



wwPDB EM Validation Summary Report ⓘ

Apr 12, 2026 – 11:22 AM UTC

PDB ID : 9NJ6 / pdb_00009nj6
EMDB ID : EMD-49475
Title : Computationally optimized broadly reactive influenza B hemagglutinin BC2 bound by antibody #3978
Authors : Dzimianski, J.V.; Kunkel, I.; Balasco Serrao, V.H.; DuBois, R.M.
Deposited on : 2025-02-26
Resolution : 2.36 Å(reported)
Based on initial model : 9NJ3

This is a wwPDB EM Validation Summary 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:

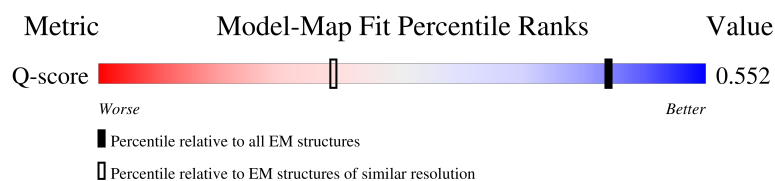
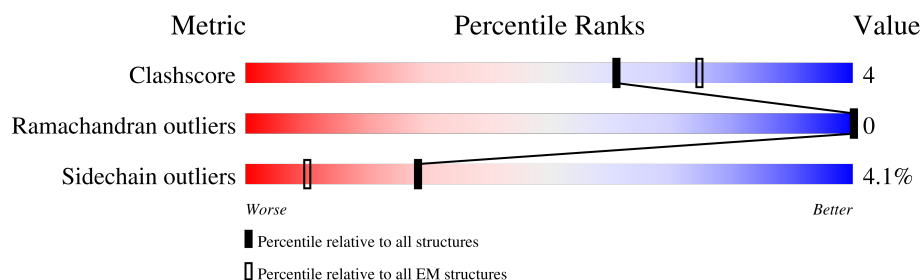
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13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

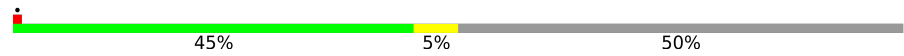
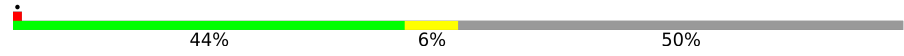
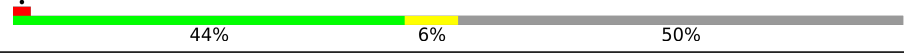
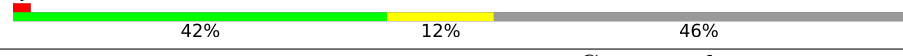
The reported resolution of this entry is 2.36 Å.

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.



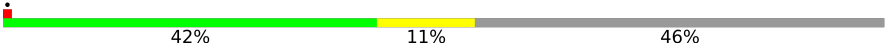
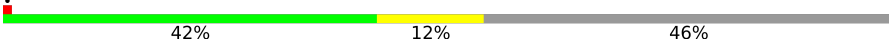
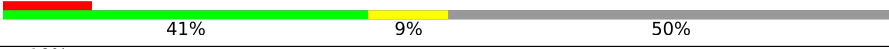
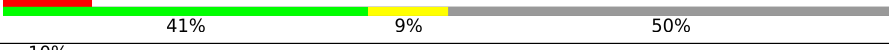
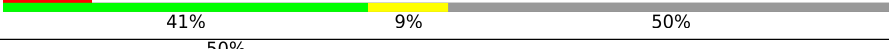
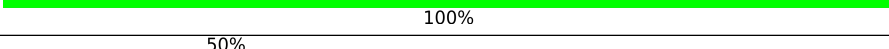
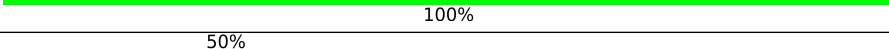
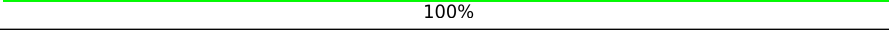
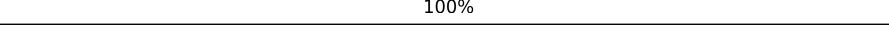
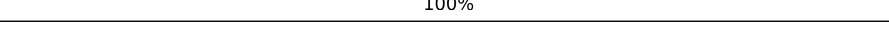
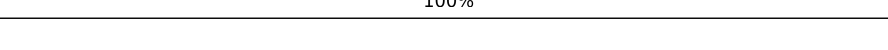
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4686 (1.86 - 2.86)

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	530	
1	B	530	
1	C	530	
2	H	239	

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Mol	Chain	Length	Quality of chain
2	J	239	
2	Q	239	
3	K	217	
3	L	217	
3	P	217	
4	D	2	
4	F	2	
4	I	2	
5	E	3	
5	G	3	
5	M	3	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11709 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	267	Total 2023	C 1269	N 362	O 377	S 15	0	0
1	B	267	Total 2023	C 1269	N 362	O 377	S 15	0	0
1	C	267	Total 2023	C 1269	N 362	O 377	S 15	0	0

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	ARG	LYS	conflict	UNP P17504
A	116	ASN	HIS	conflict	UNP P17504
A	129	LYS	THR	conflict	UNP P17504
A	136	ARG	LYS	conflict	UNP P17504
A	137	ILE	VAL	conflict	UNP P17504
A	199	THR	ALA	conflict	UNP P17504
A	202	LYS	VAL	conflict	UNP P17504
A	235	THR	ALA	conflict	UNP P17504
A	262	VAL	THR	conflict	UNP P17504
A	293	ALA	ARG	conflict	UNP P17504
A	524	SER	-	expression tag	UNP P17504
A	525	GLY	-	expression tag	UNP P17504
A	526	ARG	-	expression tag	UNP P17504
A	527	LEU	-	expression tag	UNP P17504
A	528	VAL	-	expression tag	UNP P17504
A	529	PRO	-	expression tag	UNP P17504
A	530	ARG	-	expression tag	UNP P17504
B	88	ARG	LYS	conflict	UNP P17504
B	116	ASN	HIS	conflict	UNP P17504
B	129	LYS	THR	conflict	UNP P17504
B	136	ARG	LYS	conflict	UNP P17504
B	137	ILE	VAL	conflict	UNP P17504
B	199	THR	ALA	conflict	UNP P17504
B	202	LYS	VAL	conflict	UNP P17504

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Chain	Residue	Modelled	Actual	Comment	Reference
B	235	THR	ALA	conflict	UNP P17504
B	262	VAL	THR	conflict	UNP P17504
B	293	ALA	ARG	conflict	UNP P17504
B	524	SER	-	expression tag	UNP P17504
B	525	GLY	-	expression tag	UNP P17504
B	526	ARG	-	expression tag	UNP P17504
B	527	LEU	-	expression tag	UNP P17504
B	528	VAL	-	expression tag	UNP P17504
B	529	PRO	-	expression tag	UNP P17504
B	530	ARG	-	expression tag	UNP P17504
C	88	ARG	LYS	conflict	UNP P17504
C	116	ASN	HIS	conflict	UNP P17504
C	129	LYS	THR	conflict	UNP P17504
C	136	ARG	LYS	conflict	UNP P17504
C	137	ILE	VAL	conflict	UNP P17504
C	199	THR	ALA	conflict	UNP P17504
C	202	LYS	VAL	conflict	UNP P17504
C	235	THR	ALA	conflict	UNP P17504
C	262	VAL	THR	conflict	UNP P17504
C	293	ALA	ARG	conflict	UNP P17504
C	524	SER	-	expression tag	UNP P17504
C	525	GLY	-	expression tag	UNP P17504
C	526	ARG	-	expression tag	UNP P17504
C	527	LEU	-	expression tag	UNP P17504
C	528	VAL	-	expression tag	UNP P17504
C	529	PRO	-	expression tag	UNP P17504
C	530	ARG	-	expression tag	UNP P17504

- Molecule 2 is a protein called Fab A Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	129	Total	C	N	O	S	0	0
			1001	637	167	189	8		
2	J	129	Total	C	N	O	S	0	0
			1001	637	167	189	8		
2	Q	129	Total	C	N	O	S	0	0
			1001	637	167	189	8		

- Molecule 3 is a protein called Fab A Light Chain.

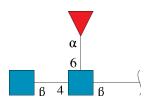
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	109	Total	C	N	O	S	0	0
			799	497	136	164	2		
3	K	109	Total	C	N	O	S	0	0
			799	497	136	164	2		
3	P	109	Total	C	N	O	S	0	0
			799	497	136	164	2		

- Molecule 4 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
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	3	Total	C	N	O	0	0
			38	22	2	14		
5	G	3	Total	C	N	O	0	0
			38	22	2	14		
5	M	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

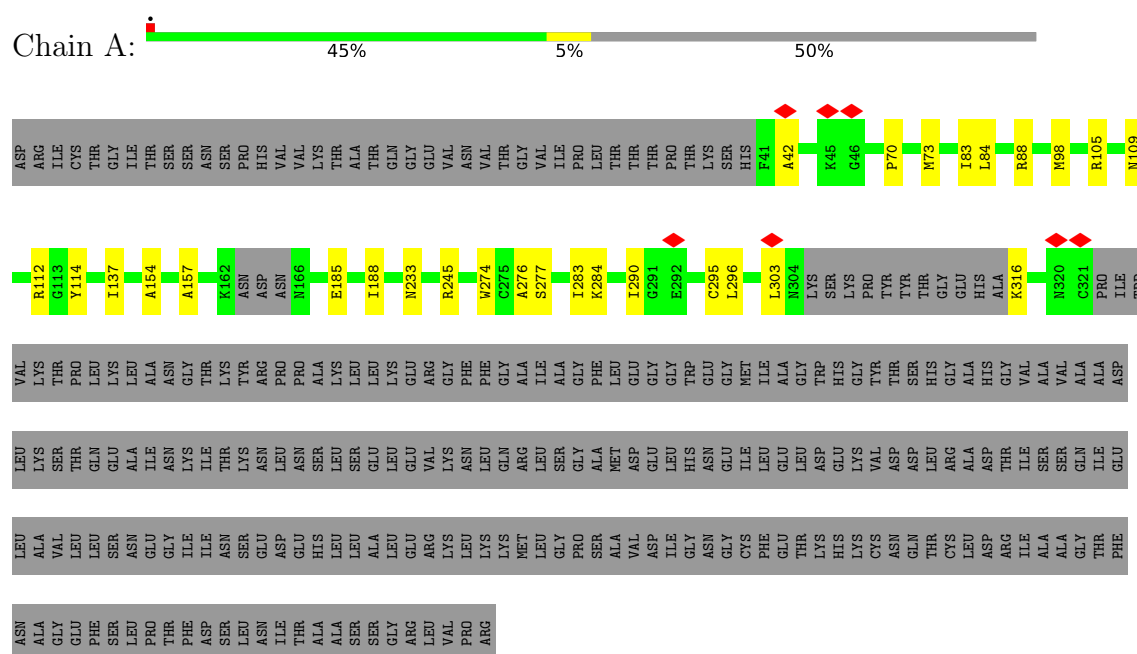


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

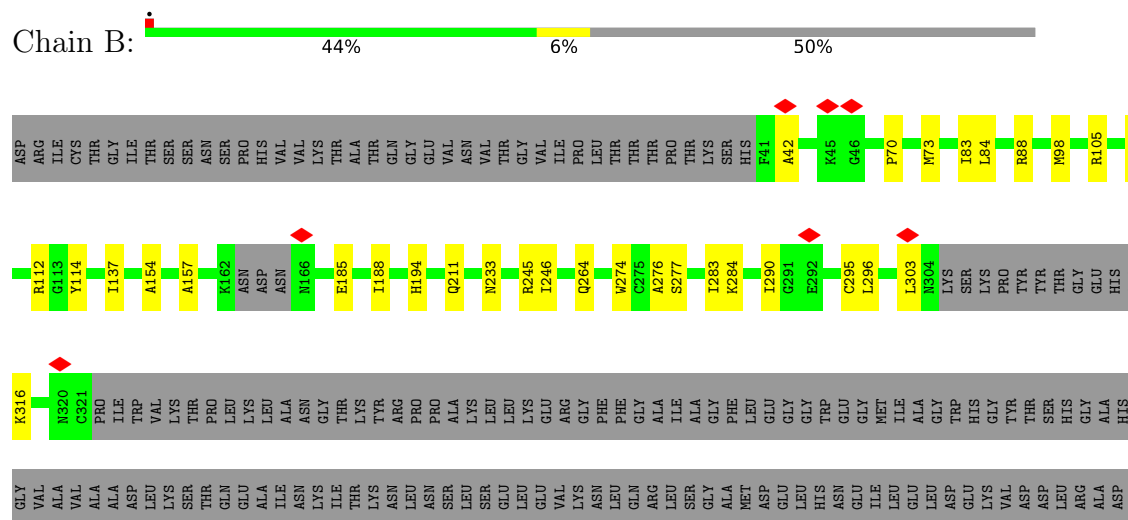
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

