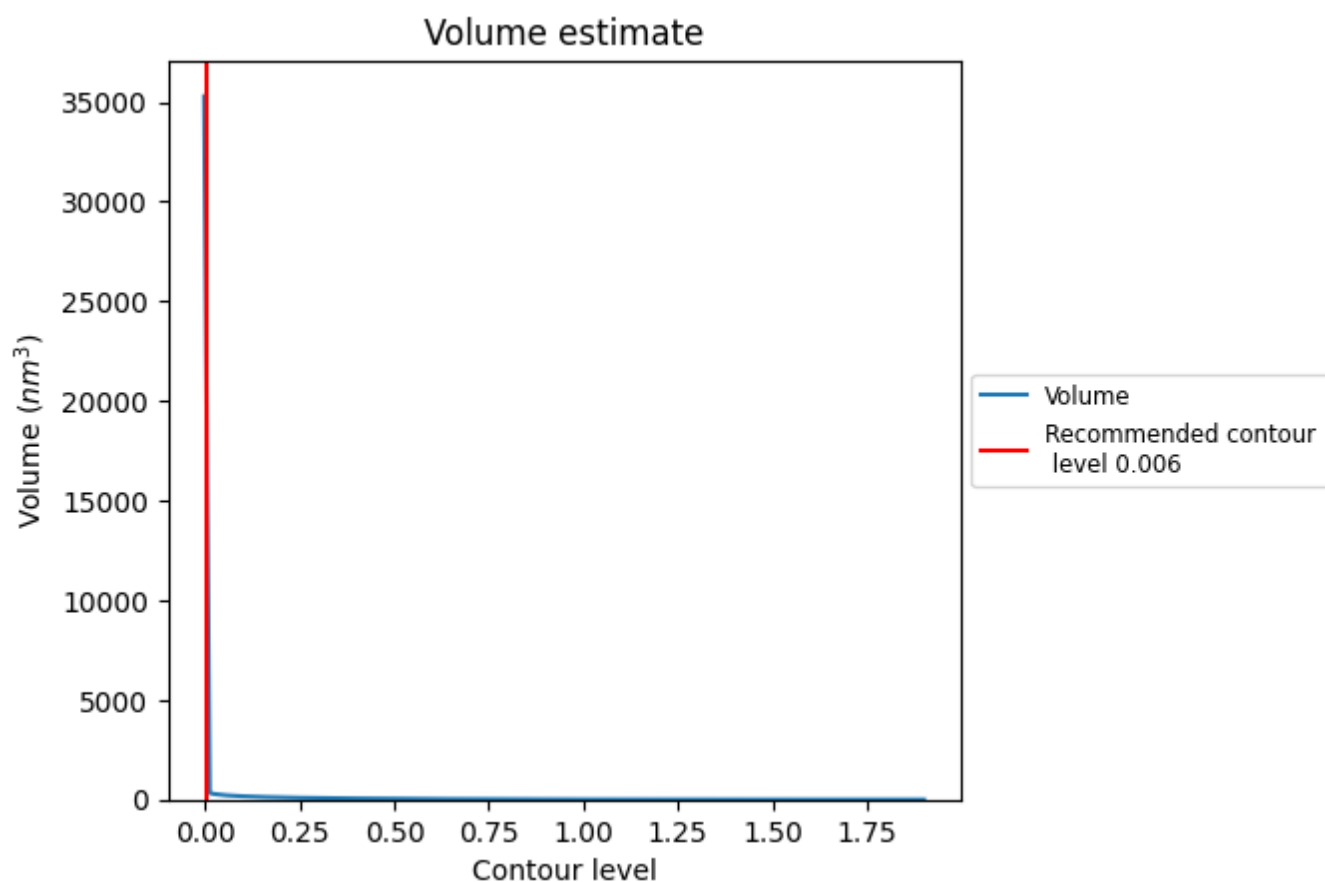
This section contains the results of statistical analysis of the map.

