



wwPDB EM Validation Summary Report ⓘ

Jul 27, 2025 – 10:36 PM EDT

PDB ID : 9MV0 / pdb_00009mv0
EMDB ID : EMD-48650
Title : Structure of HKU5 spike C-terminal domain in complex with ACE2 from *Pipistrellus abramus*
Authors : Li, N.; Tsybovsky, Y.; Teng, I.; Zhou, T.
Deposited on : 2025-01-15
Resolution : 4.20 Å(reported)

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

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
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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.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

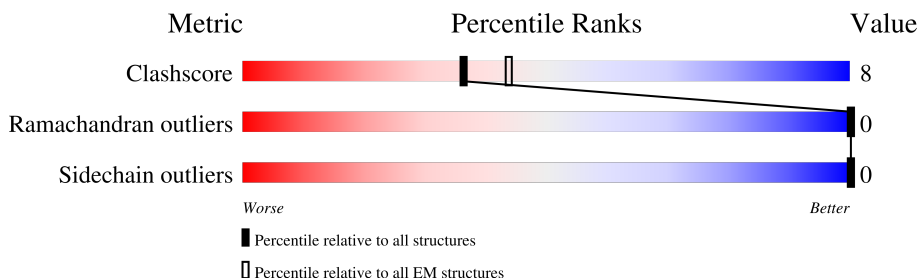
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	803	
1	C	803	
2	B	1352	
2	D	1352	
3	E	2	
3	F	2	
3	G	2	
3	H	2	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14631 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 Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	692	Total	C	N	O	S	0	0
			5686	3623	958	1071	34		
1	C	692	Total	C	N	O	S	0	0
			5686	3623	958	1071	34		

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	196	Total	C	N	O	S	0	0
			1521	970	238	301	12		
2	D	195	Total	C	N	O	S	0	0
			1514	965	237	300	12		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

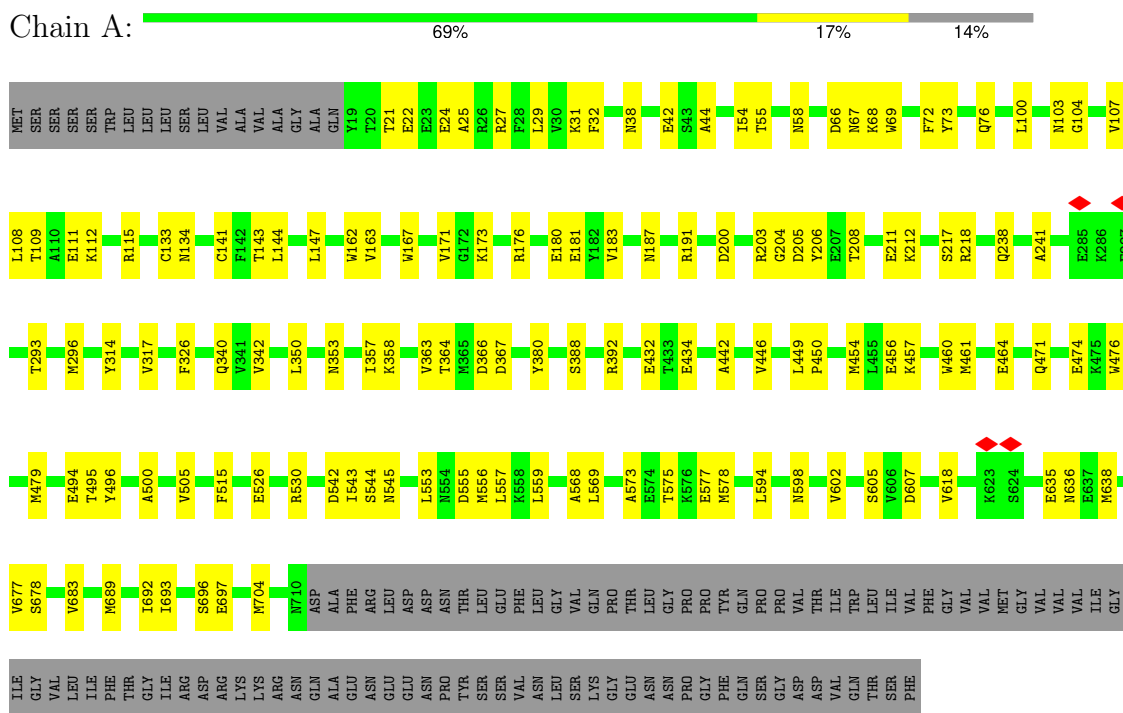


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

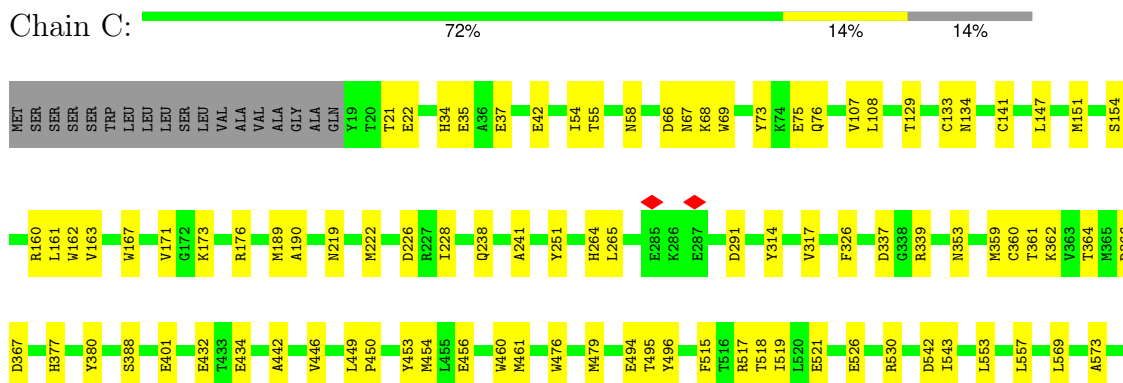
3 Residue-property plots

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: Angiotensin-converting enzyme



• Molecule 1: Angiotensin-converting enzyme



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

- Molecule 2: Spike glycoprotein

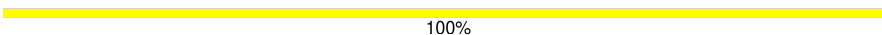


THR	TTR	ALA	SER	TYR	ASP	PRO	ASP	GLU	MET
THR	VAL	LEU	A442	THR	ASP	ASP	GLY	GLY	ILE
GLY	ARG	ARG	T443	VAL	ILE	ILE	PHE	VAL	ARG
CYS	ASN	ASN	G444	PRO	CYS	CYS	VAL	ILE	SER
ALA	ASP	ASP	C445	ARG	THR	THR	ARG	PRO	LEU
MET	CYS	SER	Y446	SER	PHE	ILE	ILE	ASN	VAL
GLY	VAL	SER	S447	ILE	ARG	THR	THR	GLY	LEU
PHE	ILE	ILE	S448	SER	THR	THR	GLY	ASN	VAL
ILE	GLU	GLU	L449	ARG	TYR	HIS	VAL	GLY	LEU
ASN	PRO	ASP		SER	ASN	ALA	ALA	SER	MET
SER	VAL	VAL	S457	PRO	THR	CYS	ALA	TYR	SER
SER	LEU	LEU	T458	PHE	THR	THR	ASN	SER	LEU
SER	SER	SER	T459	ASN	ILE	CYS	LYS	THR	THR
MET	ASP	ASP	M460	ASP	THR	VAL	THR	ILE	PHE
VAL	ILE	VAL		ARG	GLU	GLU	GLY	THR	THR
VAL	TYR	CYS	L464	LYS	ASP	HIS	THR	LEU	GLY
ASP	ASP	VAL		ALA	GLU	PRO	VAL	THR	ASN
GLU	GLU	GLU	SER	ALA	GLU	ARG	THR	THR	LEU
GLY	LYS	TYR	A469	TRP	ASN	THR	ILE	THR	THR
CYS	ALA	SER		ALA	ALA	GLN	SER	GLY	ARG
GLN	SER	LEU	GLY	ALA	GLU	GLN	GLN	GLY	THR
LEU	ASN	LEU	Y473	PHE	THR	GLN	GLN	LEU	GLY
PRO	SER	HIS	Q474	THR	PHE	THR	GLN	LEU	GLY
LEU	HIS	GLY	F475	PHE	THR	ASN	LYS	GLY	ASN
GLY	ILE	ILE	N476	ILE	GLY	CYS	THR	PRO	SER
GLN	ALA	THR		TYR	ILE	ALA	PHE	LYS	VAL
THR	THR	THR	GLU	TYR	THR	GLY	LYS	ALA	ASP
SER	LEU	GLY	Q479	LYS	THR	GLY	PRO	ASN	ASP
LEU	PHE	ARG		LEU	GLN	GLU	ASP	ASN	MET
CYS	GLY	GLY	N483	HIS	ASP	THR	ILE	ASP	GLY
ALA	VAL	VAL	T484	PRO	THR	THR	LYS	LEU	HIS
ILE	VAL	PHE	T485	LEU	GLN	PHE	LYS	GLY	ASN
PRO	ALA	HIS	E390	THR	GLY	GLY	ILE	LYS	GLY
CYS	ASN	ASN	L508	TYR	VAL	SER	TYR	GLN	THR
THR	CYS	THR	T509	LEU	HIS	LEU	PRO	TYR	GLY
THR	HIS	THR	E510	LEU	LEU	SER	ALA	LEU	SER
SER	VAL	SER	D392	ASN	TYR	LEU	PHE	PHE	CYS
SER	GLY	GLY	F393	PHE	SER	SER	LEU	SER	LEU
ARG	VAL	VAL	T394	ASP	SER	ASP	ASP	ASP	ASP
VAL	LEU	LEU	P395	VAL	ARG	THR	GLY	GLY	SER
ARG	ARG	ARG	Y517	GLU	LYS	THR	HIS	HIS	GLN
ARG	ASN	SER	A528	GLY	VAL	PRO	ALA	VAL	VAL
ALA	GLN	GLN	Y529	TYR	GLU	SER	SER	GLN	GLN
THR	PHE	ARG		ILE	VAL	ASP	GLY	PRO	PRO
SER	ARG	PHE	P403	THR	PHE	CYS	THR	ARG	TYR
GLY	VAL	VAL	Y405	LYS	ARG	VAL	THR	ARG	TYR
ALA	TYR	TYR	L535	ALA	ASN	SER	THR	LEU	PHE
SER	ASP	ASP	N567	VAL	ASN	GLY	PRO	ASN	GLU
ASP	LYS	THR	A568	ASP	MET	SER	THR	ASN	SER
VAL	PHE	PHE		CYS	PHE	TYR	ASN	VAL	VAL
ASN	ASN	ASN	T571	GLY	HIS	GLN	THR	THR	HIS
GLN	LEU	ASN		TYR	PHE	GLN	THR	VAL	THR
ILE	LEU	LEU		ASP	ALA	ALA	GLY	ASN	THR
ALA	ALA	VAL	Q574	ASP	THR	THR	ARG	ASN	TRP
THR	ARG	GLY	Y575	LEU	LEU	THR	LEU	TYR	ASN
THR	THR	TYR	G576	ALA	PRO	THR	LEU	SER	MET
ASN	ASN	HIS	T577	GLN	VAL	GLY	ASN	SER	PRO
PHE	PHE	SER	T578	LEU	THR	PHE	ALA	GLN	ILE
THR	THR	ASP	D579	CYS	GLN	LYS	HIS	VAL	ASP
PRO	PRO	ASN	T579	GLN	THR	THR	THR	GLN	THR
PRO	LEU	GLY	N580	SER	ILE	VAL	VAL	GLU	SER
LEU	THR	ASN	S581	TYR	THR	PHE	ILE	SER	LYS
		</							

