



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 10:16 PM UTC

PDB ID : 9IH8 / pdb_00009ih8
EMDB ID : EMD-52863
Title : HSV-2 postfusion glycoprotein B
Authors : Vollmer, B.; Mulvaney, T.; Ebel, H.; Nentwig, J.; Gruenewald, K.
Deposited on : 2025-02-20
Resolution : 2.21 Å(reported)
Based on initial model : .

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

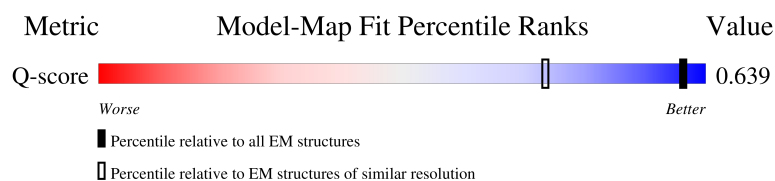
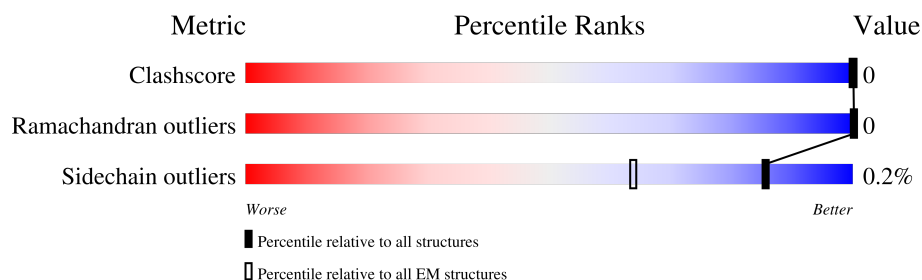
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

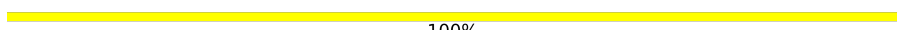
The reported resolution of this entry is 2.21 Å.

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.



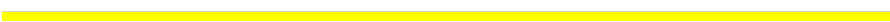
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3231 (1.71 - 2.71)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	948	 62% 38%
1	B	948	 62% 38%
1	C	948	 62% 38%
2	D	2	 100%

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Mol	Chain	Length	Quality of chain
2	E	2	 100%
2	F	2	 100%
2	G	2	 100%
2	H	2	 100%
2	I	2	 100%
2	J	2	 50% 100%
2	K	2	 50% 100%
2	L	2	 50% 100%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14487 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	588	Total	C	N	O	S	0	0
			4745	2995	833	894	23		
1	B	588	Total	C	N	O	S	0	0
			4745	2995	833	894	23		
1	C	588	Total	C	N	O	S	0	0
			4745	2995	833	894	23		

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	905	GLY	-	expression tag	UNP P06763
A	906	THR	-	expression tag	UNP P06763
A	907	LEU	-	expression tag	UNP P06763
A	908	GLU	-	expression tag	UNP P06763
A	909	VAL	-	expression tag	UNP P06763
A	910	LEU	-	expression tag	UNP P06763
A	911	PHE	-	expression tag	UNP P06763
A	912	GLN	-	expression tag	UNP P06763
A	913	GLY	-	expression tag	UNP P06763
A	914	PRO	-	expression tag	UNP P06763
A	915	GLY	-	expression tag	UNP P06763
A	916	GLY	-	expression tag	UNP P06763
A	917	SER	-	expression tag	UNP P06763
A	918	GLY	-	expression tag	UNP P06763
A	919	SER	-	expression tag	UNP P06763
A	920	ALA	-	expression tag	UNP P06763
A	921	TRP	-	expression tag	UNP P06763
A	922	SER	-	expression tag	UNP P06763
A	923	HIS	-	expression tag	UNP P06763
A	924	PRO	-	expression tag	UNP P06763
A	925	GLN	-	expression tag	UNP P06763
A	926	PHE	-	expression tag	UNP P06763
A	927	GLU	-	expression tag	UNP P06763
A	928	LYS	-	expression tag	UNP P06763

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Chain	Residue	Modelled	Actual	Comment	Reference
A	929	GLY	-	expression tag	UNP P06763
A	930	GLY	-	expression tag	UNP P06763
A	931	GLY	-	expression tag	UNP P06763
A	932	SER	-	expression tag	UNP P06763
A	933	GLY	-	expression tag	UNP P06763
A	934	GLY	-	expression tag	UNP P06763
A	935	GLY	-	expression tag	UNP P06763
A	936	SER	-	expression tag	UNP P06763
A	937	GLY	-	expression tag	UNP P06763
A	938	GLY	-	expression tag	UNP P06763
A	939	SER	-	expression tag	UNP P06763
A	940	ALA	-	expression tag	UNP P06763
A	941	TRP	-	expression tag	UNP P06763
A	942	SER	-	expression tag	UNP P06763
A	943	HIS	-	expression tag	UNP P06763
A	944	PRO	-	expression tag	UNP P06763
A	945	GLN	-	expression tag	UNP P06763
A	946	PHE	-	expression tag	UNP P06763
A	947	GLU	-	expression tag	UNP P06763
A	948	LYS	-	expression tag	UNP P06763
B	905	GLY	-	expression tag	UNP P06763
B	906	THR	-	expression tag	UNP P06763
B	907	LEU	-	expression tag	UNP P06763
B	908	GLU	-	expression tag	UNP P06763
B	909	VAL	-	expression tag	UNP P06763
B	910	LEU	-	expression tag	UNP P06763
B	911	PHE	-	expression tag	UNP P06763
B	912	GLN	-	expression tag	UNP P06763
B	913	GLY	-	expression tag	UNP P06763
B	914	PRO	-	expression tag	UNP P06763
B	915	GLY	-	expression tag	UNP P06763
B	916	GLY	-	expression tag	UNP P06763
B	917	SER	-	expression tag	UNP P06763
B	918	GLY	-	expression tag	UNP P06763
B	919	SER	-	expression tag	UNP P06763
B	920	ALA	-	expression tag	UNP P06763
B	921	TRP	-	expression tag	UNP P06763
B	922	SER	-	expression tag	UNP P06763
B	923	HIS	-	expression tag	UNP P06763
B	924	PRO	-	expression tag	UNP P06763
B	925	GLN	-	expression tag	UNP P06763
B	926	PHE	-	expression tag	UNP P06763

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Chain	Residue	Modelled	Actual	Comment	Reference
B	927	GLU	-	expression tag	UNP P06763
B	928	LYS	-	expression tag	UNP P06763
B	929	GLY	-	expression tag	UNP P06763
B	930	GLY	-	expression tag	UNP P06763
B	931	GLY	-	expression tag	UNP P06763
B	932	SER	-	expression tag	UNP P06763
B	933	GLY	-	expression tag	UNP P06763
B	934	GLY	-	expression tag	UNP P06763
B	935	GLY	-	expression tag	UNP P06763
B	936	SER	-	expression tag	UNP P06763
B	937	GLY	-	expression tag	UNP P06763
B	938	GLY	-	expression tag	UNP P06763
B	939	SER	-	expression tag	UNP P06763
B	940	ALA	-	expression tag	UNP P06763
B	941	TRP	-	expression tag	UNP P06763
B	942	SER	-	expression tag	UNP P06763
B	943	HIS	-	expression tag	UNP P06763
B	944	PRO	-	expression tag	UNP P06763
B	945	GLN	-	expression tag	UNP P06763
B	946	PHE	-	expression tag	UNP P06763
B	947	GLU	-	expression tag	UNP P06763
B	948	LYS	-	expression tag	UNP P06763
C	905	GLY	-	expression tag	UNP P06763
C	906	THR	-	expression tag	UNP P06763
C	907	LEU	-	expression tag	UNP P06763
C	908	GLU	-	expression tag	UNP P06763
C	909	VAL	-	expression tag	UNP P06763
C	910	LEU	-	expression tag	UNP P06763
C	911	PHE	-	expression tag	UNP P06763
C	912	GLN	-	expression tag	UNP P06763
C	913	GLY	-	expression tag	UNP P06763
C	914	PRO	-	expression tag	UNP P06763
C	915	GLY	-	expression tag	UNP P06763
C	916	GLY	-	expression tag	UNP P06763
C	917	SER	-	expression tag	UNP P06763
C	918	GLY	-	expression tag	UNP P06763
C	919	SER	-	expression tag	UNP P06763
C	920	ALA	-	expression tag	UNP P06763
C	921	TRP	-	expression tag	UNP P06763
C	922	SER	-	expression tag	UNP P06763
C	923	HIS	-	expression tag	UNP P06763
C	924	PRO	-	expression tag	UNP P06763

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Chain	Residue	Modelled	Actual	Comment	Reference
C	925	GLN	-	expression tag	UNP P06763
C	926	PHE	-	expression tag	UNP P06763
C	927	GLU	-	expression tag	UNP P06763
C	928	LYS	-	expression tag	UNP P06763
C	929	GLY	-	expression tag	UNP P06763
C	930	GLY	-	expression tag	UNP P06763
C	931	GLY	-	expression tag	UNP P06763
C	932	SER	-	expression tag	UNP P06763
C	933	GLY	-	expression tag	UNP P06763
C	934	GLY	-	expression tag	UNP P06763
C	935	GLY	-	expression tag	UNP P06763
C	936	SER	-	expression tag	UNP P06763
C	937	GLY	-	expression tag	UNP P06763
C	938	GLY	-	expression tag	UNP P06763
C	939	SER	-	expression tag	UNP P06763
C	940	ALA	-	expression tag	UNP P06763
C	941	TRP	-	expression tag	UNP P06763
C	942	SER	-	expression tag	UNP P06763
C	943	HIS	-	expression tag	UNP P06763
C	944	PRO	-	expression tag	UNP P06763
C	945	GLN	-	expression tag	UNP P06763
C	946	PHE	-	expression tag	UNP P06763
C	947	GLU	-	expression tag	UNP P06763
C	948	LYS	-	expression tag	UNP P06763

- Molecule 2 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		

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

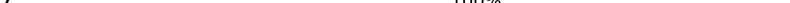
[illegible]

- Molecule 1: Envelope glycoprotein B

Chain C: 62% 38%

GLY	VAL	LYS	GLY	GLN	ALA	MET
SER	THR	THR	VAL	ARG	ARG	GLY
GLY	ASN	SER	VAL	ARG	LYS	GLY
SER	MET	PRO	SER	PRO	ARG	GLY
ALA	VAL	GLY	ALA	ASN	THR	ILE
TRP	LEU	VAL	VAL	ALA	LYS	ILE
SER	ARG	VAL	SER	ALA	LYS	CYS
HIS	LYS	GLY	GLY	THR	PRO	ALA
PRO	ARG	GLY	VAL	PRO	PRO	LEU
GLN	ASN	GLU	SER	ALA	LYS	ALA
PHE	LYS	GLY	SER	PRO	VAL	VAL
GLU	ALA	GLU	PHE	LEU	PRO	GLY
ARG	ALA	GLU	MET	ARG	GLU	ALA
LYS	TYR	GLY	SER	GLU	ALA	LEU
	SER	ALA	ASN	ALA	THR	VAL
	PRO	GLU	PRO	PRO	PRO	ALA
	LEU	GLY	PHE	SER	PRO	ALA
	HIS	GLY	GLY	ALA	VAL	ALA
	ASN	GLY	ALA	ASN	ASP	ALA
	GLU	PHE	LEU	ALA	ALA	SER
	ASP	ASP	ALA	S498	ASN	ALA
	GLU	GLU	VAL	V578	ALA	ALA
	ALA	ALA	GLY	I720	THR	PRO
	ASP	LYS	LEU	I720	VAL	ALA
	GLU	GLU	VAL	ARG	ALA	ALA
	ASP	GLU	LEU	ALA	GLY	ALA
	GLU	ALA	ALA	ASP	HIS	ALA
	LEU	ARG	GLY	ALA	ALA	ALA
	GLY	GLU	LEU	ASN	THR	ARG
	THR	MET	VAL	ALA	LEU	ALA
	LEU	ILE	ALA	ALA	ARG	ALA
	GLU	ARG	ALA	MET	GLY	GLY
	VAL	VAL	PHE	PHE	HIS	GLY
	LEU	MET	PHE	ALA	LEU	VAL
	PHE	ALA	GLY	GLY	ARG	ALA
	GLN	LEU	PHE	LEU	GLU	ALA
	GLY	VAL	ARG	PHE	GLU	ALA
	GLY	ARG	LEU	GLY	N103	ASN
	SER	THR	GLN	MET	E214	GLY
	ALA	GLU	ARG	GLY	E214	PRO
	TRP	HIS	ASN	ASP	R274	ALA
	ALA	LYS	PRO	LEU	V290	SER
	HIS	ALA	MET	GLY	V290	ARG
	PRO	ARG	LYS	ARG	E457	PRO
	GLN	LYS	ALA	ALA	E457	PRO
	PHE	LYS	LEU	VAL	LEU	PRO
	GLU	GLY	TYR	GLY	TYR	VAL
	LYS	THR	PRO	LYS	VAL	VAL
	GLY	SER	LEU	VAL	ARG	SER
	ALA	ALA	THR	VAL	GLU	PRO
	GLY	LEU	THR	MET	TYR	THR
	GLY	LEU	LYS	GLY	MET	ALA
	GLY	SER	GLU	VAL	ARG	THR
	GLY	SER	LEU	VAL	GLU	THR
	GLY	SER	LEU	VAL	VAL	THR

