



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 12:32 AM UTC

PDB ID : 9Q7B / pdb_00009q7b
EMDB ID : EMD-72293
Title : Structure of the Measles Virus Fusion Glycoprotein Ectodomain in Prefusion Conformation Bound to Neutralizing Antibody H8
Authors : Zyla, D.; Niemeyer, G.; Porotto, M.; Saphire, E.O.
Deposited on : 2025-08-22
Resolution : 2.42 Å (reported)
Based on initial models : ., 8UUP

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:

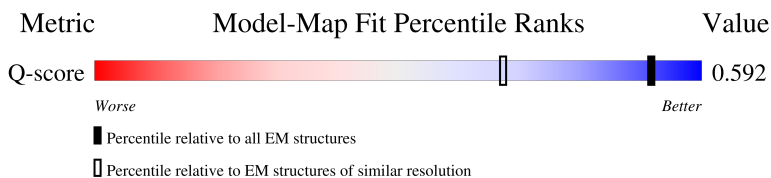
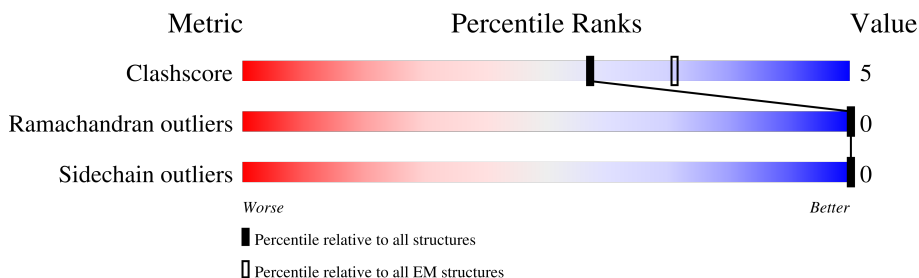
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 2.42 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.












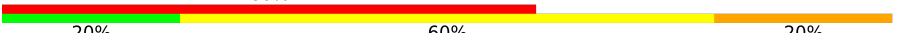

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5729 (1.92 - 2.92)

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	532	
1	B	532	
1	C	532	
1	D	532	

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Mol	Chain	Length	Quality of chain
1	E	532	
1	F	532	
2	G	476	
2	J	476	
2	L	476	
3	I	236	
3	K	236	
3	M	236	
4	H	3	
5	N	2	
5	P	2	
5	R	2	
6	O	5	
6	Q	5	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 15835 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	77	Total	C	N	O	S	0	0
			608	382	115	107	4		
1	B	372	Total	C	N	O	S	0	0
			2806	1770	476	546	14		
1	C	77	Total	C	N	O	S	0	0
			608	382	115	107	4		
1	D	372	Total	C	N	O	S	0	0
			2800	1767	473	546	14		
1	E	77	Total	C	N	O	S	0	0
			608	382	115	107	4		
1	F	372	Total	C	N	O	S	0	0
			2800	1767	473	546	14		

There are 234 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	GLY	GLU	conflict	UNP Q786F3
A	455	GLY	GLU	conflict	UNP Q786F3
A	496	GLY	-	expression tag	UNP Q786F3
A	497	VAL	-	expression tag	UNP Q786F3
A	498	ASP	-	expression tag	UNP Q786F3
A	499	ASP	-	expression tag	UNP Q786F3
A	500	ASP	-	expression tag	UNP Q786F3
A	501	ASP	-	expression tag	UNP Q786F3
A	502	LYS	-	expression tag	UNP Q786F3
A	503	ALA	-	expression tag	UNP Q786F3
A	504	GLY	-	expression tag	UNP Q786F3
A	505	TRP	-	expression tag	UNP Q786F3
A	506	SER	-	expression tag	UNP Q786F3
A	507	HIS	-	expression tag	UNP Q786F3
A	508	PRO	-	expression tag	UNP Q786F3
A	509	GLN	-	expression tag	UNP Q786F3
A	510	PHE	-	expression tag	UNP Q786F3
A	511	GLU	-	expression tag	UNP Q786F3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	512	LYS	-	expression tag	UNP Q786F3
A	513	GLY	-	expression tag	UNP Q786F3
A	514	GLY	-	expression tag	UNP Q786F3
A	515	GLY	-	expression tag	UNP Q786F3
A	516	SER	-	expression tag	UNP Q786F3
A	517	GLY	-	expression tag	UNP Q786F3
A	518	GLY	-	expression tag	UNP Q786F3
A	519	GLY	-	expression tag	UNP Q786F3
A	520	SER	-	expression tag	UNP Q786F3
A	521	GLY	-	expression tag	UNP Q786F3
A	522	GLY	-	expression tag	UNP Q786F3
A	523	GLY	-	expression tag	UNP Q786F3
A	524	SER	-	expression tag	UNP Q786F3
A	525	TRP	-	expression tag	UNP Q786F3
A	526	SER	-	expression tag	UNP Q786F3
A	527	HIS	-	expression tag	UNP Q786F3
A	528	PRO	-	expression tag	UNP Q786F3
A	529	GLN	-	expression tag	UNP Q786F3
A	530	PHE	-	expression tag	UNP Q786F3
A	531	GLU	-	expression tag	UNP Q786F3
A	532	LYS	-	expression tag	UNP Q786F3
B	170	GLY	GLU	conflict	UNP Q786F3
B	455	GLY	GLU	conflict	UNP Q786F3
B	496	GLY	-	expression tag	UNP Q786F3
B	497	VAL	-	expression tag	UNP Q786F3
B	498	ASP	-	expression tag	UNP Q786F3
B	499	ASP	-	expression tag	UNP Q786F3
B	500	ASP	-	expression tag	UNP Q786F3
B	501	ASP	-	expression tag	UNP Q786F3
B	502	LYS	-	expression tag	UNP Q786F3
B	503	ALA	-	expression tag	UNP Q786F3
B	504	GLY	-	expression tag	UNP Q786F3
B	505	TRP	-	expression tag	UNP Q786F3
B	506	SER	-	expression tag	UNP Q786F3
B	507	HIS	-	expression tag	UNP Q786F3
B	508	PRO	-	expression tag	UNP Q786F3
B	509	GLN	-	expression tag	UNP Q786F3
B	510	PHE	-	expression tag	UNP Q786F3
B	511	GLU	-	expression tag	UNP Q786F3
B	512	LYS	-	expression tag	UNP Q786F3
B	513	GLY	-	expression tag	UNP Q786F3
B	514	GLY	-	expression tag	UNP Q786F3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	515	GLY	-	expression tag	UNP Q786F3
B	516	SER	-	expression tag	UNP Q786F3
B	517	GLY	-	expression tag	UNP Q786F3
B	518	GLY	-	expression tag	UNP Q786F3
B	519	GLY	-	expression tag	UNP Q786F3
B	520	SER	-	expression tag	UNP Q786F3
B	521	GLY	-	expression tag	UNP Q786F3
B	522	GLY	-	expression tag	UNP Q786F3
B	523	GLY	-	expression tag	UNP Q786F3
B	524	SER	-	expression tag	UNP Q786F3
B	525	TRP	-	expression tag	UNP Q786F3
B	526	SER	-	expression tag	UNP Q786F3
B	527	HIS	-	expression tag	UNP Q786F3
B	528	PRO	-	expression tag	UNP Q786F3
B	529	GLN	-	expression tag	UNP Q786F3
B	530	PHE	-	expression tag	UNP Q786F3
B	531	GLU	-	expression tag	UNP Q786F3
B	532	LYS	-	expression tag	UNP Q786F3
C	170	GLY	GLU	conflict	UNP Q786F3
C	455	GLY	GLU	conflict	UNP Q786F3
C	496	GLY	-	expression tag	UNP Q786F3
C	497	VAL	-	expression tag	UNP Q786F3
C	498	ASP	-	expression tag	UNP Q786F3
C	499	ASP	-	expression tag	UNP Q786F3
C	500	ASP	-	expression tag	UNP Q786F3
C	501	ASP	-	expression tag	UNP Q786F3
C	502	LYS	-	expression tag	UNP Q786F3
C	503	ALA	-	expression tag	UNP Q786F3
C	504	GLY	-	expression tag	UNP Q786F3
C	505	TRP	-	expression tag	UNP Q786F3
C	506	SER	-	expression tag	UNP Q786F3
C	507	HIS	-	expression tag	UNP Q786F3
C	508	PRO	-	expression tag	UNP Q786F3
C	509	GLN	-	expression tag	UNP Q786F3
C	510	PHE	-	expression tag	UNP Q786F3
C	511	GLU	-	expression tag	UNP Q786F3
C	512	LYS	-	expression tag	UNP Q786F3
C	513	GLY	-	expression tag	UNP Q786F3
C	514	GLY	-	expression tag	UNP Q786F3
C	515	GLY	-	expression tag	UNP Q786F3
C	516	SER	-	expression tag	UNP Q786F3
C	517	GLY	-	expression tag	UNP Q786F3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	518	GLY	-	expression tag	UNP Q786F3
C	519	GLY	-	expression tag	UNP Q786F3
C	520	SER	-	expression tag	UNP Q786F3
C	521	GLY	-	expression tag	UNP Q786F3
C	522	GLY	-	expression tag	UNP Q786F3
C	523	GLY	-	expression tag	UNP Q786F3
C	524	SER	-	expression tag	UNP Q786F3
C	525	TRP	-	expression tag	UNP Q786F3
C	526	SER	-	expression tag	UNP Q786F3
C	527	HIS	-	expression tag	UNP Q786F3
C	528	PRO	-	expression tag	UNP Q786F3
C	529	GLN	-	expression tag	UNP Q786F3
C	530	PHE	-	expression tag	UNP Q786F3
C	531	GLU	-	expression tag	UNP Q786F3
C	532	LYS	-	expression tag	UNP Q786F3
D	170	GLY	GLU	conflict	UNP Q786F3
D	455	GLY	GLU	conflict	UNP Q786F3
D	496	GLY	-	expression tag	UNP Q786F3
D	497	VAL	-	expression tag	UNP Q786F3
D	498	ASP	-	expression tag	UNP Q786F3
D	499	ASP	-	expression tag	UNP Q786F3
D	500	ASP	-	expression tag	UNP Q786F3
D	501	ASP	-	expression tag	UNP Q786F3
D	502	LYS	-	expression tag	UNP Q786F3
D	503	ALA	-	expression tag	UNP Q786F3
D	504	GLY	-	expression tag	UNP Q786F3
D	505	TRP	-	expression tag	UNP Q786F3
D	506	SER	-	expression tag	UNP Q786F3
D	507	HIS	-	expression tag	UNP Q786F3
D	508	PRO	-	expression tag	UNP Q786F3
D	509	GLN	-	expression tag	UNP Q786F3
D	510	PHE	-	expression tag	UNP Q786F3
D	511	GLU	-	expression tag	UNP Q786F3
D	512	LYS	-	expression tag	UNP Q786F3
D	513	GLY	-	expression tag	UNP Q786F3
D	514	GLY	-	expression tag	UNP Q786F3
D	515	GLY	-	expression tag	UNP Q786F3
D	516	SER	-	expression tag	UNP Q786F3
D	517	GLY	-	expression tag	UNP Q786F3
D	518	GLY	-	expression tag	UNP Q786F3
D	519	GLY	-	expression tag	UNP Q786F3
D	520	SER	-	expression tag	UNP Q786F3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	521	GLY	-	expression tag	UNP Q786F3
D	522	GLY	-	expression tag	UNP Q786F3
D	523	GLY	-	expression tag	UNP Q786F3
D	524	SER	-	expression tag	UNP Q786F3
D	525	TRP	-	expression tag	UNP Q786F3
D	526	SER	-	expression tag	UNP Q786F3
D	527	HIS	-	expression tag	UNP Q786F3
D	528	PRO	-	expression tag	UNP Q786F3
D	529	GLN	-	expression tag	UNP Q786F3
D	530	PHE	-	expression tag	UNP Q786F3
D	531	GLU	-	expression tag	UNP Q786F3
D	532	LYS	-	expression tag	UNP Q786F3
E	170	GLY	GLU	conflict	UNP Q786F3
E	455	GLY	GLU	conflict	UNP Q786F3
E	496	GLY	-	expression tag	UNP Q786F3
E	497	VAL	-	expression tag	UNP Q786F3
E	498	ASP	-	expression tag	UNP Q786F3
E	499	ASP	-	expression tag	UNP Q786F3
E	500	ASP	-	expression tag	UNP Q786F3
E	501	ASP	-	expression tag	UNP Q786F3
E	502	LYS	-	expression tag	UNP Q786F3
E	503	ALA	-	expression tag	UNP Q786F3
E	504	GLY	-	expression tag	UNP Q786F3
E	505	TRP	-	expression tag	UNP Q786F3
E	506	SER	-	expression tag	UNP Q786F3
E	507	HIS	-	expression tag	UNP Q786F3
E	508	PRO	-	expression tag	UNP Q786F3
E	509	GLN	-	expression tag	UNP Q786F3
E	510	PHE	-	expression tag	UNP Q786F3
E	511	GLU	-	expression tag	UNP Q786F3
E	512	LYS	-	expression tag	UNP Q786F3
E	513	GLY	-	expression tag	UNP Q786F3
E	514	GLY	-	expression tag	UNP Q786F3
E	515	GLY	-	expression tag	UNP Q786F3
E	516	SER	-	expression tag	UNP Q786F3
E	517	GLY	-	expression tag	UNP Q786F3
E	518	GLY	-	expression tag	UNP Q786F3
E	519	GLY	-	expression tag	UNP Q786F3
E	520	SER	-	expression tag	UNP Q786F3
E	521	GLY	-	expression tag	UNP Q786F3
E	522	GLY	-	expression tag	UNP Q786F3
E	523	GLY	-	expression tag	UNP Q786F3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	524	SER	-	expression tag	UNP Q786F3
E	525	TRP	-	expression tag	UNP Q786F3
E	526	SER	-	expression tag	UNP Q786F3
E	527	HIS	-	expression tag	UNP Q786F3
E	528	PRO	-	expression tag	UNP Q786F3
E	529	GLN	-	expression tag	UNP Q786F3
E	530	PHE	-	expression tag	UNP Q786F3
E	531	GLU	-	expression tag	UNP Q786F3
E	532	LYS	-	expression tag	UNP Q786F3
F	170	GLY	GLU	conflict	UNP Q786F3
F	455	GLY	GLU	conflict	UNP Q786F3
F	496	GLY	-	expression tag	UNP Q786F3
F	497	VAL	-	expression tag	UNP Q786F3
F	498	ASP	-	expression tag	UNP Q786F3
F	499	ASP	-	expression tag	UNP Q786F3
F	500	ASP	-	expression tag	UNP Q786F3
F	501	ASP	-	expression tag	UNP Q786F3
F	502	LYS	-	expression tag	UNP Q786F3
F	503	ALA	-	expression tag	UNP Q786F3
F	504	GLY	-	expression tag	UNP Q786F3
F	505	TRP	-	expression tag	UNP Q786F3
F	506	SER	-	expression tag	UNP Q786F3
F	507	HIS	-	expression tag	UNP Q786F3
F	508	PRO	-	expression tag	UNP Q786F3
F	509	GLN	-	expression tag	UNP Q786F3
F	510	PHE	-	expression tag	UNP Q786F3
F	511	GLU	-	expression tag	UNP Q786F3
F	512	LYS	-	expression tag	UNP Q786F3
F	513	GLY	-	expression tag	UNP Q786F3
F	514	GLY	-	expression tag	UNP Q786F3
F	515	GLY	-	expression tag	UNP Q786F3
F	516	SER	-	expression tag	UNP Q786F3
F	517	GLY	-	expression tag	UNP Q786F3
F	518	GLY	-	expression tag	UNP Q786F3
F	519	GLY	-	expression tag	UNP Q786F3
F	520	SER	-	expression tag	UNP Q786F3
F	521	GLY	-	expression tag	UNP Q786F3
F	522	GLY	-	expression tag	UNP Q786F3
F	523	GLY	-	expression tag	UNP Q786F3
F	524	SER	-	expression tag	UNP Q786F3
F	525	TRP	-	expression tag	UNP Q786F3
F	526	SER	-	expression tag	UNP Q786F3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	527	HIS	-	expression tag	UNP Q786F3
F	528	PRO	-	expression tag	UNP Q786F3
F	529	GLN	-	expression tag	UNP Q786F3
F	530	PHE	-	expression tag	UNP Q786F3
F	531	GLU	-	expression tag	UNP Q786F3
F	532	LYS	-	expression tag	UNP Q786F3

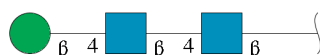
- Molecule 2 is a protein called Mab H8 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	117	Total	C	N	O	S	0	0
			899	572	150	174	3		
2	J	117	Total	C	N	O	S	0	0
			899	572	150	174	3		
2	L	116	Total	C	N	O	S	0	0
			893	569	149	172	3		

- Molecule 3 is a protein called mAb H8 light chain.