### 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.

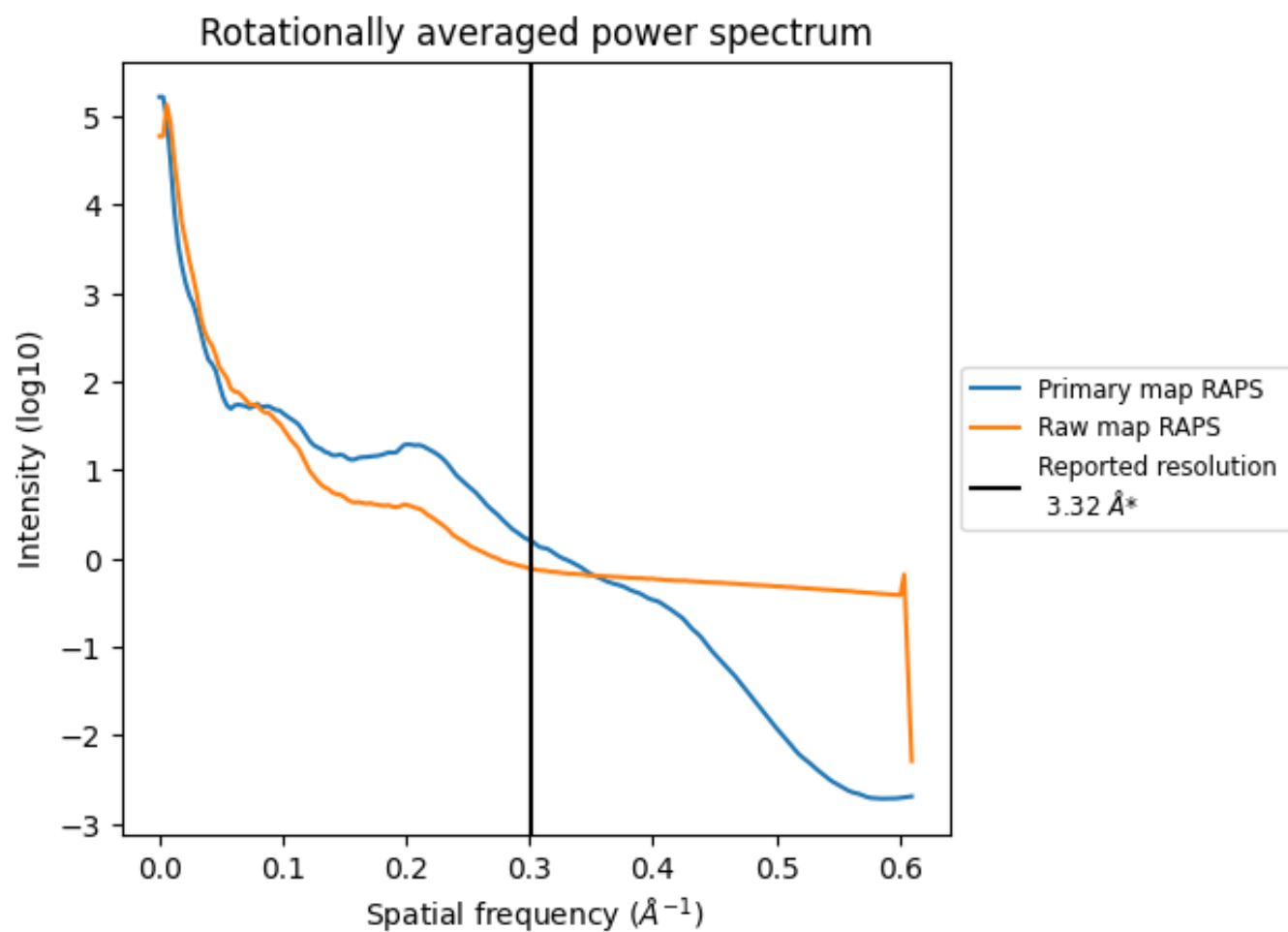
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 16612  $\text{nm}^3$ ; this corresponds to an approximate mass of 15006 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 ⓘ