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

Chain D:  100%

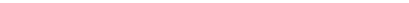
NAG1
NAG2

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

Chain E: 100%

NAG1
NAG2

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

Chain F:  100%

MAG1
MAG2

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

Chain G:  100%MAG1
MAG2

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

Chain H:  100%MAG1
MAG2

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

Chain I:  100%MAG1
MAG2

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

Chain J:  50% 100%MAG1
MAG2

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

Chain K:  50% 100%MAG1
MAG2

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

Chain L:  50% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	323536	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.825	Depositor
Minimum map value	-0.294	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.102	Depositor
Map size (Å)	348.6, 348.6, 348.6	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	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: 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	0.56	0/4862	1.21	1/6605 (0.0%)
1	B	0.56	0/4862	1.21	0/6605
1	C	0.56	0/4862	1.22	2/6605 (0.0%)
All	All	0.56	0/14586	1.22	3/19815 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	290	VAL	CA-CB-CG2	-6.83	98.79	110.40
1	C	290	VAL	N-CA-CB	6.16	119.66	111.90
1	A	581	GLN	OE1-CD-NE2	-5.05	117.55	122.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	274	ARG	Sidechain

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	4745	0	4569	0	0
1	B	4745	0	4569	1	0
1	C	4745	0	4569	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
All	All	14487	0	13932	1	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 0.

All (1) 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:111:CYS:HB3	1:B:557:SER:HB3	2.03	0.41

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	584/948 (62%)	575 (98%)	9 (2%)	0	100	100
1	B	584/948 (62%)	576 (99%)	8 (1%)	0	100	100
1	C	584/948 (62%)	577 (99%)	7 (1%)	0	100	100
All	All	1752/2844 (62%)	1728 (99%)	24 (1%)	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	512/769 (67%)	511 (100%)	1 (0%)	87	94
1	B	512/769 (67%)	512 (100%)	0	100	100
1	C	512/769 (67%)	510 (100%)	2 (0%)	84	91
All	All	1536/2307 (67%)	1533 (100%)	3 (0%)	85	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	496	SER
1	C	214	GLU
1	C	578	VAL

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

Mol	Chain	Res	Type
1	A	107	GLN
1	A	655	GLN
1	A	703	GLN
1	C	258	HIS
1	C	634	HIS
1	C	703	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 ⓘ

18 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	D	1	2,1	14,14,15	1.70	3 (21%)	17,19,21	0.51	0
2	NAG	D	2	2	14,14,15	1.73	4 (28%)	17,19,21	1.13	1 (5%)
2	NAG	E	1	2,1	14,14,15	1.72	3 (21%)	17,19,21	0.64	0
2	NAG	E	2	2	14,14,15	1.79	4 (28%)	17,19,21	1.17	1 (5%)
2	NAG	F	1	2,1	14,14,15	1.70	3 (21%)	17,19,21	0.58	0
2	NAG	F	2	2	14,14,15	1.76	3 (21%)	17,19,21	1.00	1 (5%)
2	NAG	G	1	2,1	14,14,15	1.74	4 (28%)	17,19,21	0.79	0
2	NAG	G	2	2	14,14,15	1.77	3 (21%)	17,19,21	0.93	1 (5%)
2	NAG	H	1	2,1	14,14,15	1.76	3 (21%)	17,19,21	0.70	0
2	NAG	H	2	2	14,14,15	1.76	4 (28%)	17,19,21	1.05	1 (5%)
2	NAG	I	1	2,1	14,14,15	1.78	5 (35%)	17,19,21	0.81	0
2	NAG	I	2	2	14,14,15	1.79	4 (28%)	17,19,21	0.96	1 (5%)
2	NAG	J	1	2,1	14,14,15	1.78	3 (21%)	17,19,21	0.76	0
2	NAG	J	2	2	14,14,15	1.79	4 (28%)	17,19,21	1.12	1 (5%)
2	NAG	K	1	2,1	14,14,15	1.78	4 (28%)	17,19,21	1.07	2 (11%)
2	NAG	K	2	2	14,14,15	1.78	3 (21%)	17,19,21	0.91	1 (5%)
2	NAG	L	1	2,1	14,14,15	1.76	3 (21%)	17,19,21	0.86	0
2	NAG	L	2	2	14,14,15	1.78	4 (28%)	17,19,21	1.03	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	NAG	O5-C5	3.41	1.50	1.43
2	I	2	NAG	O5-C5	3.41	1.50	1.43
2	J	2	NAG	O5-C5	3.22	1.49	1.43
2	J	2	NAG	C1-C2	3.21	1.56	1.52
2	F	2	NAG	O5-C5	3.21	1.49	1.43
2	E	2	NAG	O5-C5	3.21	1.49	1.43
2	H	1	NAG	O5-C5	3.21	1.49	1.43
2	H	2	NAG	O5-C5	3.19	1.49	1.43
2	L	2	NAG	O5-C5	3.18	1.49	1.43
2	I	1	NAG	O5-C5	3.14	1.49	1.43
2	D	2	NAG	O5-C5	3.14	1.49	1.43
2	K	2	NAG	C1-C2	3.13	1.56	1.52
2	G	1	NAG	O5-C5	3.13	1.49	1.43
2	L	2	NAG	C1-C2	3.11	1.56	1.52
2	I	1	NAG	C1-C2	3.11	1.56	1.52
2	L	1	NAG	C1-C2	3.10	1.56	1.52
2	K	2	NAG	O5-C5	3.10	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	O5-C5	3.08	1.49	1.43
2	D	1	NAG	O5-C5	3.06	1.49	1.43
2	L	1	NAG	O5-C5	3.05	1.49	1.43
2	E	2	NAG	C1-C2	3.04	1.56	1.52
2	H	2	NAG	C1-C2	3.04	1.56	1.52
2	J	1	NAG	C1-C2	3.02	1.56	1.52
2	F	2	NAG	C1-C2	3.01	1.56	1.52
2	J	1	NAG	O5-C5	2.99	1.49	1.43
2	G	2	NAG	C1-C2	2.97	1.56	1.52
2	I	2	NAG	C1-C2	2.96	1.56	1.52
2	G	1	NAG	C1-C2	2.95	1.56	1.52
2	E	1	NAG	O5-C5	2.94	1.49	1.43
2	D	2	NAG	C1-C2	2.93	1.56	1.52
2	K	1	NAG	O5-C5	2.86	1.49	1.43
2	H	1	NAG	C1-C2	2.84	1.56	1.52
2	K	1	NAG	C1-C2	2.82	1.56	1.52
2	J	1	NAG	O4-C4	2.81	1.49	1.43
2	E	1	NAG	C1-C2	2.79	1.56	1.52
2	F	1	NAG	C1-C2	2.79	1.56	1.52
2	K	1	NAG	O4-C4	2.77	1.49	1.43
2	D	1	NAG	O4-C4	2.76	1.49	1.43
2	E	1	NAG	O4-C4	2.72	1.49	1.43
2	H	2	NAG	O5-C1	2.69	1.48	1.43
2	G	2	NAG	O5-C1	2.68	1.48	1.43
2	H	1	NAG	O4-C4	2.67	1.49	1.43
2	F	1	NAG	O4-C4	2.66	1.49	1.43
2	F	2	NAG	O5-C1	2.65	1.48	1.43
2	K	2	NAG	O5-C1	2.64	1.48	1.43
2	I	1	NAG	O4-C4	2.64	1.49	1.43
2	D	1	NAG	C1-C2	2.63	1.55	1.52
2	I	2	NAG	O5-C1	2.62	1.48	1.43
2	G	1	NAG	O4-C4	2.62	1.49	1.43
2	J	2	NAG	O5-C1	2.60	1.48	1.43
2	L	2	NAG	O5-C1	2.58	1.48	1.43
2	E	2	NAG	O5-C1	2.58	1.48	1.43
2	L	1	NAG	O4-C4	2.56	1.49	1.43
2	D	2	NAG	O5-C1	2.48	1.47	1.43
2	J	2	NAG	C8-C7	2.07	1.54	1.50
2	E	2	NAG	C8-C7	2.07	1.54	1.50
2	G	1	NAG	C8-C7	2.05	1.54	1.50
2	H	2	NAG	C8-C7	2.05	1.54	1.50
2	L	2	NAG	C8-C7	2.04	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	NAG	C8-C7	2.02	1.54	1.50
2	I	1	NAG	C8-C7	2.01	1.54	1.50
2	I	1	NAG	O5-C1	2.01	1.47	1.43
2	D	2	NAG	C8-C7	2.00	1.54	1.50
2	I	2	NAG	C8-C7	2.00	1.54	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	4.11	117.69	112.19
2	E	2	NAG	C1-O5-C5	4.09	117.67	112.19
2	H	2	NAG	C1-O5-C5	3.72	117.18	112.19
2	J	2	NAG	C1-O5-C5	3.65	117.08	112.19
2	F	2	NAG	C1-O5-C5	3.50	116.88	112.19
2	L	2	NAG	C1-O5-C5	3.13	116.38	112.19
2	G	2	NAG	C1-O5-C5	2.80	115.94	112.19
2	K	1	NAG	C4-C3-C2	2.77	115.08	111.02
2	I	2	NAG	C1-O5-C5	2.54	115.59	112.19
2	K	2	NAG	C1-O5-C5	2.49	115.53	112.19
2	K	1	NAG	C3-C4-C5	2.25	114.31	110.23

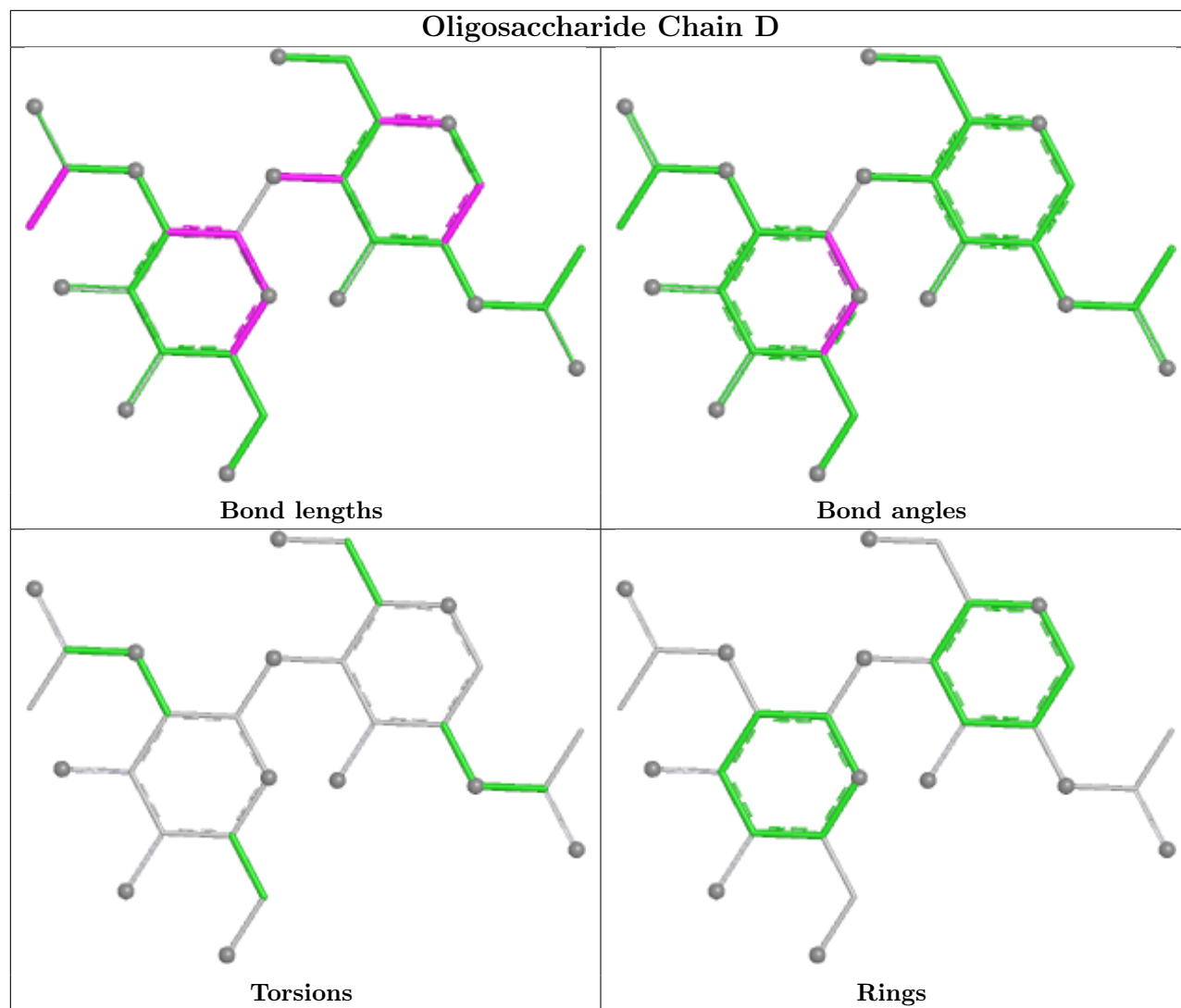
There are no chirality outliers.

