



## Full wwPDB EM Validation Report ⓘ

Sep 18, 2025 – 12:36 PM EDT

PDB ID : 9MKZ / pdb\_00009mkz  
EMDB ID : EMD-48343  
Title : Structure of acid-sensing ion channel 5 without calcium, open  
Authors : Freitas, M.M.; Gouaux, E.  
Deposited on : 2024-12-18  
Resolution : 3.47 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev126  
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

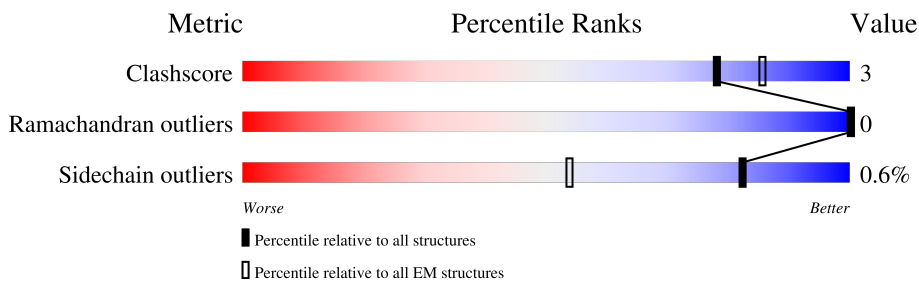
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.47 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	435	<div> <div>17%</div> <div>72%</div> <div>24%</div> <div>• •</div> </div>
1	B	435	<div> <div>17%</div> <div>70%</div> <div>26%</div> <div>• •</div> </div>
1	C	435	<div> <div>17%</div> <div>70%</div> <div>26%</div> <div>• •</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18852 atoms, of which 9225 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.

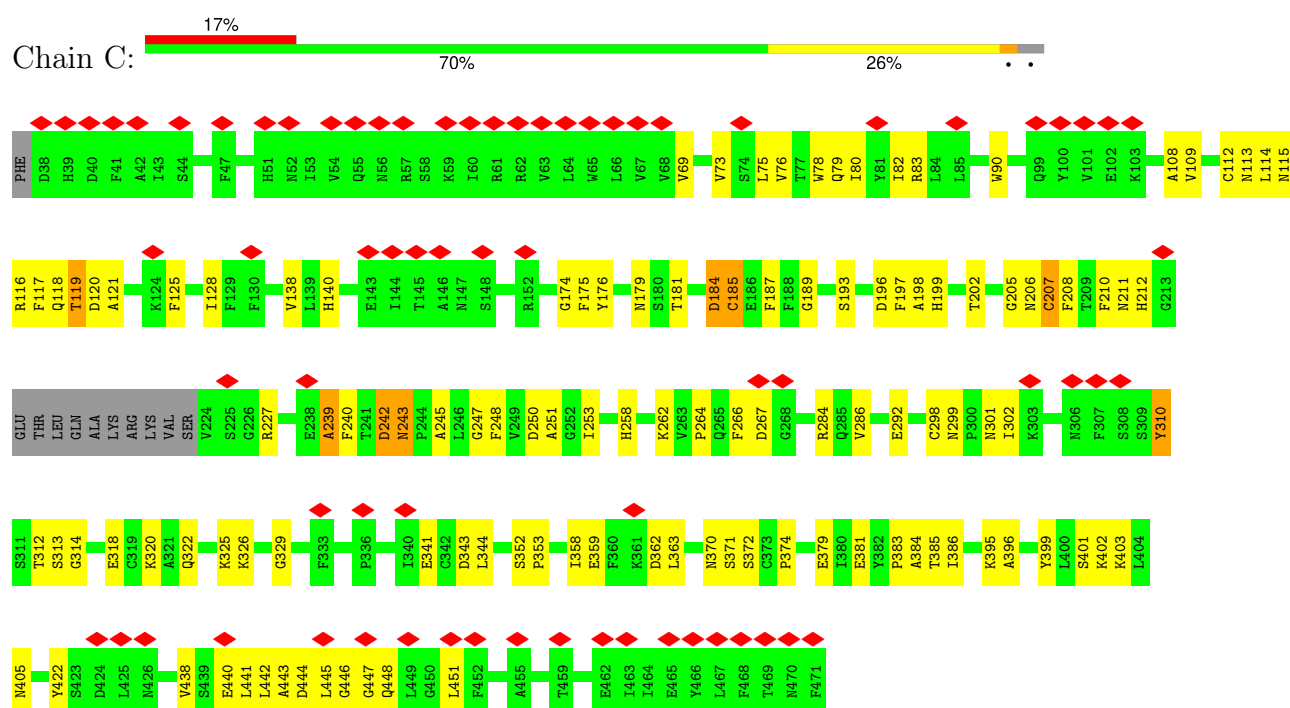
- Molecule 1 is a protein called Acid-sensing ion channel 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	424	Total	C	H	N	O	S	0	0
			6284	2059	3075	543	598	9		
1	B	424	Total	C	H	N	O	S	0	0
			6284	2059	3075	543	598	9		
1	A	424	Total	C	H	N	O	S	0	0
			6284	2059	3075	543	598	9		