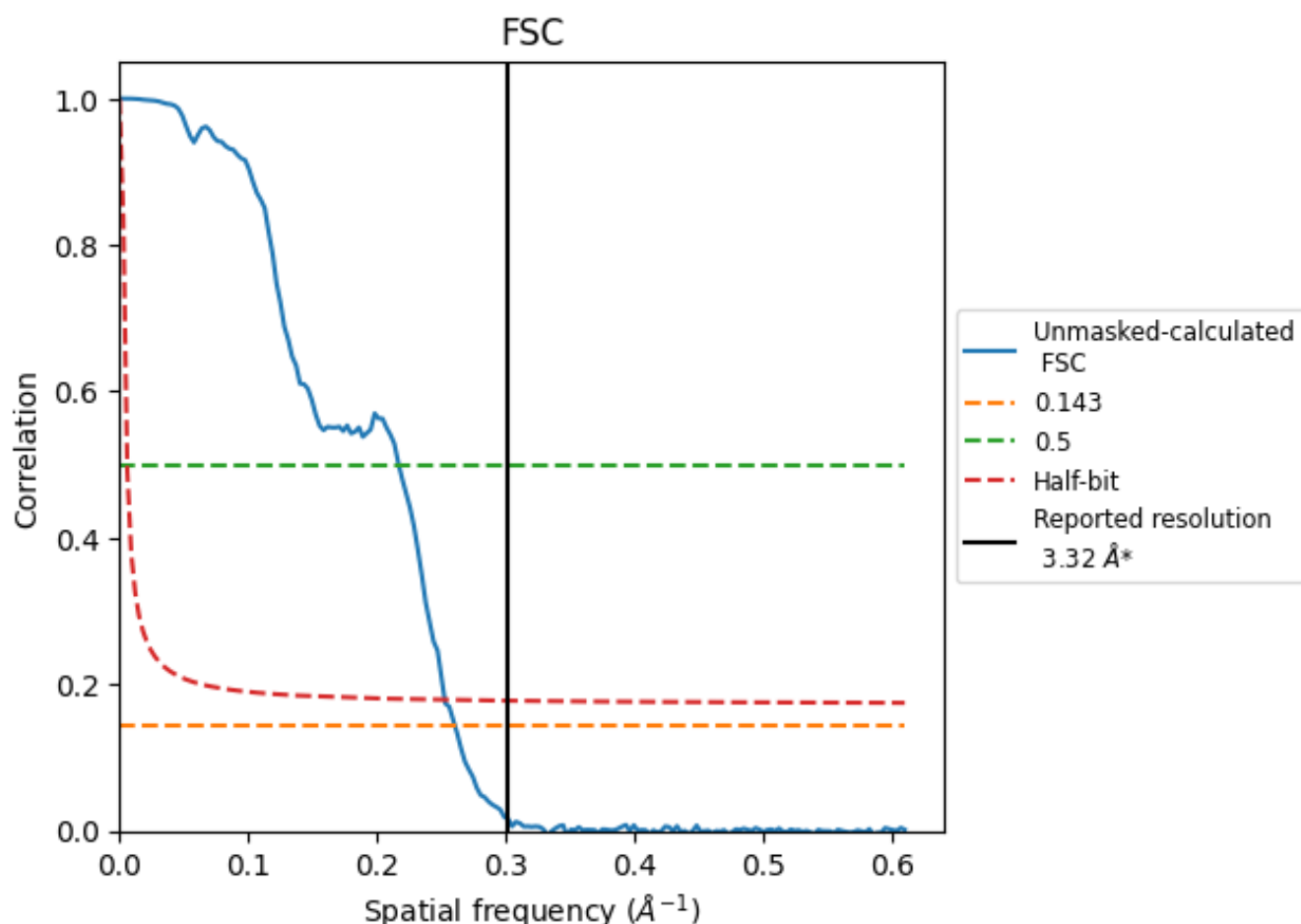


\*Reported resolution corresponds to spatial frequency of 0.301 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

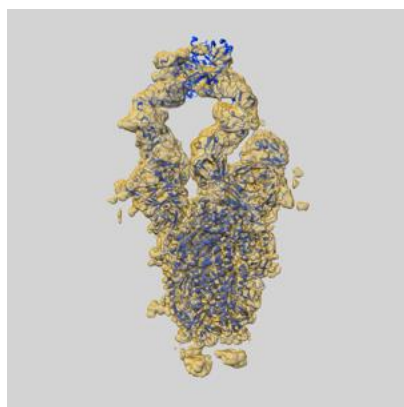
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.32	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.84	4.61	3.96

\*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 3.84 differs from the reported value 3.32 by more than 10 %

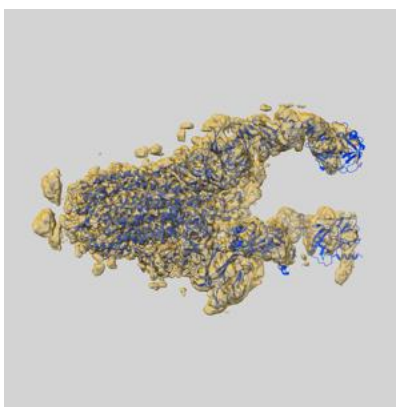
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39038 and PDB model 8Y89. Per-residue inclusion information can be found in section [3](#) on page [8](#).