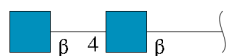
Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	109	Total	C	N	O	S	0	0
			829	525	138	164	2		
3	K	109	Total	C	N	O	S	0	0
			829	525	138	164	2		
3	M	109	Total	C	N	O	S	0	0
			829	525	138	164	2		

- 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.



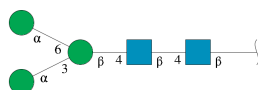
Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



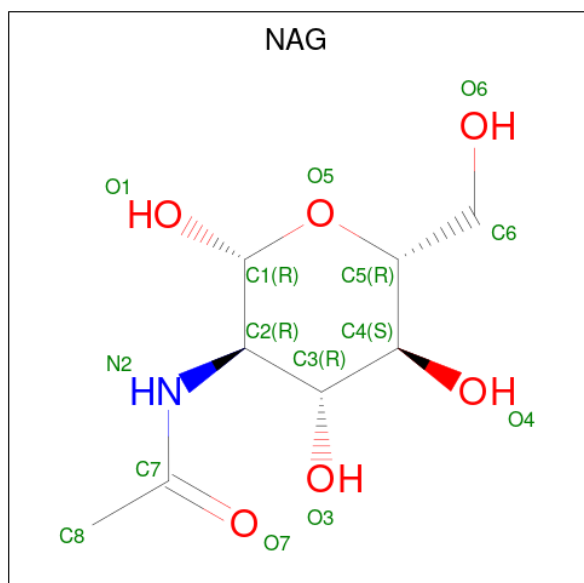
Mol	Chain	Residues	Atoms				AltConf	Trace
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 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
6	O	5	Total	C	N	O	0	0
			61	34	2	25		
6	Q	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

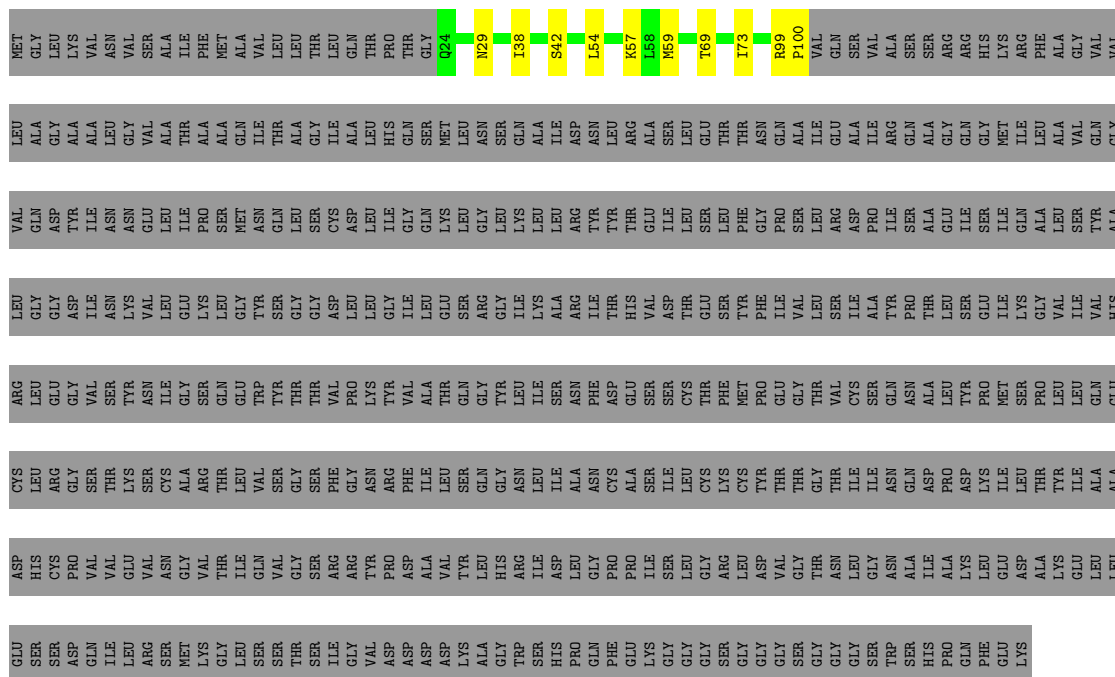


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	

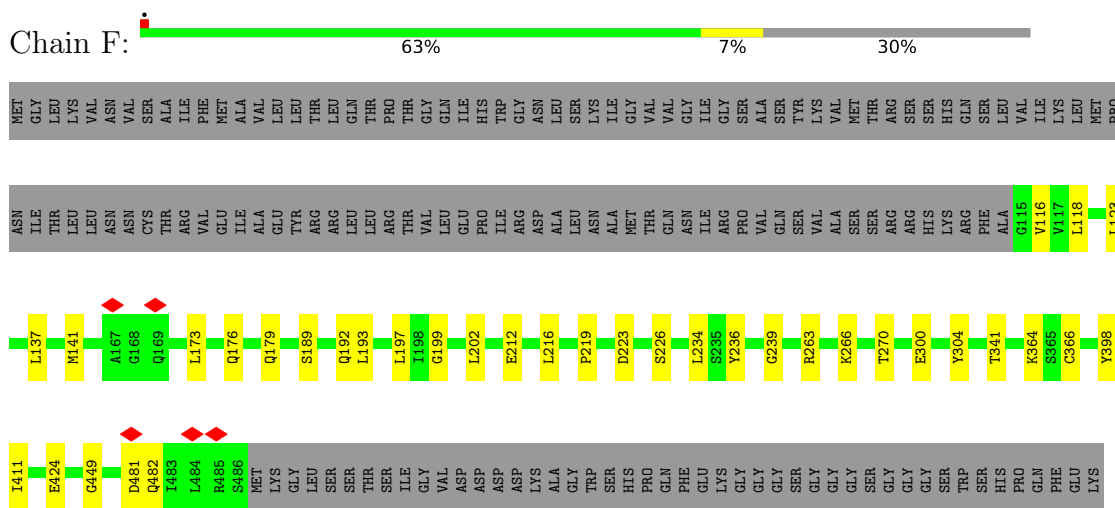
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	11	Total	O	0
			11	11	
8	B	71	Total	O	0
			71	71	
8	C	7	Total	O	0
			7	7	
8	D	20	Total	O	0
			20	20	
8	E	3	Total	O	0
			3	3	
8	F	26	Total	O	0
			26	26	
8	I	2	Total	O	0
			2	2	

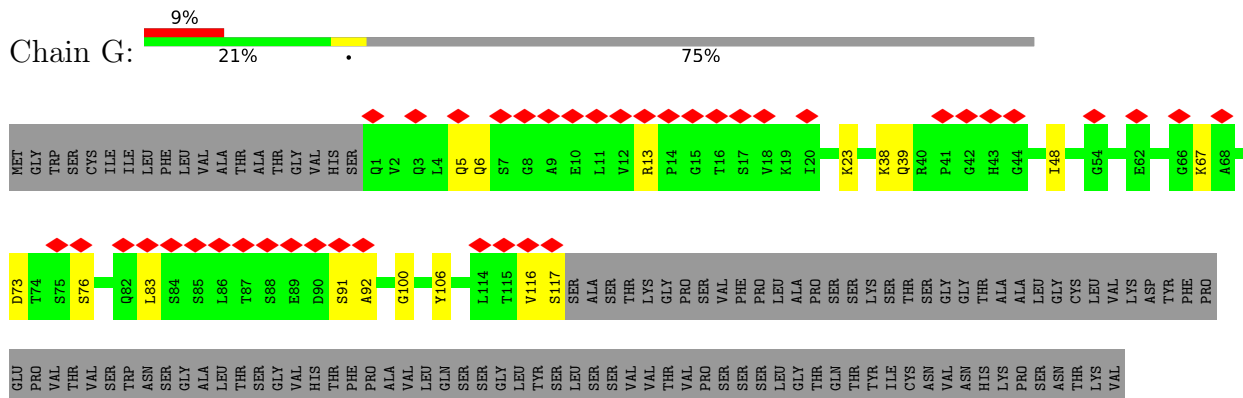




- Molecule 1: Fusion glycoprotein F0

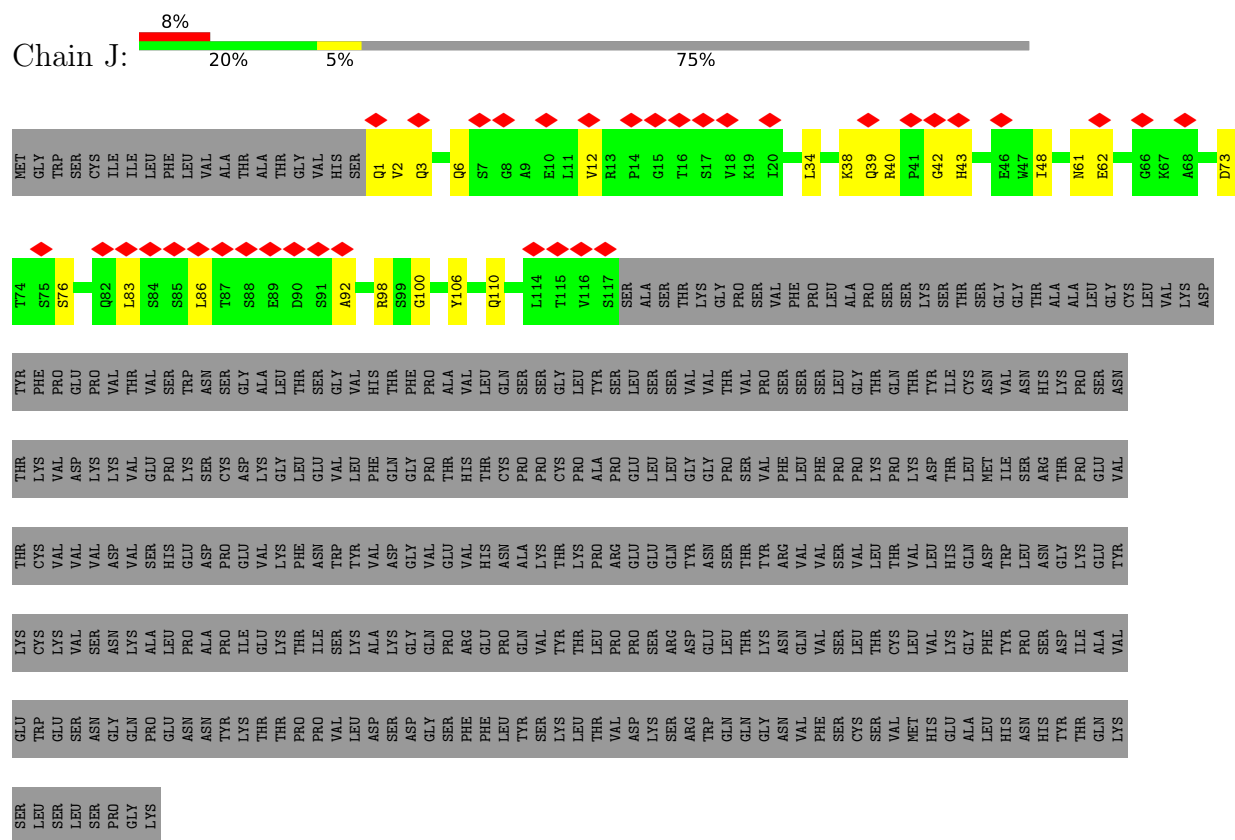


- Molecule 2: Mab H8 heavy chain

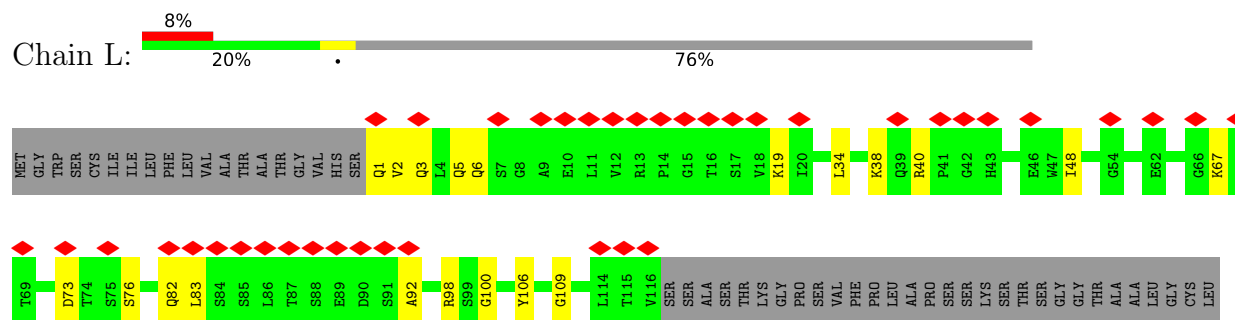


LEU	SER	SER	ASP
PRO	GLY	ASN	VAL
GLY	GLN	LYS	VAL
LYS	PRO	ALA	SER
	GLU	LEU	HIS
	ASN	PRO	GLU
	ASN	ALA	ASP
	TYR	PRO	PRO
	LYS	ILE	GLU
	THR	GLY	VAL
	THR	LYS	LYS
	PRO	THR	LYS
	PRO	ILE	PHE
	VAL	SER	ASN
	LEU	LYS	VAL
	ASP	ALA	VAL
	SER	LYS	ASP
	ASP	GLY	GLY
	GLY	GLN	VAL
	SER	PRO	GLU
	PHE	ARG	VAL
	PHE	GLU	HIS
	LEU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