[illegible]

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

Chain E:



NAG1
NAG2

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

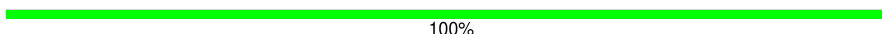
Chain F:



NAG1
NAG2

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

Chain G:



NAG1
NAG2

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

Chain H:

100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	242675	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	47000	Depositor
Image detector	DIRECT ELECTRON APOLLO (4k x 4k)	Depositor
Maximum map value	1.881	Depositor
Minimum map value	-1.155	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.23	Depositor
Map size (Å)	360.0, 360.0, 360.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/5834	0.33	0/7888
1	C	0.13	0/5834	0.30	0/7888
2	B	0.13	0/1562	0.35	0/2133
2	D	0.13	0/1554	0.34	0/2120
All	All	0.13	0/14784	0.32	0/20029

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	446	TYR	Peptide

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	5686	0	5510	94	0
1	C	5686	0	5510	77	0
2	B	1521	0	1444	23	0
2	D	1514	0	1434	25	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	2	0
4	A	56	0	52	0	0
4	C	56	0	52	0	0
All	All	14631	0	14102	216	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 8.

The worst 5 of 216 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ALA:O	1:A:29:LEU:HD23	1.79	0.81
1:C:226:ASP:OD1	1:C:453:TYR:OH	2.03	0.76
1:A:55:THR:OG1	1:A:58:ASN:OD1	2.05	0.75
1:C:683:VAL:CG2	1:C:693:ILE:HG21	2.17	0.75
1:C:21:THR:HG22	1:C:22:GLU:OE1	1.87	0.74

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	690/803 (86%)	633 (92%)	57 (8%)	0	100	100
1	C	690/803 (86%)	645 (94%)	45 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	192/1352 (14%)	175 (91%)	17 (9%)	0	100	100
2	D	189/1352 (14%)	171 (90%)	18 (10%)	0	100	100
All	All	1761/4310 (41%)	1624 (92%)	137 (8%)	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	621/716 (87%)	621 (100%)	0	100	100
1	C	621/716 (87%)	621 (100%)	0	100	100
2	B	174/1174 (15%)	174 (100%)	0	100	100
2	D	173/1174 (15%)	173 (100%)	0	100	100
All	All	1589/3780 (42%)	1589 (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. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	51	ASN
1	C	400	HIS
1	C	504	HIS
1	A	539	HIS
1	A	614	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 ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	E	1	3,1	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
3	NAG	E	2	3	14,14,15	0.69	0	17,19,21	1.14	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.74	0	17,19,21	0.80	0
3	NAG	F	2	3	14,14,15	0.70	0	17,19,21	0.85	0
3	NAG	G	1	3,1	14,14,15	0.72	0	17,19,21	1.01	0
3	NAG	G	2	3	14,14,15	0.70	0	17,19,21	0.83	0
3	NAG	H	1	3,1	14,14,15	0.74	0	17,19,21	0.93	1 (5%)
3	NAG	H	2	3	14,14,15	0.73	0	17,19,21	1.68	2 (11%)

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

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	C2-N2-C7	5.48	130.24	122.90
3	E	2	NAG	C2-N2-C7	3.40	127.46	122.90
3	H	1	NAG	O5-C1-C2	-2.33	107.68	111.29
3	H	2	NAG	C8-C7-N2	2.15	119.69	116.12
3	E	1	NAG	C1-O5-C5	2.08	114.97	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

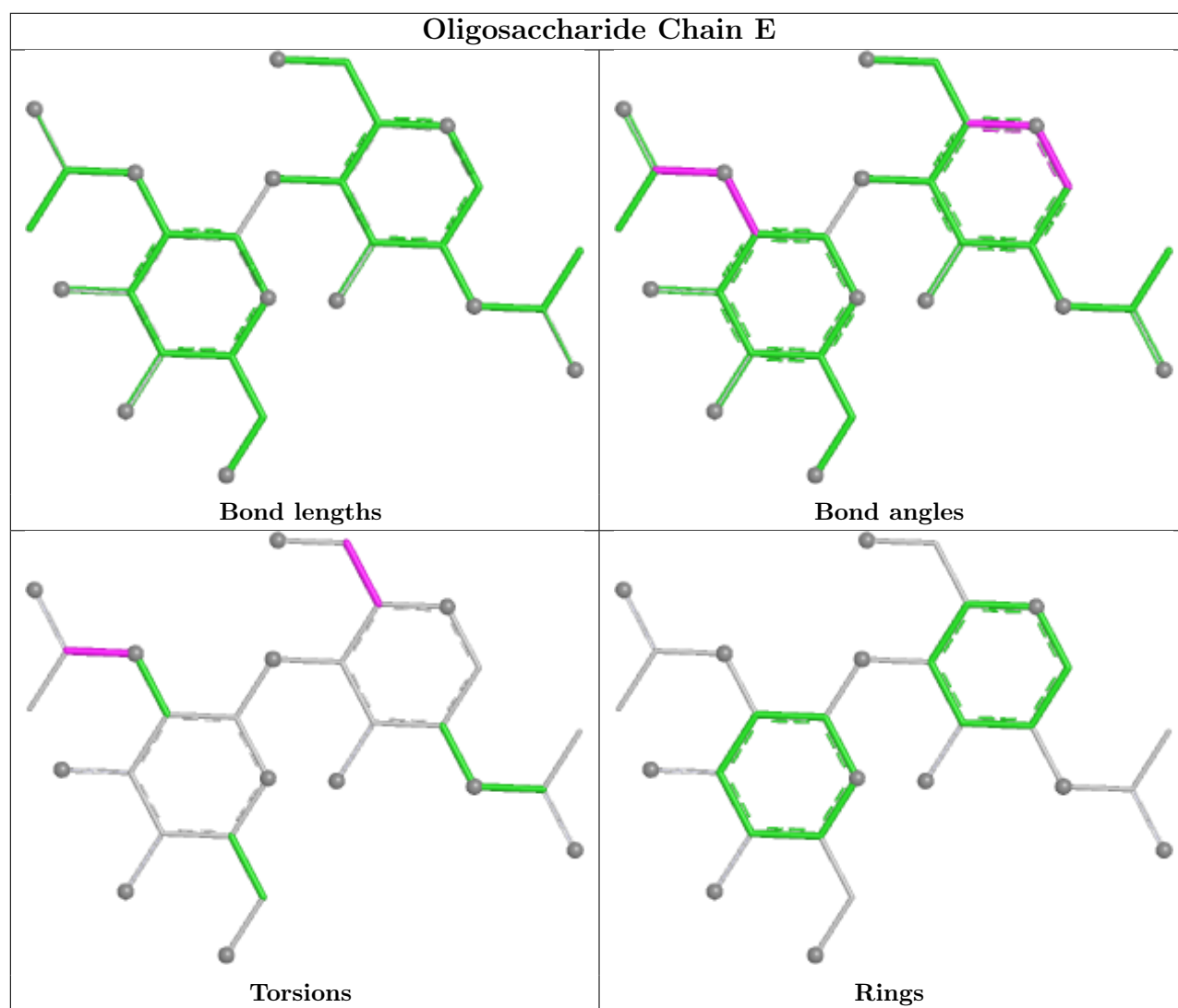
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	E	1	NAG	O5-C5-C6-O6