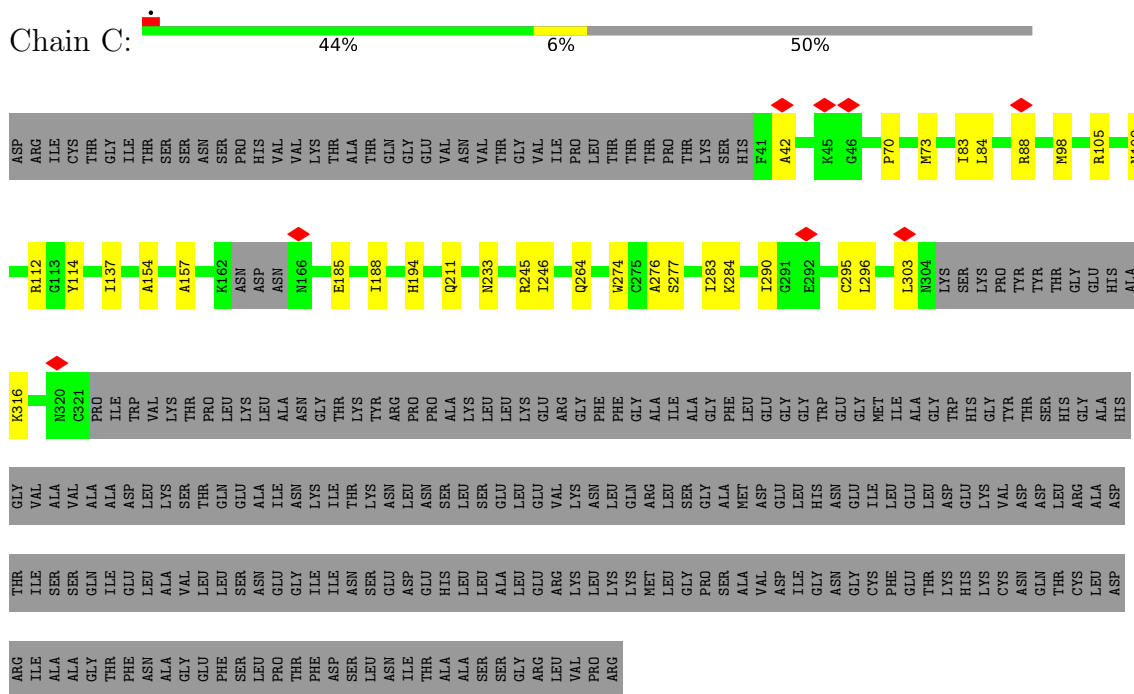
• Molecule 1: Hemagglutinin



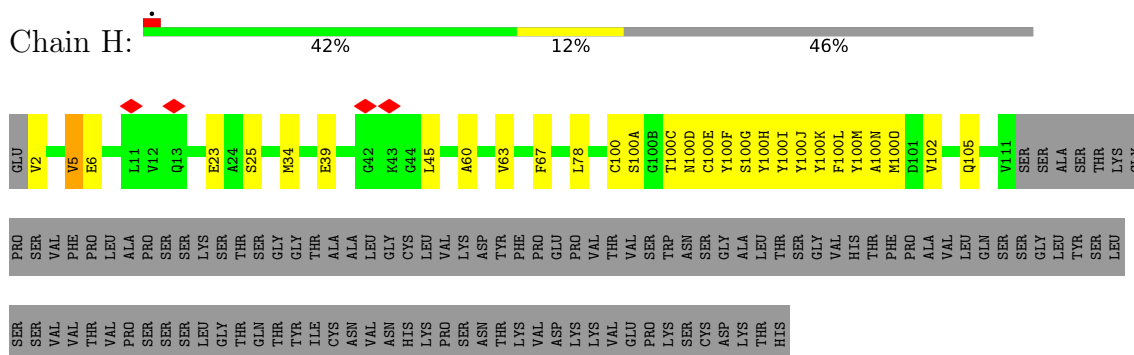
• Molecule 1: Hemagglutinin



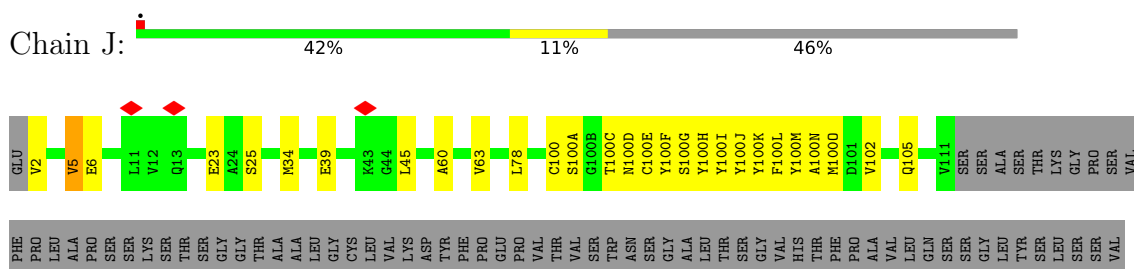
- Molecule 1: Hemagglutinin



- Molecule 2: Fab A Heavy Chain



- Molecule 2: Fab A Heavy Chain



VAL THR VAL PRO SER SER LEU GLY THR GLN THR TYR THR ILE CYS ASN VAL ASN HIS LYS PRO ASN SER ASN THR LYS VAL ASP LYS VAL GLU PRO LYS CYS ASP LYS THR HIS

• Molecule 2: Fab A Heavy Chain

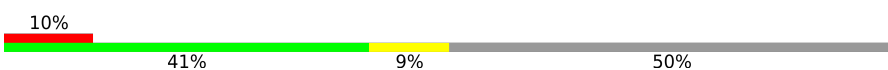
Chain Q:  42% 12% 46%

GLU V2 V5 E6 L11 V12 Q13 E23 A24 S25 M34 E39 K43 G44 L45 A60 V63 F67 L78 C100 S100A G100B T100C N100D C100E Y100F S100G Y100H Y100I Y100J Y100K F100L Y100M A100N M100D D101 V102 Q105 V111 SER SER ALA THR LYS PRO

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

SER VAL VAL THR PRO SER SER SER GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS THR LYS VAL ASP LYS LYS VAL GLU PRO LYS CYS SER ASP LYS THR HIS

• Molecule 3: Fab A Light Chain

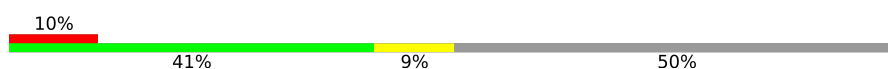
Chain L:  10% 41% 9% 50%

GLN S2 P8 S9 V11 S12 G13 A14 P15 G16 Q17 G18 V19 C23 S27 S28 N29 L30 G30A Y31 H34 W35 Y36 Q37 H38 L39 P40 G41 K42 K43 P44 L47 I48 N51 D52 D60 R66 F69 S70 A71 I75 S76 G77 L78 Q79 Q80 E81 D82 E83

Q89 S96 V106 VAL LEU GLY GLN SER PRO LYS ALA PRO VAL THR LEU PHE PRO PRO PRO SER SER SER GLU GLU GLN ALA ASN LYS ALA THR VAL CYS VAL ILE SER ASP PHE TYR PRO GLY ALA VAL THR VAL TRP LYS ASP ALA PRO VAL LYS VAL GLY

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

• Molecule 3: Fab A Light Chain

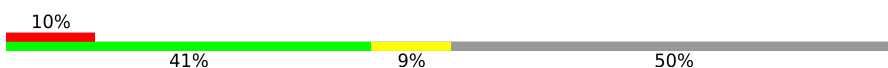
Chain K:  10% 41% 9% 50%

GLN S2 P8 S9 V11 S12 G13 A14 P15 G16 Q17 G18 V19 C23 S27 S28 N29 L30 G30A Y31 H34 W35 Y36 Q37 H38 G41 K42 K43 P44 L47 I48 N51 D52 D60 R66 F69 S70 A71 I75 S76 G77 L78 Q79 Q80 E81 D82 E83

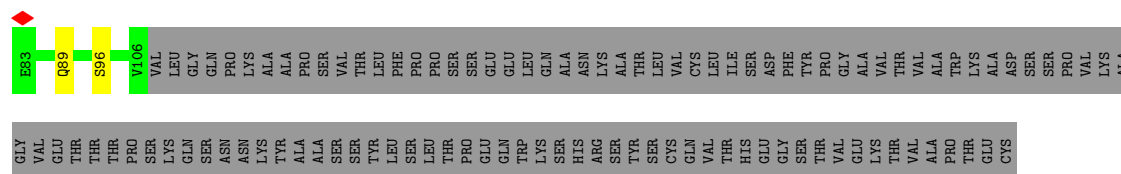
Q89 S96 K103 V105 VAL LEU GLY GLN SER PRO LYS ALA PRO VAL THR SER LEU PHE PRO PRO SER SER SER GLU GLU GLN ALA ASN LYS ALA THR VAL CYS VAL ILE SER ASP PHE TYR THR VAL GLY THR THR VAL ALA ALA TRP LYS ASP ALA PRO VAL LYS VAL GLY

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

• Molecule 3: Fab A Light Chain

Chain P:  10% 41% 9% 50%

GLN S2 P7 P8 S9 V11 S12 G13 A14 P15 G16 Q17 G18 V19 C23 S27 S28 N29 L30 G30A Y31 H34 W35 Y36 Q37 H38 L39 P40 G41 K42 K43 P44 L47 I48 N51 D52 D60 R66 F69 S70 A71 I75 S76 G77 L78 Q79 Q80 E81 D82



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



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



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



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



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

Chain M:  100%

MAG1
MAG2
FUC3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	185640	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	3.016	Depositor
Minimum map value	-1.795	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	329.8752, 329.8752, 329.8752	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5727, 0.5727, 0.5727	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, FUC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.09	0/2064	0.26	0/2791
1	B	0.09	0/2064	0.26	0/2791
1	C	0.09	0/2064	0.26	0/2791
2	H	0.08	0/1028	0.27	0/1391
2	J	0.08	0/1028	0.27	0/1391
2	Q	0.08	0/1028	0.27	0/1391
3	K	0.08	0/820	0.28	0/1117
3	L	0.09	0/820	0.28	0/1117
3	P	0.09	0/820	0.28	0/1117
All	All	0.09	0/11736	0.27	0/15897

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	2023	0	2025	14	0
1	B	2023	0	2025	16	0
1	C	2023	0	2025	16	0
2	H	1001	0	941	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1001	0	941	9	0
2	Q	1001	0	941	10	0
3	K	799	0	754	10	0
3	L	799	0	754	10	0
3	P	799	0	754	10	0
4	D	28	0	25	0	0
4	F	28	0	25	0	0
4	I	28	0	25	0	0
5	E	38	0	34	0	0
5	G	38	0	34	0	0
5	M	38	0	34	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
All	All	11709	0	11376	102	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 4.