- Molecule 2: Mab H8 heavy chain

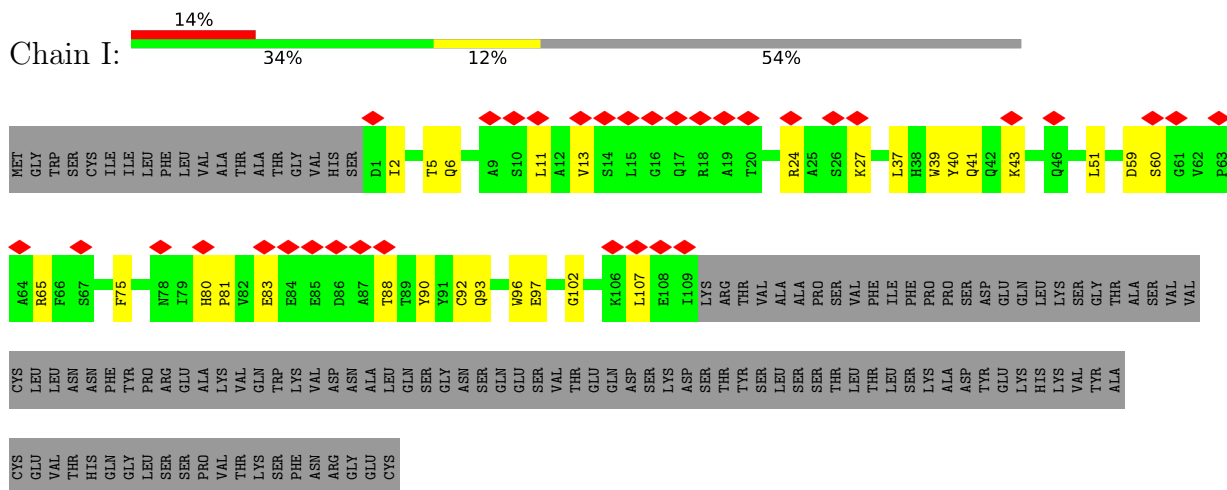


- Molecule 2: Mab H8 heavy chain

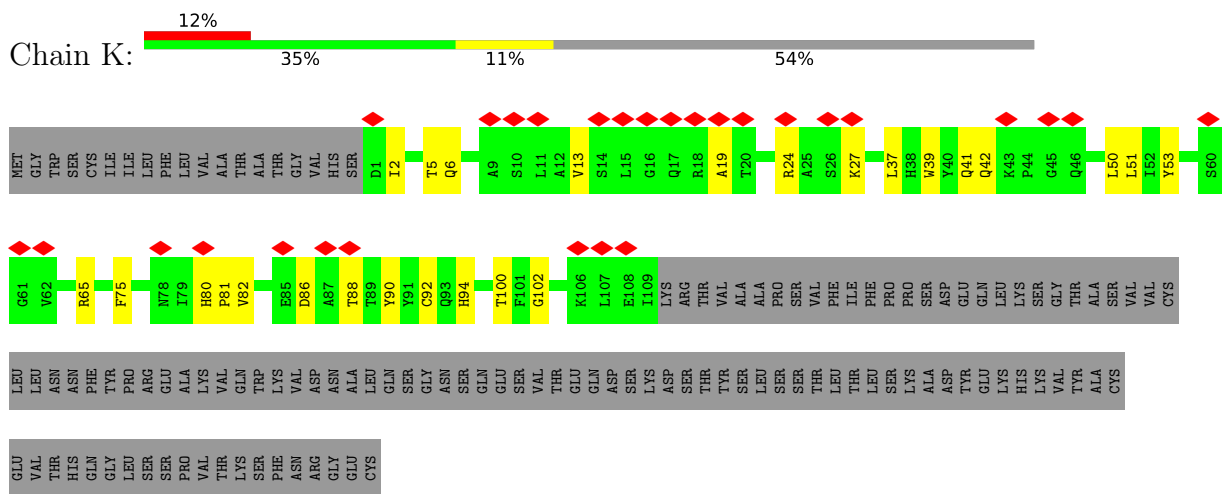


[illegible]

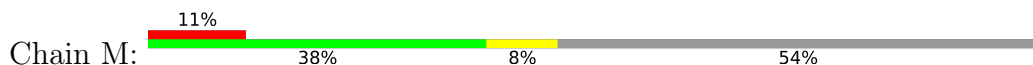
- Molecule 3: mAb H8 light chain

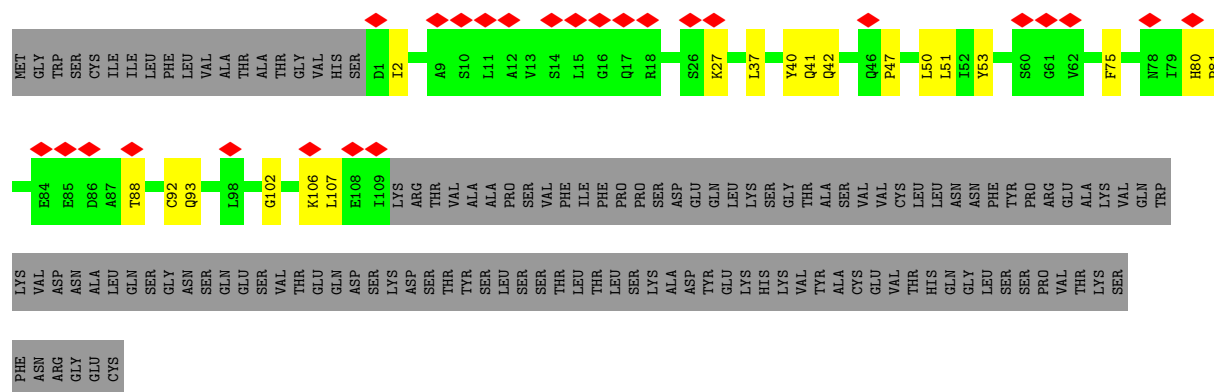


- Molecule 3: mAb H8 light chain



- Molecule 3: mAb H8 light chain

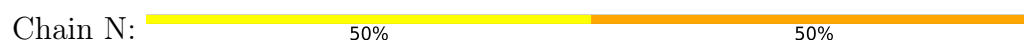




- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



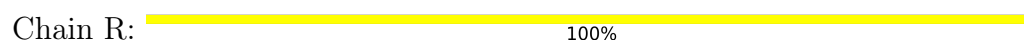
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

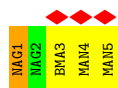


- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 6: 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	210000	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.615	Depositor
Minimum map value	-1.508	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.209	Depositor
Map size (Å)	337.91998, 337.91998, 337.91998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	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, MAN, BMA

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	0.22	0/616	0.34	0/833
1	B	0.21	0/2847	0.28	0/3866
1	C	0.21	0/616	0.31	0/833
1	D	0.21	0/2841	0.29	0/3859
1	E	0.22	0/616	0.32	0/833
1	F	0.21	0/2841	0.28	0/3859
2	G	0.12	0/923	0.25	0/1251
2	J	0.12	0/923	0.25	0/1251
2	L	0.12	0/917	0.25	0/1243
3	I	0.13	0/851	0.32	0/1159
3	K	0.13	0/851	0.30	0/1159
3	M	0.14	0/851	0.31	0/1159
All	All	0.19	0/15693	0.29	0/21305

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	608	0	640	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2806	0	2841	19	0
1	C	608	0	640	8	0
1	D	2800	0	2830	25	0
1	E	608	0	640	10	0
1	F	2800	0	2830	25	0
2	G	899	0	863	9	0
2	J	899	0	863	14	0
2	L	893	0	858	11	0
3	I	829	0	800	15	0
3	K	829	0	800	16	0
3	M	829	0	800	10	0
4	H	39	0	34	0	0
5	N	28	0	25	1	0
5	P	28	0	25	1	0
5	R	28	0	25	0	0
6	O	61	0	52	1	0
6	Q	61	0	52	1	0
7	A	14	0	13	0	0
7	C	14	0	13	1	0
7	E	14	0	13	0	0
8	A	11	0	0	0	0
8	B	71	0	0	1	0
8	C	7	0	0	0	0
8	D	20	0	0	0	0
8	E	3	0	0	0	0
8	F	26	0	0	0	0
8	I	2	0	0	0	0
All	All	15835	0	15657	149	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 (149) 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)
3:I:43:LYS:HG2	3:I:88:THR:HG21	1.73	0.68
1:A:100:PRO:HG2	1:B:116:VAL:HA	1.76	0.68
1:E:57:LYS:O	1:F:176:GLN:NE2	2.27	0.68
2:G:67:LYS:HZ3	2:G:83:LEU:HD22	1.61	0.66
3:I:41:GLN:HB2	3:I:51:LEU:HD11	1.79	0.65
2:L:67:LYS:HE2	2:L:83:LEU:HD22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:SER:HB2	1:F:192:GLN:HE21	1.62	0.64
1:F:212:GLU:HG2	1:F:236:TYR:HB3	1.80	0.63
1:F:193:LEU:HD22	1:F:197:LEU:HD23	1.79	0.63
1:B:228:GLU:OE2	1:B:268:ARG:NH1	2.31	0.63
1:C:98:ILE:HG23	1:D:116:VAL:HG13	1.80	0.62
3:M:80:HIS:HB3	3:M:81:PRO:HD3	1.81	0.62
1:D:389:ASN:O	1:D:406:GLN:NE2	2.32	0.62
1:E:100:PRO:HG2	1:F:116:VAL:HA	1.82	0.62
1:C:57:LYS:O	1:D:176:GLN:NE2	2.33	0.61
1:D:193:LEU:HD22	1:D:197:LEU:HD23	1.81	0.61
1:F:216:LEU:HD21	1:F:234:LEU:HD23	1.82	0.60
2:J:100:GLY:HA3	2:J:106:TYR:HB2	1.82	0.60
1:C:96:GLN:O	1:C:99:ARG:NH2	2.34	0.60
2:L:100:GLY:HA3	2:L:106:TYR:HB2	1.84	0.60
2:G:23:LYS:NZ	2:G:76:SER:O	2.34	0.59
2:L:73:ASP:HB3	2:L:76:SER:HB3	1.84	0.59
2:G:100:GLY:HA3	2:G:106:TYR:HB2	1.84	0.59
3:I:13:VAL:HG12	3:I:107:LEU:HD11	1.85	0.59
2:L:38:LYS:HB2	2:L:48:ILE:HD11	1.86	0.58
1:A:96:GLN:O	1:A:99:ARG:NH2	2.37	0.58
2:G:13:ARG:NH1	2:G:117:SER:O	2.37	0.58
3:K:65:ARG:NE	3:K:86:ASP:OD2	2.38	0.57
3:K:80:HIS:HB3	3:K:81:PRO:HD3	1.86	0.56
1:A:57:LYS:O	1:B:176:GLN:NE2	2.38	0.56
2:J:38:LYS:HB2	2:J:48:ILE:HD11	1.88	0.55
3:I:59:ASP:OD1	3:I:60:SER:N	2.38	0.55
1:D:398:TYR:HE2	1:D:424:GLU:HB2	1.71	0.55
2:G:91:SER:HB3	2:G:116:VAL:HG23	1.88	0.55
2:L:40:ARG:HG2	2:L:92:ALA:HB2	1.88	0.55
2:J:1:GLN:NE2	2:J:2:VAL:O	2.40	0.54
1:B:304:TYR:HB2	1:B:411:ILE:HB	1.89	0.54
3:M:2:ILE:HG13	3:M:27:LYS:HE2	1.88	0.54
3:I:80:HIS:HB3	3:I:81:PRO:HD3	1.88	0.54
3:I:65:ARG:NH1	3:I:83:GLU:OE1	2.41	0.54
2:J:73:ASP:HB3	2:J:76:SER:HB3	1.90	0.54
3:K:92:CYS:O	3:K:102:GLY:N	2.40	0.54
3:M:50:LEU:HD21	3:M:53:TYR:HB3	1.90	0.53
1:E:38:ILE:HD13	1:F:300:GLU:HB2	1.91	0.53
3:I:2:ILE:HG12	3:I:27:LYS:HE2	1.89	0.53
1:D:471:GLU:HA	1:D:474:LYS:HE3	1.90	0.53
3:I:6:GLN:NE2	3:I:90:TYR:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASN:OD1	1:B:144:SER:N	2.42	0.53
2:G:5:GLN:NE2	2:G:6:GLN:O	2.38	0.52
3:K:13:VAL:HG11	3:K:82:VAL:HG21	1.91	0.52
2:L:1:GLN:OE1	2:L:3:GLN:NE2	2.43	0.52
3:I:92:CYS:O	3:I:102:GLY:N	2.42	0.52
2:J:40:ARG:HG2	2:J:42:GLY:H	1.75	0.52
1:E:69:THR:HG22	1:F:199:GLY:HA2	1.92	0.52
2:G:73:ASP:HB3	2:G:76:SER:HB3	1.91	0.51
3:I:5:THR:HB	3:I:24:ARG:HB2	1.93	0.51
2:J:83:LEU:HD13	2:J:86:LEU:HD21	1.92	0.51
1:C:29:ASN:OD1	6:O:1:NAG:N2	2.44	0.51
2:L:1:GLN:NE2	2:L:2:VAL:O	2.45	0.51
1:E:69:THR:HG21	1:F:202:LEU:HD23	1.93	0.50
3:K:2:ILE:HG12	3:K:27:LYS:HB2	1.92	0.50
1:B:208:ARG:NH2	1:F:239:GLY:O	2.44	0.50
1:E:29:ASN:OD1	6:Q:1:NAG:N2	2.44	0.50
2:G:38:LYS:HB2	2:G:48:ILE:HD11	1.94	0.49
3:K:65:ARG:HD2	3:K:81:PRO:O	2.12	0.49
1:F:137:LEU:HD11	1:F:270:THR:HA	1.95	0.49
3:M:92:CYS:O	3:M:102:GLY:N	2.45	0.49
2:L:19:LYS:HG2	2:L:82:GLN:HB2	1.95	0.48
1:D:304:TYR:HB2	1:D:411:ILE:HB	1.95	0.48
2:J:12:VAL:HG11	2:J:86:LEU:HD12	1.95	0.48
1:B:118:LEU:HD11	1:B:123:LEU:HD22	1.96	0.48
3:M:106:LYS:NZ	3:M:107:LEU:O	2.47	0.48
1:C:38:ILE:HD13	1:D:300:GLU:HB2	1.96	0.48
1:D:241:ASP:OD2	1:D:243:ASN:ND2	2.44	0.48
1:F:263:ARG:O	1:F:266:LYS:HE3	2.13	0.47
2:J:1:GLN:OE1	2:J:3:GLN:NE2	2.46	0.47
1:B:366:CYS:O	1:B:449:GLY:HA3	2.15	0.47
1:B:263:ARG:O	1:B:266:LYS:HE3	2.15	0.47
1:D:364:LYS:HB3	1:D:447:ASP:HB3	1.97	0.47
1:E:99:ARG:HD3	1:E:99:ARG:HA	1.64	0.47
3:I:40:TYR:HE2	3:I:93:GLN:HB3	1.79	0.47
2:J:6:GLN:H	2:J:110:GLN:HE22	1.62	0.47
1:D:223:ASP:OD2	1:D:226:SER:OG	2.32	0.47
1:F:366:CYS:O	1:F:449:GLY:HA3	2.15	0.47
1:D:310:GLU:HB3	1:D:371:VAL:HG22	1.97	0.47
1:D:212:GLU:HG3	1:D:236:TYR:CG	2.50	0.46
1:B:386:LEU:HD21	1:B:425:VAL:HG21	1.98	0.46
1:F:137:LEU:O	1:F:141:MET:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:13:VAL:HG21	3:K:19:ALA:HB2	1.98	0.46
2:J:61:ASN:OD1	2:J:62:GLU:N	2.49	0.46
3:M:42:GLN:O	3:M:88:THR:OG1	2.33	0.46
1:B:268:ARG:NH1	8:B:606:HOH:O	2.31	0.46
1:D:306:ILE:HD12	1:D:311:TRP:CD1	2.50	0.46
1:D:366:CYS:O	1:D:449:GLY:HA3	2.16	0.46
1:B:156:THR:HB	5:N:2:NAG:H62	1.97	0.45
1:D:191:ASN:OD1	1:D:192:GLN:N	2.49	0.45
1:F:304:TYR:HB2	1:F:411:ILE:HB	1.98	0.45
1:B:481:ASP:OD1	1:B:482:GLN:N	2.49	0.45
1:D:378:ARG:HD3	1:D:393:ILE:HG23	1.98	0.45
2:J:39:GLN:O	2:J:92:ALA:HB1	2.16	0.45
3:I:11:LEU:HD23	3:I:11:LEU:HA	1.87	0.45
3:K:50:LEU:HD21	3:K:53:TYR:HB3	1.97	0.44
2:G:39:GLN:O	2:G:92:ALA:HB1	2.17	0.44
1:B:310:GLU:HB3	1:B:371:VAL:HG22	1.98	0.44
1:C:63:THR:OG1	5:P:1:NAG:H82	2.17	0.44
1:E:54:LEU:HD12	1:F:173:LEU:HB3	1.99	0.44
1:D:369:THR:HG22	1:D:452:ILE:O	2.18	0.44
3:K:6:GLN:HE22	3:K:90:TYR:C	2.26	0.44
1:F:118:LEU:HD11	1:F:123:LEU:HD22	2.00	0.44
3:K:37:LEU:HD13	3:K:75:PHE:CD1	2.53	0.43
1:E:42:SER:O	1:F:341:THR:HG22	2.18	0.43
3:M:40:TYR:HE2	3:M:93:GLN:HB3	1.84	0.43
1:F:398:TYR:HE2	1:F:424:GLU:HB2	1.83	0.43
2:J:40:ARG:HH11	2:J:43:HIS:CG	2.37	0.43
3:I:37:LEU:HD13	3:I:75:PHE:CD1	2.54	0.43
1:C:70:ARG:NH2	7:C:601:NAG:O7	2.52	0.43
1:F:398:TYR:CE2	1:F:424:GLU:HB2	2.53	0.43
3:K:42:GLN:O	3:K:88:THR:OG1	2.38	0.42
1:B:176:GLN:CG	1:B:179:GLN:HB2	2.49	0.42
1:F:364:LYS:HD3	1:F:364:LYS:H	1.84	0.42
2:J:34:LEU:HD23	2:J:98:ARG:HA	2.01	0.42
1:E:59:MET:HE1	1:E:73:ILE:HG23	2.01	0.42
1:B:193:LEU:HD22	1:B:197:LEU:HD23	2.02	0.42
1:D:212:GLU:HG3	1:D:236:TYR:CD1	2.54	0.42
1:F:176:GLN:HG3	1:F:179:GLN:HB2	2.02	0.42
1:F:223:ASP:OD2	1:F:226:SER:OG	2.33	0.42
3:M:41:GLN:HB2	3:M:51:LEU:HD11	2.01	0.42
3:K:39:TRP:CZ3	3:K:92:CYS:HB3	2.55	0.42
3:M:37:LEU:HD13	3:M:75:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:41:GLN:HB3	3:K:51:LEU:HD11	2.01	0.42
3:I:96:TRP:CD1	3:I:97:GLU:HG2	2.55	0.42
1:D:398:TYR:CE2	1:D:424:GLU:HB2	2.52	0.42
2:L:109:GLY:O	3:M:47:PRO:HG3	2.20	0.42
1:F:481:ASP:OD1	1:F:482:GLN:N	2.53	0.41
1:B:155:GLU:O	1:B:155:GLU:HG3	2.19	0.41
1:B:212:GLU:HG3	1:B:236:TYR:CD1	2.55	0.41
1:D:228:GLU:HB3	1:D:266:LYS:HD3	2.02	0.41
3:K:5:THR:OG1	3:K:24:ARG:HB2	2.21	0.41
3:I:39:TRP:CZ3	3:I:92:CYS:HB3	2.55	0.41
2:J:86:LEU:HD23	2:J:86:LEU:HA	1.84	0.41
3:K:65:ARG:HG3	3:K:81:PRO:HD2	2.02	0.41
1:A:38:ILE:HA	1:D:125:VAL:HG11	2.03	0.41
3:K:94:HIS:NE2	3:K:100:THR:HB	2.35	0.41
1:B:212:GLU:HG3	1:B:236:TYR:CG	2.56	0.40
2:L:5:GLN:NE2	2:L:6:GLN:O	2.43	0.40
1:C:87:ILE:HD11	1:D:217:PHE:HB3	2.04	0.40
1:D:261:GLU:HG3	1:F:219:PRO:HD2	2.03	0.40
1:D:176:GLN:CG	1:D:179:GLN:HB2	2.52	0.40
2:L:34:LEU:HD23	2:L:98:ARG:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	75/532 (14%)	75 (100%)	0	0	100	100
1	B	370/532 (70%)	367 (99%)	3 (1%)	0	100	100
1	C	75/532 (14%)	75 (100%)	0	0	100	100
1	D	370/532 (70%)	364 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	75/532 (14%)	72 (96%)	3 (4%)	0	100	100
1	F	370/532 (70%)	366 (99%)	4 (1%)	0	100	100
2	G	115/476 (24%)	113 (98%)	2 (2%)	0	100	100
2	J	115/476 (24%)	113 (98%)	2 (2%)	0	100	100
2	L	114/476 (24%)	113 (99%)	1 (1%)	0	100	100
3	I	107/236 (45%)	97 (91%)	10 (9%)	0	100	100
3	K	107/236 (45%)	100 (94%)	7 (6%)	0	100	100
3	M	107/236 (45%)	103 (96%)	4 (4%)	0	100	100
All	All	2000/5328 (38%)	1958 (98%)	42 (2%)	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	69/442 (16%)	69 (100%)	0	100	100
1	B	309/442 (70%)	309 (100%)	0	100	100
1	C	69/442 (16%)	69 (100%)	0	100	100
1	D	308/442 (70%)	308 (100%)	0	100	100
1	E	69/442 (16%)	69 (100%)	0	100	100
1	F	308/442 (70%)	308 (100%)	0	100	100
2	G	95/417 (23%)	95 (100%)	0	100	100
2	J	95/417 (23%)	95 (100%)	0	100	100
2	L	94/417 (22%)	94 (100%)	0	100	100
3	I	92/204 (45%)	92 (100%)	0	100	100
3	K	92/204 (45%)	92 (100%)	0	100	100
3	M	92/204 (45%)	92 (100%)	0	100	100
All	All	1692/4515 (38%)	1692 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	149	ASN
1	B	169	GLN
1	B	243	ASN
1	B	346	ASN
1	B	444	HIS
1	D	149	ASN
1	D	346	ASN
1	D	356	GLN
1	D	406	GLN
1	D	444	HIS
1	F	130	GLN
1	F	192	GLN
1	F	243	ASN
1	F	328	ASN
1	F	346	ASN
1	F	405	ASN
1	F	419	HIS
1	F	444	HIS
1	F	465	ASN
2	J	3	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 ⓘ