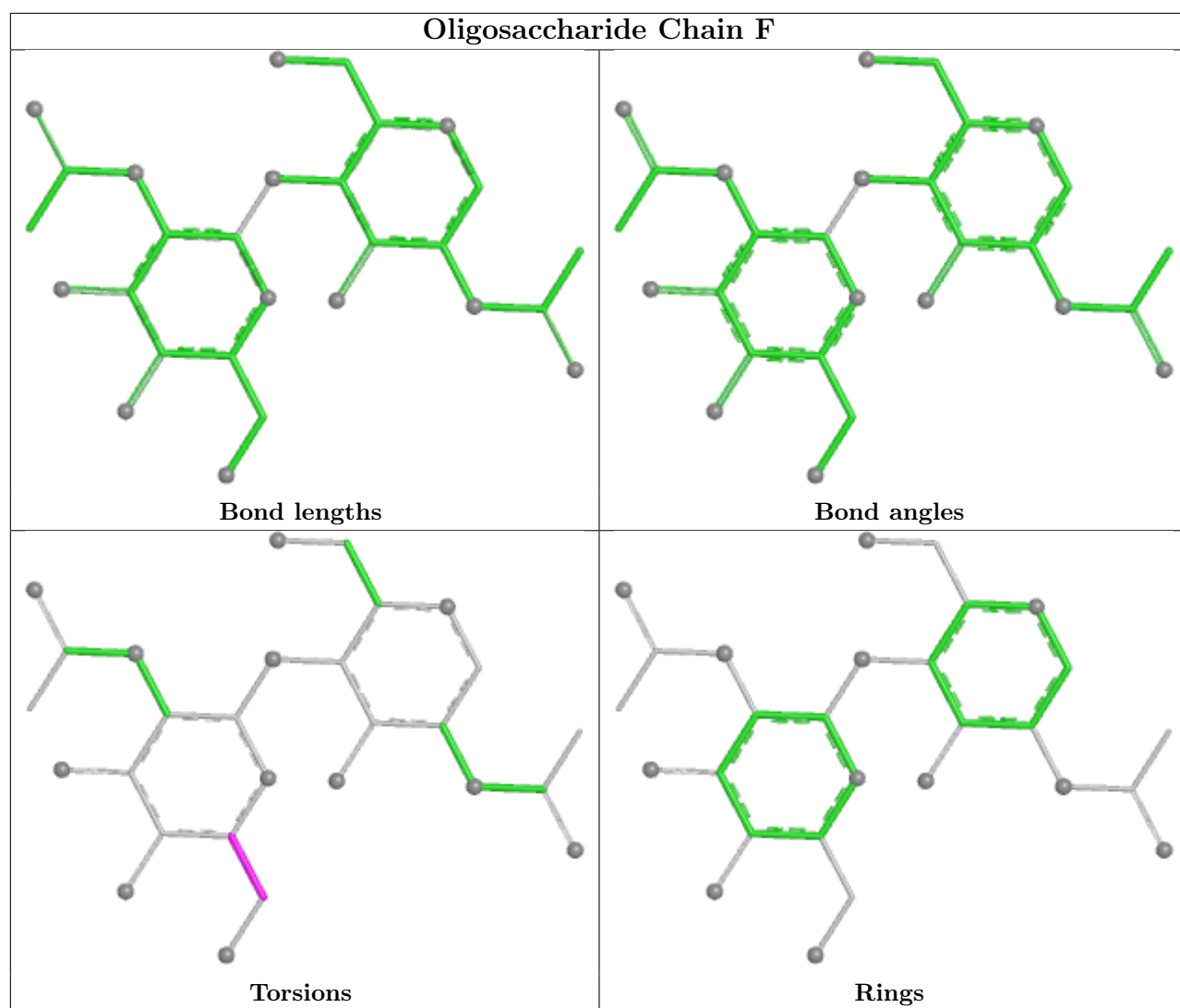
There are no ring outliers.

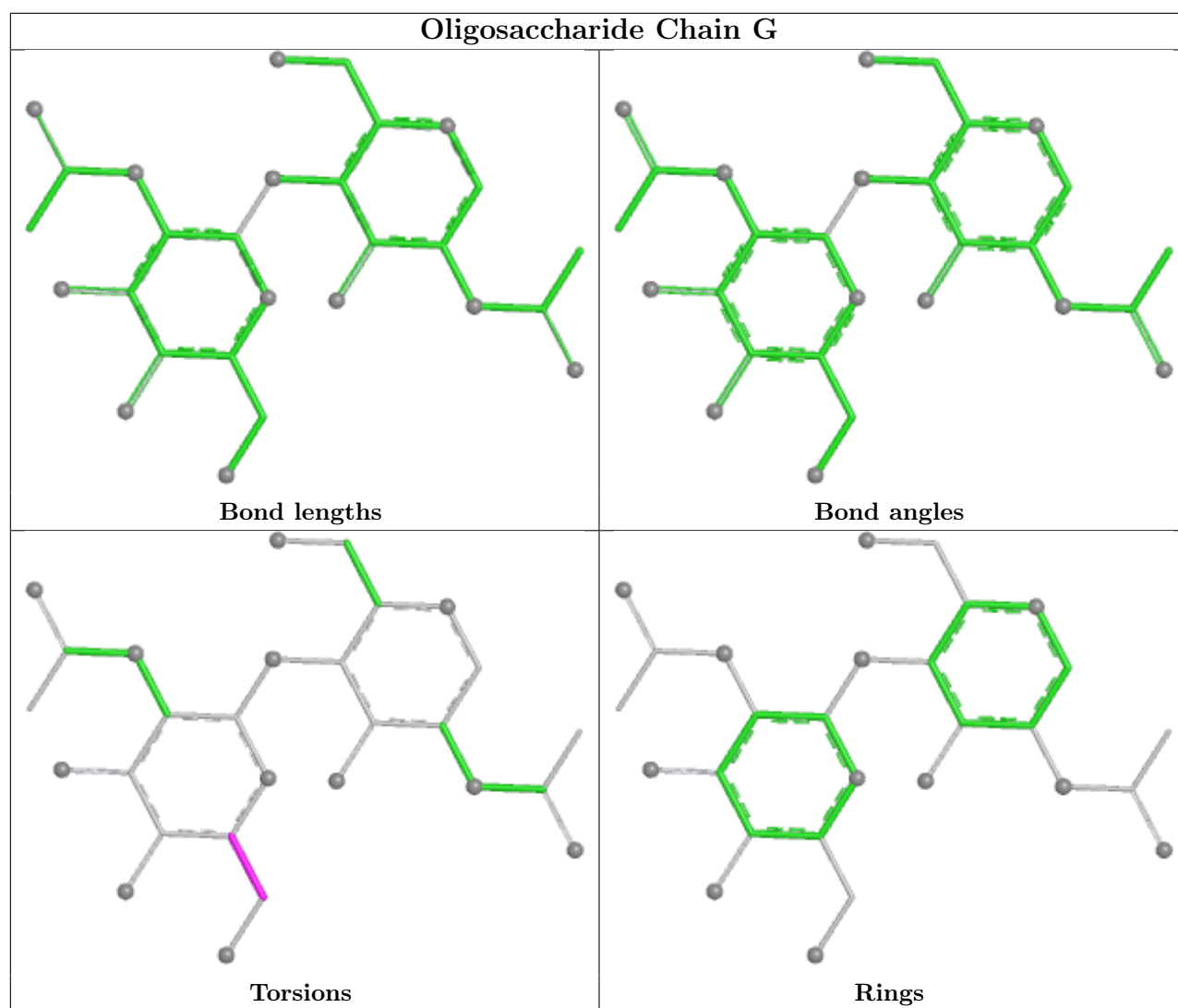
2 monomers are involved in 2 short contacts:

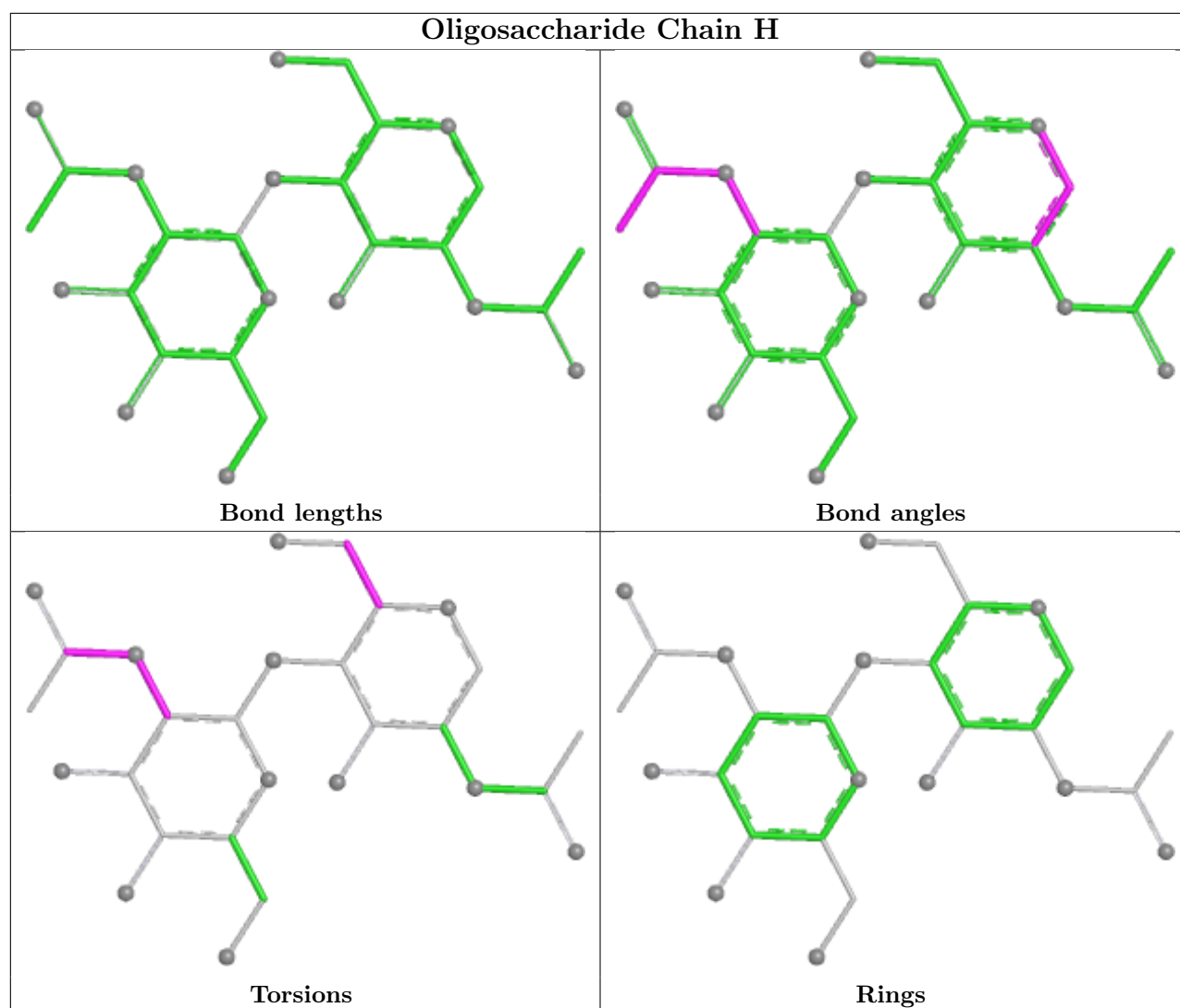
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0
3	H	2	NAG	1	0

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](#)

8 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	$\# Z > 2$
4	NAG	A	901	1	14,14,15	0.72	0	17,19,21	0.83	0
4	NAG	C	902	1	14,14,15	0.74	0	17,19,21	0.99	1 (5%)
4	NAG	C	904	1	14,14,15	0.72	0	17,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	903	1	14,14,15	0.71	0	17,19,21	1.10	1 (5%)
4	NAG	A	903	1	14,14,15	0.69	0	17,19,21	1.11	2 (11%)
4	NAG	C	901	1	14,14,15	0.72	0	17,19,21	0.93	0
4	NAG	A	902	1	14,14,15	0.73	0	17,19,21	1.02	1 (5%)
4	NAG	A	904	1	14,14,15	0.70	0	17,19,21	0.70	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	A	901	1	-	1/6/23/26	0/1/1/1
4	NAG	C	902	1	-	1/6/23/26	0/1/1/1
4	NAG	C	904	1	-	0/6/23/26	0/1/1/1
4	NAG	C	903	1	-	1/6/23/26	0/1/1/1
4	NAG	A	903	1	-	1/6/23/26	0/1/1/1
4	NAG	C	901	1	-	0/6/23/26	0/1/1/1
4	NAG	A	902	1	-	1/6/23/26	0/1/1/1
4	NAG	A	904	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	903	NAG	C2-N2-C7	2.57	126.35	122.90
4	A	903	NAG	C2-N2-C7	2.50	126.25	122.90
4	A	902	NAG	C2-N2-C7	2.28	125.95	122.90
4	C	902	NAG	C2-N2-C7	2.10	125.72	122.90
4	A	903	NAG	O5-C1-C2	-2.03	108.15	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	NAG	C1-C2-N2-C7
4	A	903	NAG	C1-C2-N2-C7
4	C	902	NAG	C1-C2-N2-C7
4	C	903	NAG	C1-C2-N2-C7
4	A	901	NAG	O5-C5-C6-O6

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.

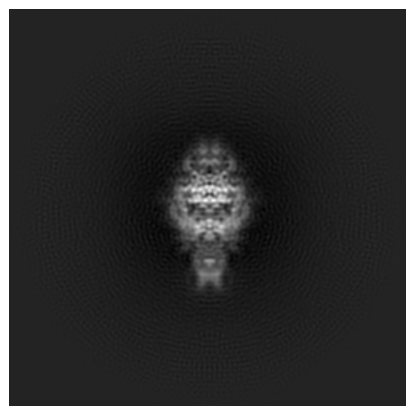
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48650. These allow visual inspection of the internal detail of the map and identification of artifacts.

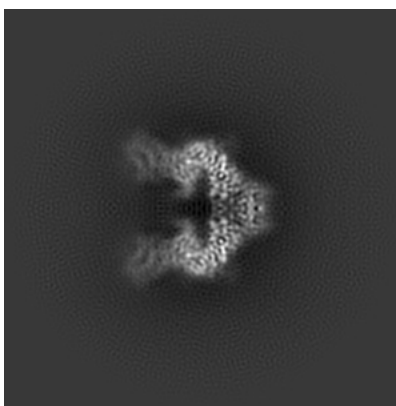
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

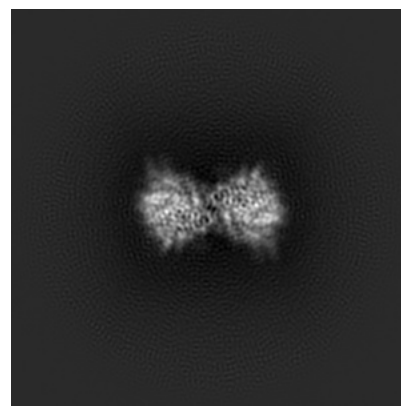
6.1.1 Primary map



X

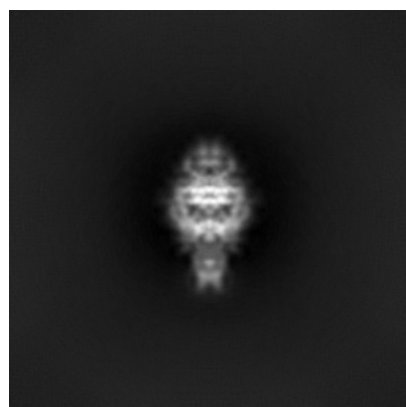


Y

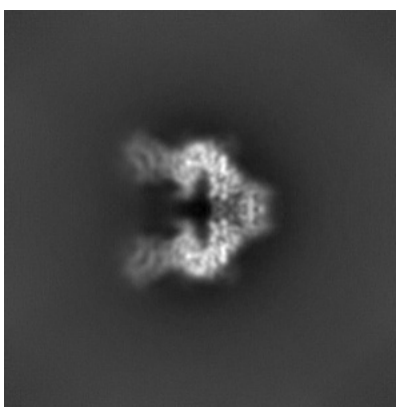


Z

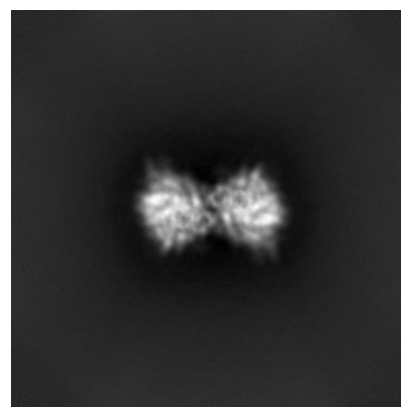
6.1.2 Raw map



X



Y

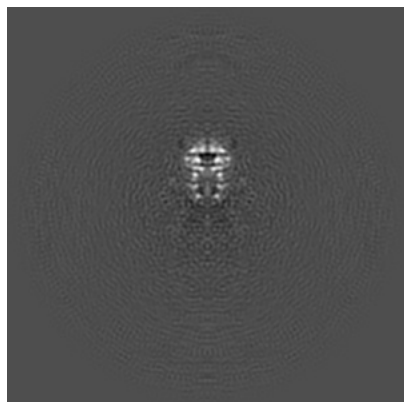


Z

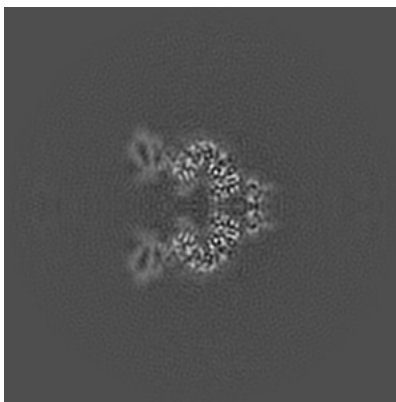
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