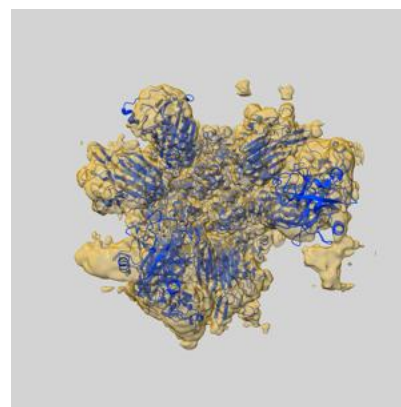
### 9.1 Map-model overlay [i](#)



X



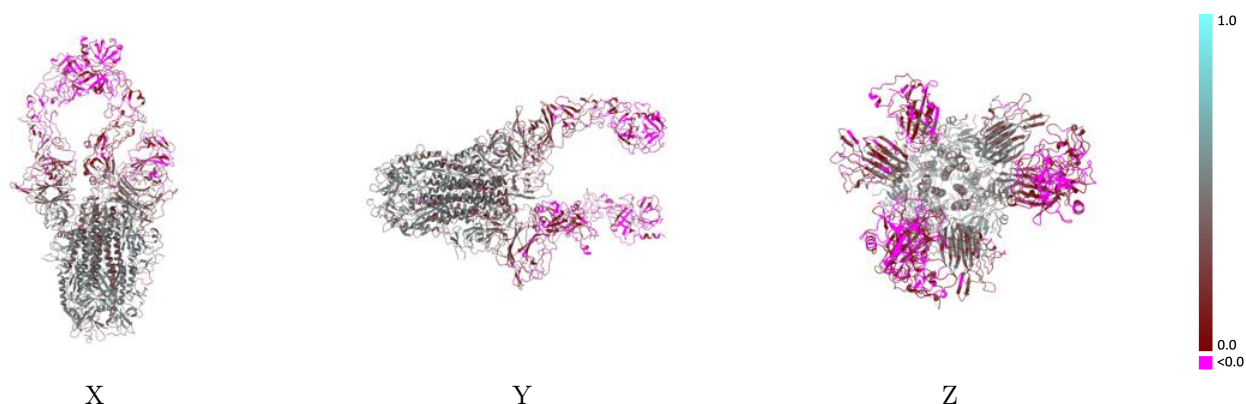
Y



Z

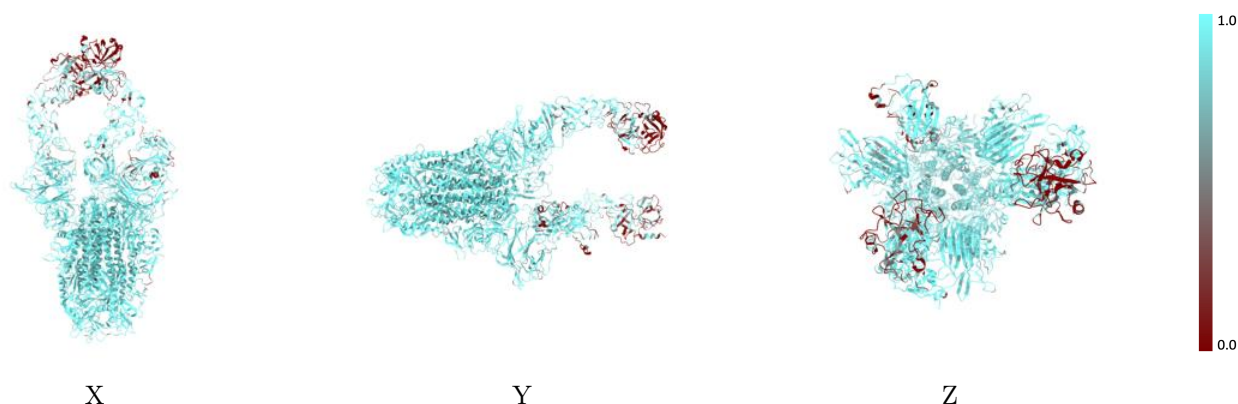
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