19 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	$\# Z > 2$
4	NAG	H	1	4,1	14,14,15	0.76	0	17,19,21	1.38	2 (11%)
4	NAG	H	2	4	14,14,15	0.75	0	17,19,21	0.95	0
4	BMA	H	3	4	11,11,12	0.84	0	15,15,17	2.01	3 (20%)
5	NAG	N	1	1,5	14,14,15	0.86	0	17,19,21	1.78	2 (11%)
5	NAG	N	2	5	14,14,15	0.73	0	17,19,21	0.87	1 (5%)
6	NAG	O	1	1,6	14,14,15	0.79	0	17,19,21	1.21	1 (5%)
6	NAG	O	2	6	14,14,15	0.74	0	17,19,21	0.96	0
6	BMA	O	3	6	11,11,12	0.83	0	15,15,17	2.03	3 (20%)
6	MAN	O	4	6	11,11,12	0.69	0	15,15,17	1.19	1 (6%)
6	MAN	O	5	6	11,11,12	0.72	0	15,15,17	1.06	1 (6%)
5	NAG	P	1	1,5	14,14,15	0.78	0	17,19,21	2.72	4 (23%)
5	NAG	P	2	5	14,14,15	0.73	0	17,19,21	0.84	1 (5%)
6	NAG	Q	1	1,6	14,14,15	0.79	0	17,19,21	1.27	2 (11%)
6	NAG	Q	2	6	14,14,15	0.74	0	17,19,21	0.96	0
6	BMA	Q	3	6	11,11,12	0.83	0	15,15,17	2.03	3 (20%)
6	MAN	Q	4	6	11,11,12	0.68	0	15,15,17	1.17	1 (6%)
6	MAN	Q	5	6	11,11,12	0.73	0	15,15,17	1.03	1 (6%)
5	NAG	R	1	1,5	14,14,15	0.86	0	17,19,21	1.65	1 (5%)
5	NAG	R	2	5	14,14,15	0.73	0	17,19,21	0.85	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
4	NAG	H	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
5	NAG	N	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
6	NAG	O	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	MAN	O	4	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	O	5	6	-	0/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
6	NAG	Q	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	0/2/19/22	0/1/1/1
6	MAN	Q	4	6	-	1/2/19/22	0/1/1/1
6	MAN	Q	5	6	-	0/2/19/22	0/1/1/1
5	NAG	R	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	1	NAG	C2-N2-C7	9.87	136.12	122.90
6	Q	3	BMA	C1-O5-C5	6.03	120.26	112.19
6	O	3	BMA	C1-O5-C5	6.02	120.25	112.19
4	H	3	BMA	C1-O5-C5	5.84	120.01	112.19
5	N	1	NAG	C2-N2-C7	5.55	130.34	122.90
5	R	1	NAG	C2-N2-C7	5.01	129.62	122.90
4	H	1	NAG	C1-O5-C5	4.20	117.82	112.19
6	O	4	MAN	C1-O5-C5	3.61	117.02	112.19
6	Q	4	MAN	C1-O5-C5	3.48	116.85	112.19
6	Q	1	NAG	C1-O5-C5	3.45	116.81	112.19
6	O	1	NAG	C1-O5-C5	3.17	116.44	112.19
5	P	1	NAG	C8-C7-N2	3.06	121.20	116.12
6	O	5	MAN	C1-O5-C5	2.96	116.15	112.19
6	Q	5	MAN	C1-O5-C5	2.81	115.95	112.19
4	H	3	BMA	C3-C4-C5	2.55	114.85	110.23
4	H	1	NAG	C3-C4-C5	-2.53	105.64	110.23
6	O	3	BMA	C3-C4-C5	2.50	114.77	110.23
6	Q	3	BMA	C3-C4-C5	2.46	114.69	110.23
5	P	1	NAG	C1-O5-C5	2.22	115.16	112.19
4	H	3	BMA	C2-C3-C4	2.20	114.72	110.86
5	N	2	NAG	O5-C1-C2	-2.13	108.00	111.29
5	N	1	NAG	C4-C3-C2	2.12	114.13	111.02
5	P	1	NAG	O7-C7-C8	-2.10	118.31	122.05
5	P	2	NAG	O5-C1-C2	-2.08	108.07	111.29
5	R	2	NAG	O5-C1-C2	-2.07	108.08	111.29
6	Q	3	BMA	C2-C3-C4	2.03	114.44	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	3	BMA	C2-C3-C4	2.00	114.39	110.86
6	Q	1	NAG	O5-C1-C2	-2.00	108.19	111.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

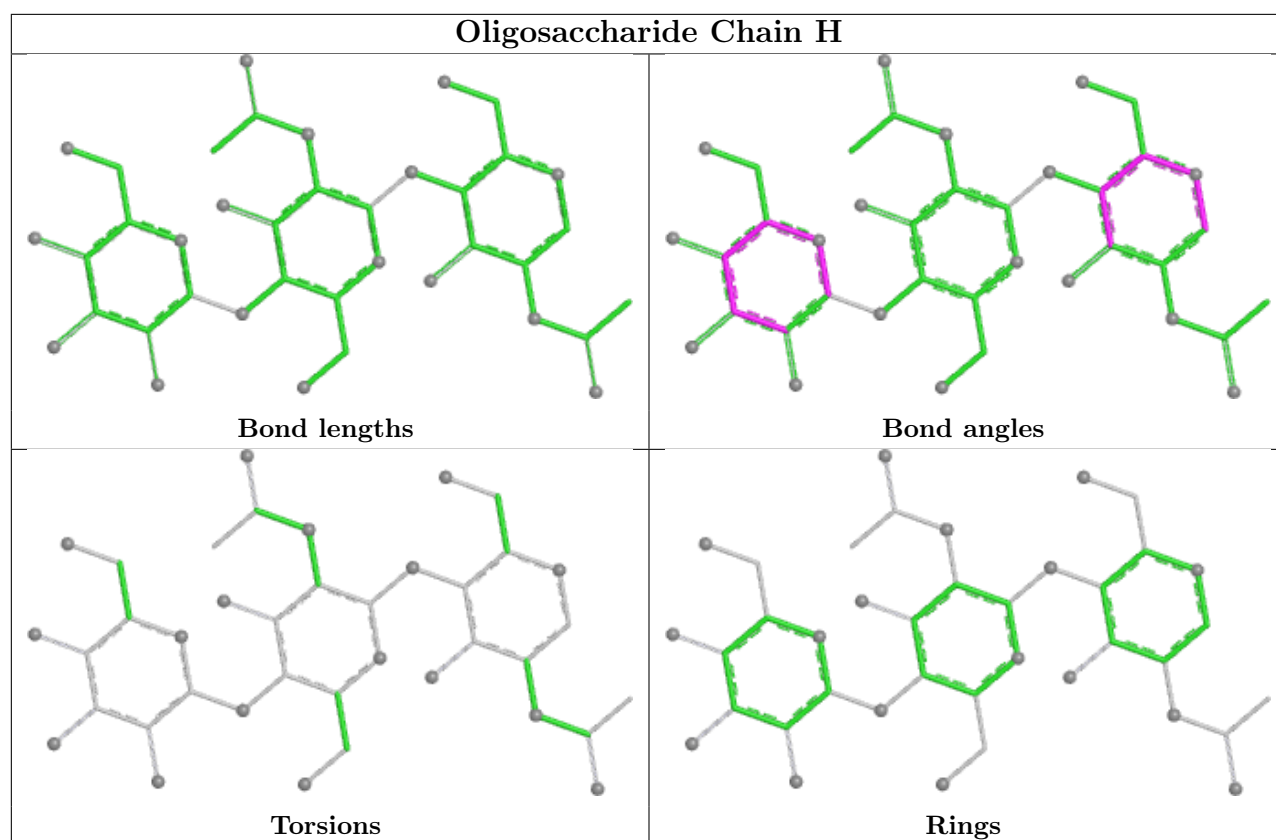
Mol	Chain	Res	Type	Atoms
5	N	1	NAG	C8-C7-N2-C2
5	N	1	NAG	O7-C7-N2-C2
5	P	1	NAG	C8-C7-N2-C2
5	P	1	NAG	O7-C7-N2-C2
5	R	1	NAG	C8-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2
6	O	2	NAG	C8-C7-N2-C2
6	O	2	NAG	O7-C7-N2-C2
6	Q	2	NAG	C8-C7-N2-C2
6	Q	2	NAG	O7-C7-N2-C2
6	Q	4	MAN	O5-C5-C6-O6
5	P	1	NAG	C3-C2-N2-C7
6	O	1	NAG	C4-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
6	Q	1	NAG	C4-C5-C6-O6
6	Q	1	NAG	O5-C5-C6-O6