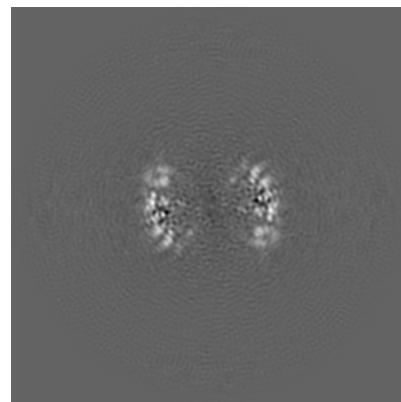
6.2.1 Primary map



X Index: 180

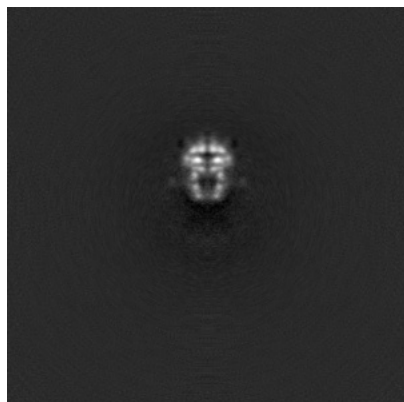


Y Index: 180

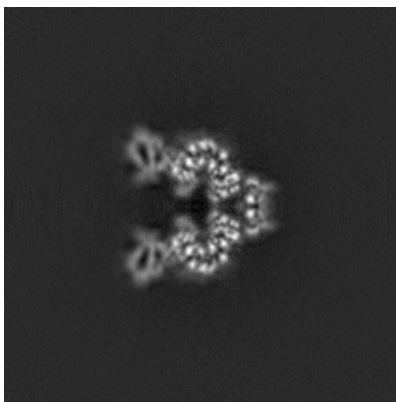


Z Index: 180

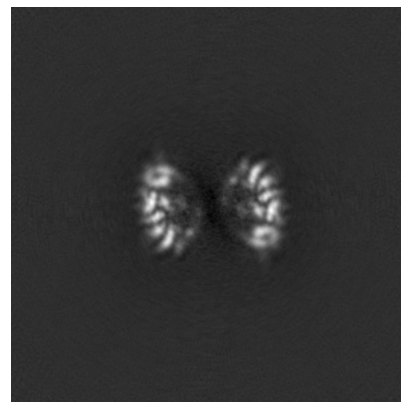
6.2.2 Raw map



X Index: 180



Y Index: 180

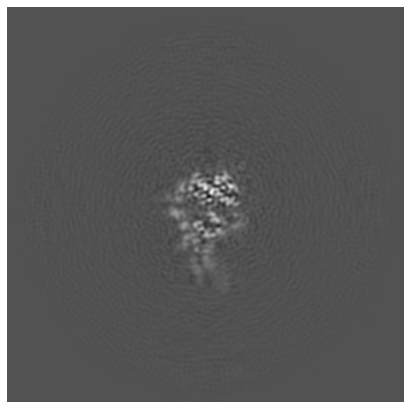


Z Index: 180

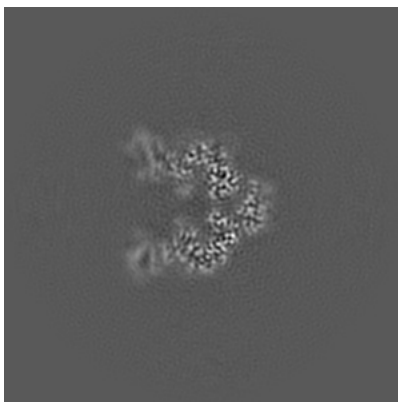
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

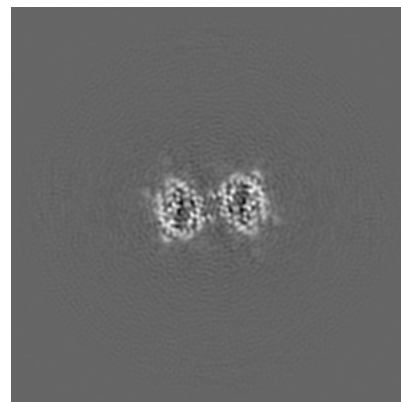
6.3.1 Primary map



X Index: 214

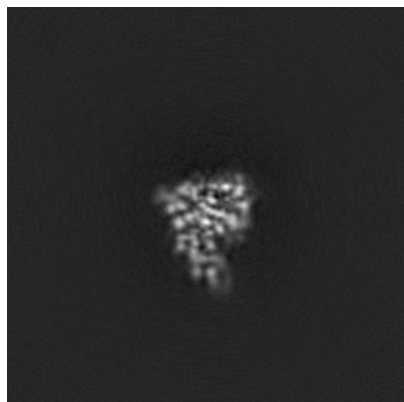


Y Index: 177

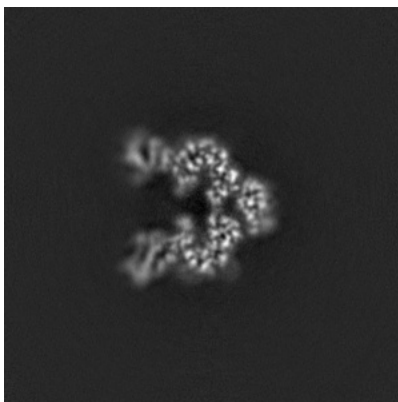


Z Index: 197

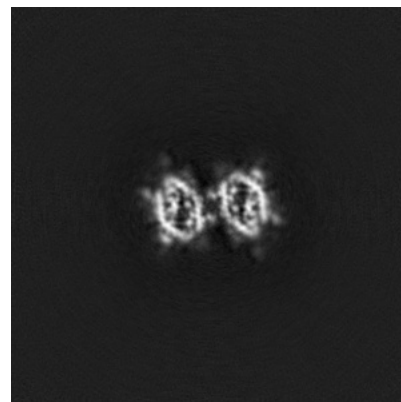
6.3.2 Raw map



X Index: 221



Y Index: 184

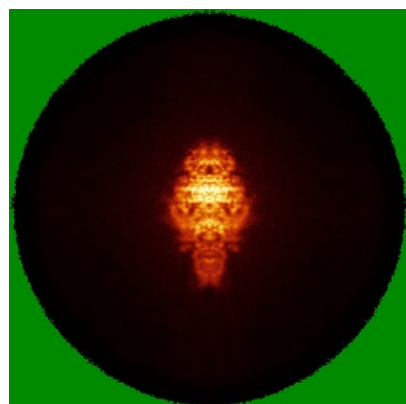


Z Index: 197

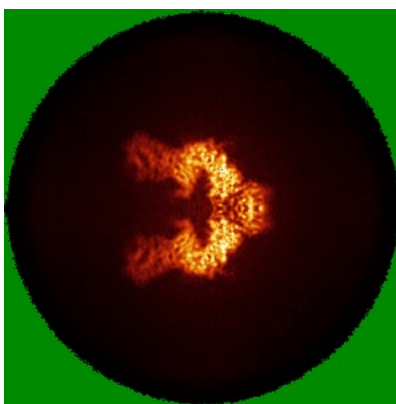
The images above show the largest variance slices of the map in three orthogonal directions.

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

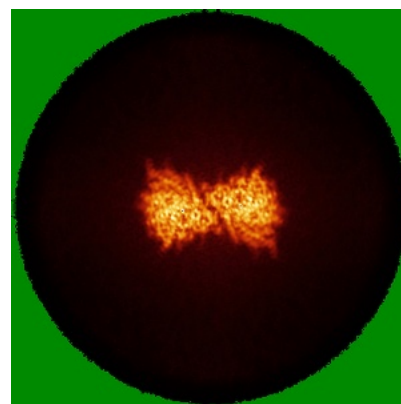
6.4.1 Primary map



X

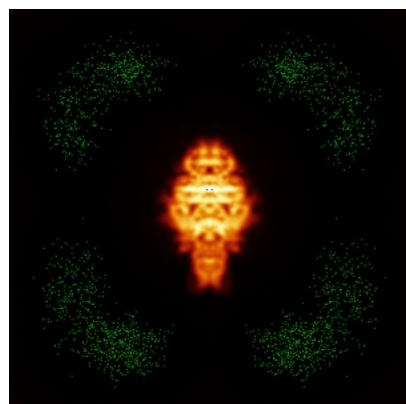


Y

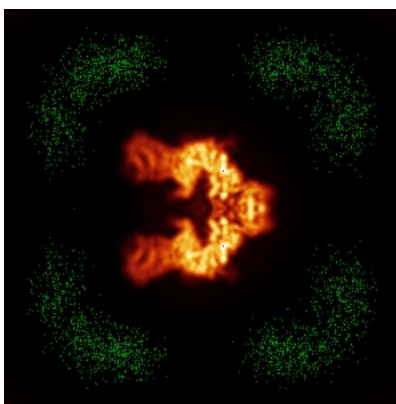


Z

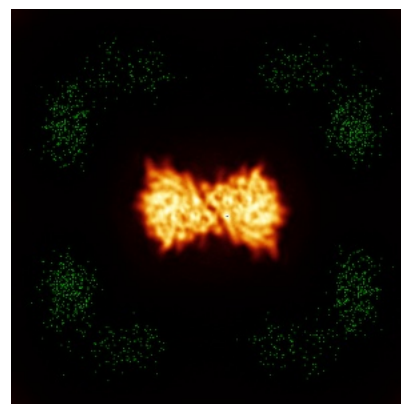
6.4.2 Raw map



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.