The worst 5 of 102 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:L:18:GLY:HA2	3:L:75:ILE:O	1.83	0.79
3:P:18:GLY:HA2	3:P:75:ILE:O	1.83	0.79
3:K:18:GLY:HA2	3:K:75:ILE:O	1.83	0.78
1:A:283:ILE:HG22	1:A:316:LYS:HE2	1.79	0.65
1:C:283:ILE:HG22	1:C:316:LYS:HE2	1.79	0.64

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	261/530 (49%)	256 (98%)	5 (2%)	0	100	100
1	B	261/530 (49%)	256 (98%)	5 (2%)	0	100	100
1	C	261/530 (49%)	256 (98%)	5 (2%)	0	100	100
2	H	127/239 (53%)	126 (99%)	1 (1%)	0	100	100
2	J	127/239 (53%)	126 (99%)	1 (1%)	0	100	100
2	Q	127/239 (53%)	126 (99%)	1 (1%)	0	100	100
3	K	107/217 (49%)	103 (96%)	4 (4%)	0	100	100
3	L	107/217 (49%)	103 (96%)	4 (4%)	0	100	100
3	P	107/217 (49%)	103 (96%)	4 (4%)	0	100	100
All	All	1485/2958 (50%)	1455 (98%)	30 (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	223/441 (51%)	221 (99%)	2 (1%)	70	82
1	B	223/441 (51%)	221 (99%)	2 (1%)	70	82
1	C	223/441 (51%)	221 (99%)	2 (1%)	70	82
2	H	102/198 (52%)	87 (85%)	15 (15%)	3	2
2	J	102/198 (52%)	87 (85%)	15 (15%)	3	2
2	Q	102/198 (52%)	87 (85%)	15 (15%)	3	2
3	K	88/181 (49%)	88 (100%)	0	100	100
3	L	88/181 (49%)	88 (100%)	0	100	100
3	P	88/181 (49%)	88 (100%)	0	100	100
All	All	1239/2460 (50%)	1188 (96%)	51 (4%)	28	36

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	100(I)	TYR
1	C	290	ILE
2	Q	100(M)	TYR
2	J	100(J)	TYR
2	J	100(M)	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	271	GLN
3	P	37	GLN
1	B	200	GLN
1	B	271	GLN
3	K	37	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

15 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	D	1	4,1	14,14,15	0.69	0	17,19,21	0.86	0
4	NAG	D	2	4	14,14,15	0.72	0	17,19,21	0.84	0
5	NAG	E	1	5,1	14,14,15	0.70	0	17,19,21	0.95	0
5	NAG	E	2	5	14,14,15	0.71	0	17,19,21	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FUC	E	3	5	10,10,11	0.80	0	14,14,16	0.88	0
4	NAG	F	1	4,1	14,14,15	0.69	0	17,19,21	0.86	0
4	NAG	F	2	4	14,14,15	0.72	0	17,19,21	0.84	0
5	NAG	G	1	5,1	14,14,15	0.70	0	17,19,21	0.95	0
5	NAG	G	2	5	14,14,15	0.71	0	17,19,21	0.90	0
5	FUC	G	3	5	10,10,11	0.80	0	14,14,16	0.88	0
4	NAG	I	1	4,1	14,14,15	0.69	0	17,19,21	0.86	0
4	NAG	I	2	4	14,14,15	0.72	0	17,19,21	0.84	0
5	NAG	M	1	5,1	14,14,15	0.70	0	17,19,21	0.95	0
5	NAG	M	2	5	14,14,15	0.71	0	17,19,21	0.90	0
5	FUC	M	3	5	10,10,11	0.80	0	14,14,16	0.88	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
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
5	NAG	E	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	FUC	E	3	5	-	-	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
5	NAG	G	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	FUC	G	3	5	-	-	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	FUC	M	3	5	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

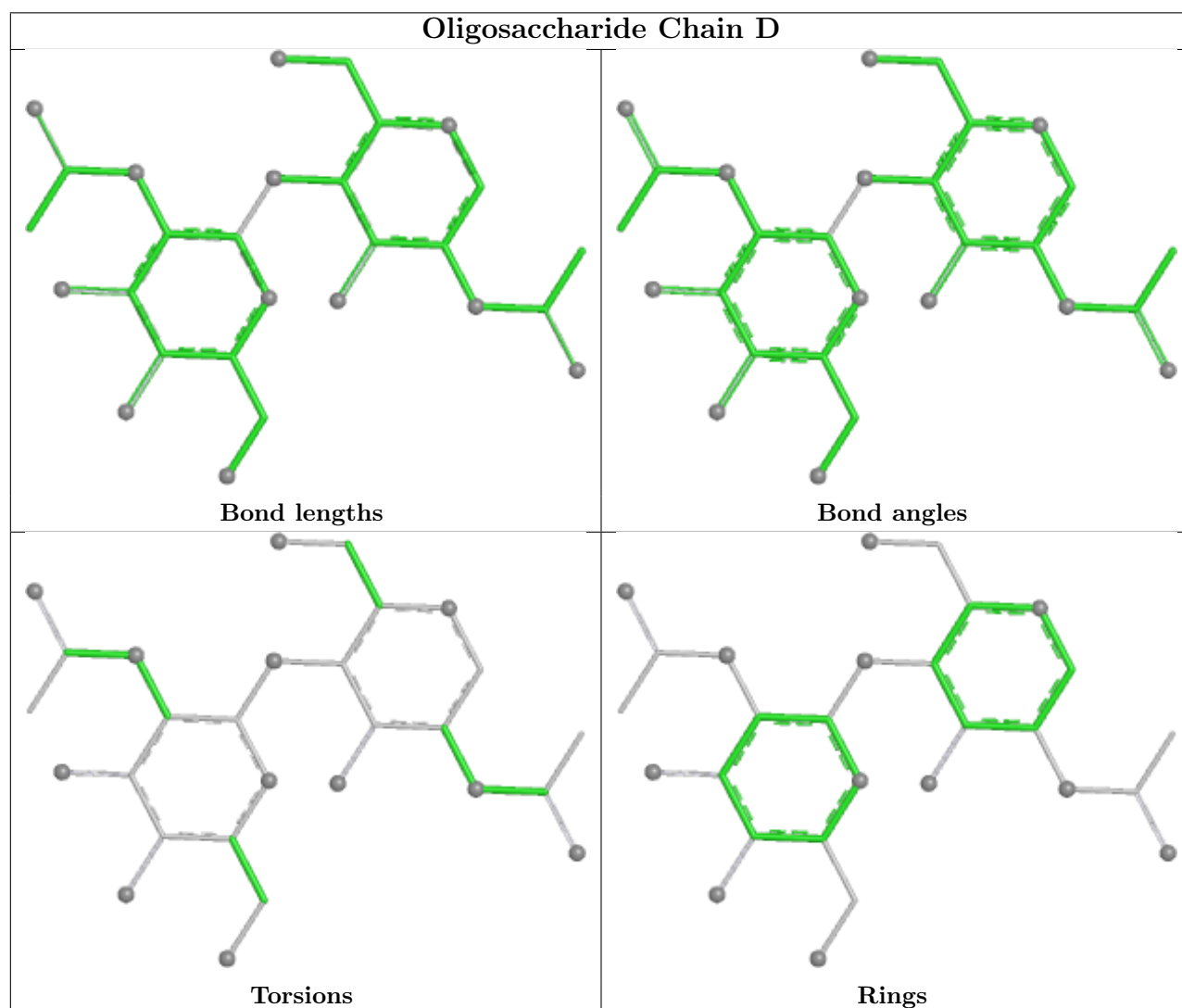
5 of 12 torsion outliers are listed below:

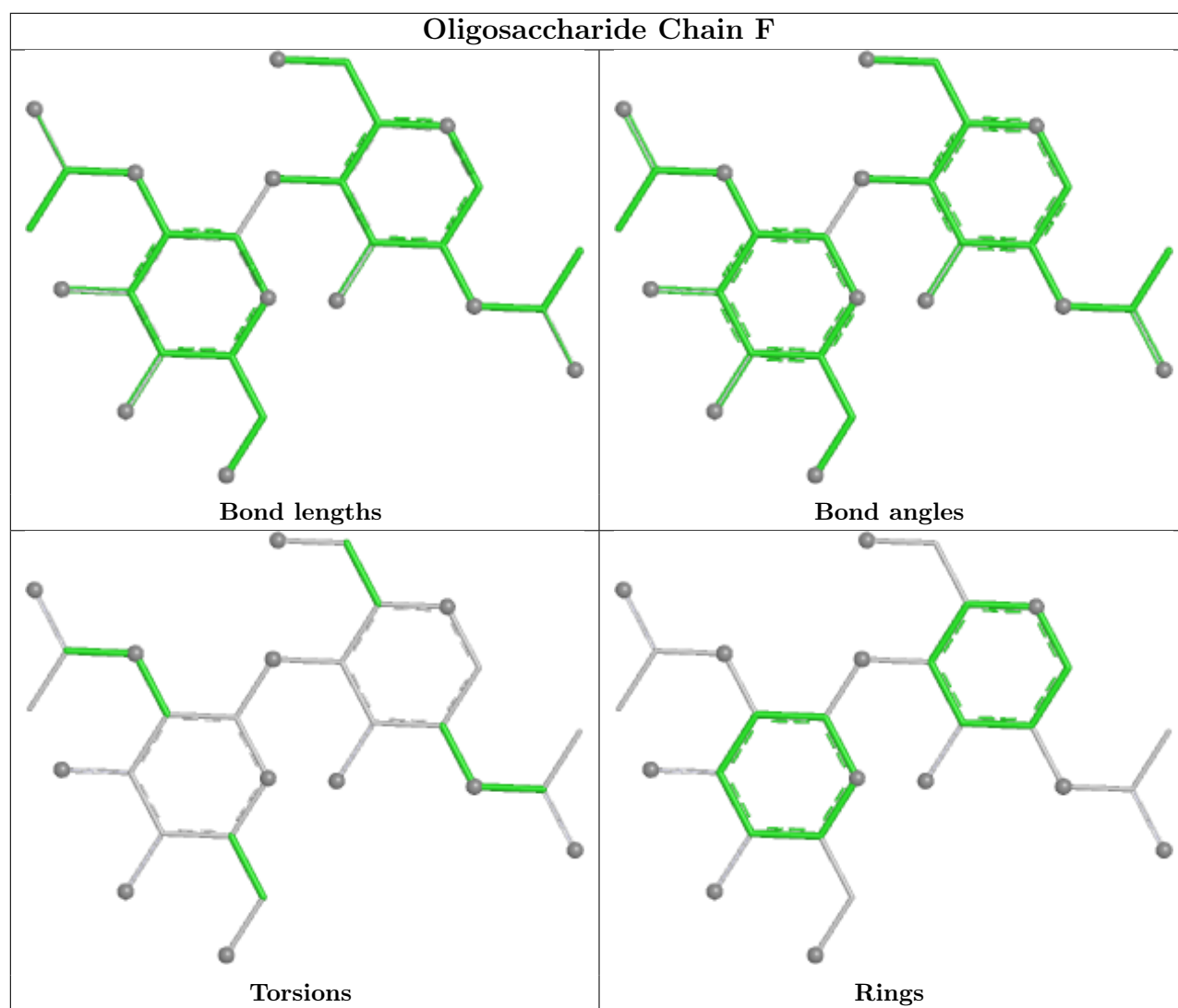
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	G	1	NAG	C8-C7-N2-C2