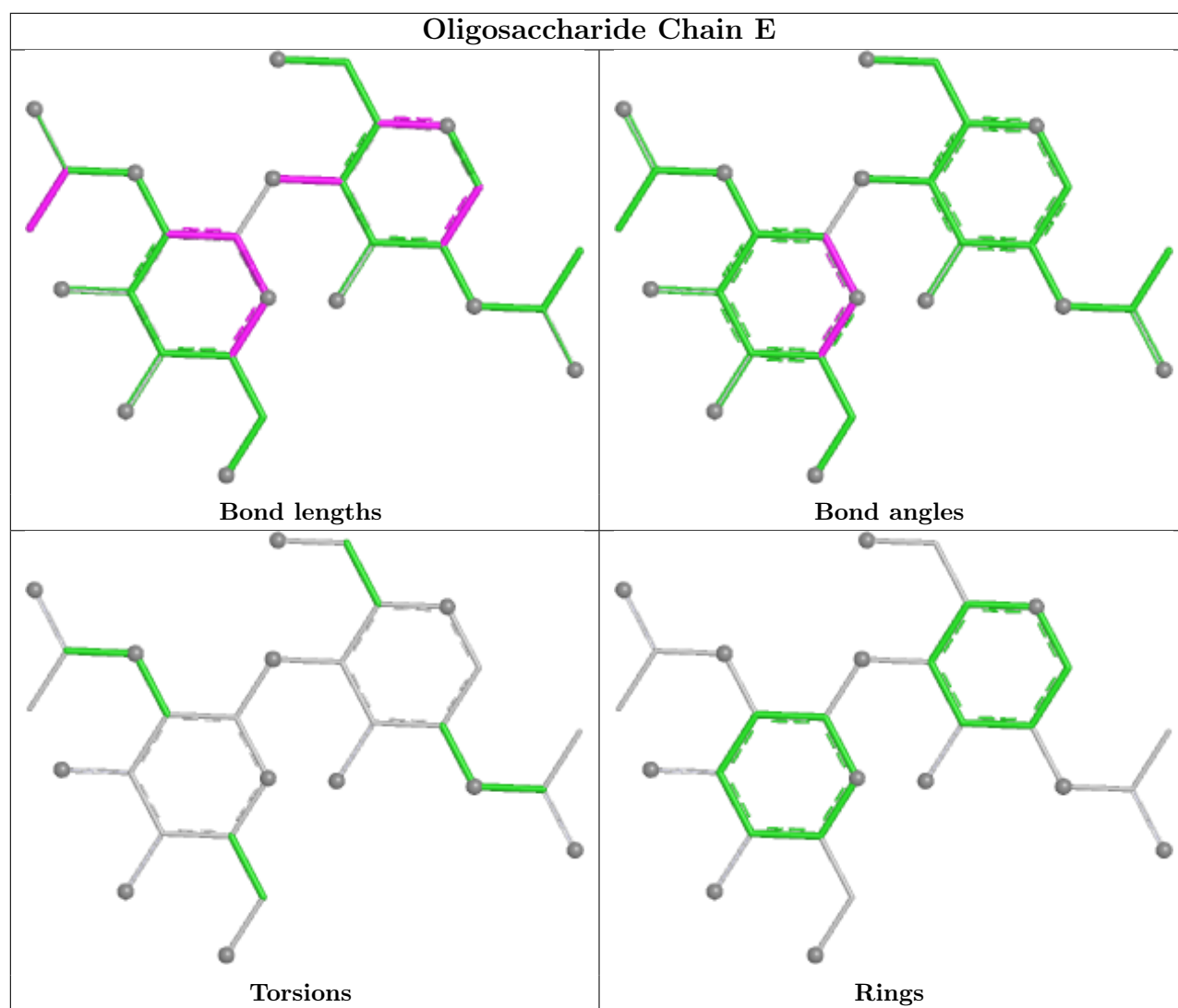
There are no torsion outliers.

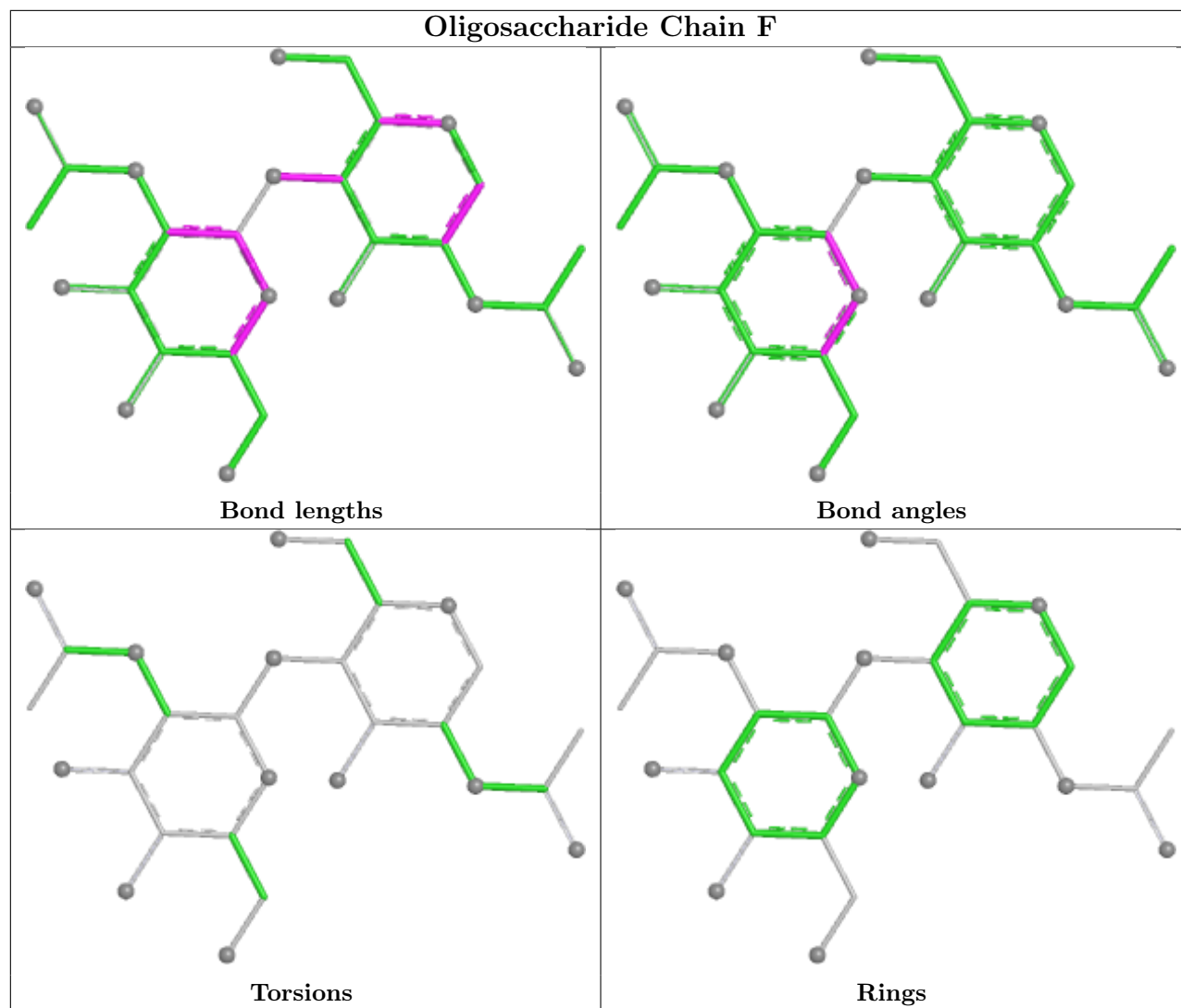
There are no ring outliers.

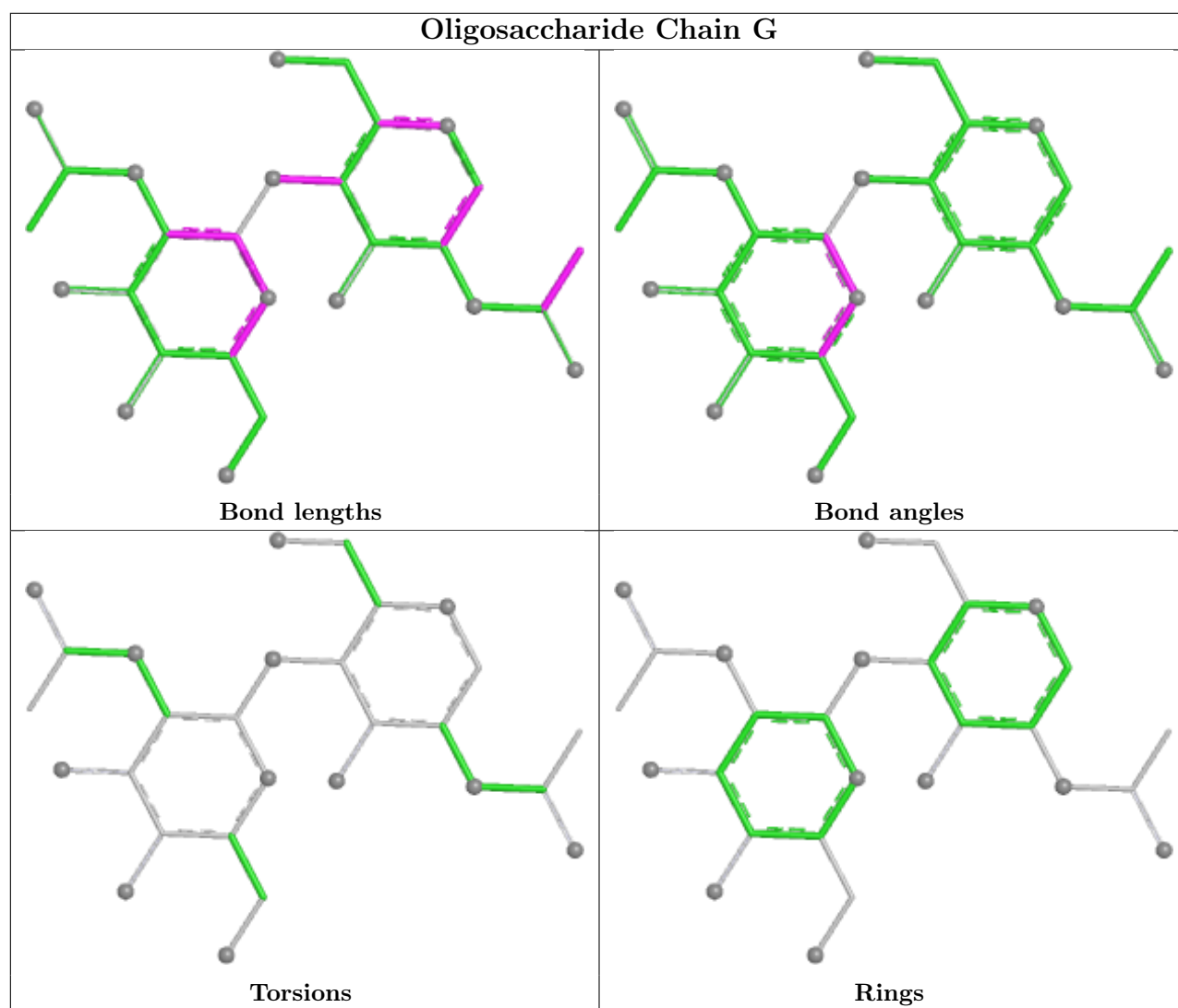
No monomer is involved in short contacts.