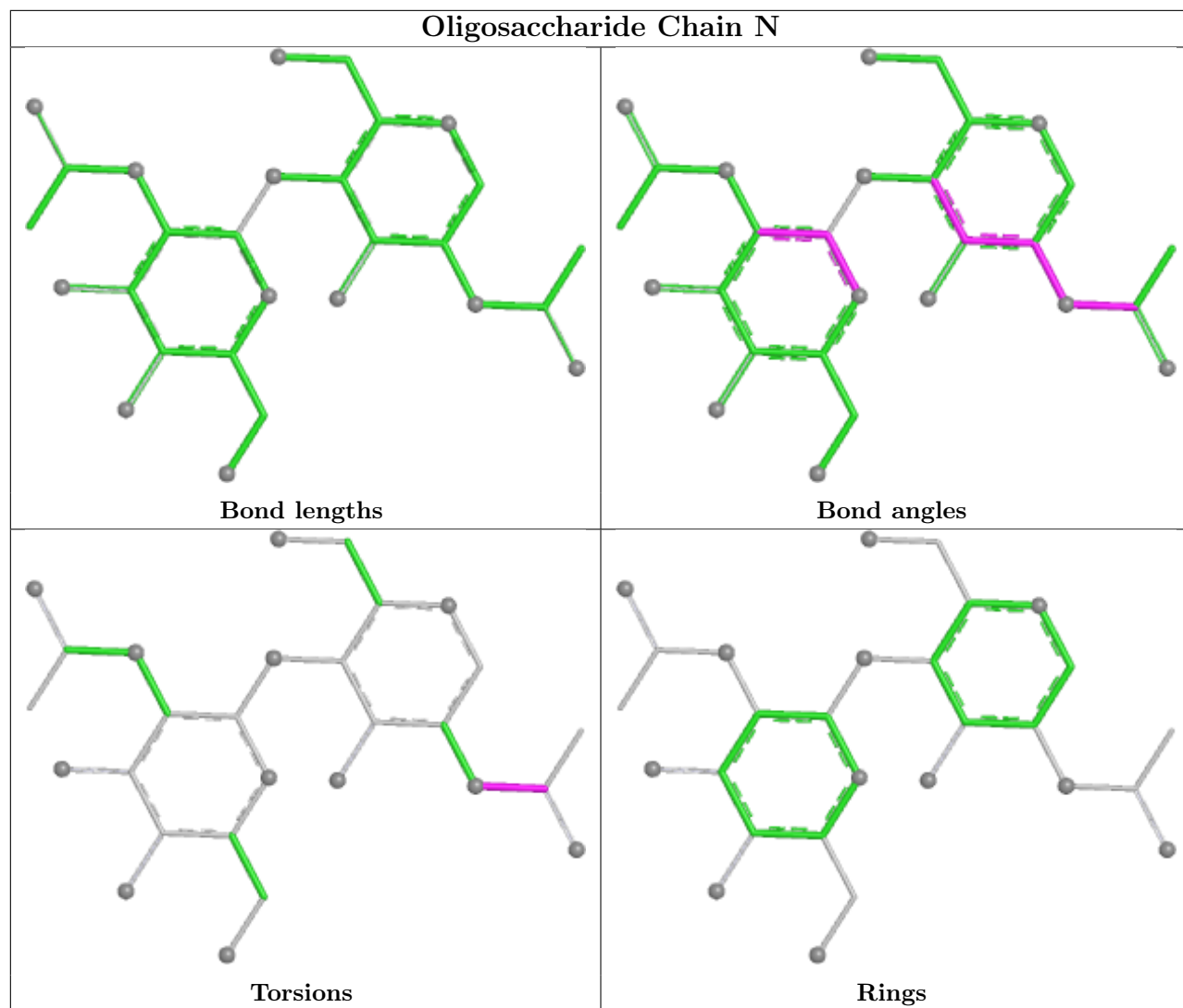
There are no ring outliers.

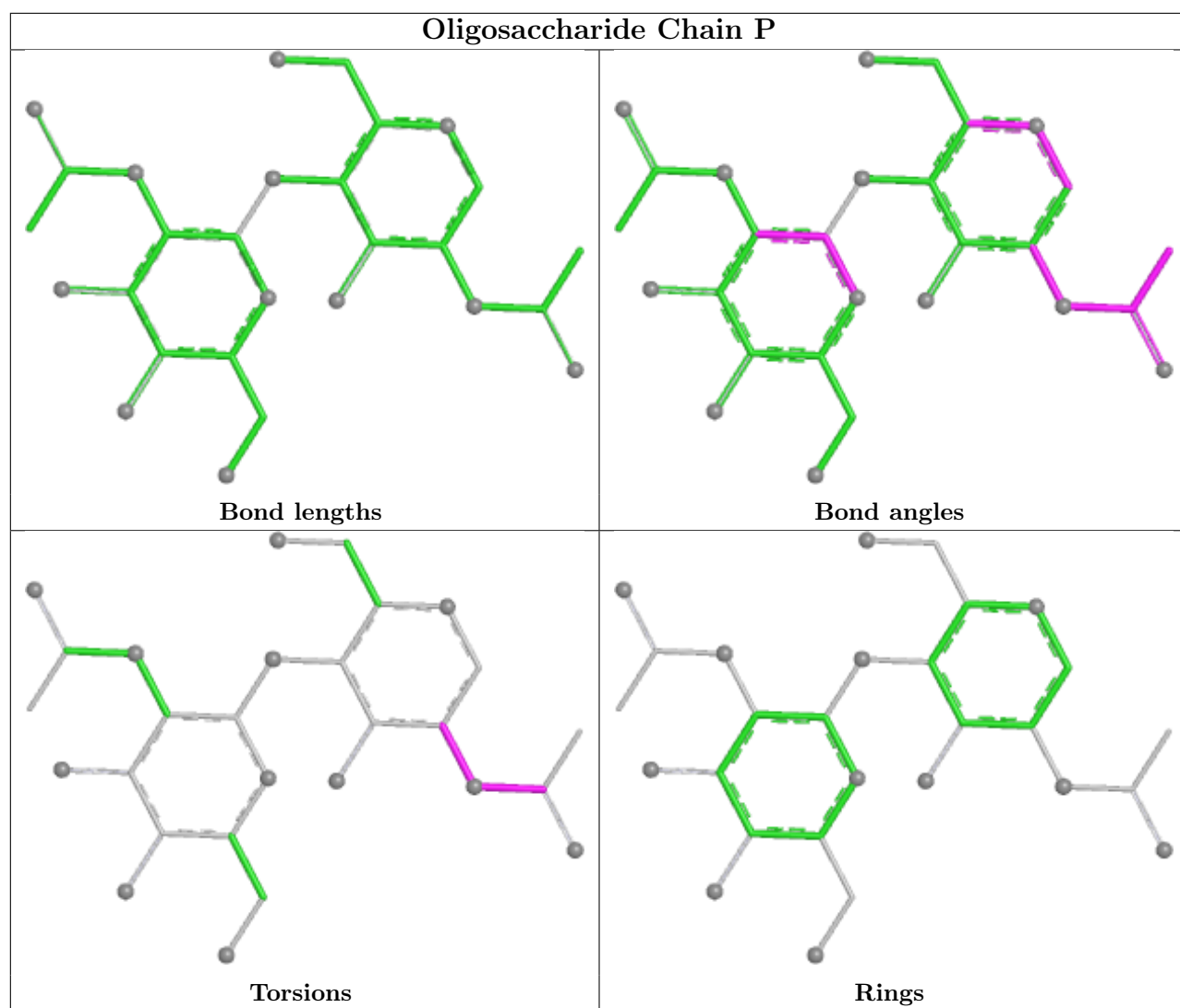
4 monomers are involved in 4 short contacts:

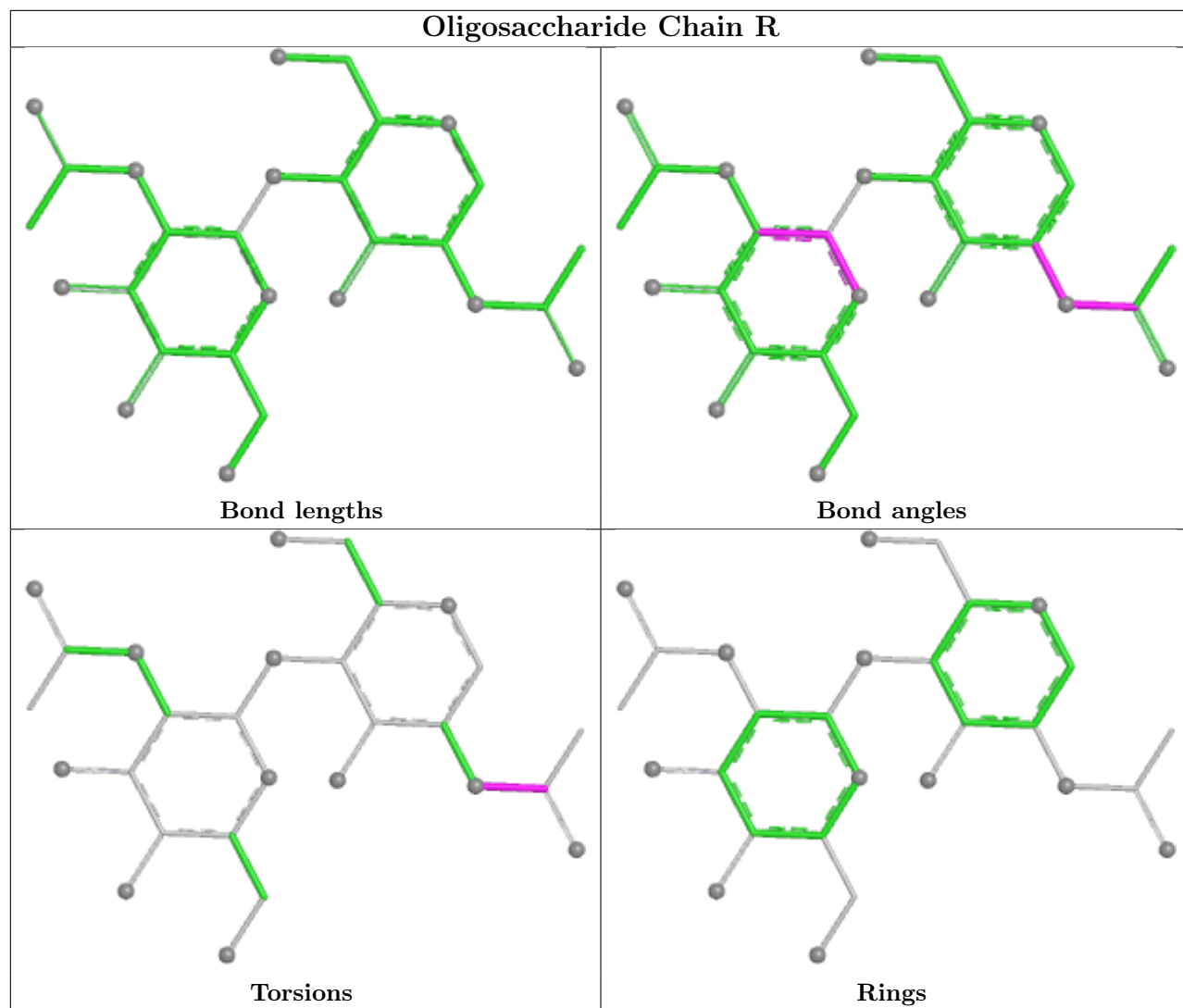
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	O	1	NAG	1	0
5	P	1	NAG	1	0
6	Q	1	NAG	1	0
5	N	2	NAG	1	0

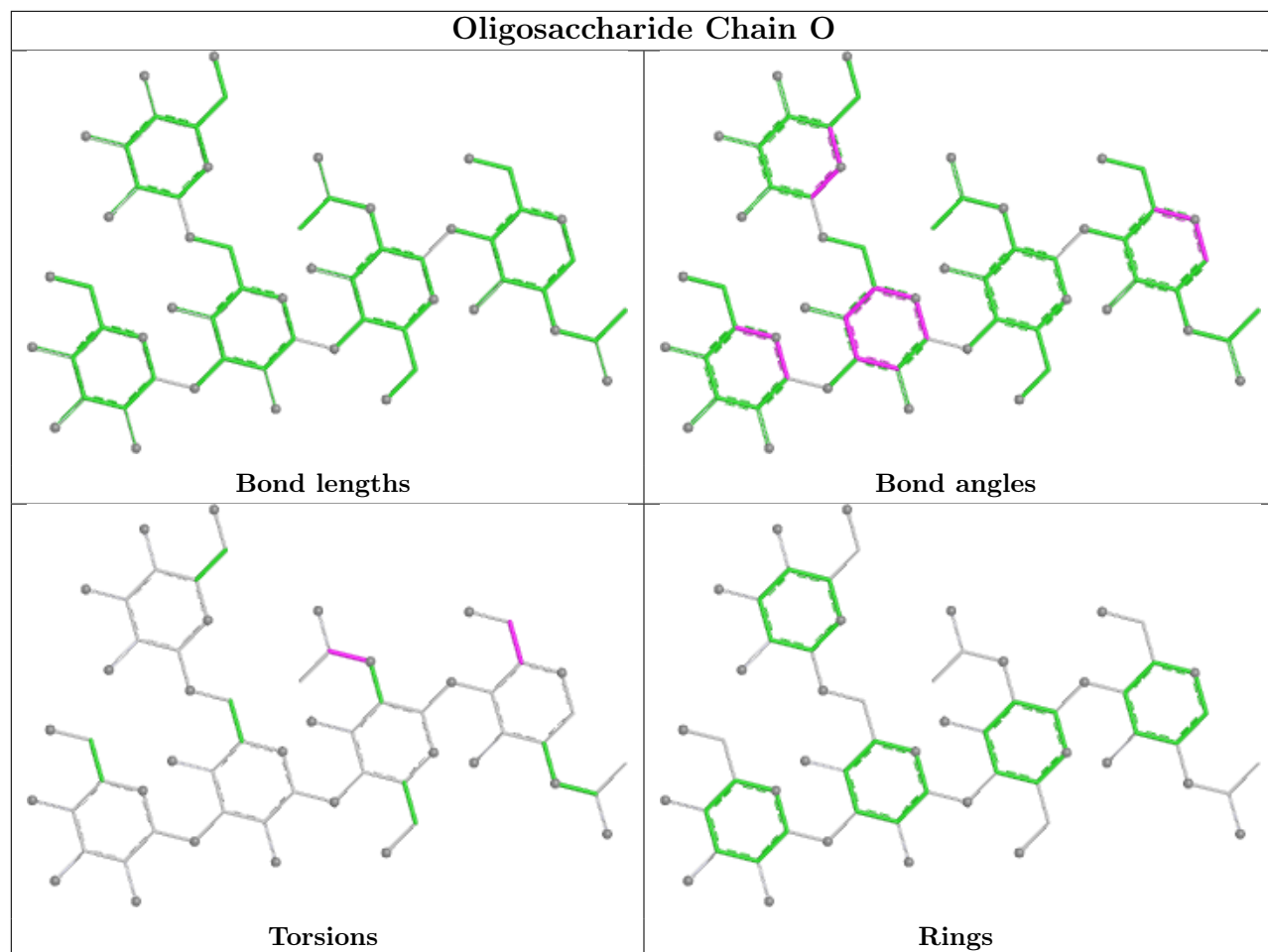
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