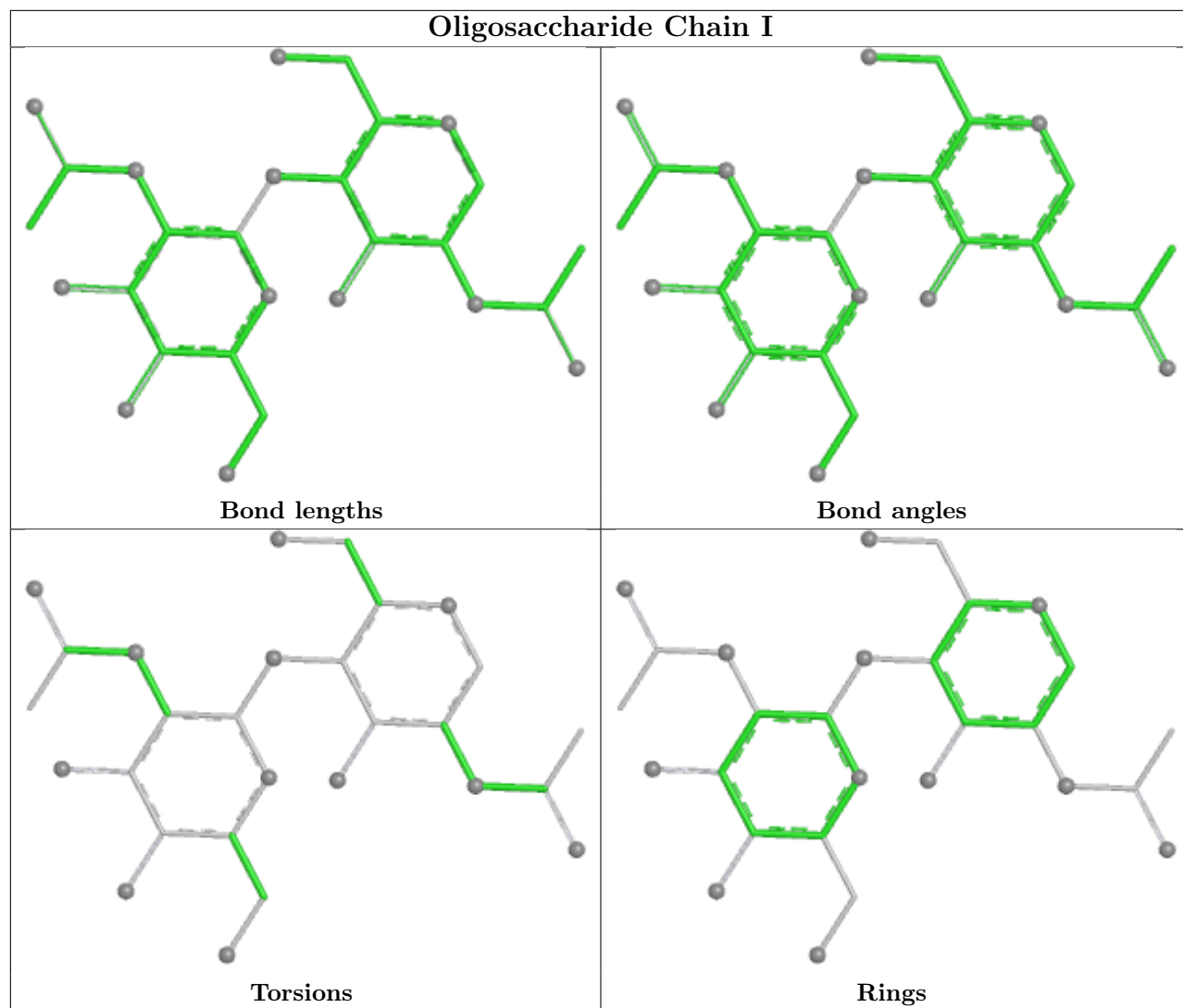
There are no ring outliers.

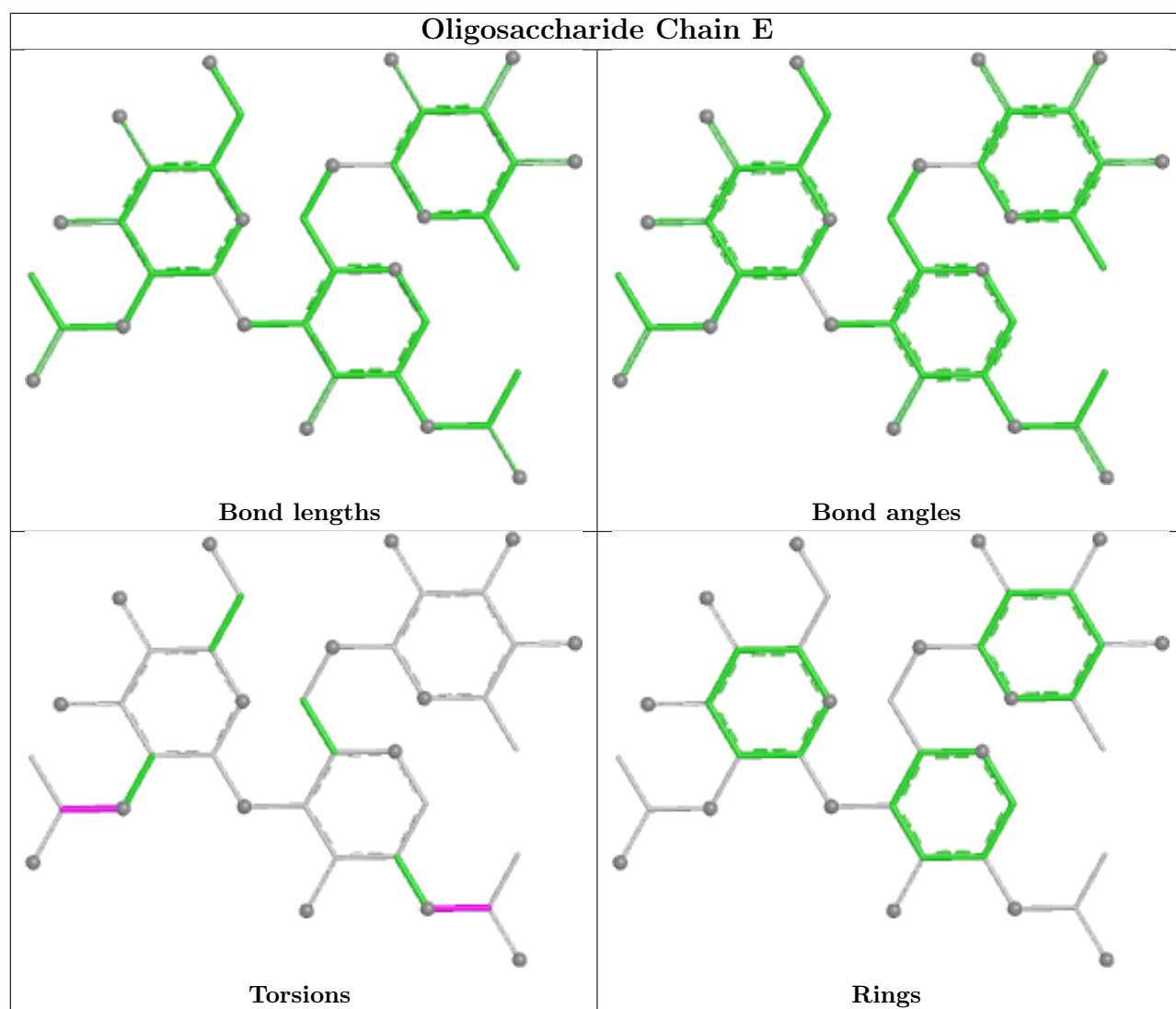
No monomer is involved in short contacts.

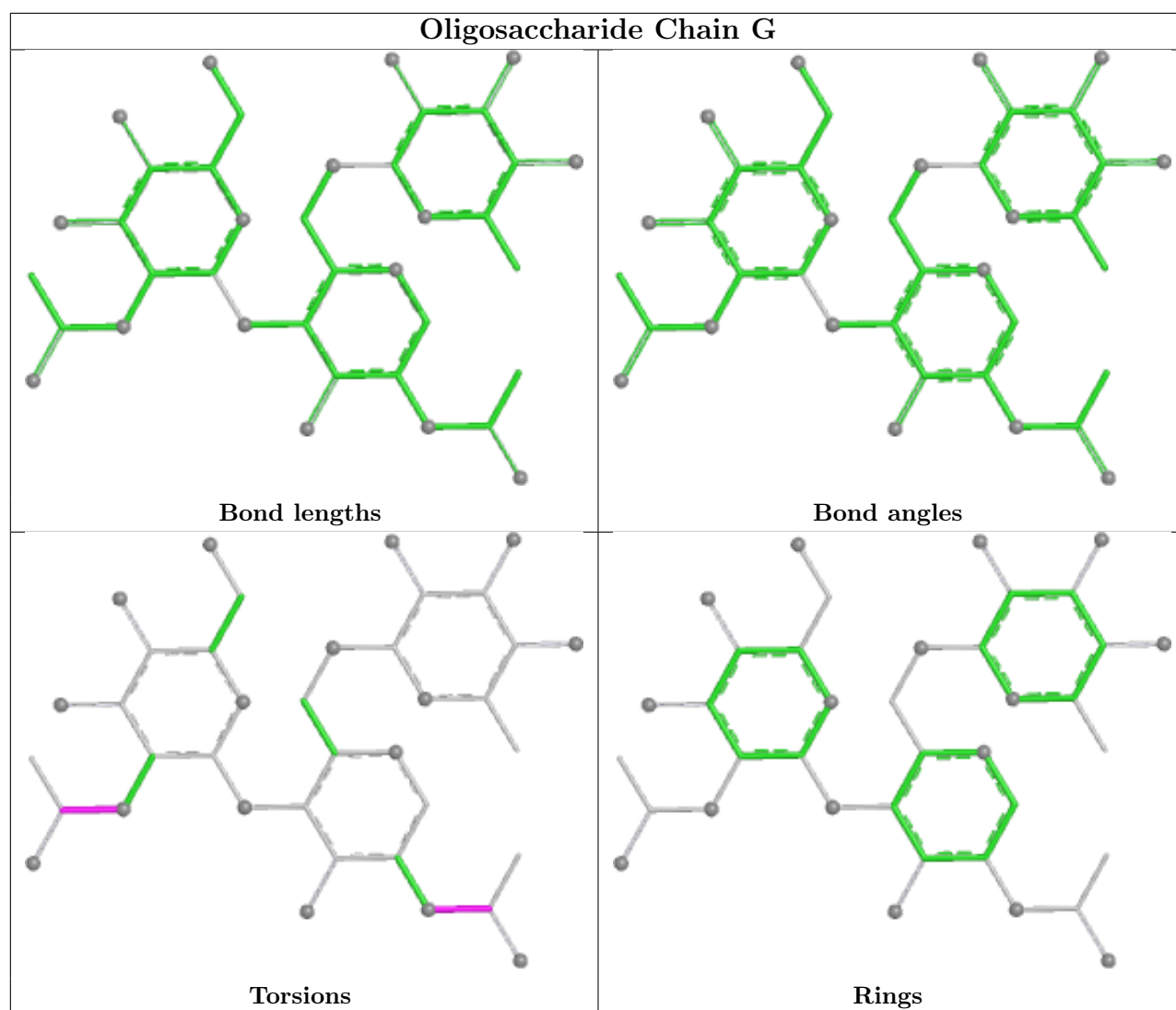
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