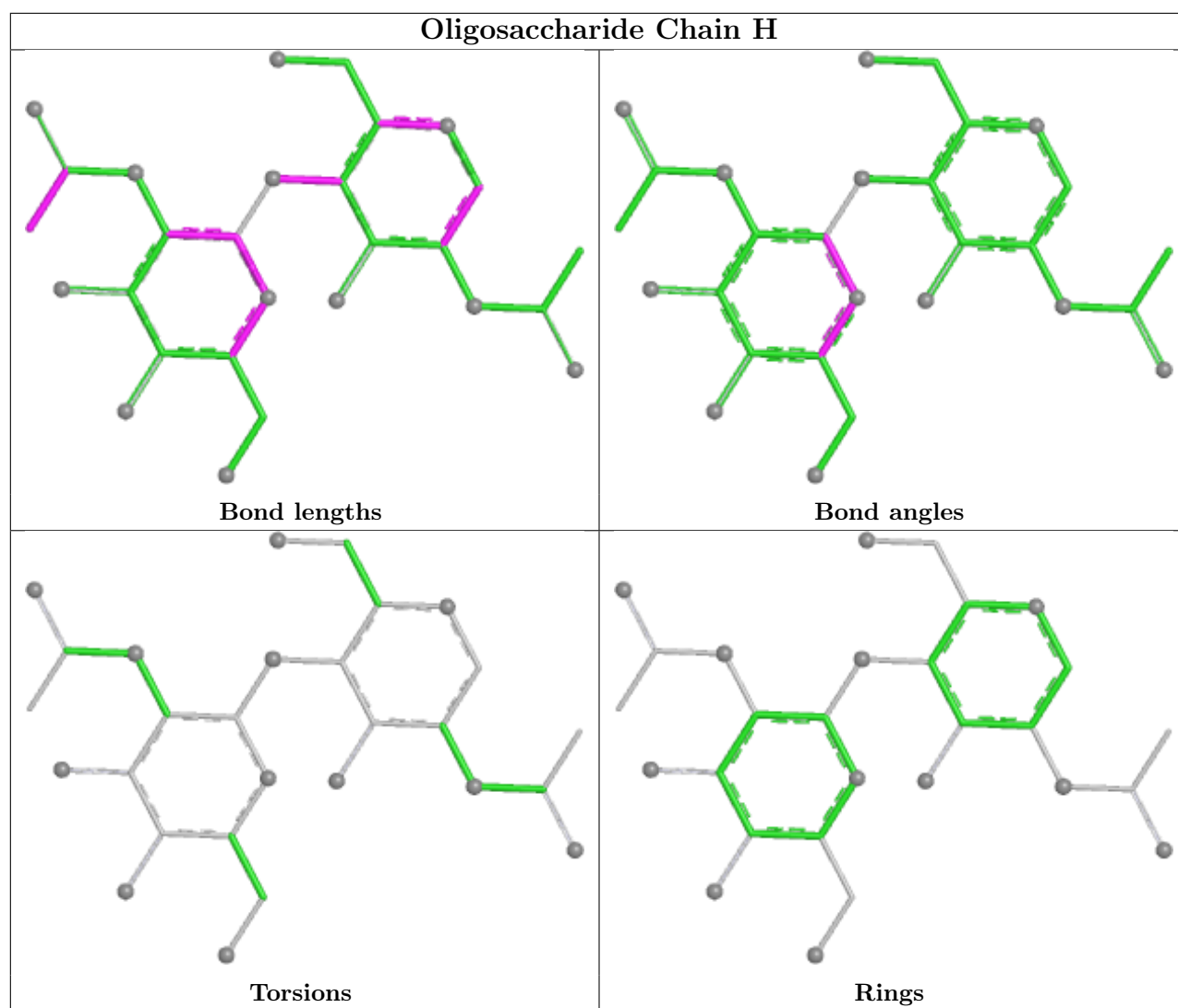
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