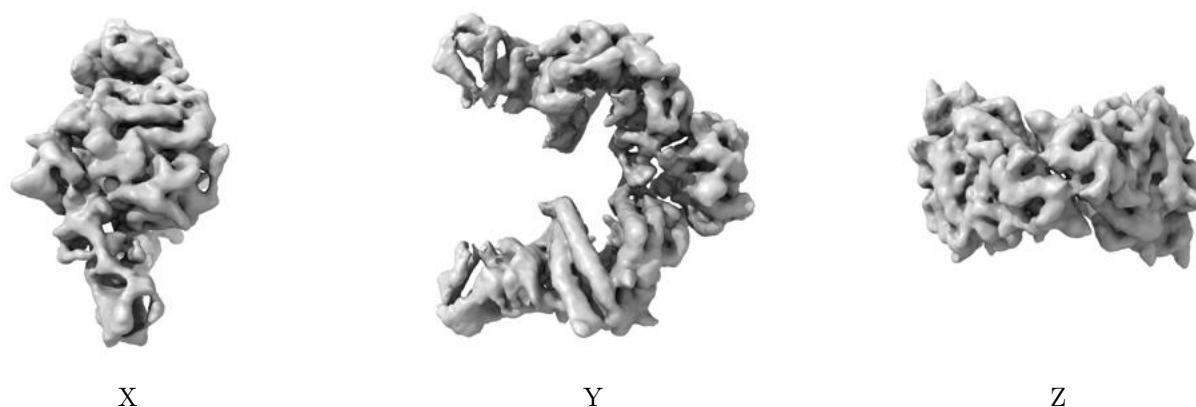
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.23. 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.

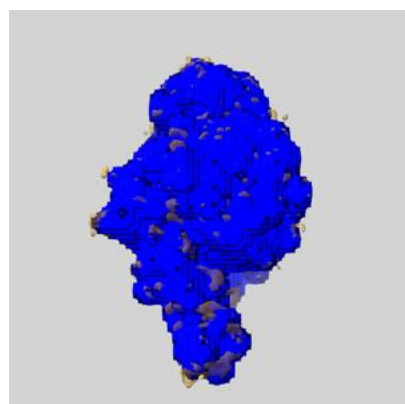
6.6 Mask visualisation [i](#)

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

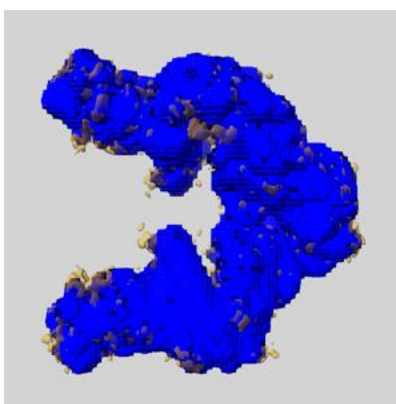
A mask typically either:

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

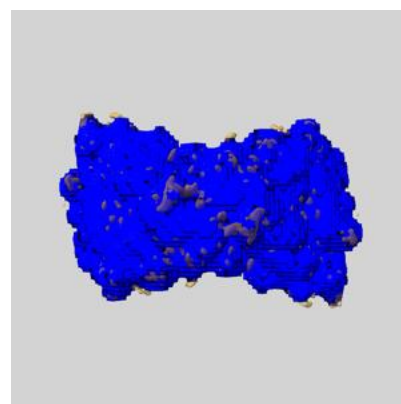
6.6.1 emd_48650_msk_1.map [i](#)



X



Y

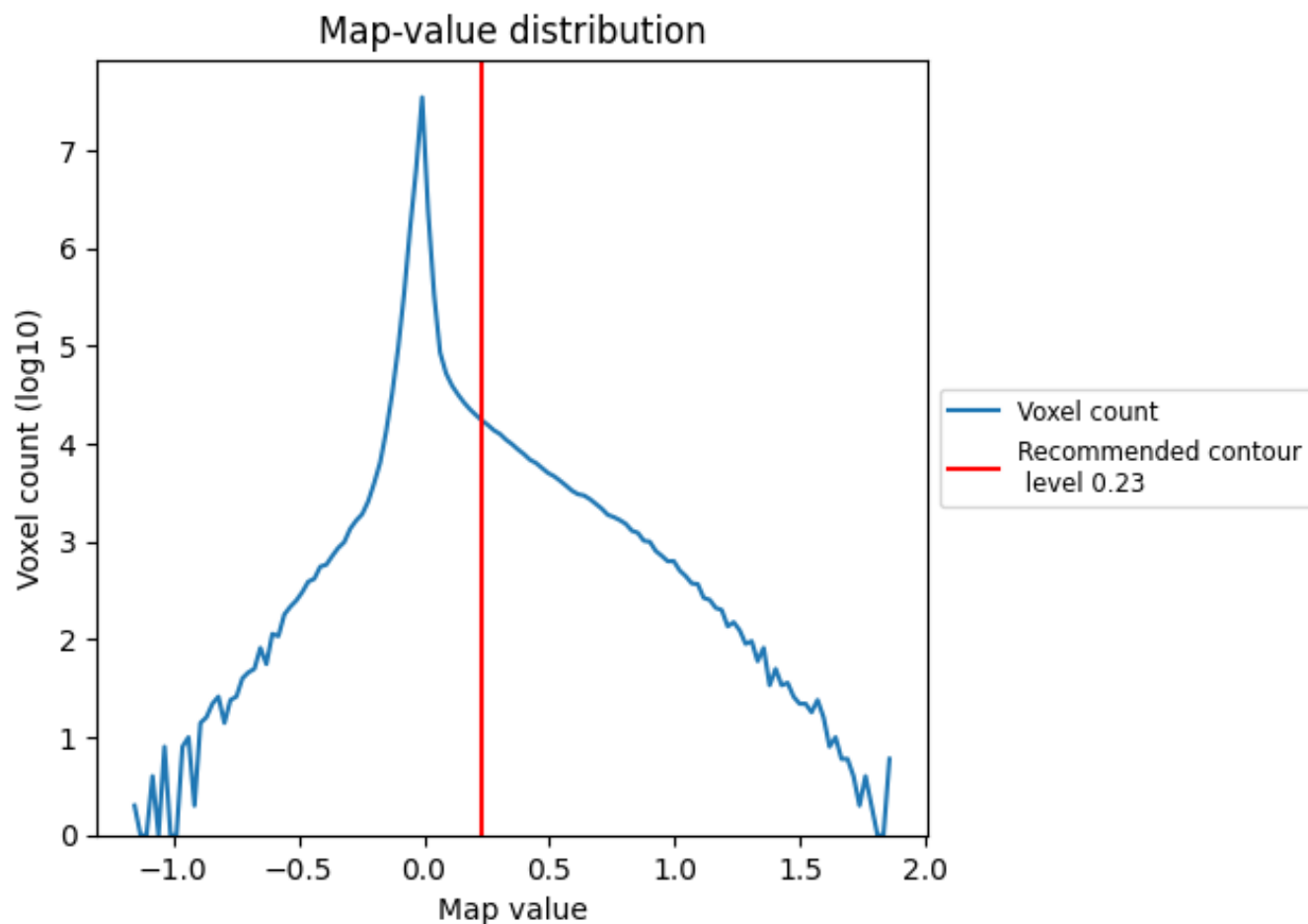


Z

7 Map analysis [i](#)

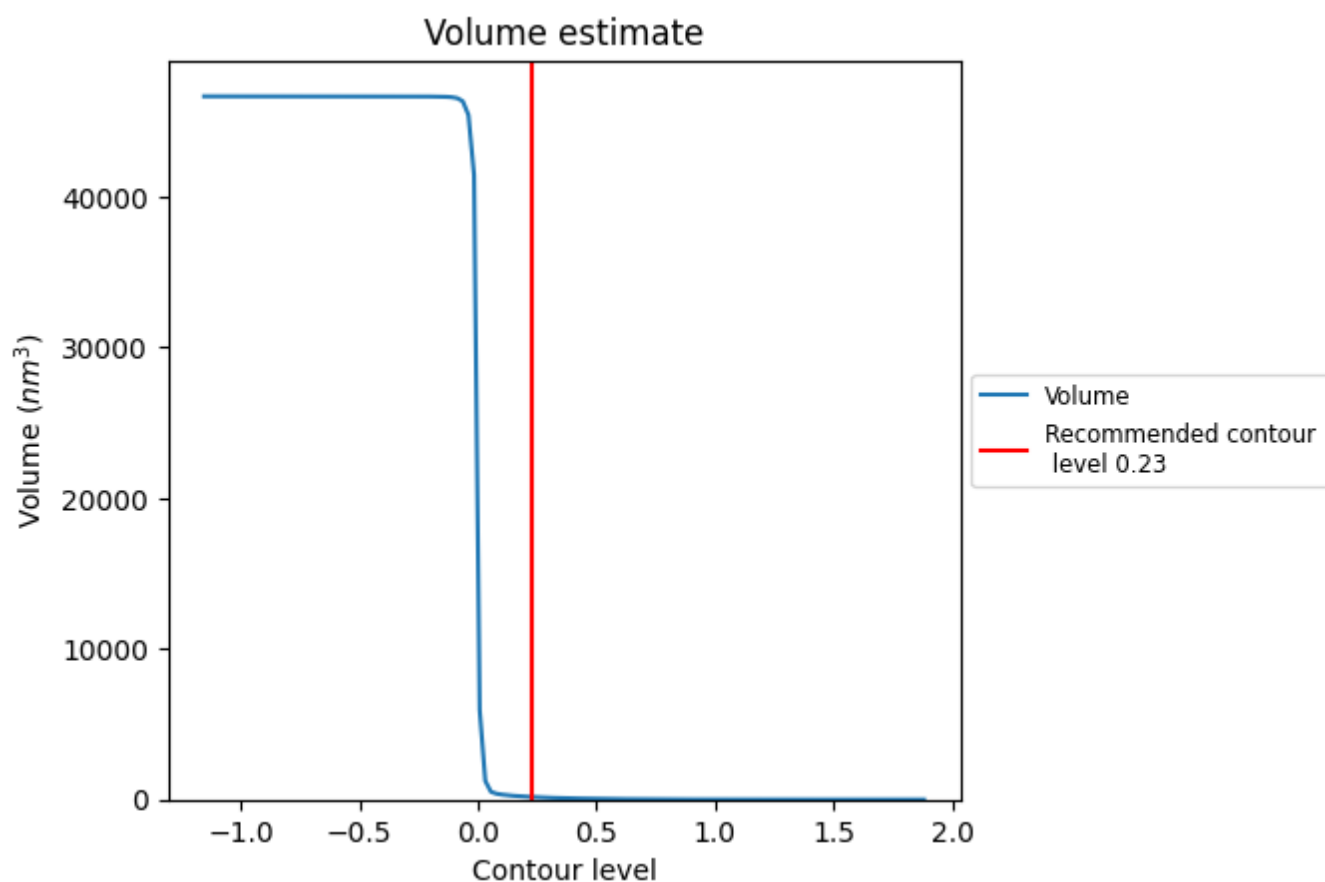
This section contains the results of statistical analysis of the map.