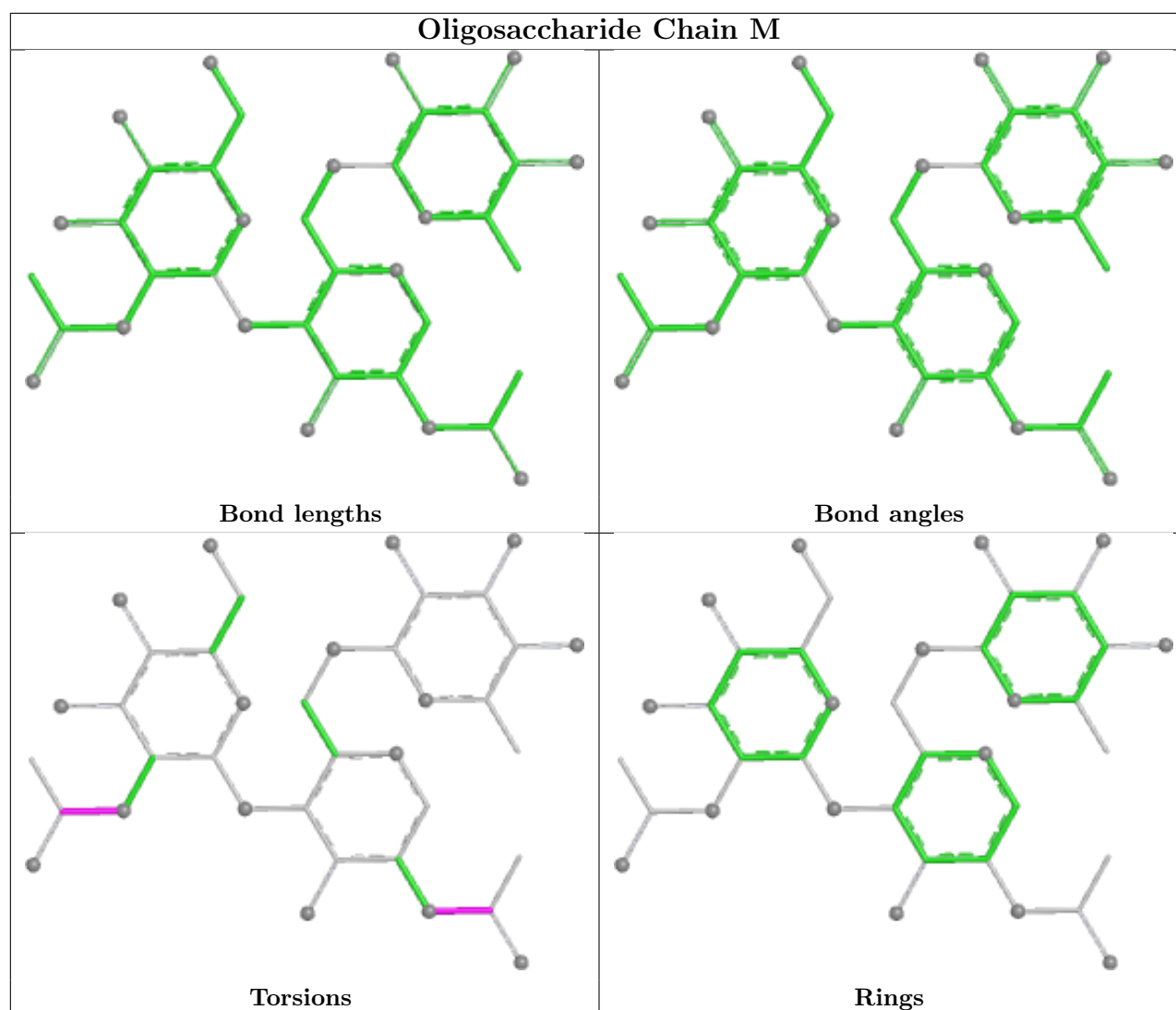












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
6	NAG	A	601	1	14,14,15	0.65	0	17,19,21	1.36	1 (5%)
6	NAG	B	601	1	14,14,15	0.65	0	17,19,21	1.36	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	601	1	14,14,15	0.65	0	17,19,21	1.36	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
6	NAG	A	601	1	-	1/6/23/26	0/1/1/1
6	NAG	B	601	1	-	1/6/23/26	0/1/1/1
6	NAG	C	601	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	601	NAG	C2-N2-C7	3.67	127.82	122.90
6	B	601	NAG	C2-N2-C7	3.67	127.82	122.90
6	A	601	NAG	C2-N2-C7	3.67	127.82	122.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	601	NAG	C3-C2-N2-C7
6	B	601	NAG	C3-C2-N2-C7
6	C	601	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

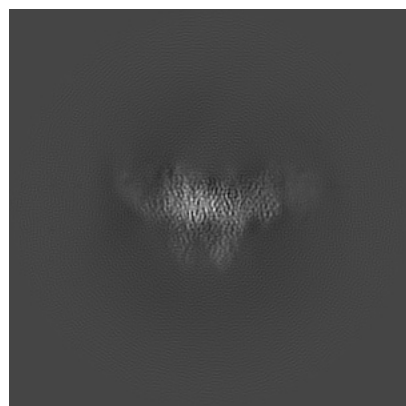
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49475. These allow visual inspection of the internal detail of the map and identification of artifacts.

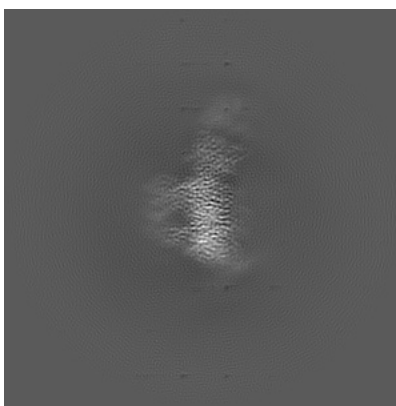
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

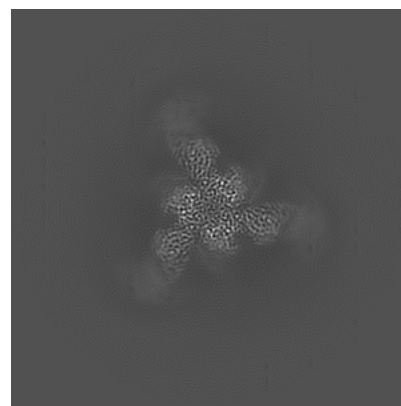
6.1.1 Primary map



X

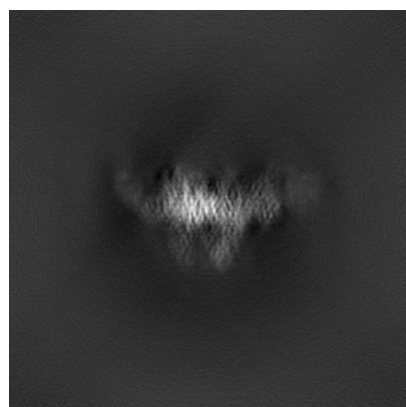


Y

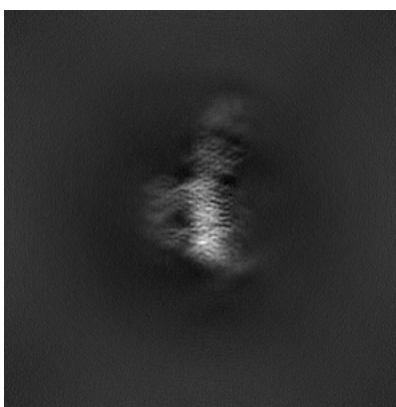


Z

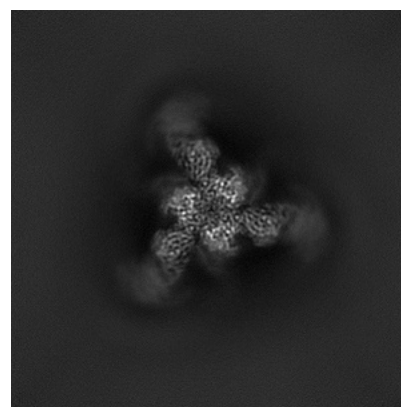
6.1.2 Raw map



X



Y

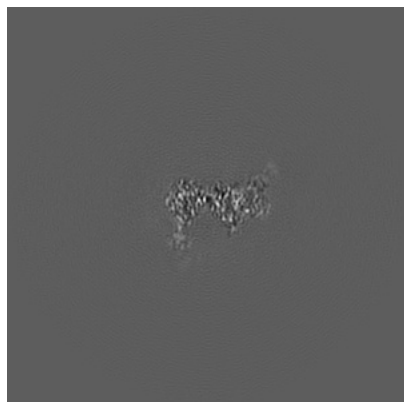


Z

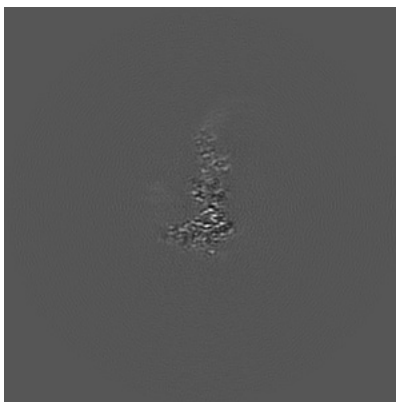
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

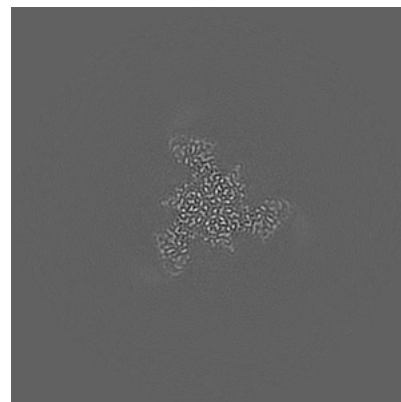
6.2.1 Primary map



X Index: 288

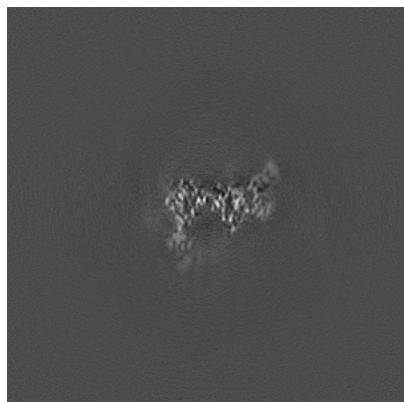


Y Index: 288

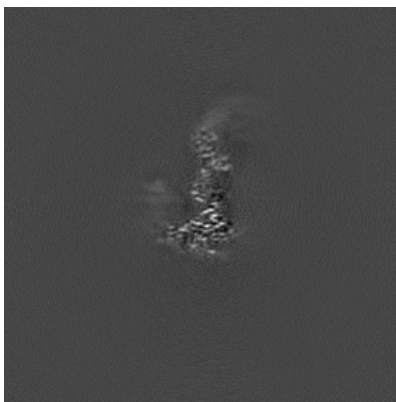


Z Index: 288

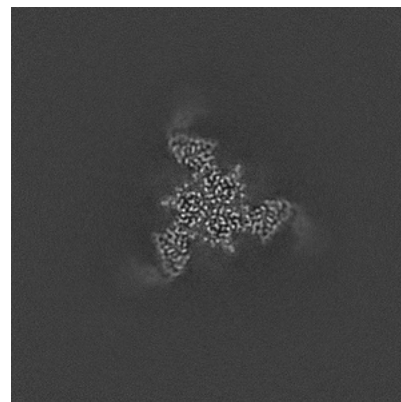
6.2.2 Raw map



X Index: 288



Y Index: 288

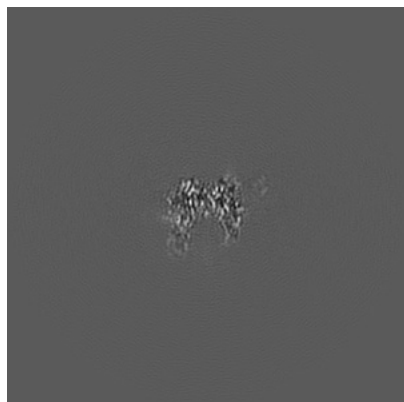


Z Index: 288

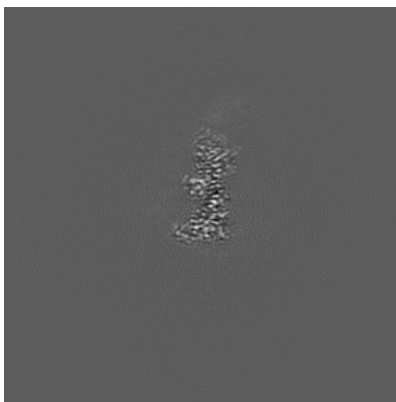
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