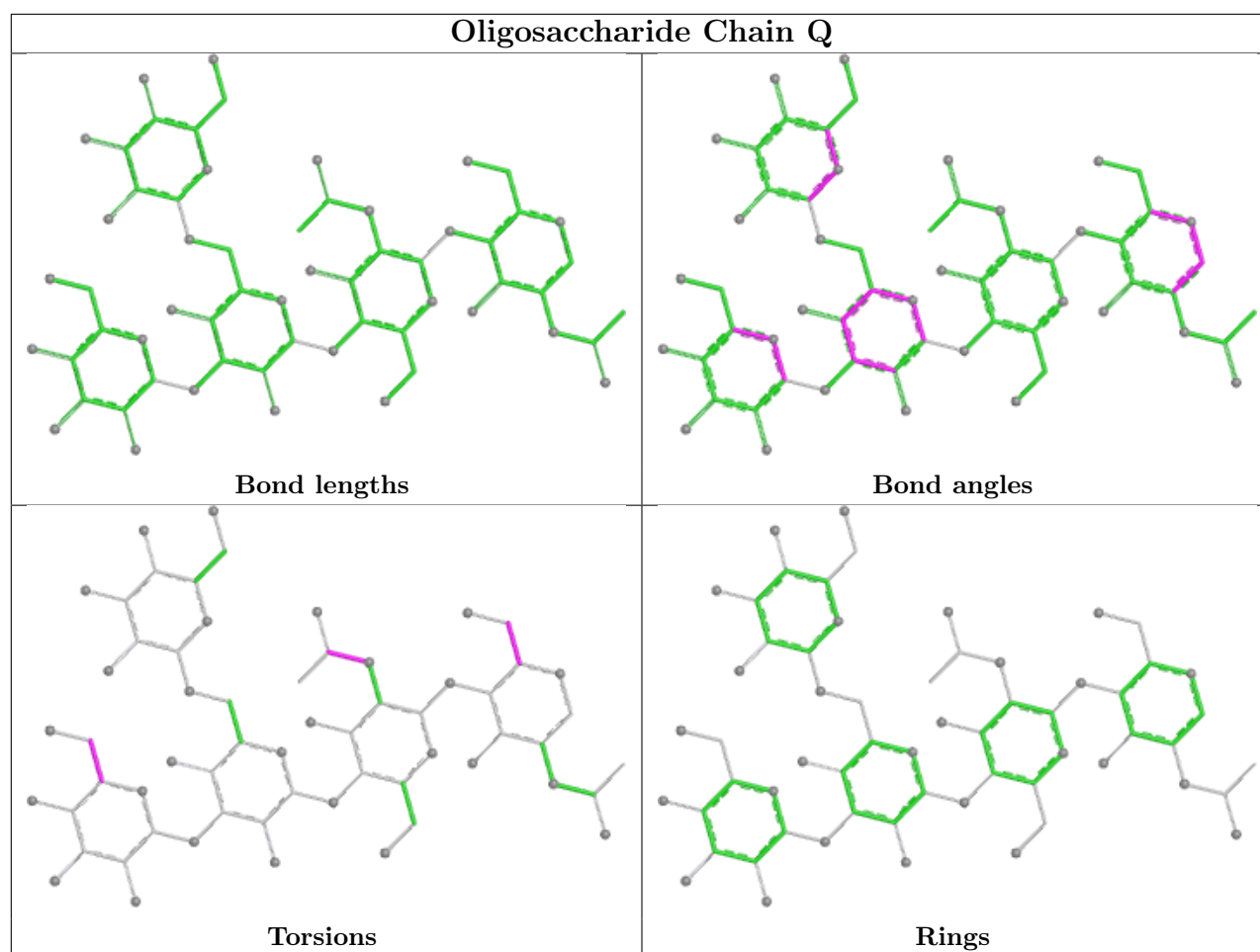












5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
7	NAG	A	601	1	14,14,15	0.71	0	17,19,21	0.79	0
7	NAG	E	601	1	14,14,15	0.70	0	17,19,21	0.82	0
7	NAG	C	601	1	14,14,15	0.71	0	17,19,21	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	601	1	-	0/6/23/26	0/1/1/1
7	NAG	E	601	1	-	2/6/23/26	0/1/1/1
7	NAG	C	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	601	NAG	C8-C7-N2-C2
7	E	601	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	601	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

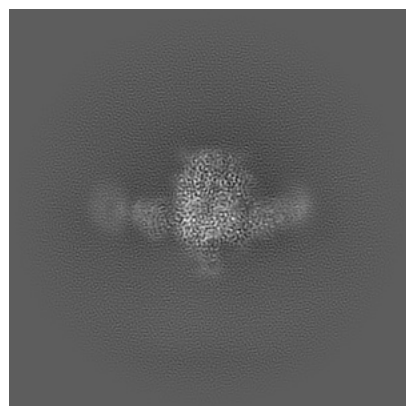
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72293. These allow visual inspection of the internal detail of the map and identification of artifacts.

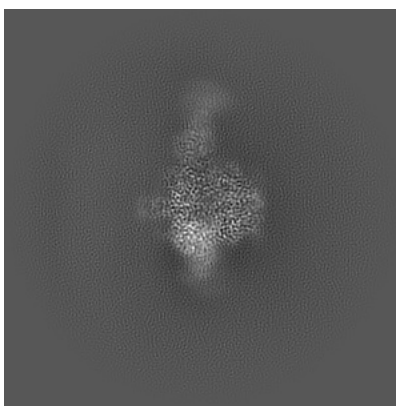
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

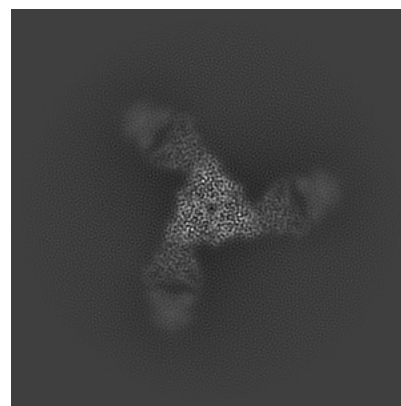
6.1.1 Primary map



X

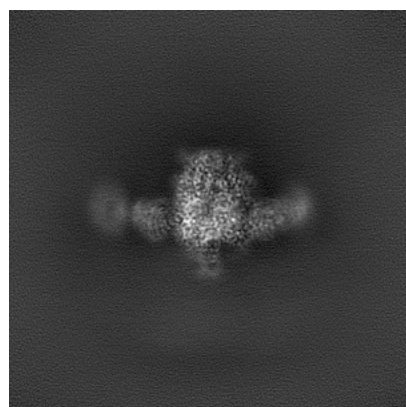


Y

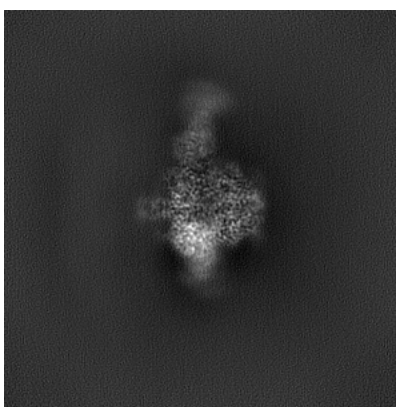


Z

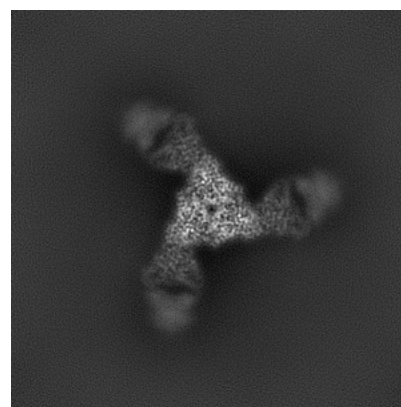
6.1.2 Raw map



X



Y

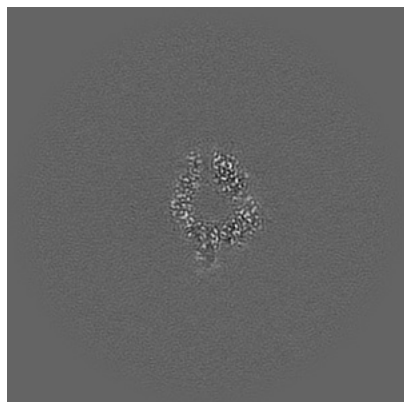


Z

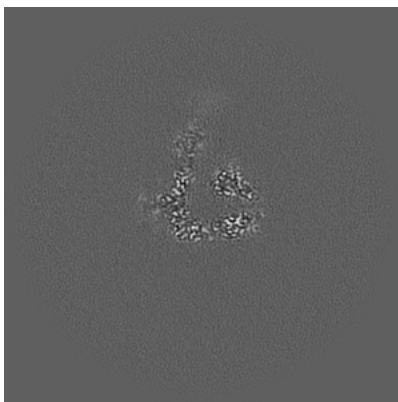
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

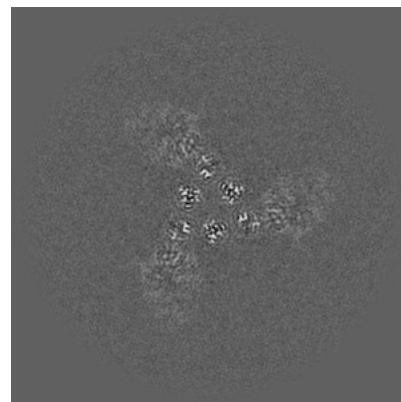
6.2.1 Primary map



X Index: 160

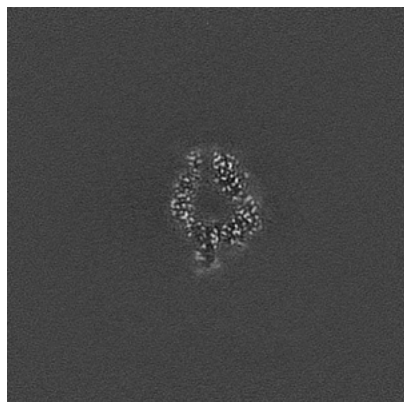


Y Index: 160

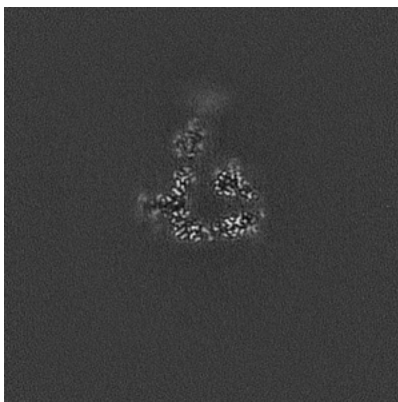


Z Index: 160

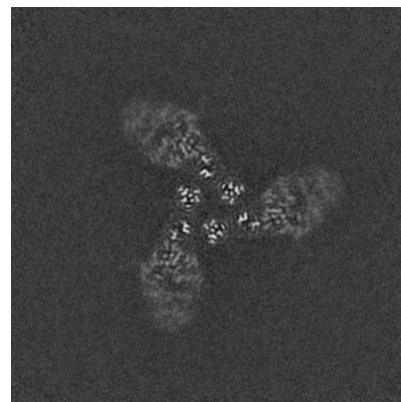
6.2.2 Raw map



X Index: 160



Y Index: 160

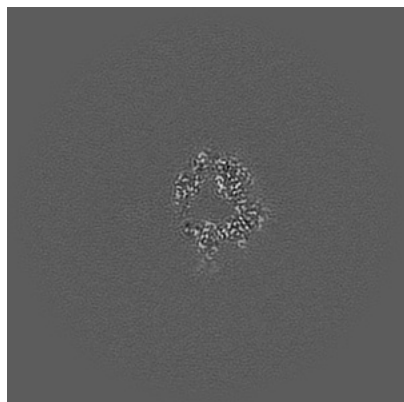


Z Index: 160

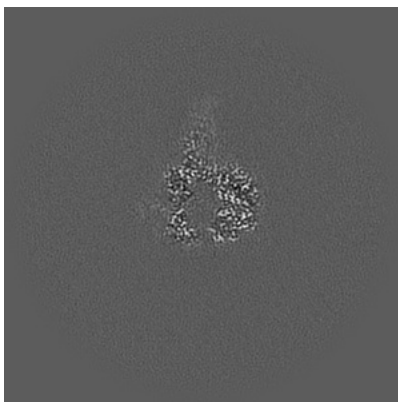
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

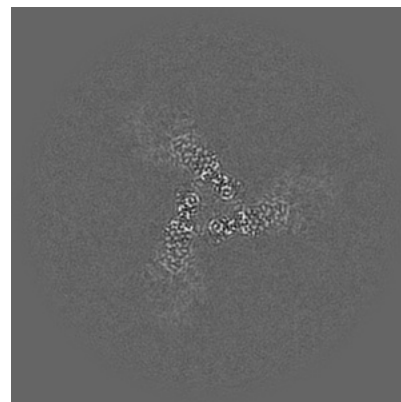
6.3.1 Primary map



X Index: 155

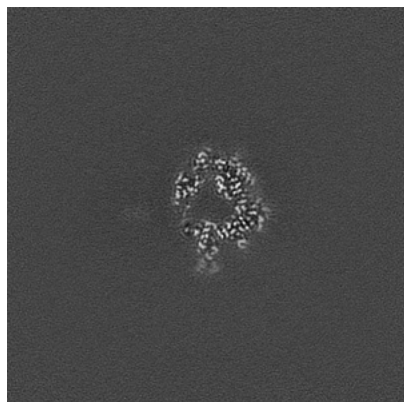


Y Index: 151

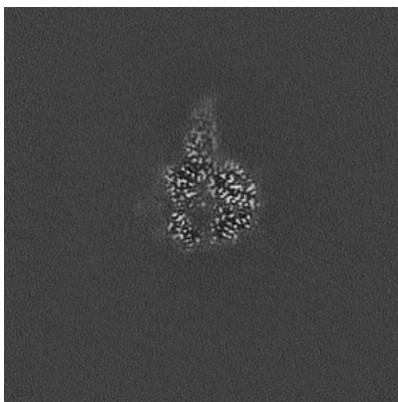


Z Index: 150

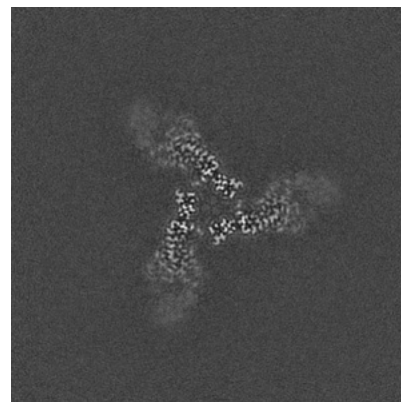
6.3.2 Raw map



X Index: 155



Y Index: 149

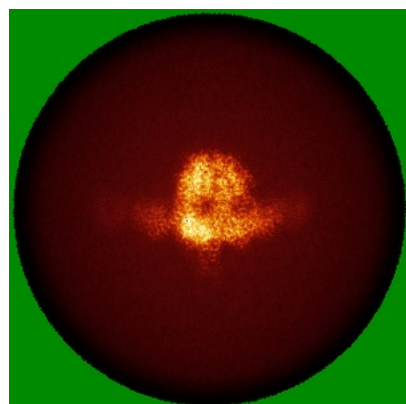


Z Index: 151

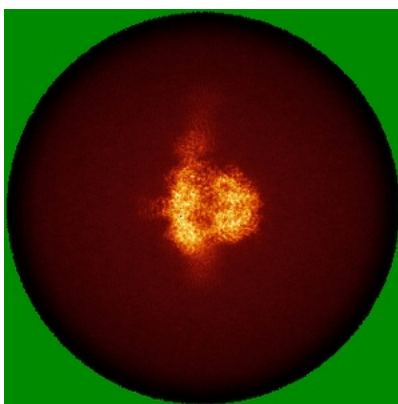
The images above show the largest variance slices of the map in three orthogonal directions.