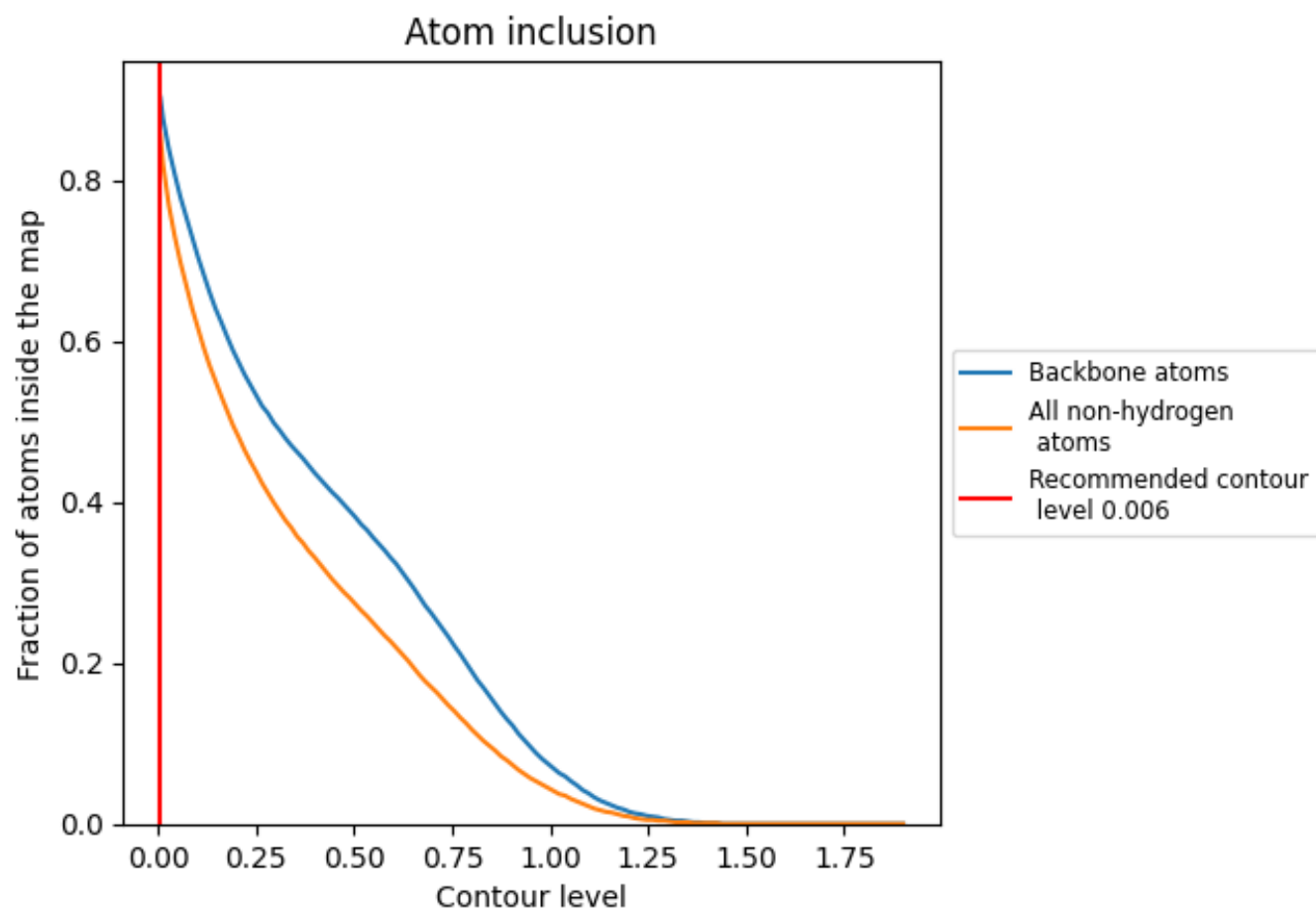
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.2960
A	 0.9020	 0.3430
B	 0.9280	 0.3530
C	 0.9150	 0.3170
D	 0.8570	 0.1440
E	 0.9640	 0.4230
F	 0.9290	 0.3940
G	 0.3160	 -0.0280
H	 0.8570	 0.3430
I	 0.8570	 0.2950
J	 0.7860	 0.2760
K	 0.9290	 0.3530
L	 0.7860	 0.2490
M	 0.7860	 0.2630
N	 0.7860	 0.2980
O	 0.8720	 0.1610
T	 0.4600	 -0.0310