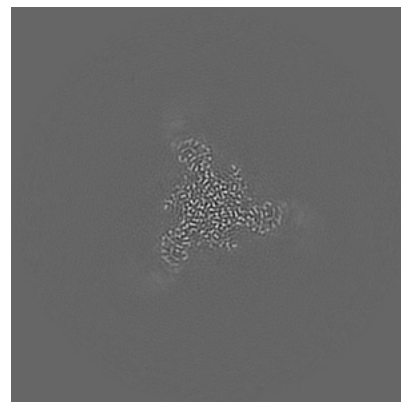
6.3.1 Primary map



X Index: 300

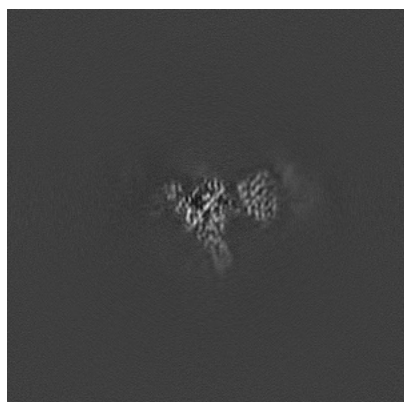


Y Index: 277

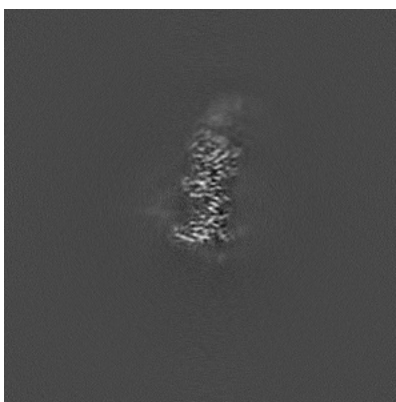


Z Index: 300

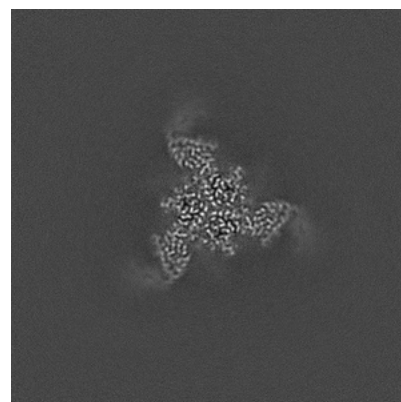
6.3.2 Raw map



X Index: 260



Y Index: 276

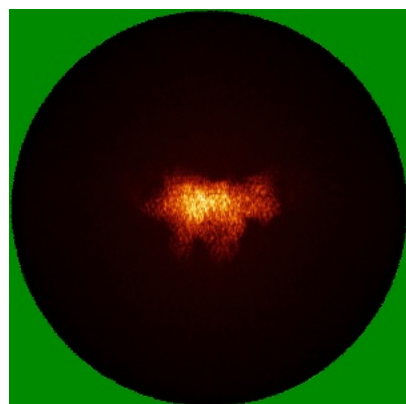


Z Index: 290

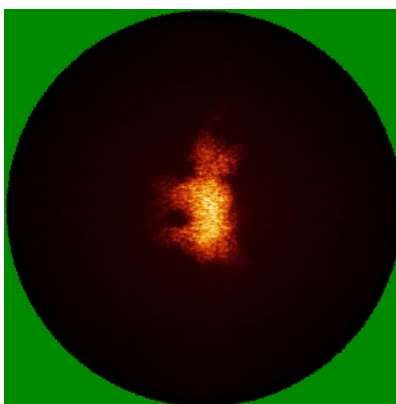
The images above show the largest variance slices of the map in three orthogonal directions.

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

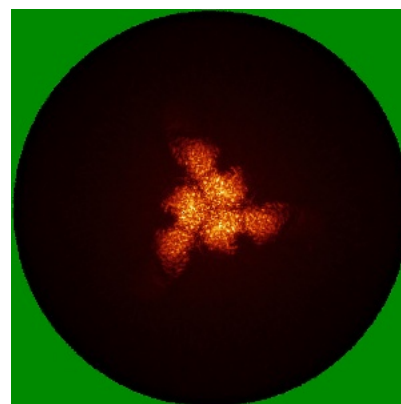
6.4.1 Primary map



X

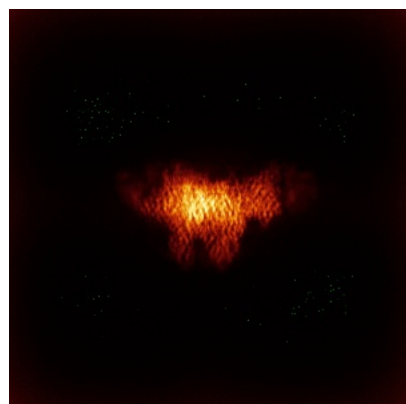


Y

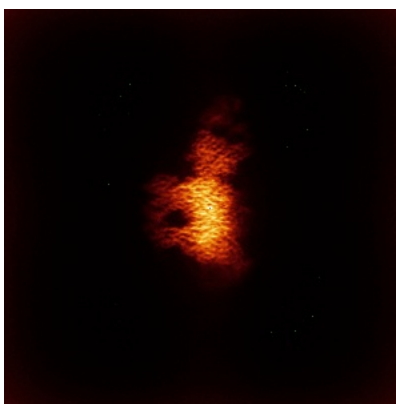


Z

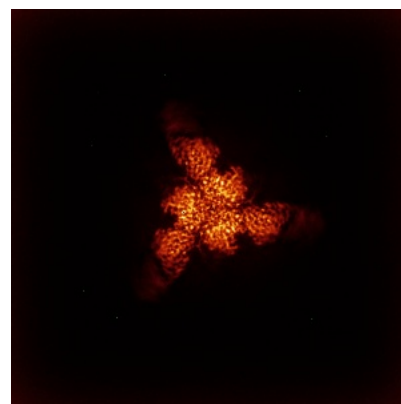
6.4.2 Raw map



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.

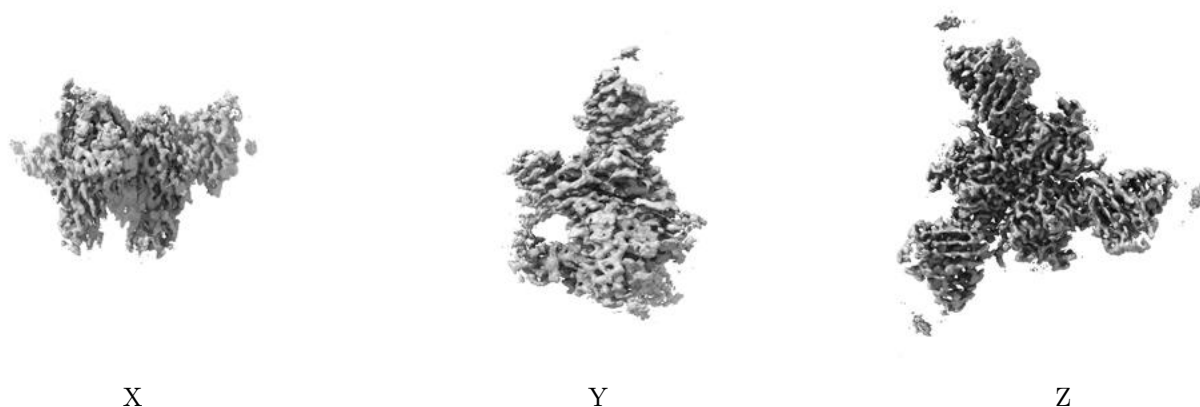
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

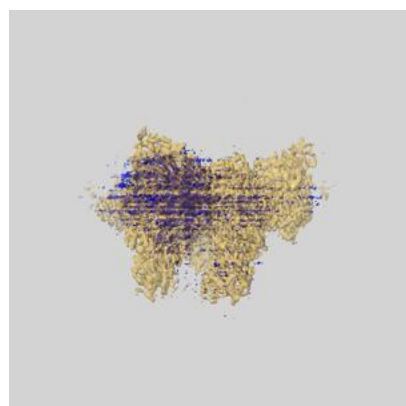
6.6 Mask visualisation [i](#)

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

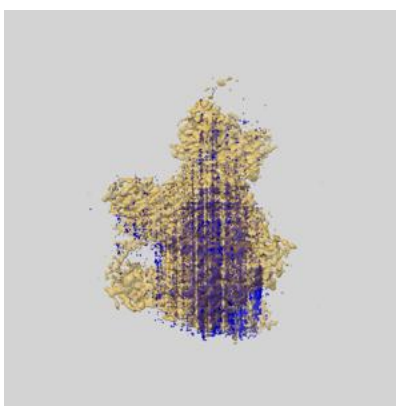
A mask typically either:

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

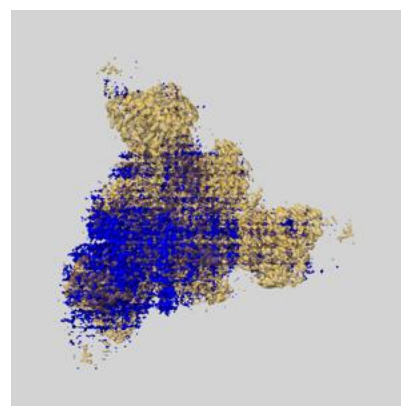
6.6.1 emd_49475_msk_1.map [i](#)