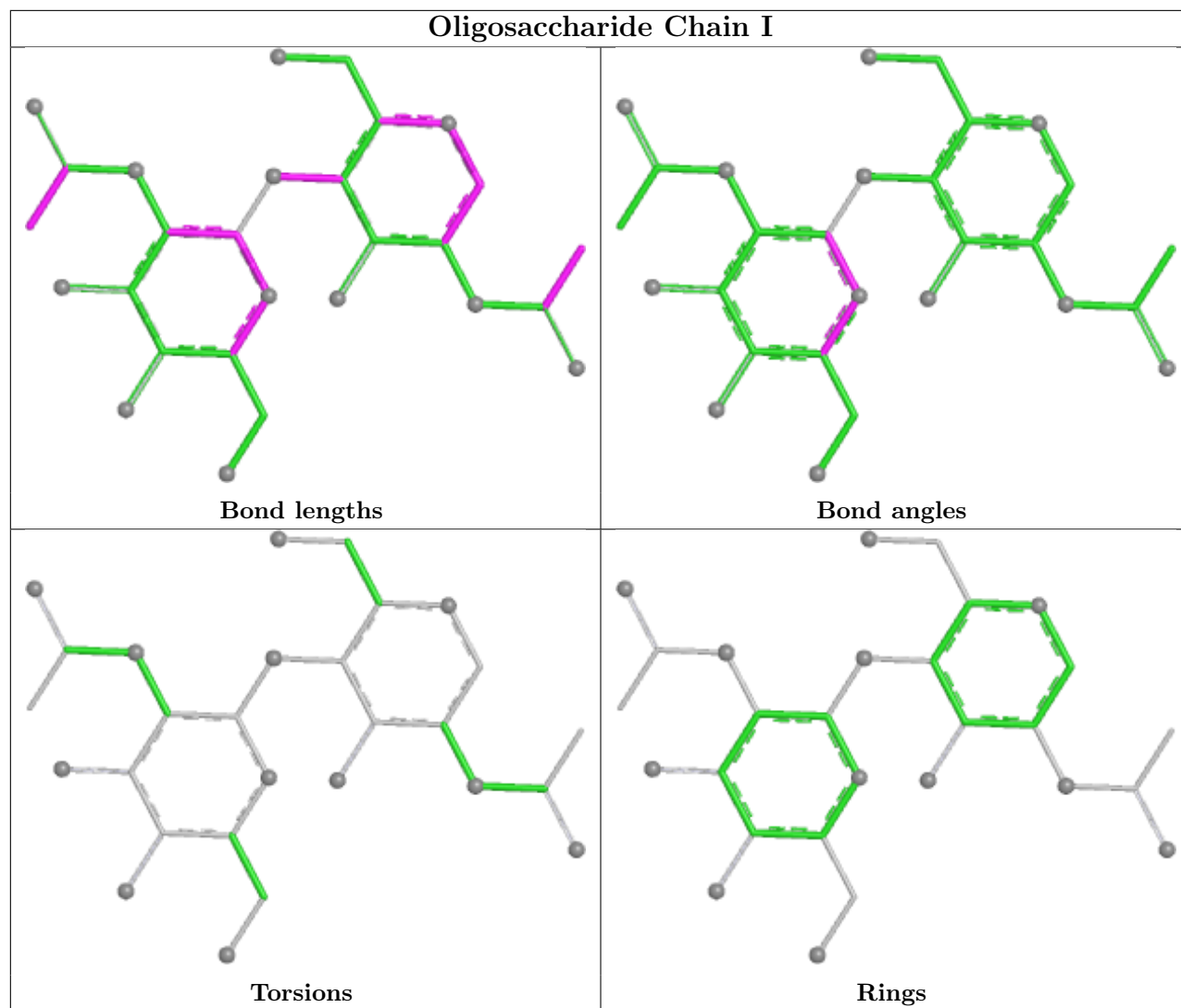


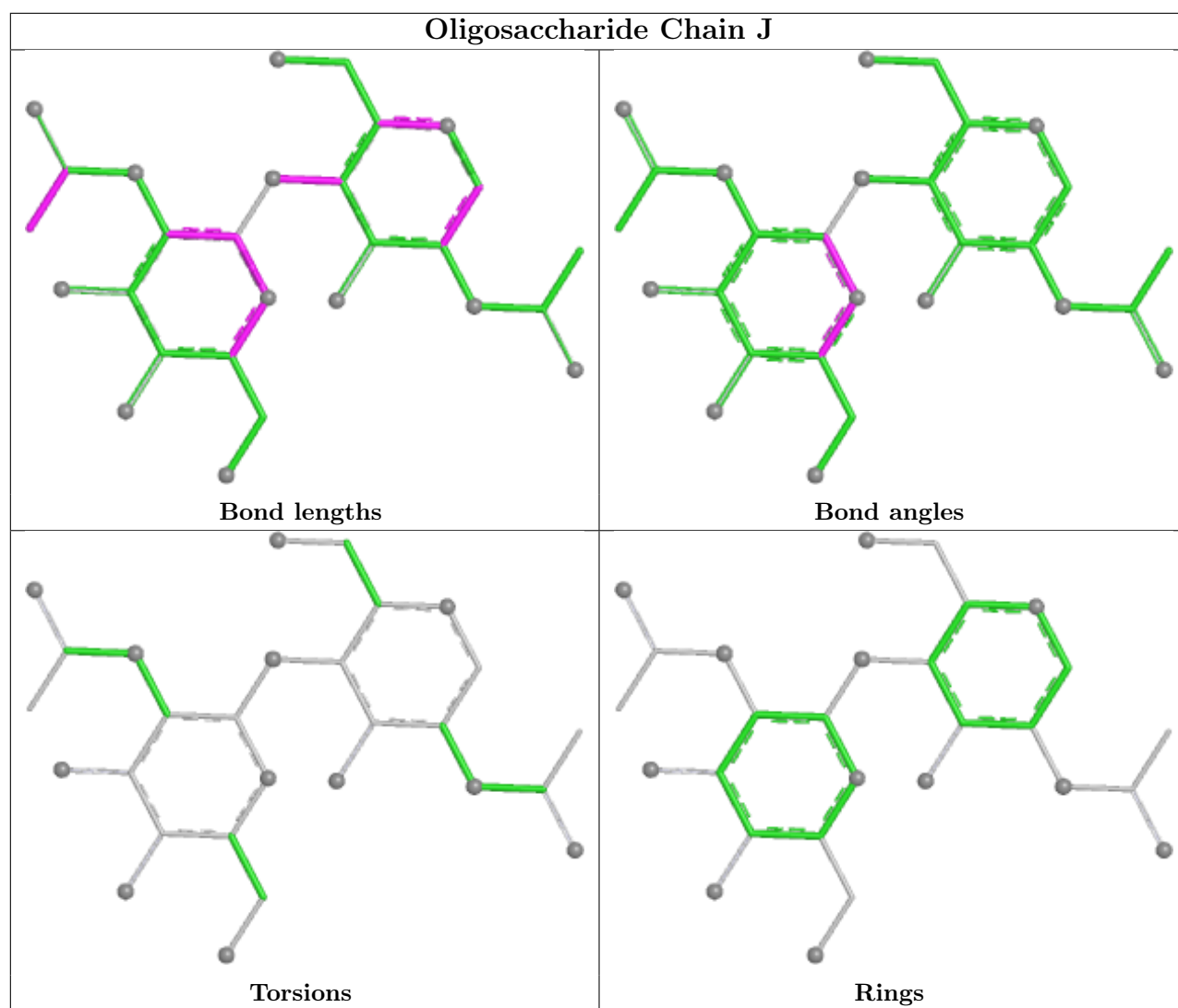


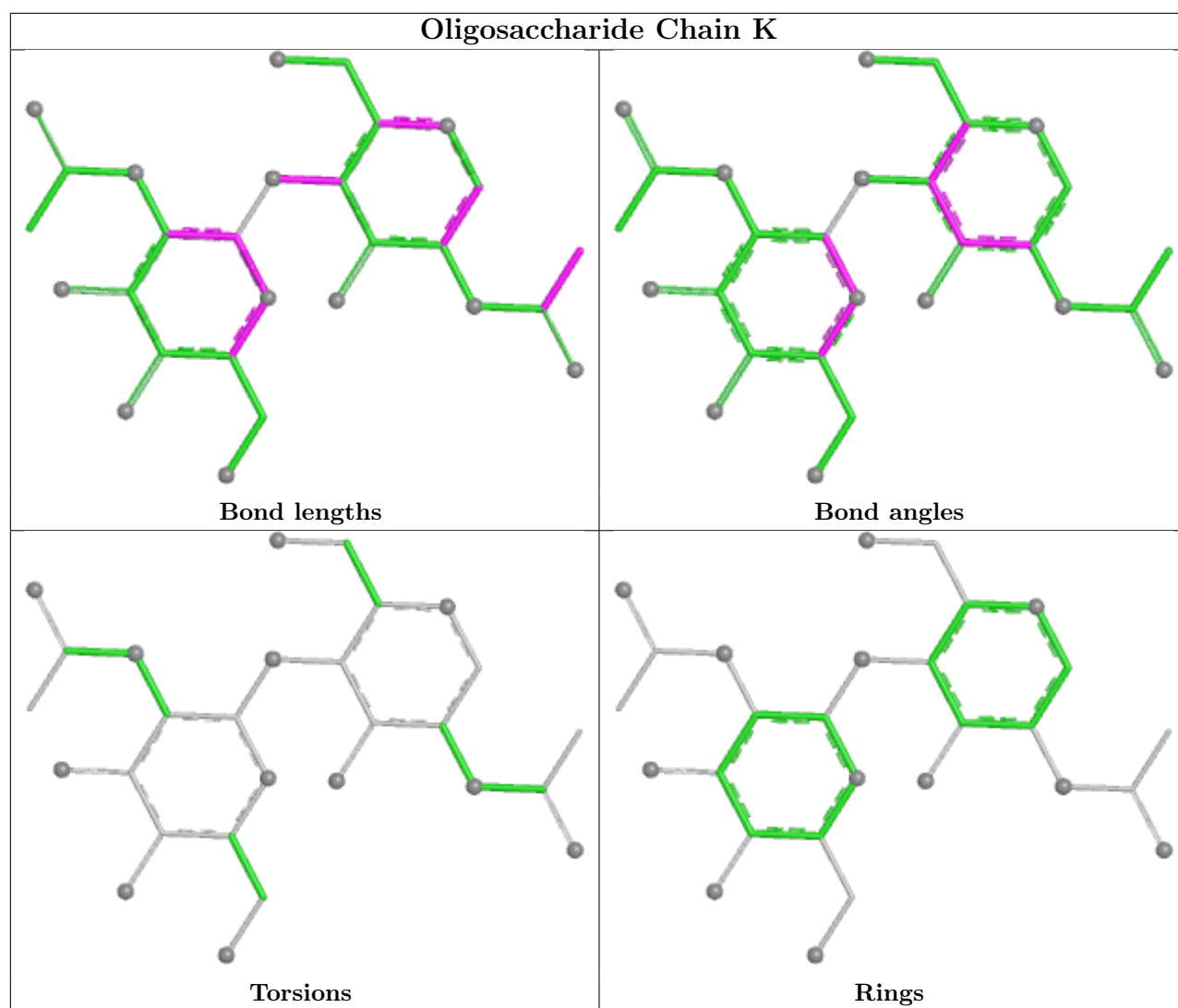


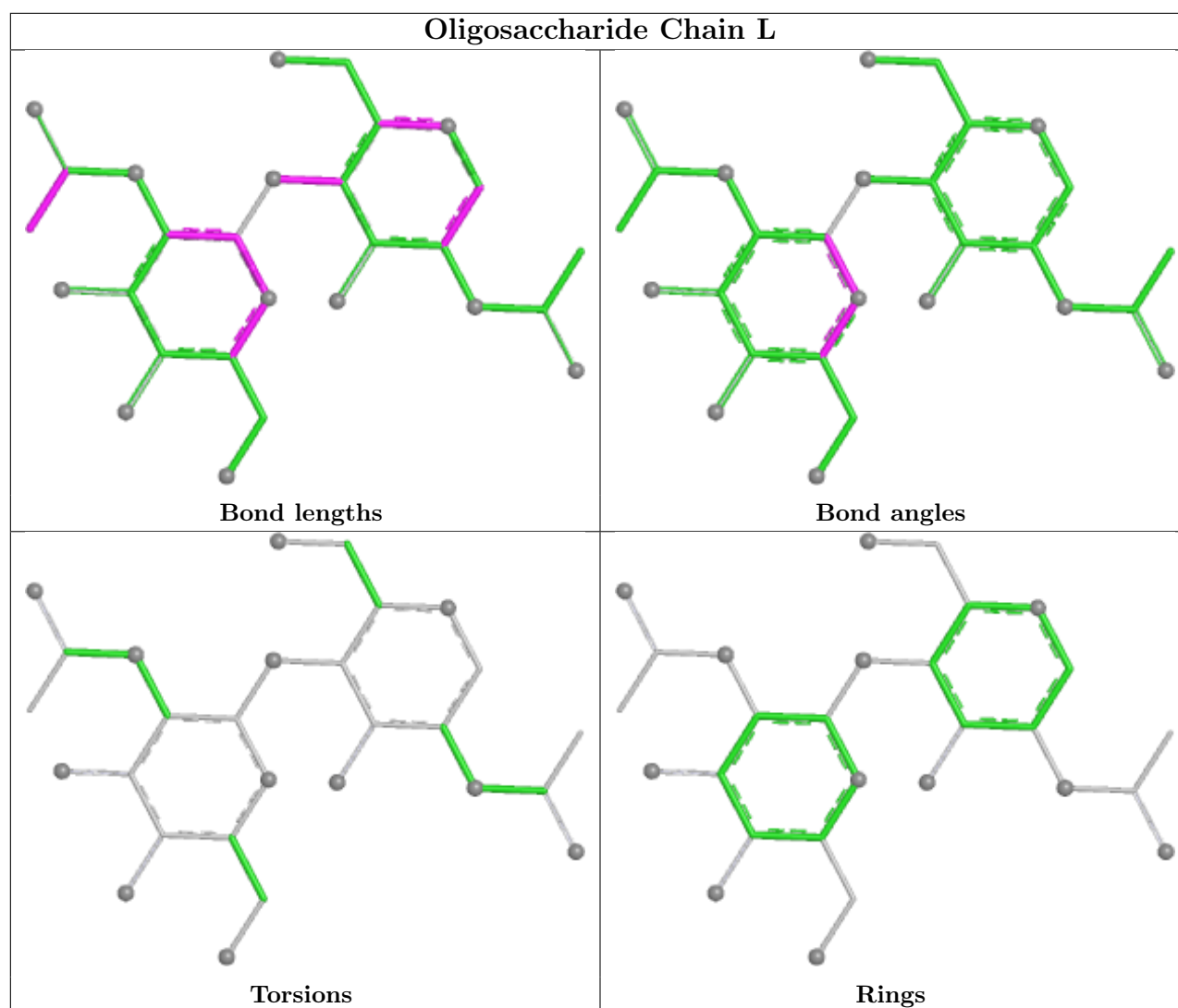












5.6 Ligand geometry [i](#)

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.

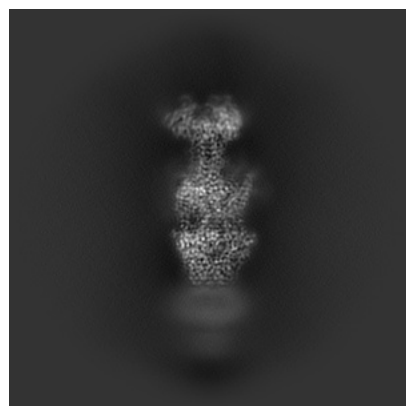
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52863. These allow visual inspection of the internal detail of the map and identification of artifacts.

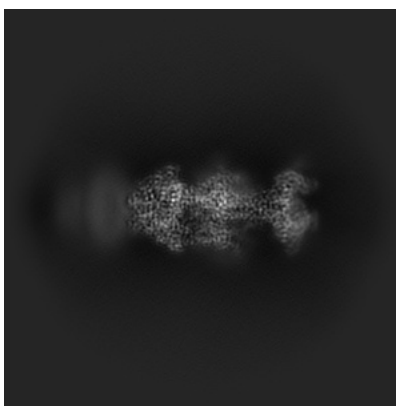
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

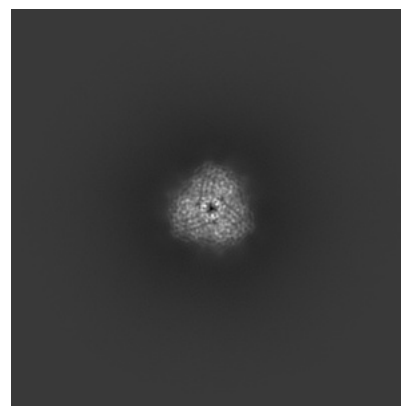
6.1.1 Primary map



X

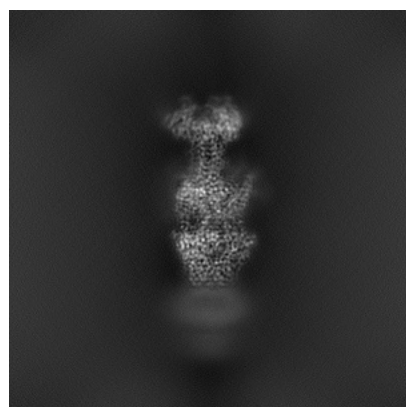


Y

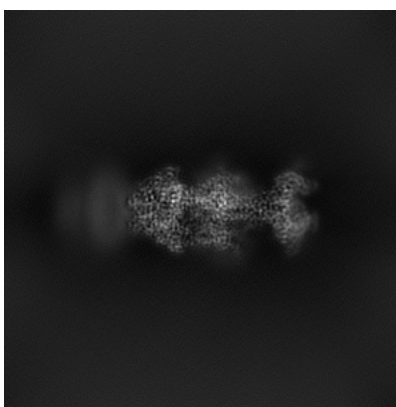


Z

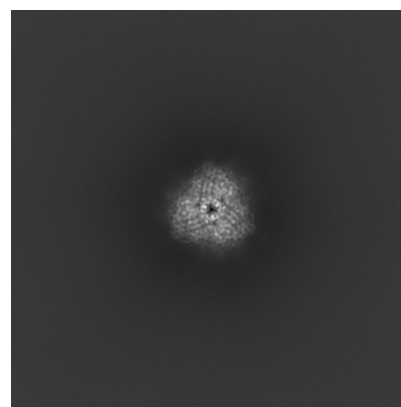
6.1.2 Raw map



X



Y

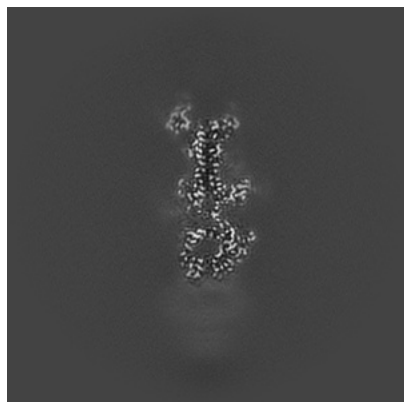


Z

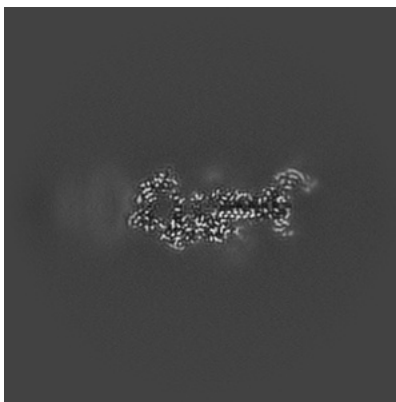
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