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.

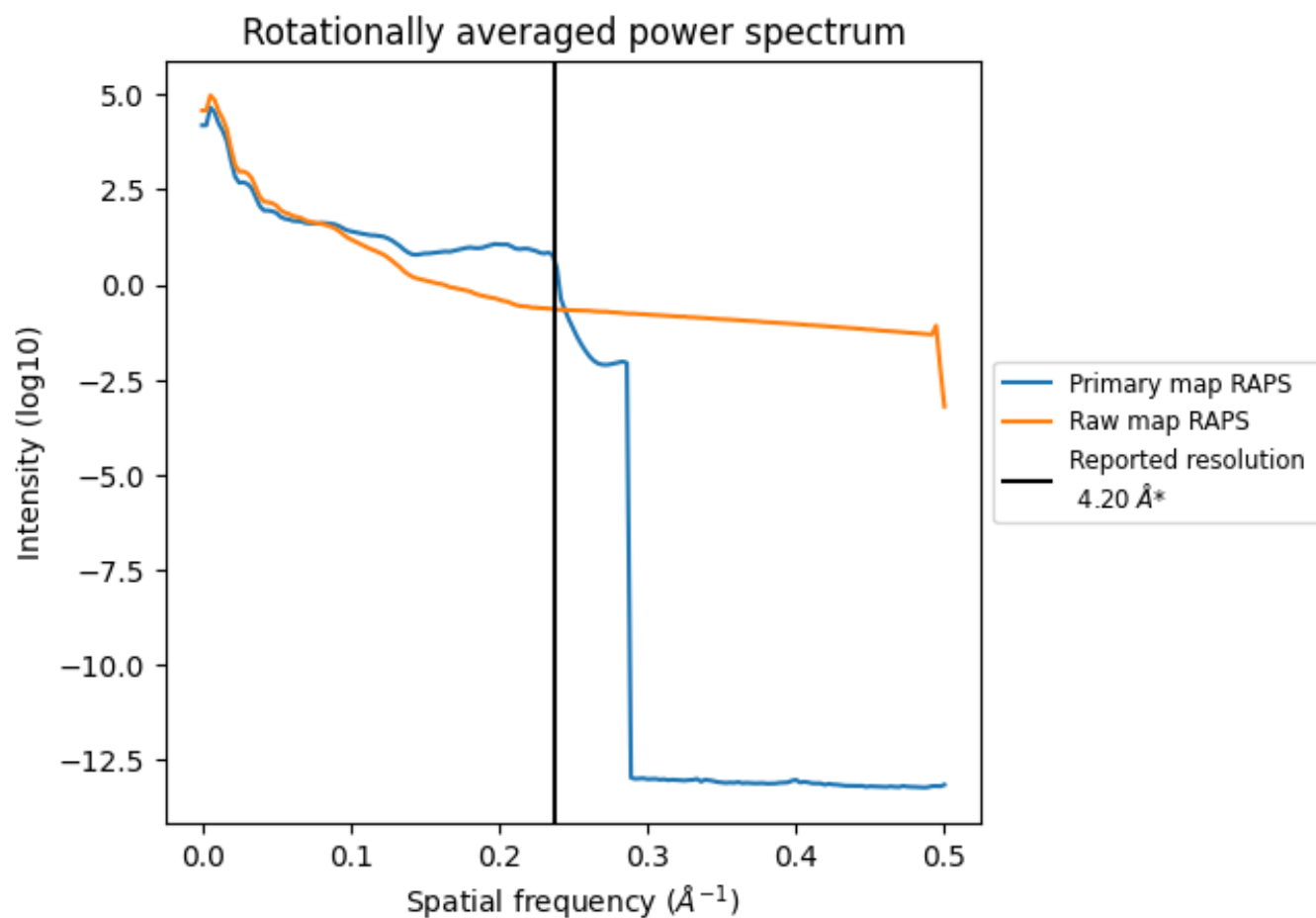
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 169 nm³; this corresponds to an approximate mass of 153 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 ⓘ

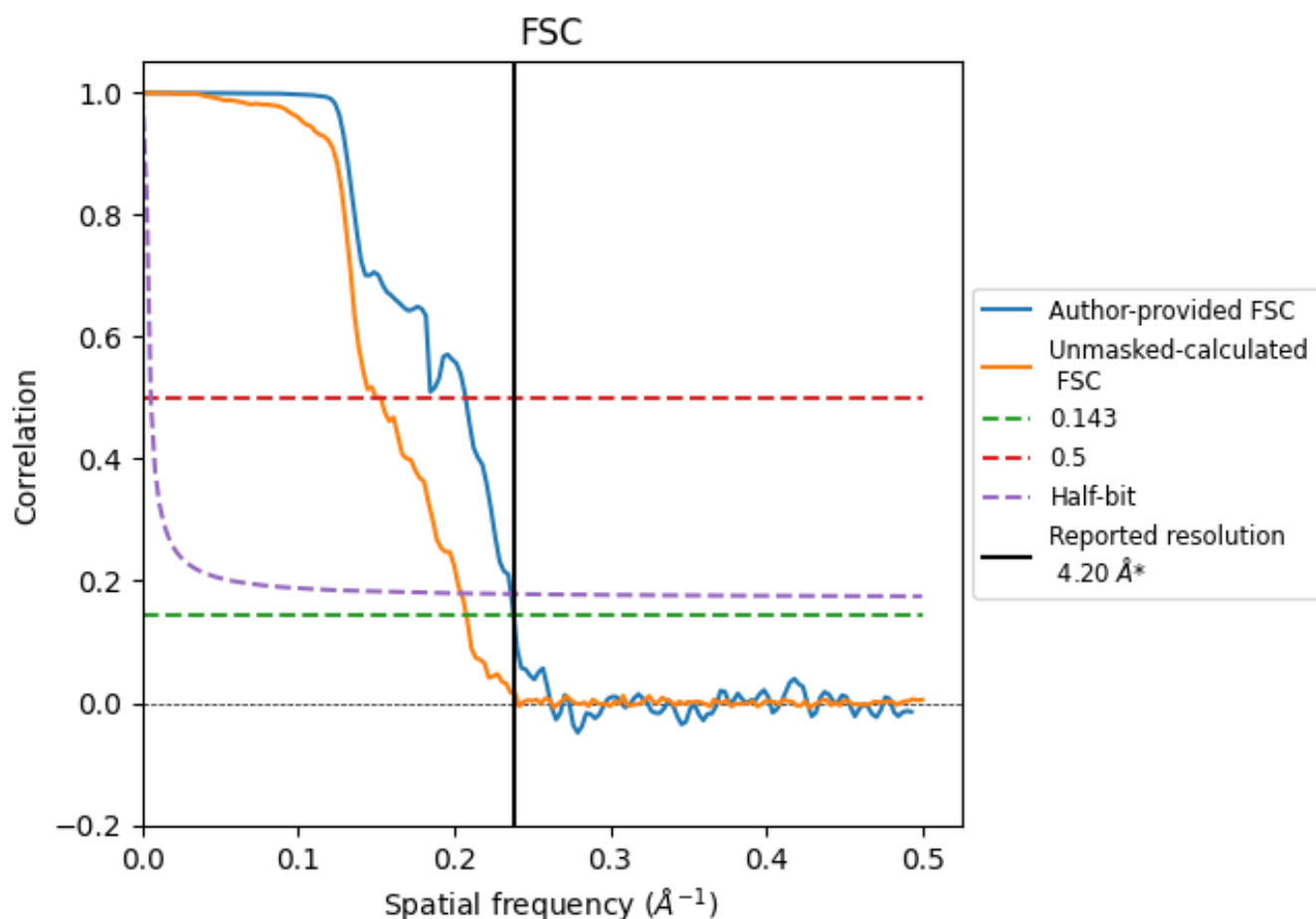


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 \AA^{-1}

8.2 Resolution estimates [i](#)

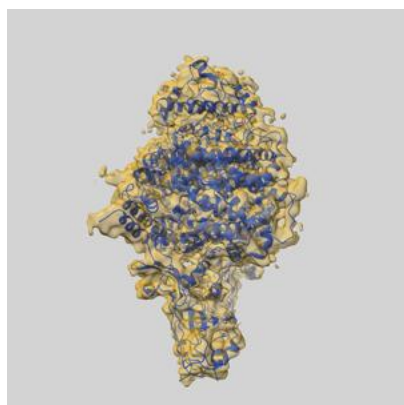
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.20	4.82	4.23
Unmasked-calculated*	4.81	6.67	4.89

*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 4.81 differs from the reported value 4.2 by more than 10 %

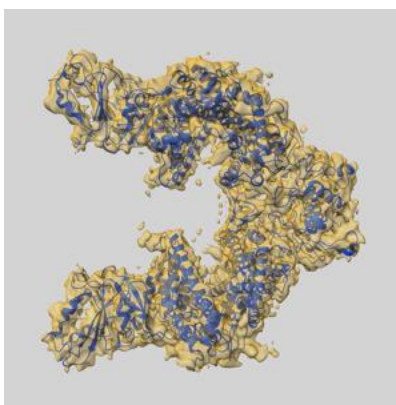
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48650 and PDB model 9MV0. Per-residue inclusion information can be found in section [3](#) on page [5](#).