X



Y

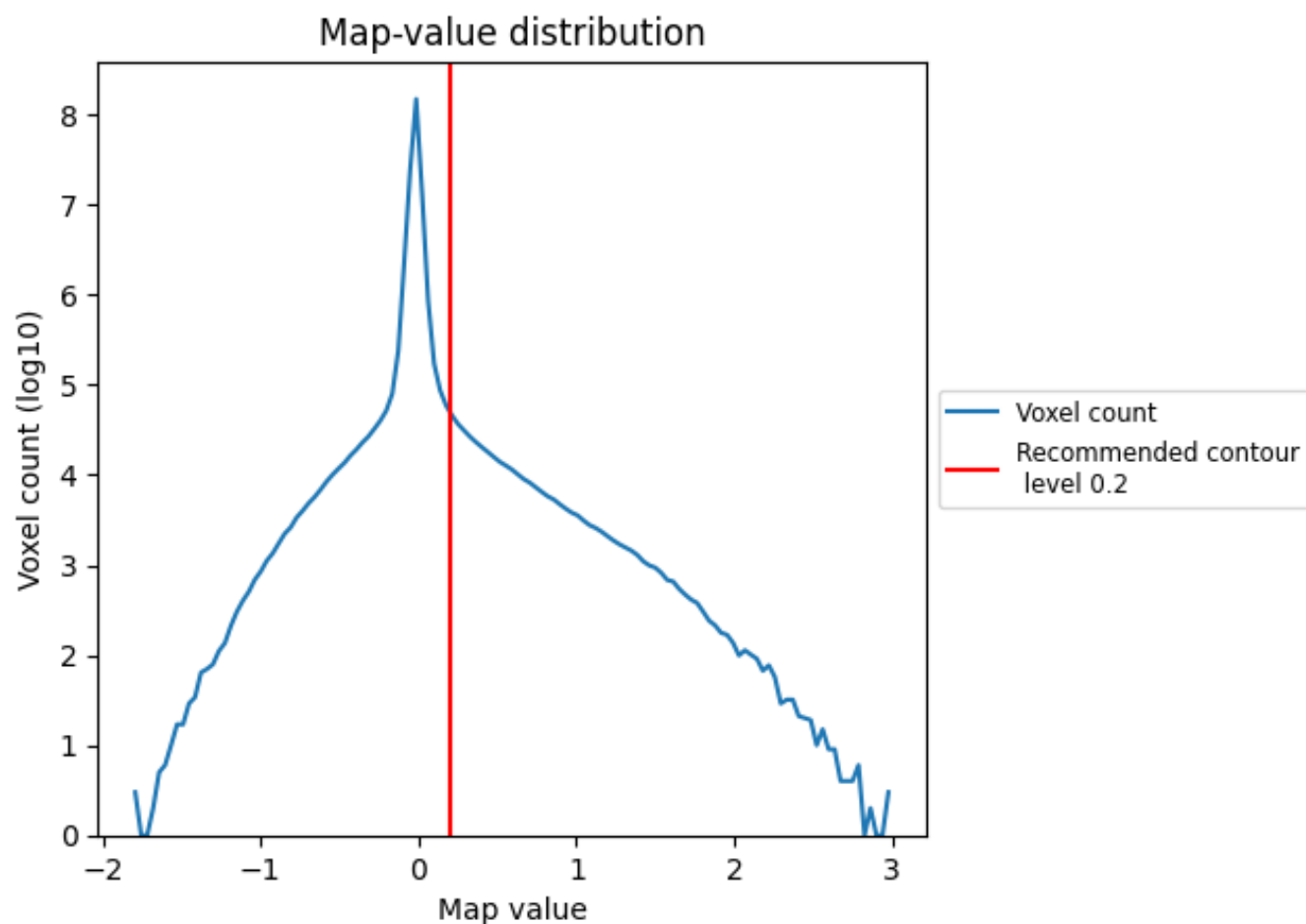


Z

7 Map analysis [i](#)

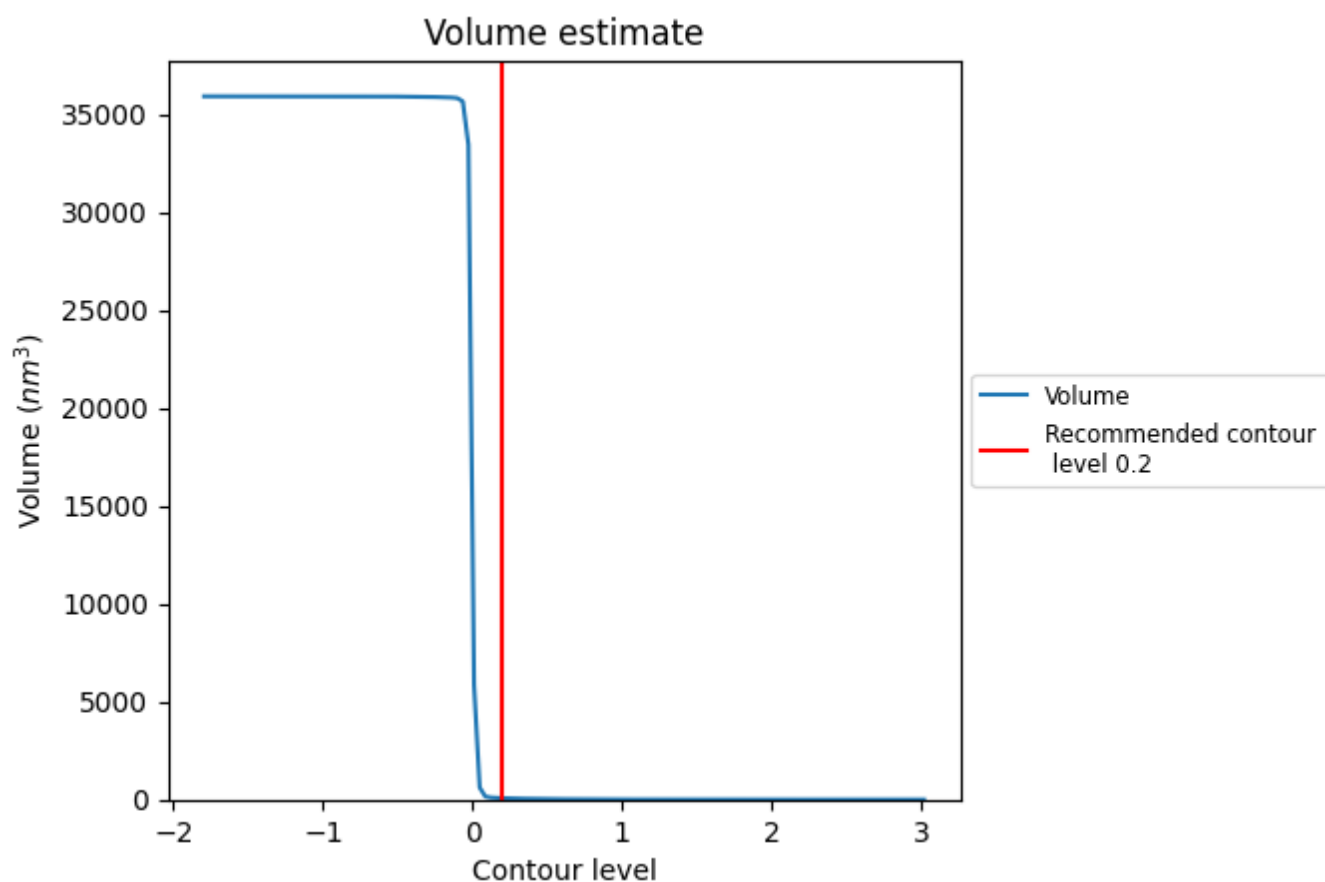
This section contains the results of statistical analysis of the map.

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.

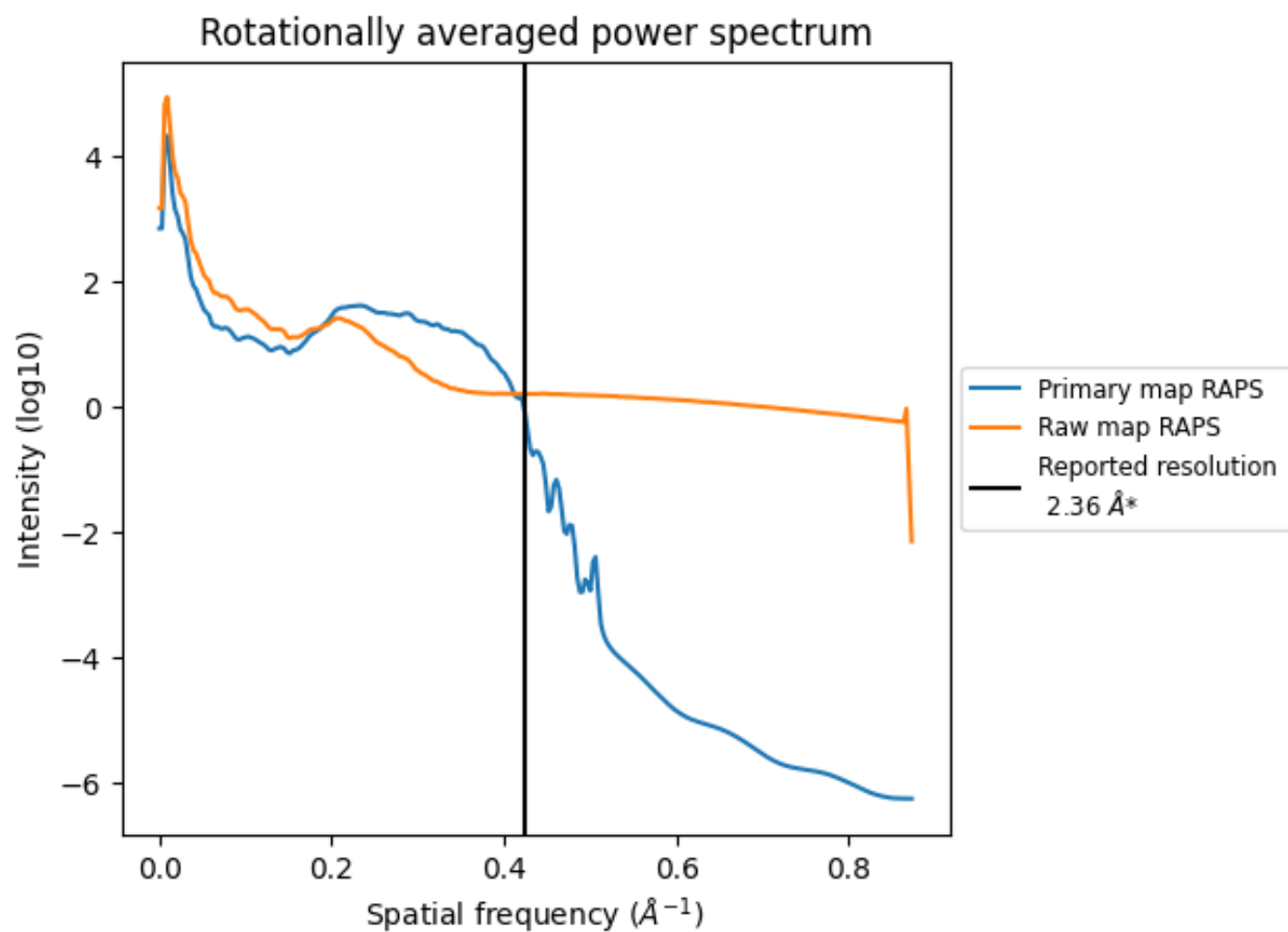
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm^3 ; this corresponds to an approximate mass of 63 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 ⓘ