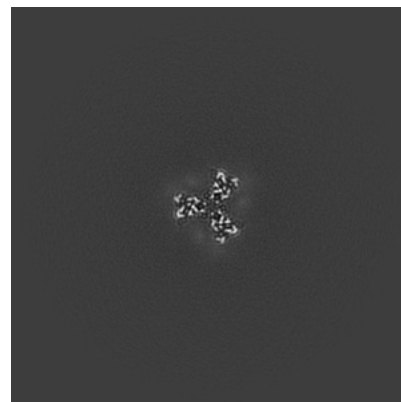
6.2.1 Primary map



X Index: 210

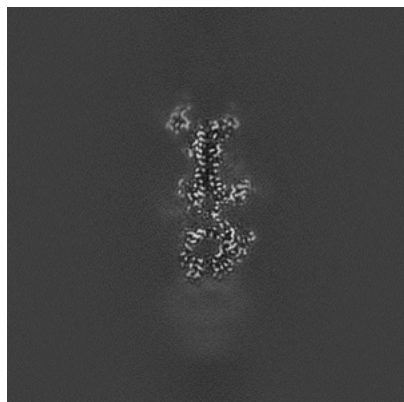


Y Index: 210

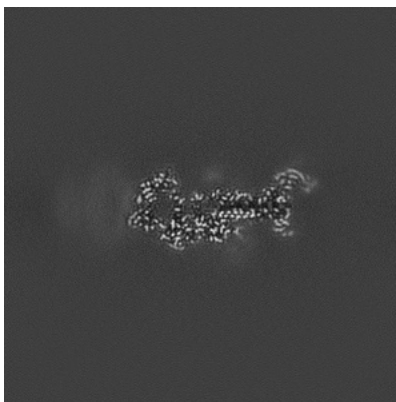


Z Index: 210

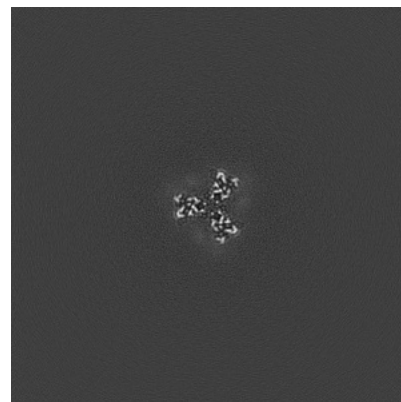
6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

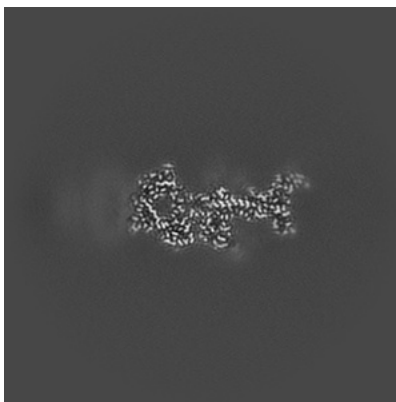
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

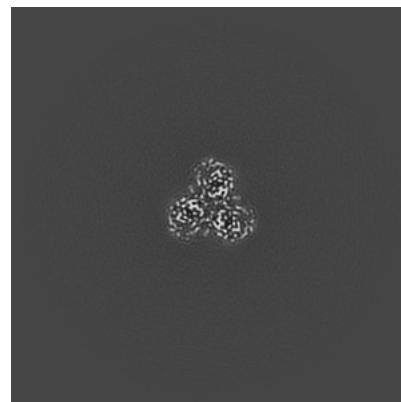
6.3.1 Primary map



X Index: 219

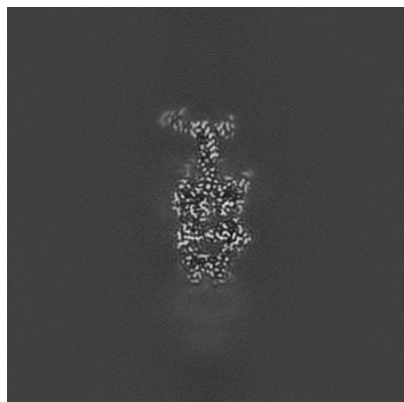


Y Index: 204

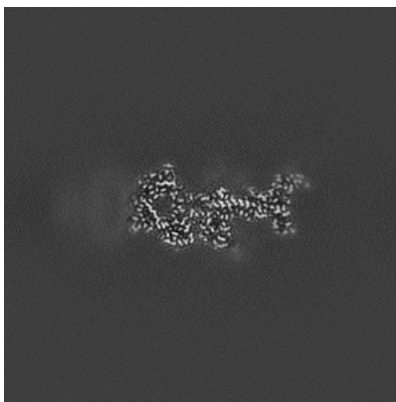


Z Index: 177

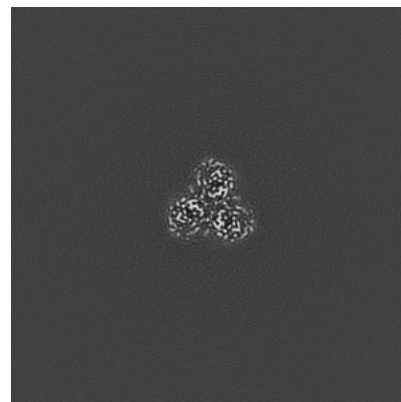
6.3.2 Raw map



X Index: 219



Y Index: 204

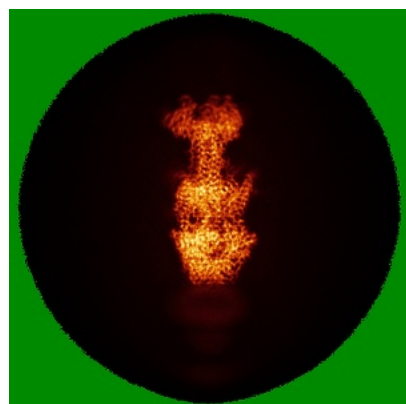


Z Index: 177

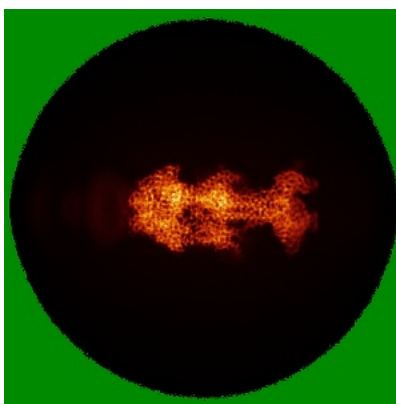
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

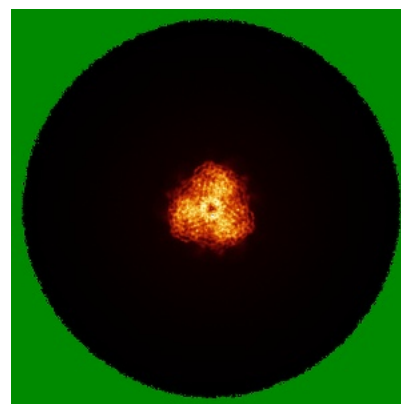
6.4.1 Primary map



X

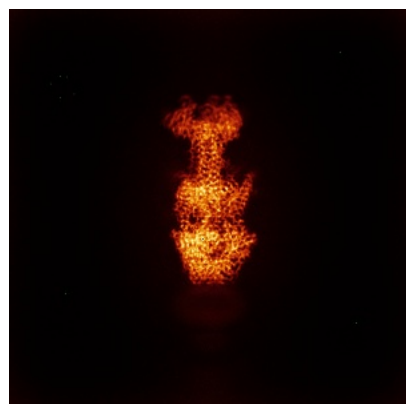


Y

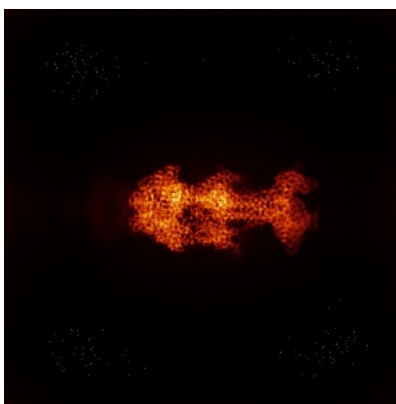


Z

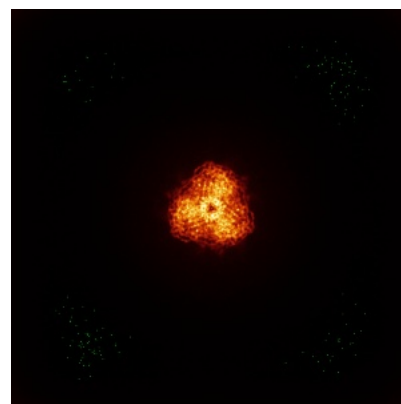
6.4.2 Raw map



X



Y

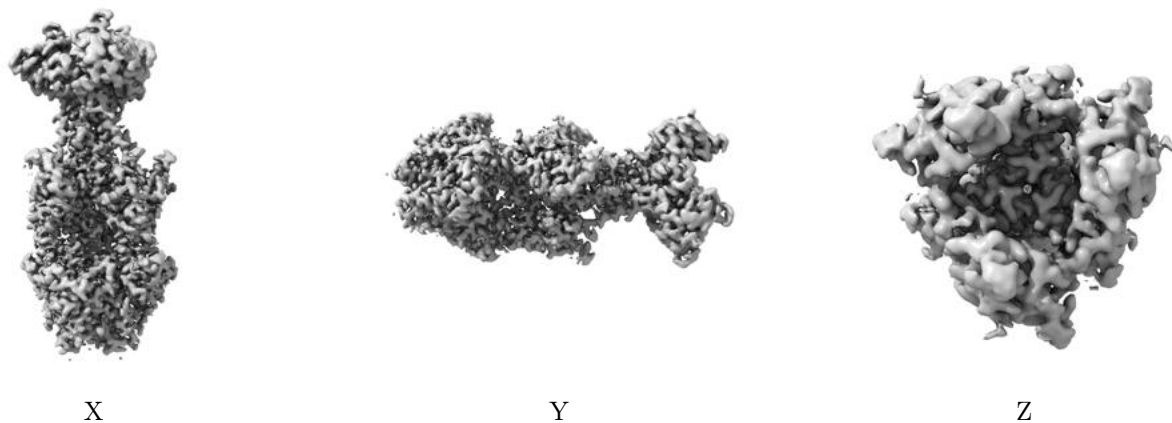


Z

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.

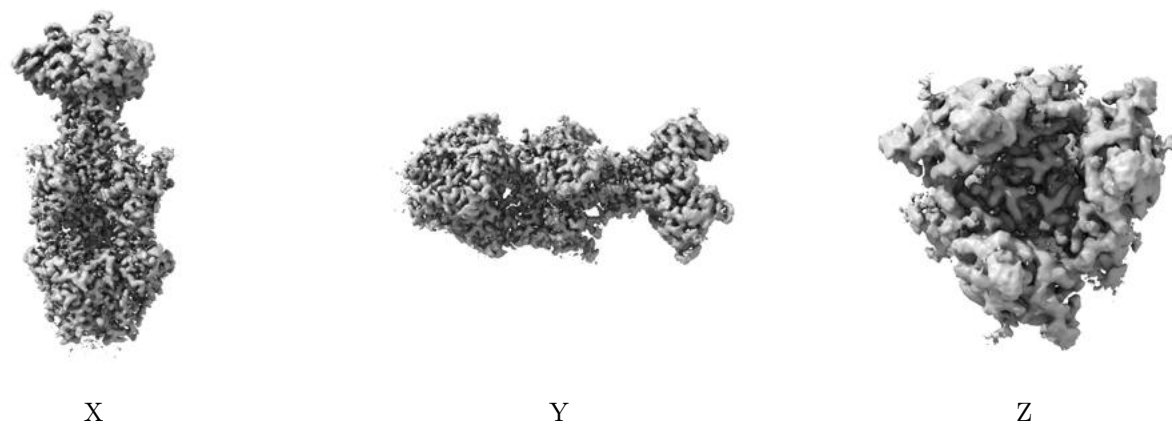
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.102. 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.