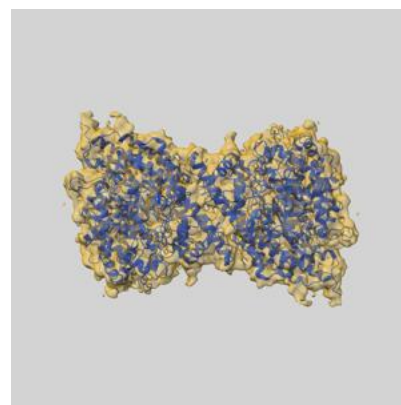
9.1 Map-model overlay [i](#)



X



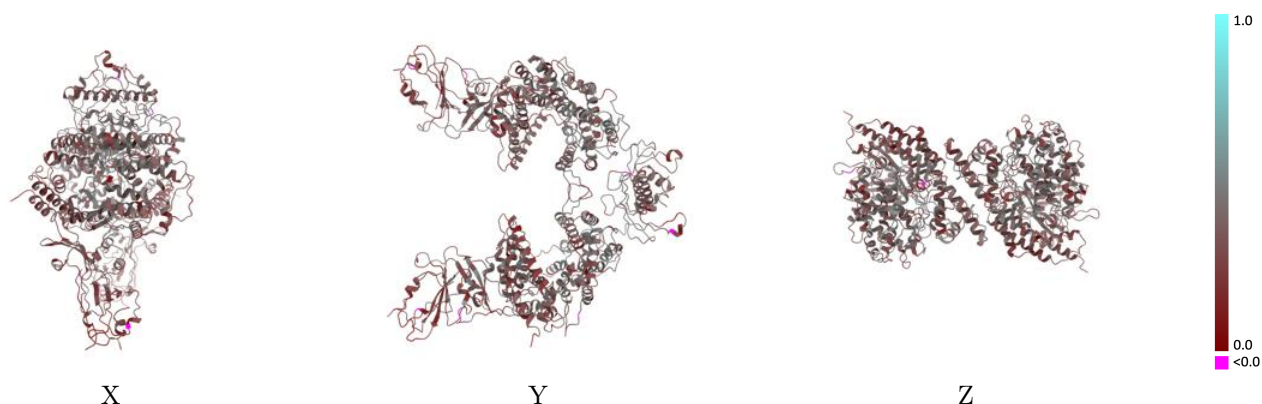
Y



Z

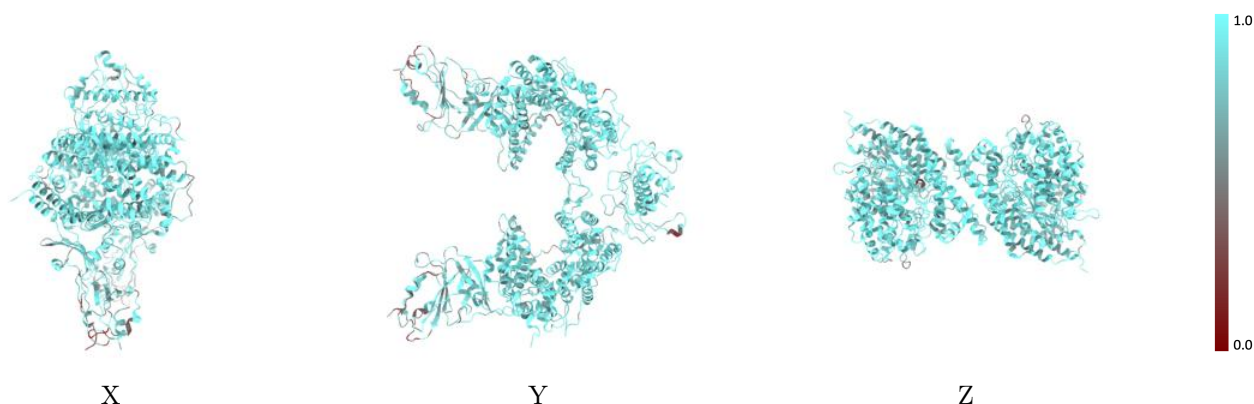
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



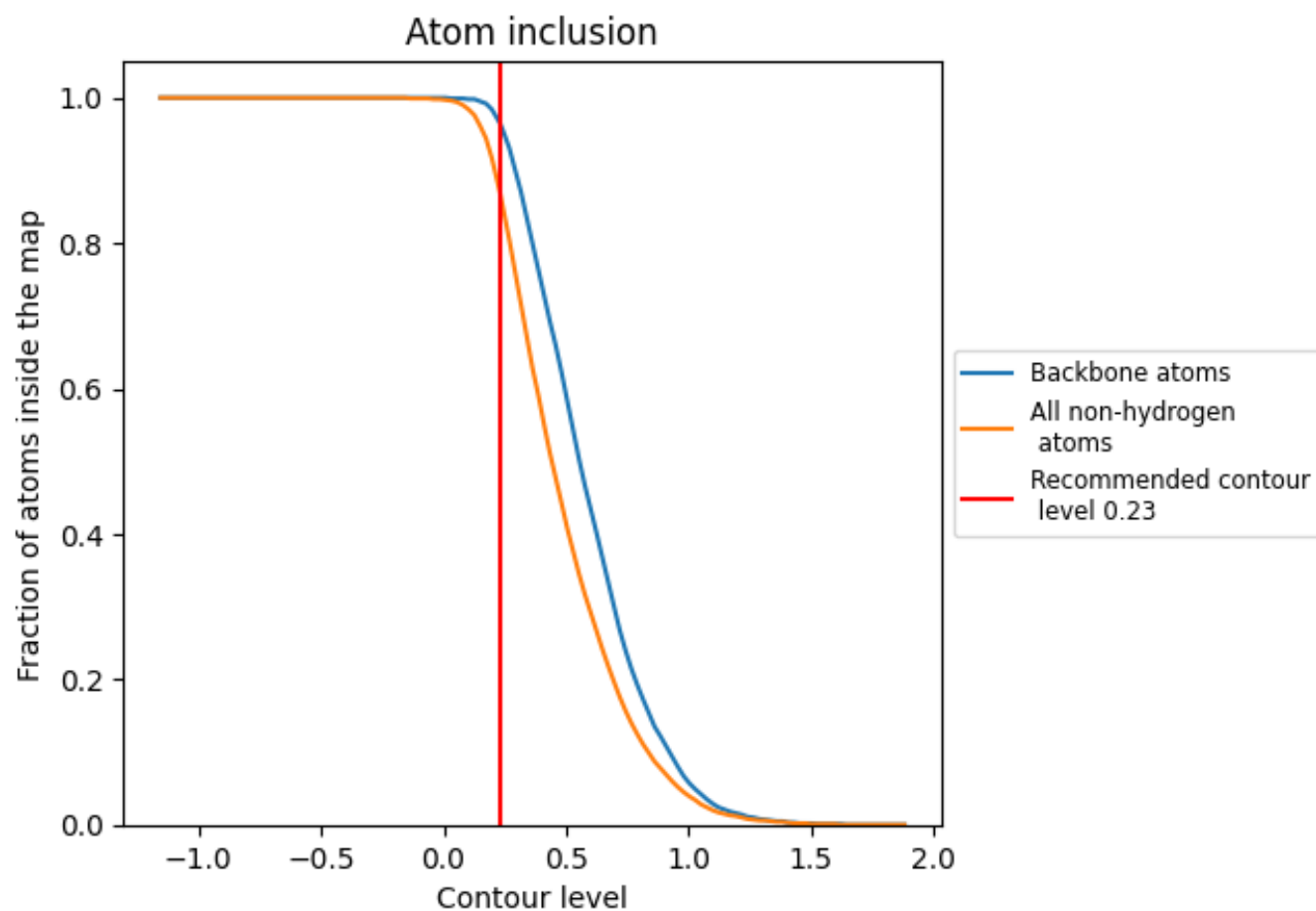
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.23).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8700	<div><div></div></div> 0.3560
A	<div><div></div></div> 0.9040	<div><div></div></div> 0.3720
B	<div><div></div></div> 0.7410	<div><div></div></div> 0.2940
C	<div><div></div></div> 0.9050	<div><div></div></div> 0.3740
D	<div><div></div></div> 0.7390	<div><div></div></div> 0.2910
E	<div><div></div></div> 0.8570	<div><div></div></div> 0.3710
F	<div><div></div></div> 0.8210	<div><div></div></div> 0.4200
G	<div><div></div></div> 0.7140	<div><div></div></div> 0.2900
H	<div><div></div></div> 0.8210	<div><div></div></div> 0.3940

1.0

0.0

<0.0