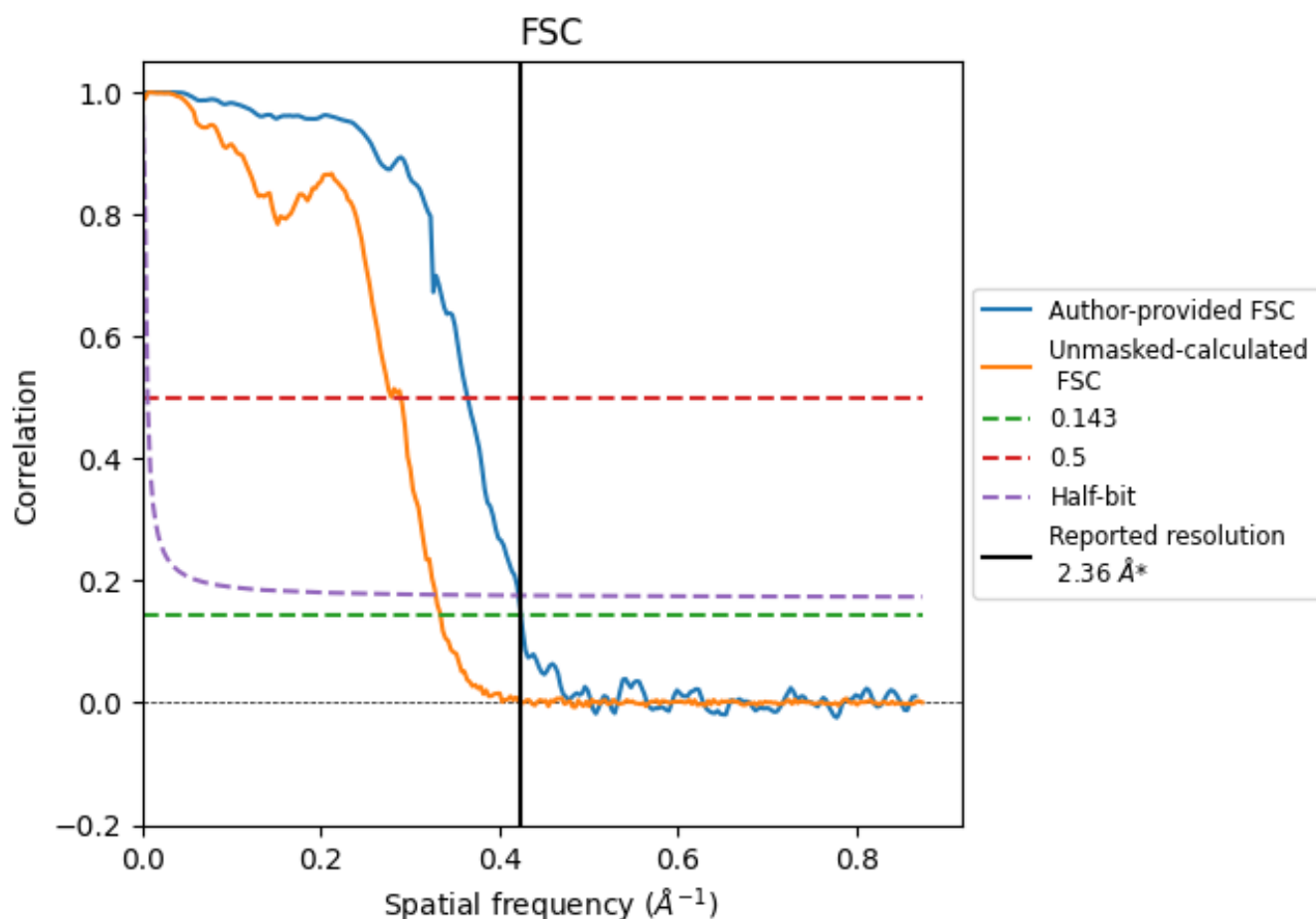


*Reported resolution corresponds to spatial frequency of 0.424 \AA^{-1}

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 0.424 \AA^{-1}

8.2 Resolution estimates [i](#)

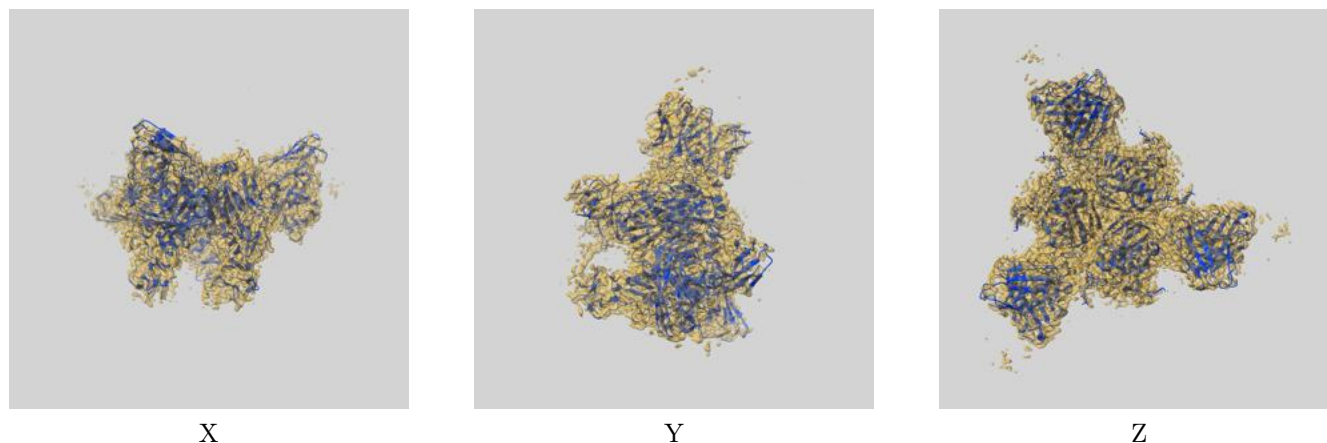
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.36	-	-
Author-provided FSC curve	2.36	2.75	2.37
Unmasked-calculated*	3.00	3.45	3.04

*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 3.00 differs from the reported value 2.36 by more than 10 %

9 Map-model fit [i](#)

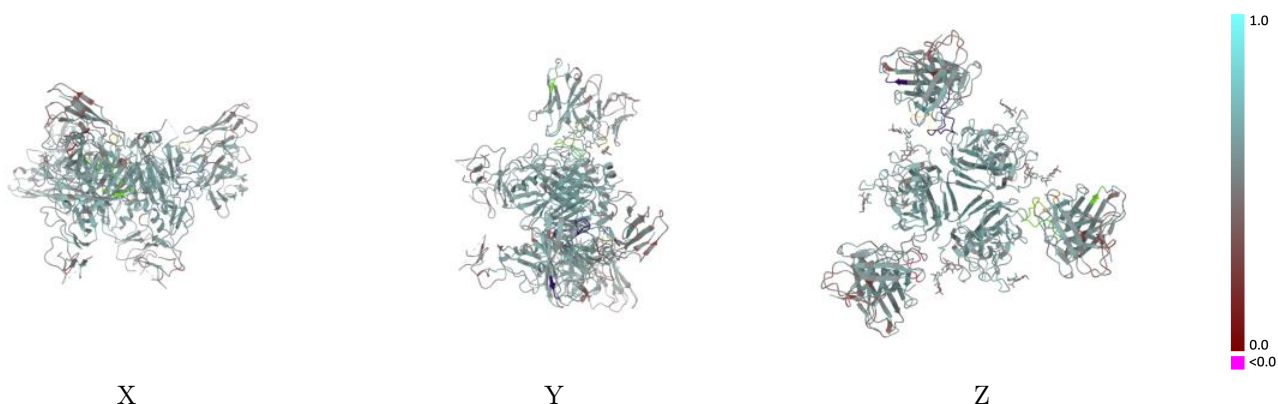
This section contains information regarding the fit between EMDB map EMD-49475 and PDB model 9NJ6. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



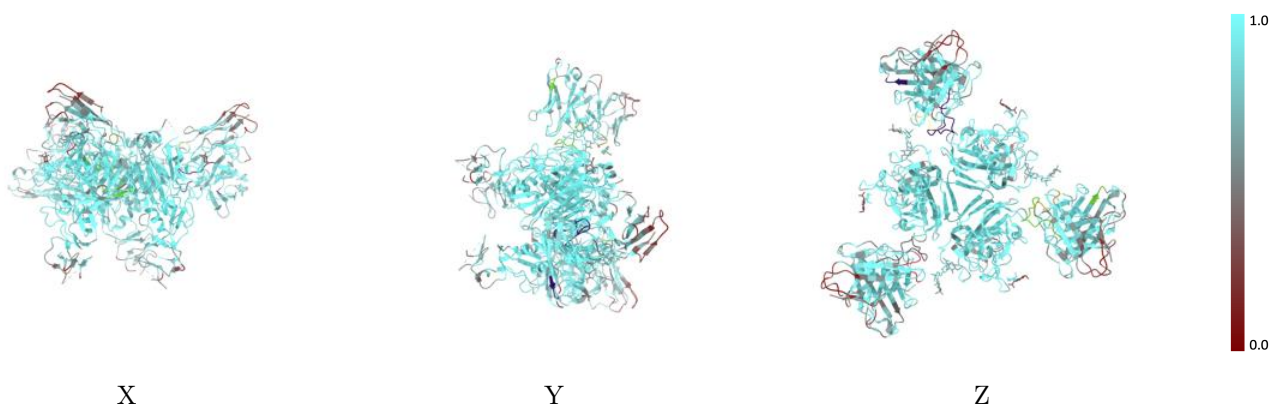
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



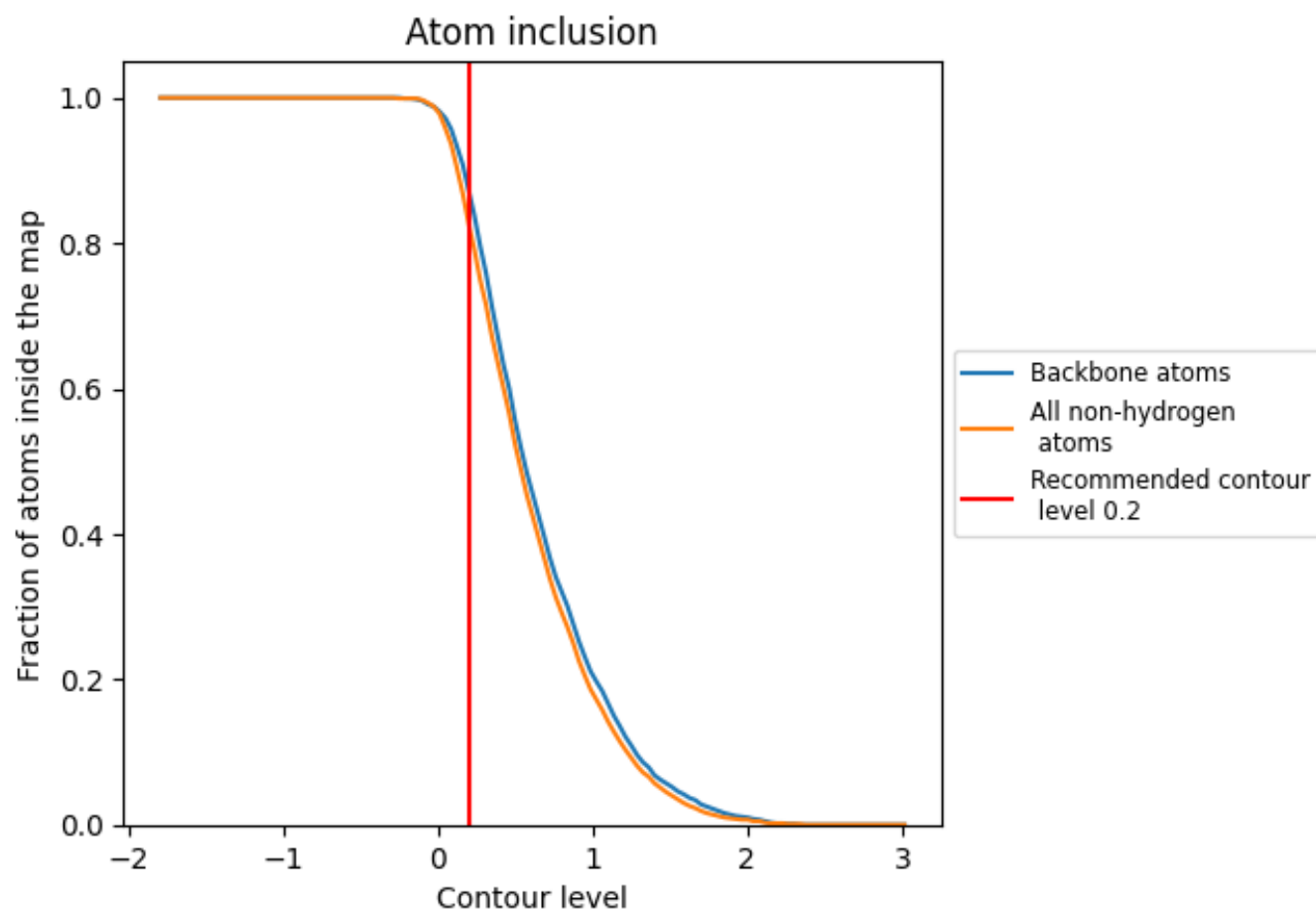
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 82% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.5520
A	 0.8750	 0.5740
B	 0.8750	 0.5720
C	 0.8750	 0.5710
D	 0.6070	 0.4900
E	 0.6580	 0.5060
F	 0.5710	 0.4960
G	 0.6840	 0.4980
H	 0.8430	 0.5550
I	 0.6070	 0.4990
J	 0.8470	 0.5560
K	 0.6810	 0.5010
L	 0.6830	 0.5010
M	 0.7110	 0.5040
P	 0.6820	 0.5000
Q	 0.8490	 0.5540