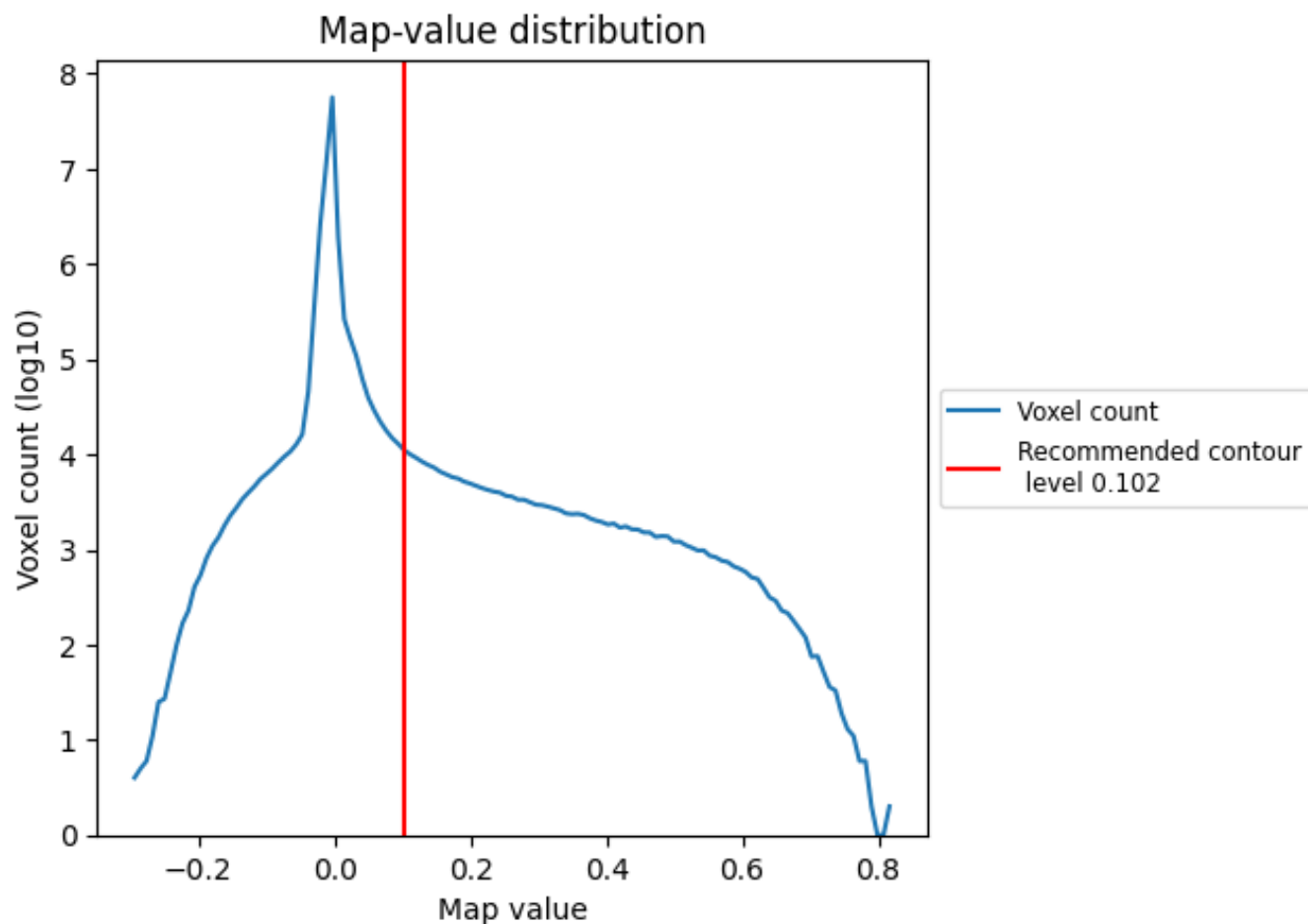
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

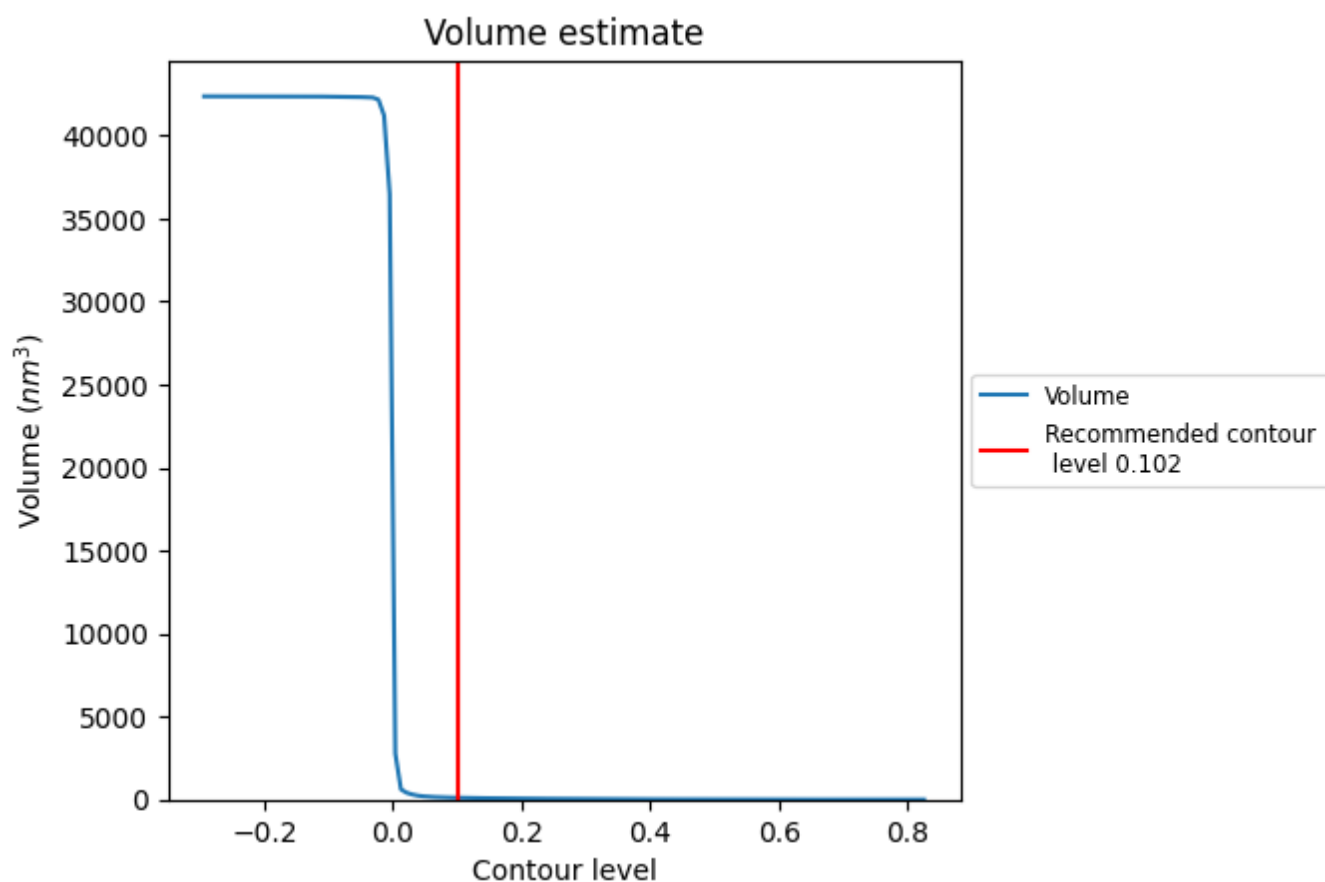
This section contains the results of statistical analysis of the map.

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.

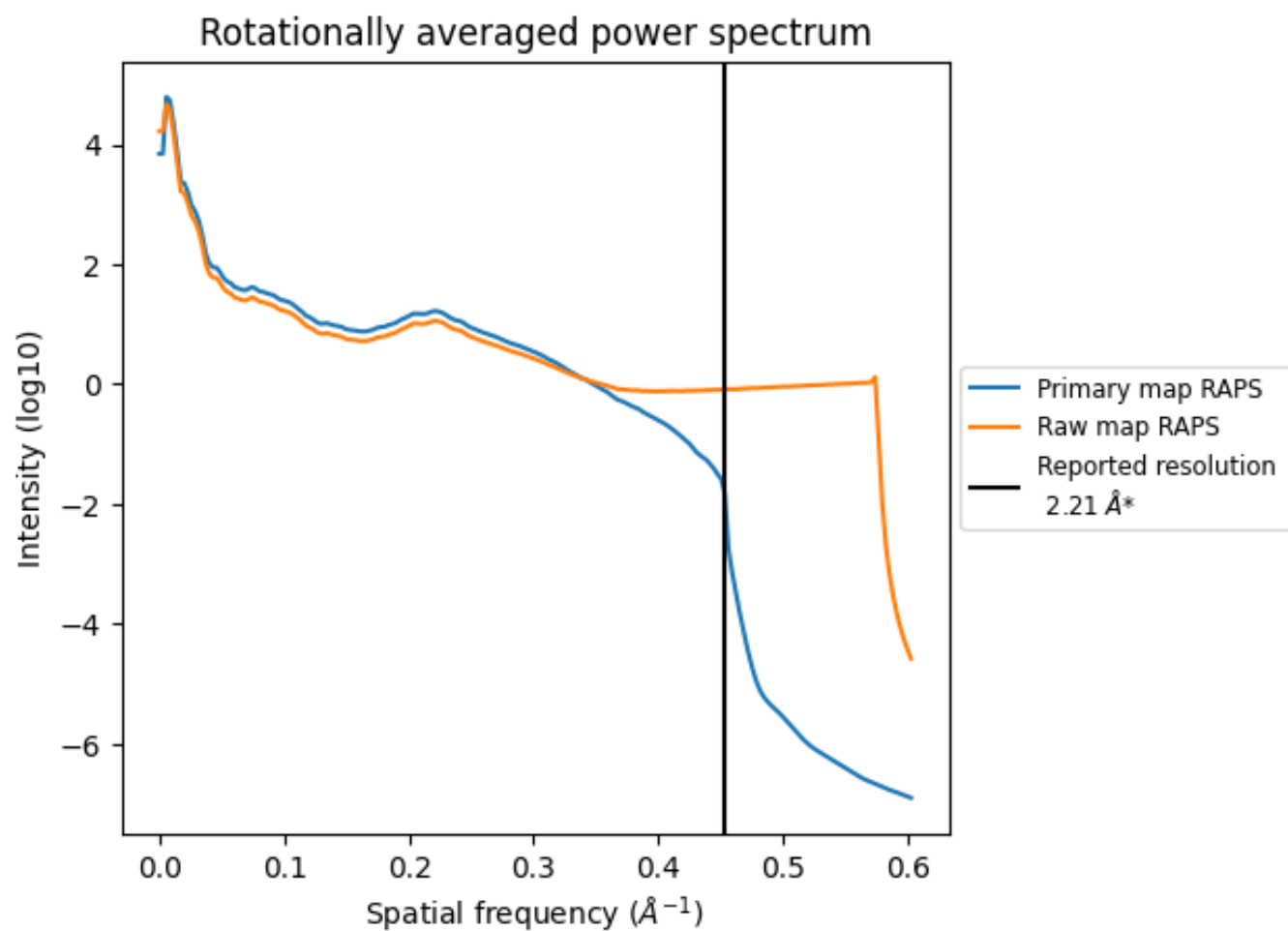
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108 nm³; this corresponds to an approximate mass of 98 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 ⓘ