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

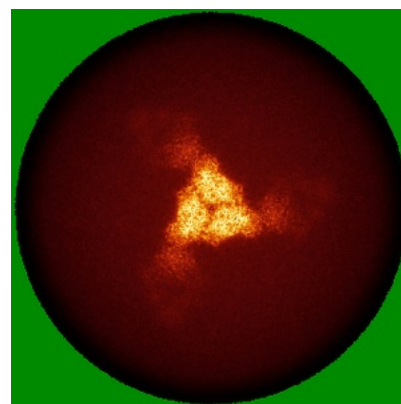
6.4.1 Primary map



X

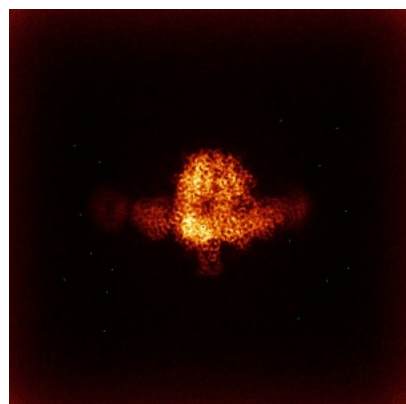


Y

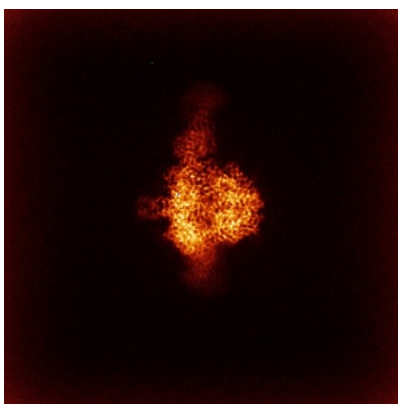


Z

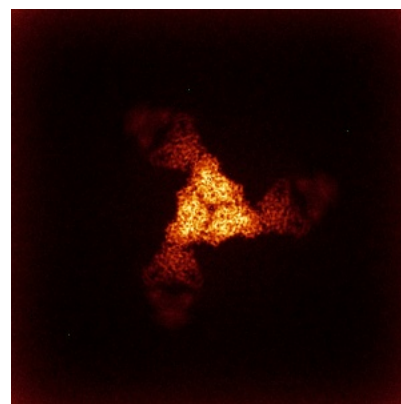
6.4.2 Raw map



X



Y

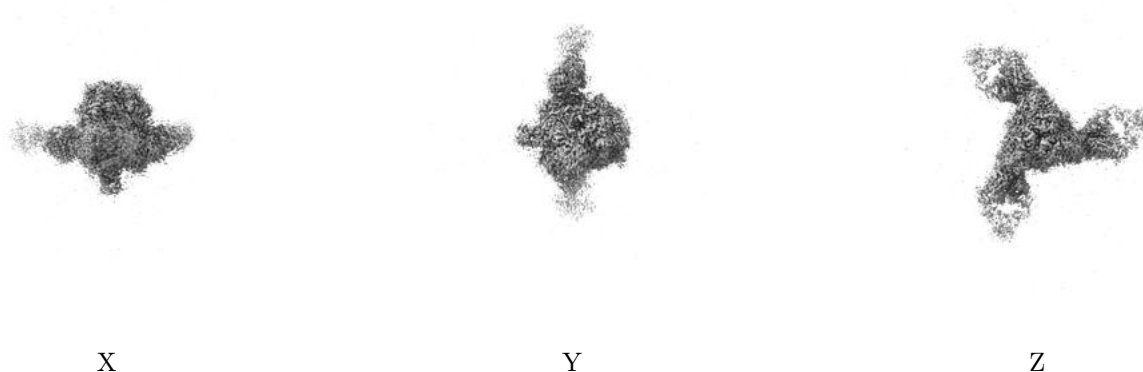


Z

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.

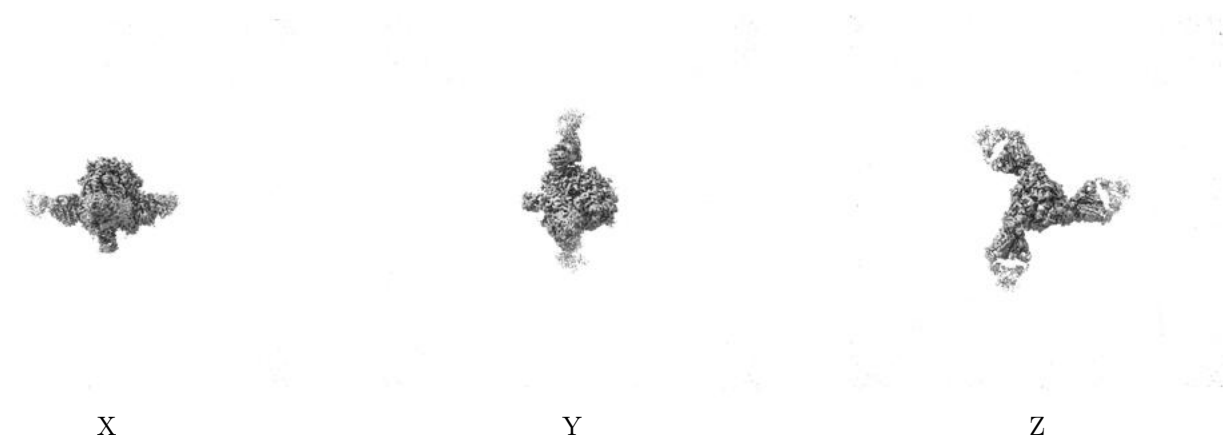
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.209. 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.

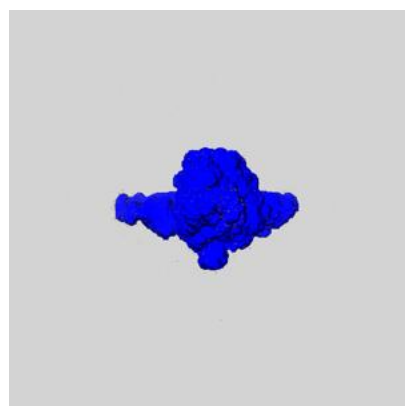
6.6 Mask visualisation [i](#)

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

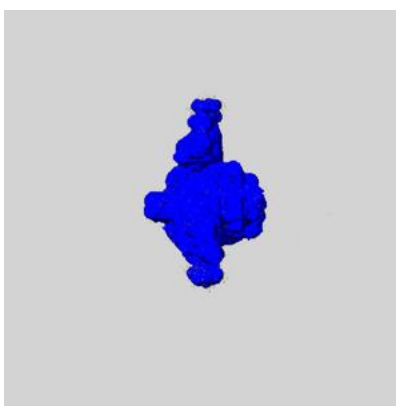
A mask typically either:

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

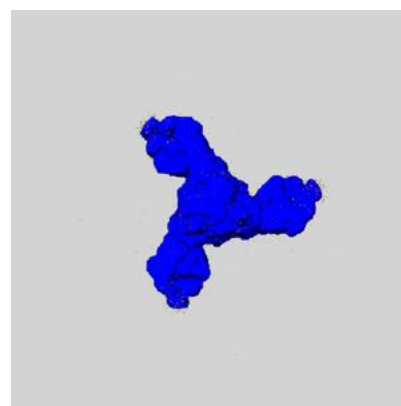
6.6.1 emd_72293_msk_1.map [i](#)



X



Y

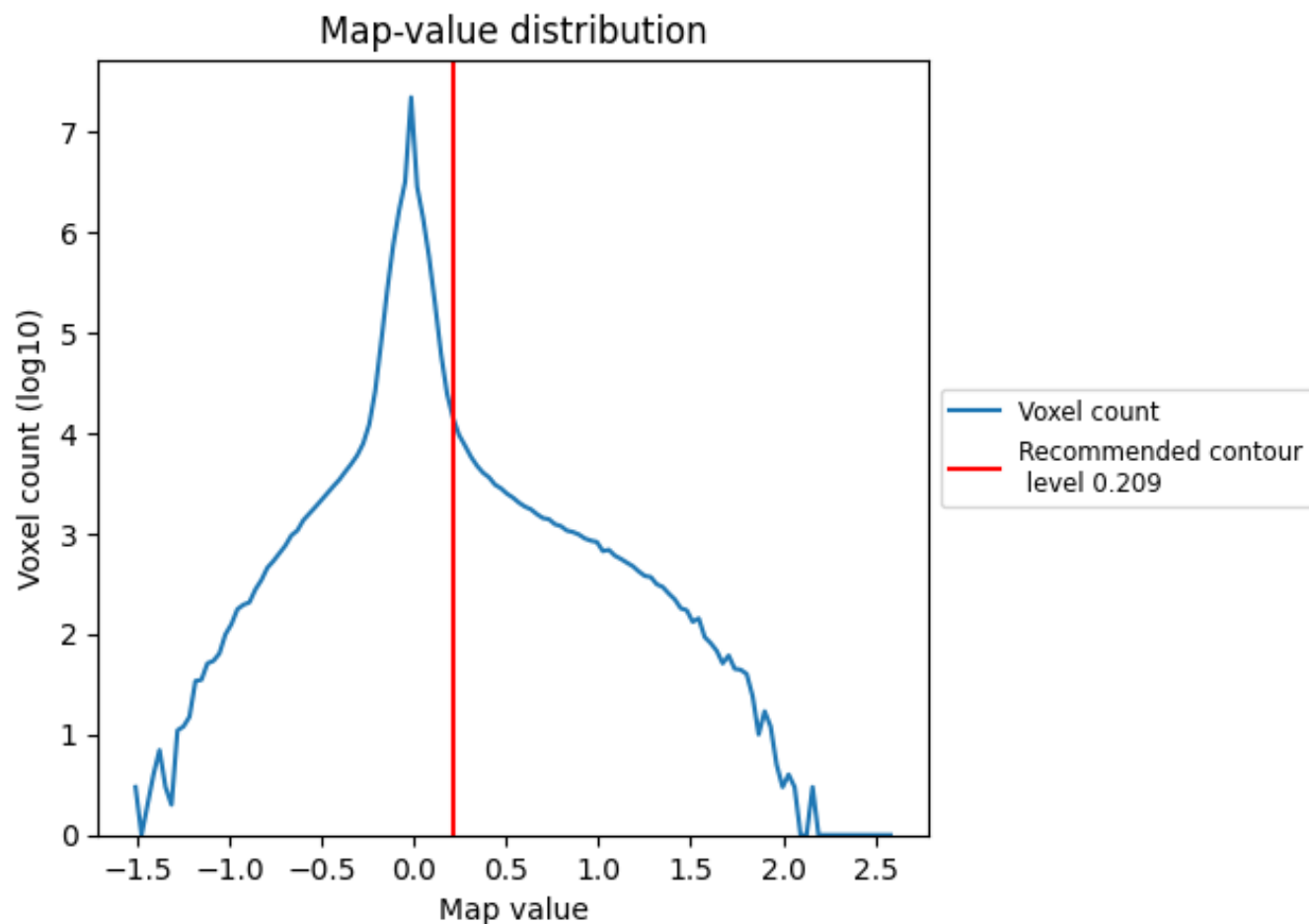


Z

7 Map analysis [i](#)

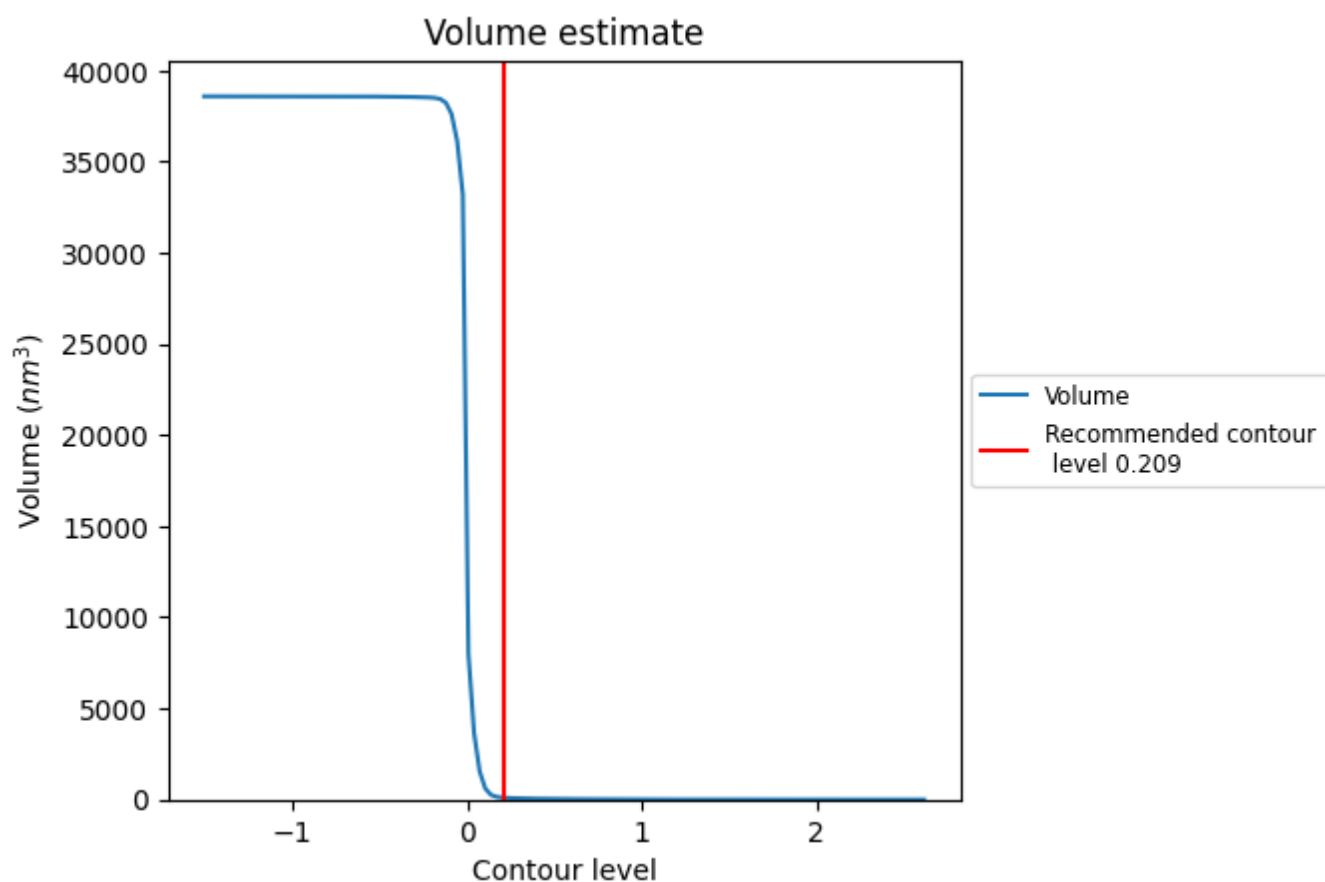
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

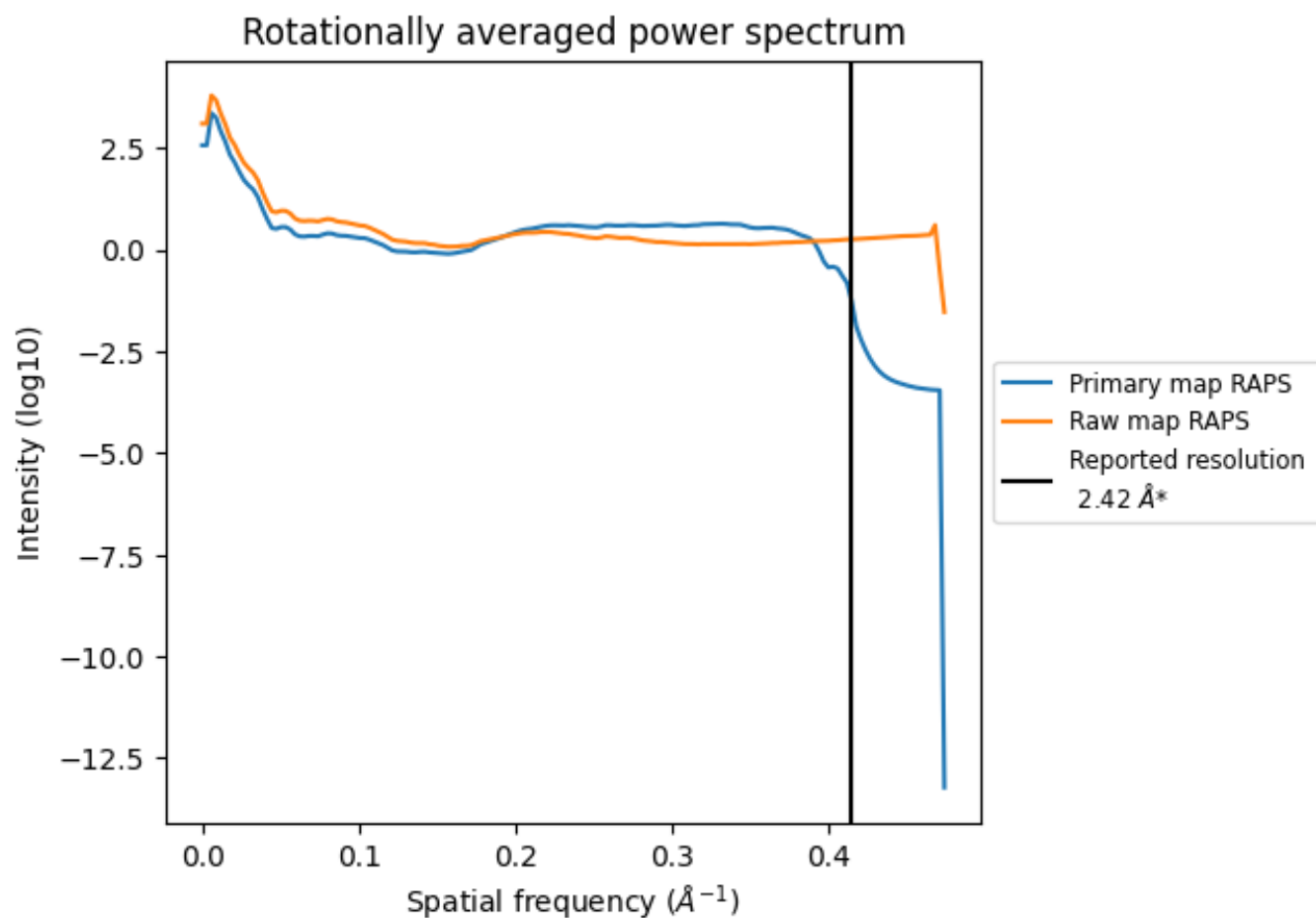
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; this corresponds to an approximate mass of 93 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 ⓘ

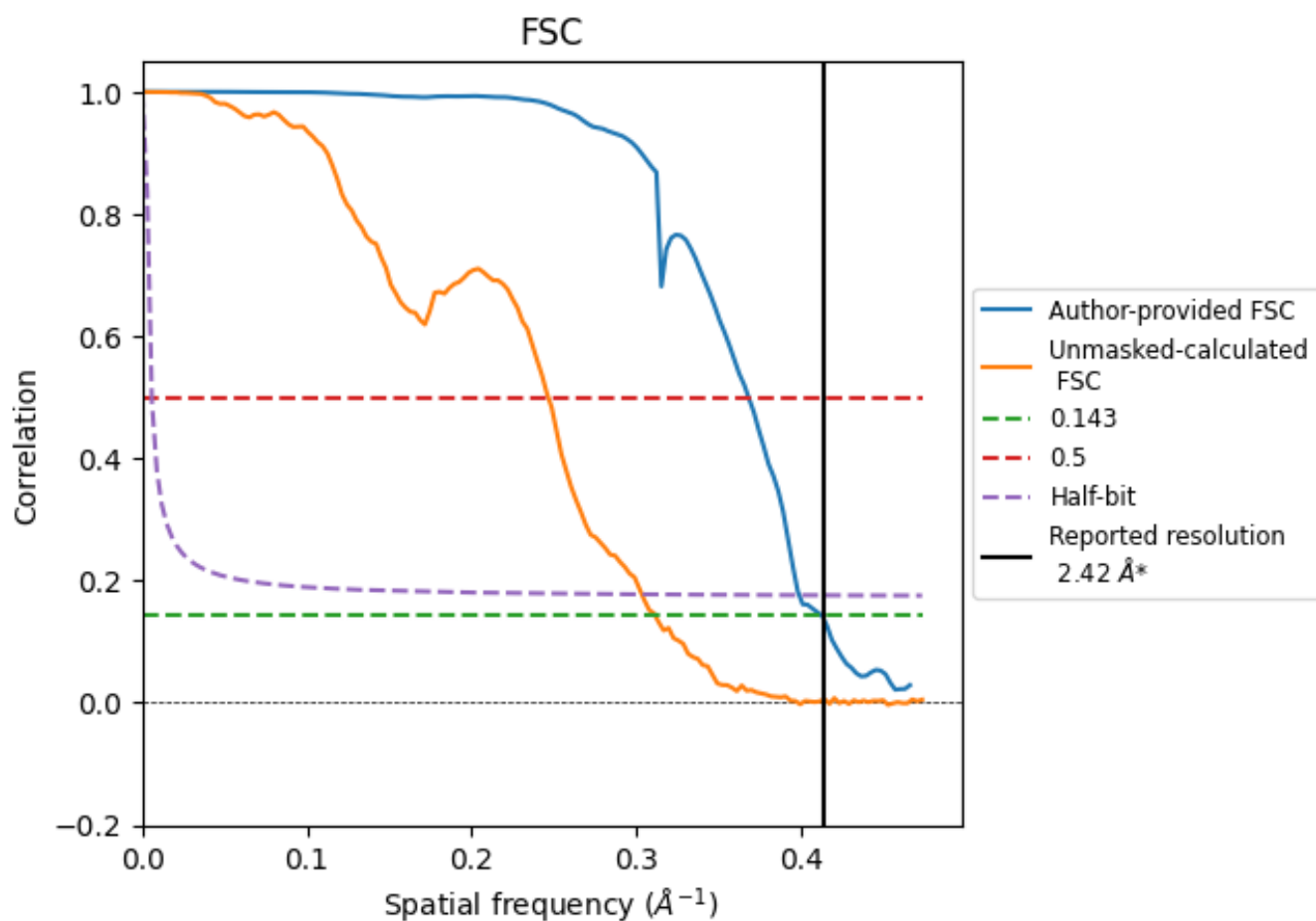


*Reported resolution corresponds to spatial frequency of 0.413 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.413 \AA^{-1}

8.2 Resolution estimates [i](#)

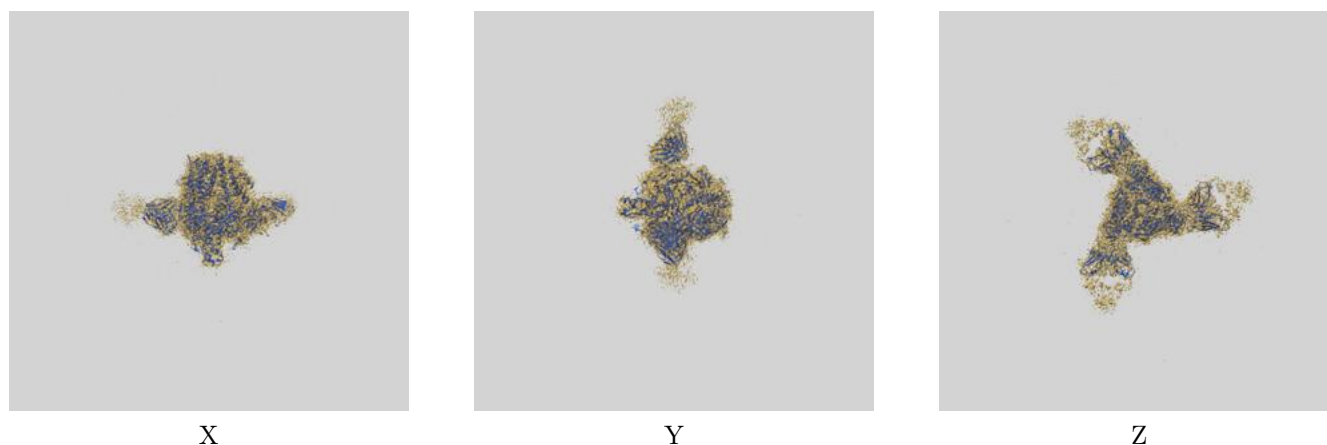
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.42	2.72	2.51
Unmasked-calculated*	3.21	4.06	3.30

*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 3.21 differs from the reported value 2.42 by more than 10 %

9 Map-model fit [i](#)

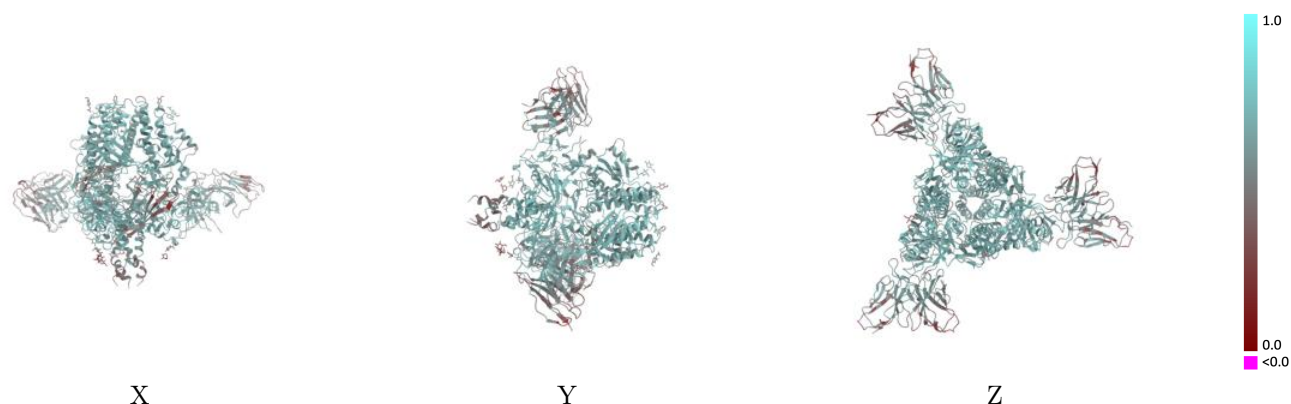
This section contains information regarding the fit between EMDB map EMD-72293 and PDB model 9Q7B. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



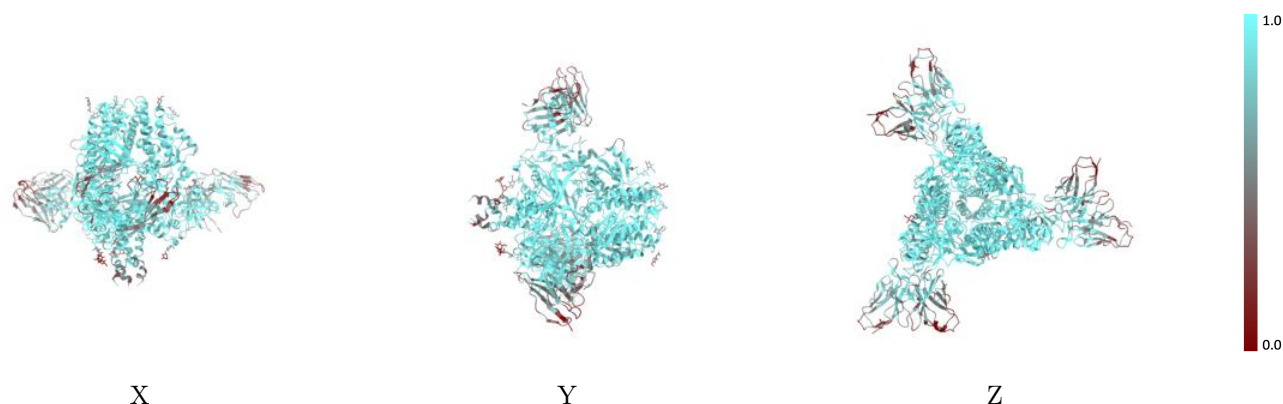
The images above show the 3D surface view of the map at the recommended contour level 0.209 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



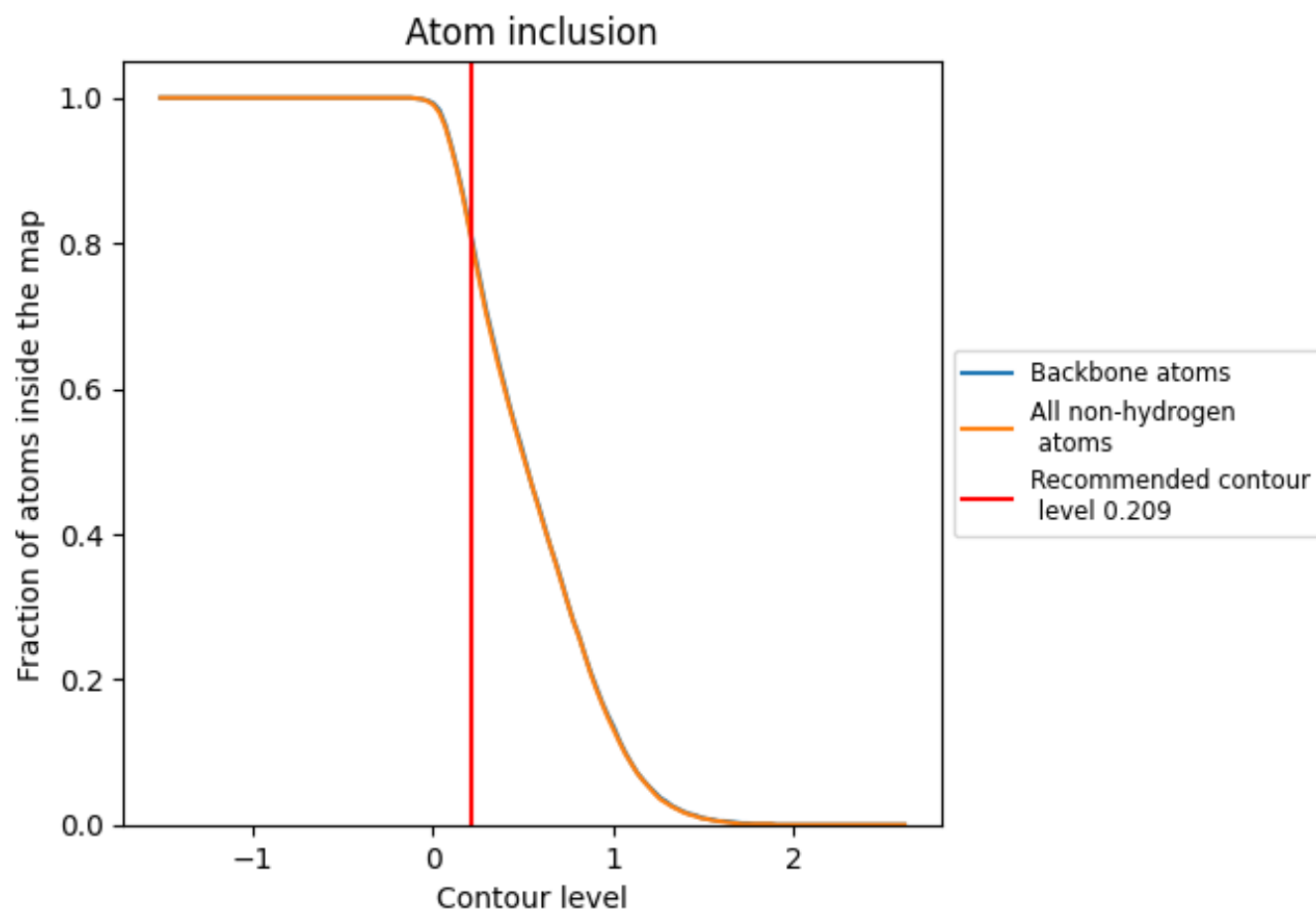
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.209).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 81% 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 (0.209) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8120	<div></div> 0.5920
A	<div></div> 0.9350	<div></div> 0.6420
B	<div></div> 0.9320	<div></div> 0.6460
C	<div></div> 0.9440	<div></div> 0.6420
D	<div></div> 0.9290	<div></div> 0.6440
E	<div></div> 0.9210	<div></div> 0.6360
F	<div></div> 0.9260	<div></div> 0.6430
G	<div></div> 0.6050	<div></div> 0.4960
H	<div></div> 0.5380	<div></div> 0.4490
I	<div></div> 0.5940	<div></div> 0.4900
J	<div></div> 0.6080	<div></div> 0.4970
K	<div></div> 0.5990	<div></div> 0.4960
L	<div></div> 0.5950	<div></div> 0.4930
M	<div></div> 0.6080	<div></div> 0.5000
N	<div></div> 0.7140	<div></div> 0.6040
O	<div></div> 0.3440	<div></div> 0.3770
P	<div></div> 0.7140	<div></div> 0.5930
Q	<div></div> 0.3280	<div></div> 0.3660
R	<div></div> 0.6790	<div></div> 0.5850