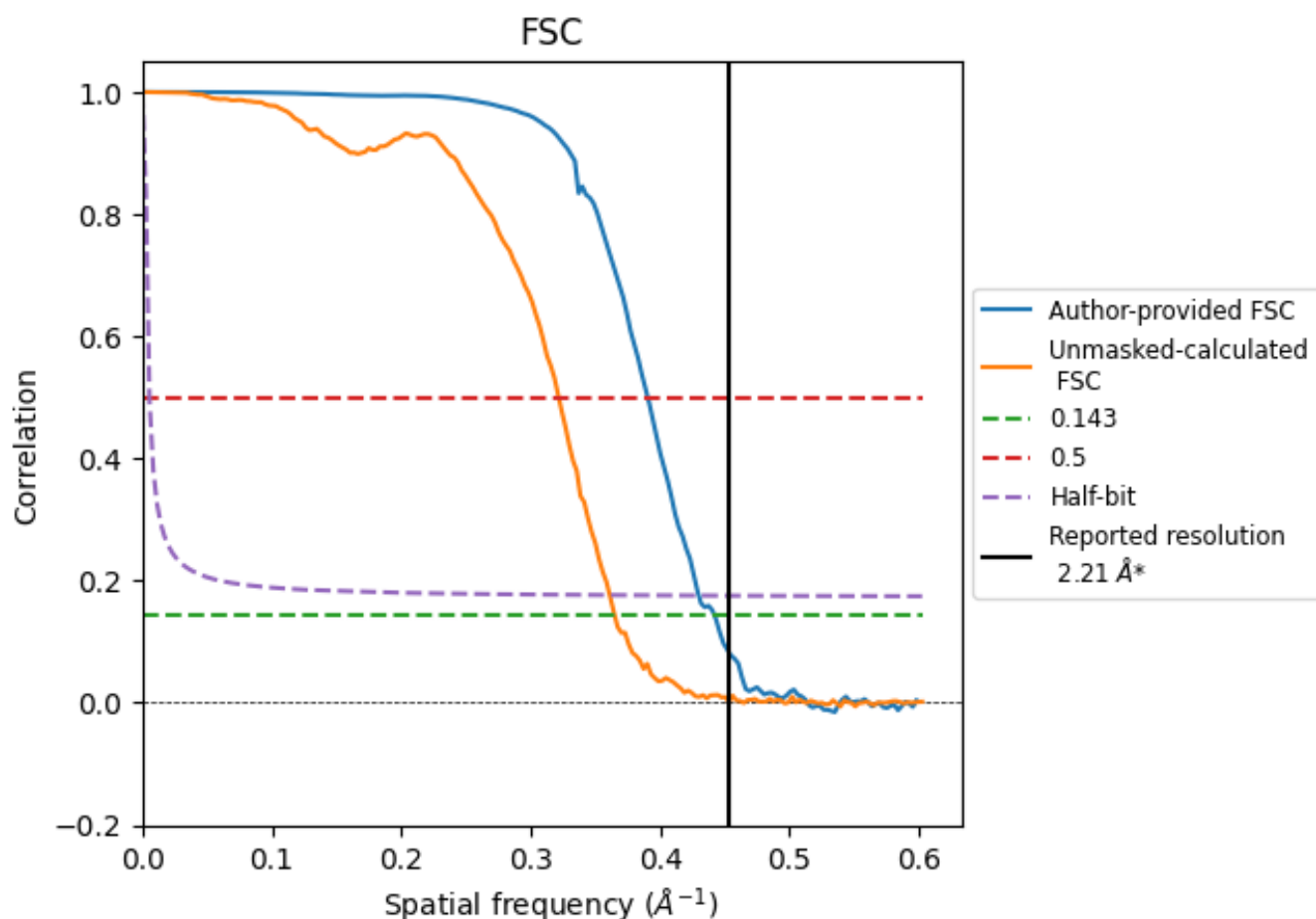


*Reported resolution corresponds to spatial frequency of $0.452 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.452 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

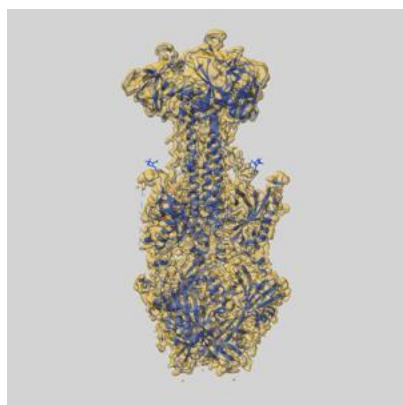
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.21	-	-
Author-provided FSC curve	2.26	2.56	2.33
Unmasked-calculated*	2.74	3.11	2.77

*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 2.74 differs from the reported value 2.21 by more than 10 %

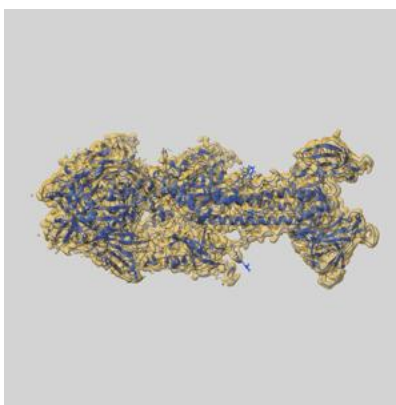
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52863 and PDB model 9IH8. Per-residue inclusion information can be found in section 3 on page 9.

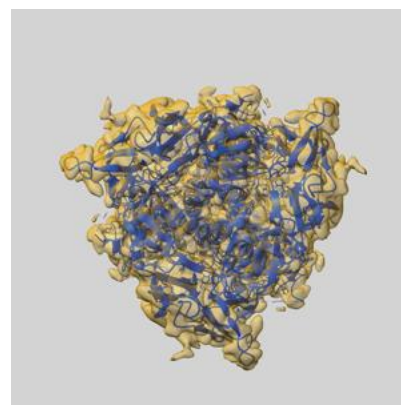
9.1 Map-model overlay [i](#)



X



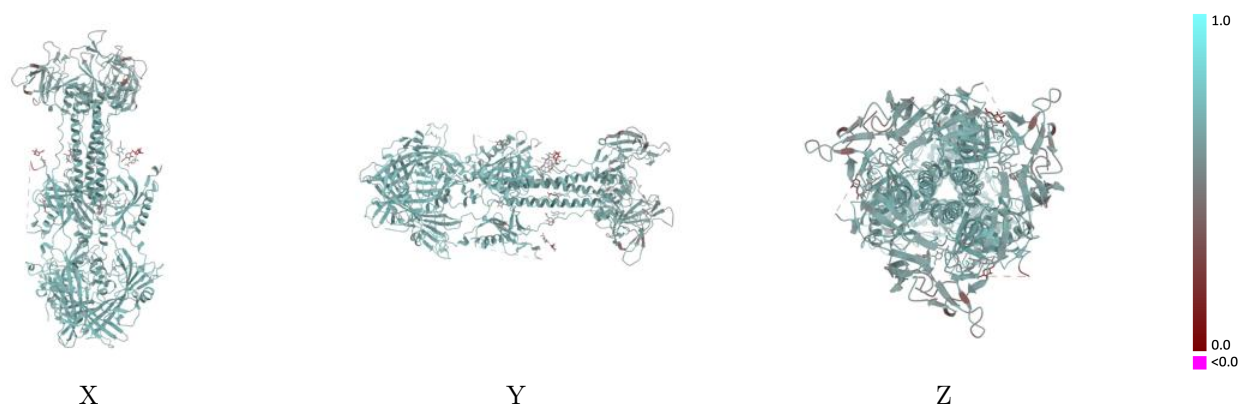
Y



Z

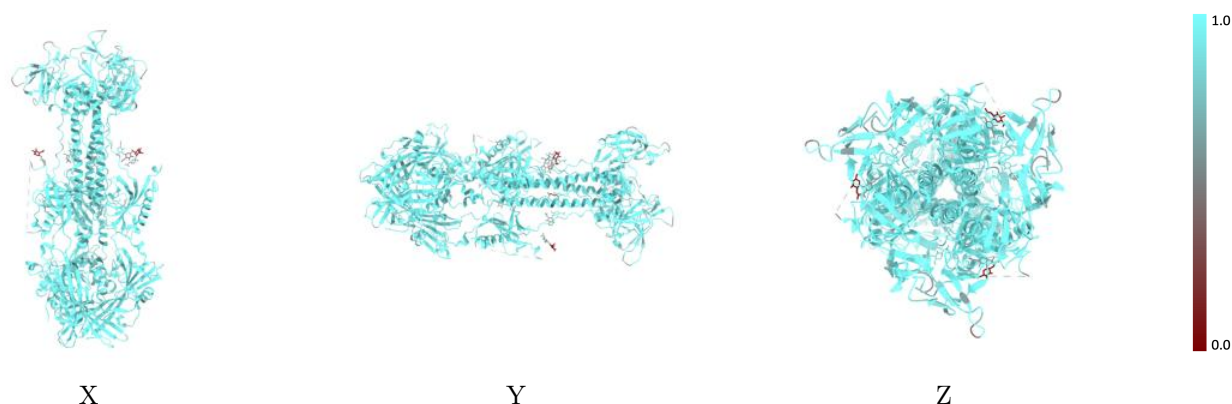
The images above show the 3D surface view of the map at the recommended contour level 0.102 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



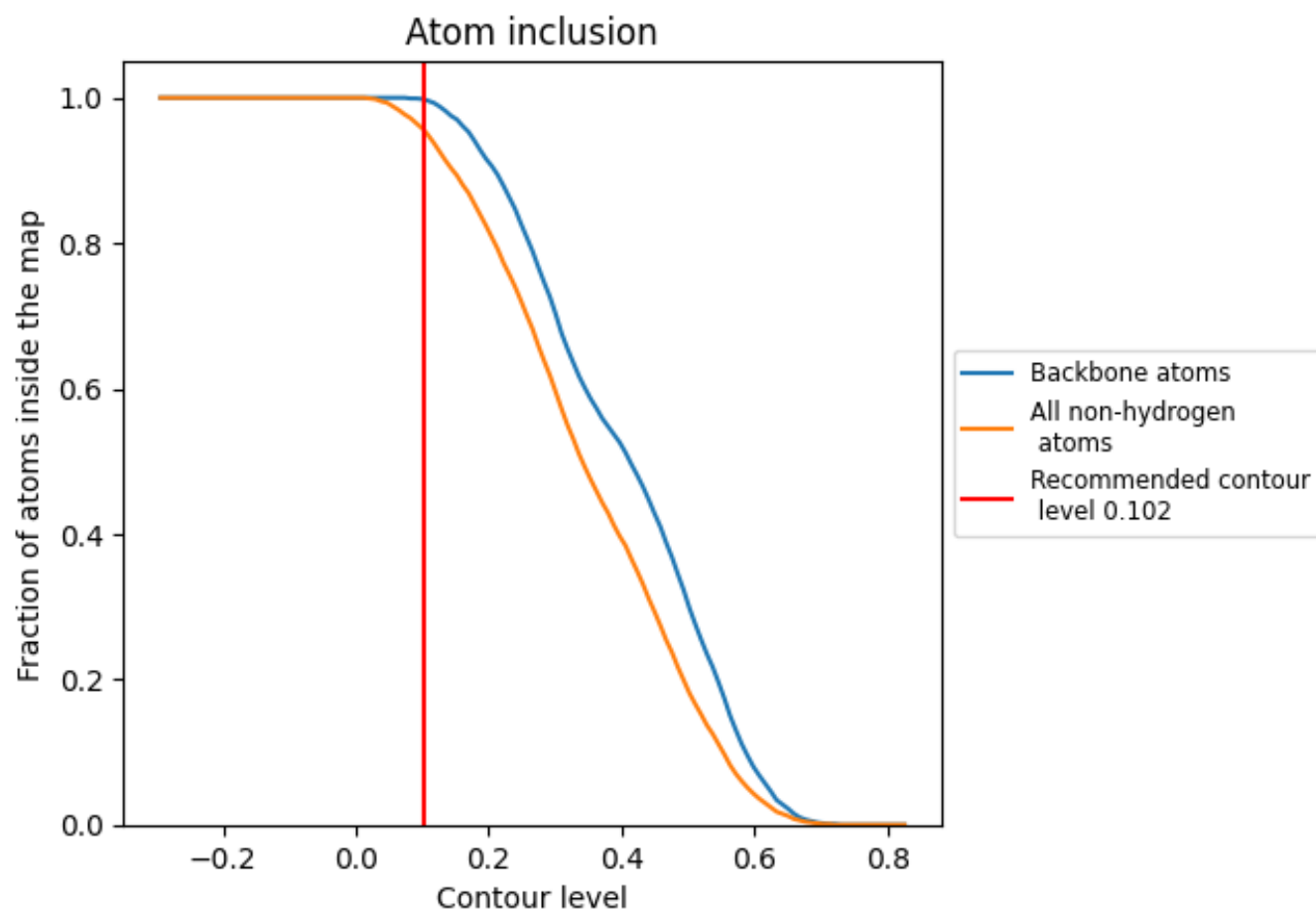
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.102).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 96% 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 (0.102) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9560	0.6390
A	0.9630	0.6430
B	0.9620	0.6430
C	0.9630	0.6420
D	0.7500	0.5050
E	0.6430	0.4570
F	0.7860	0.4850
G	0.7500	0.4220
H	0.7500	0.4290
I	0.7140	0.4230
J	0.2860	0.3670
K	0.2860	0.2620
L	0.2860	0.3280