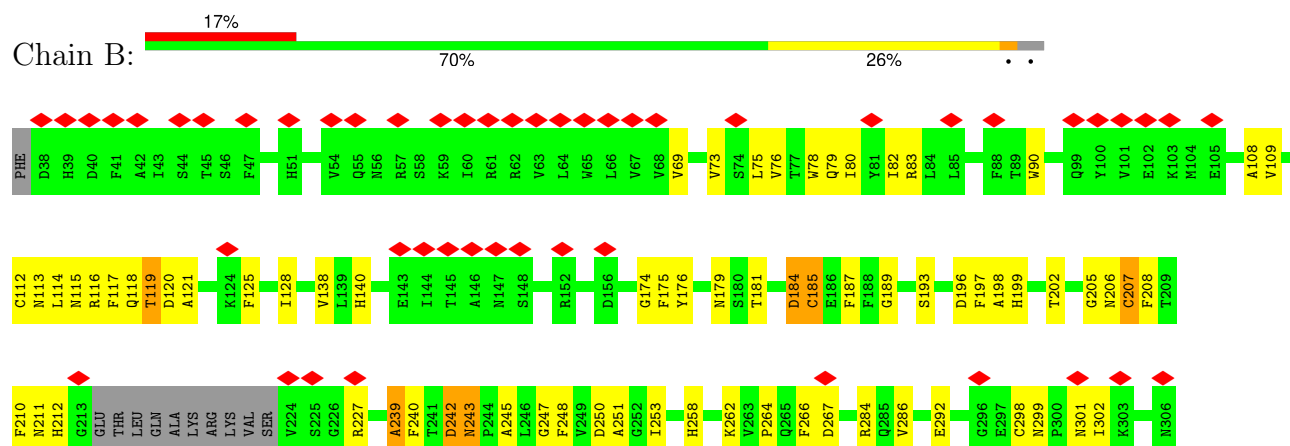
### 3 Residue-property plots

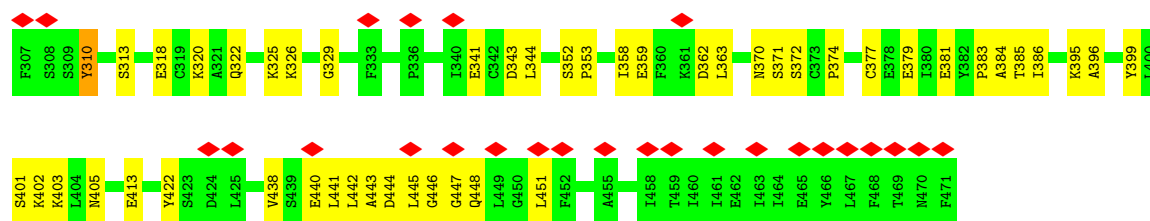
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Acid-sensing ion channel 5

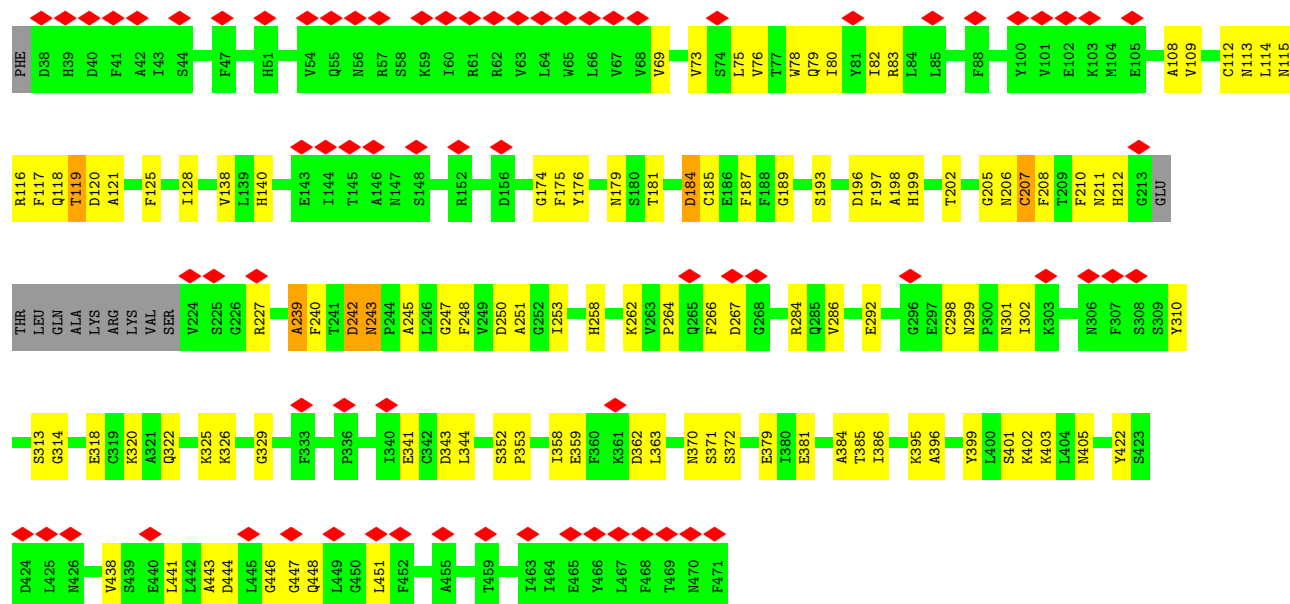


#### • Molecule 1: Acid-sensing ion channel 5





• Molecule 1: Acid-sensing ion channel 5



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18596	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)	400	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.636	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	283.58398, 283.58398, 283.58398	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.844, 0.844, 0.844	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	1.77	32/3286 (1.0%)	1.83	130/4469 (2.9%)
1	B	1.77	32/3286 (1.0%)	1.82	138/4469 (3.1%)
1	C	1.78	34/3286 (1.0%)	1.83	139/4469 (3.1%)
All	All	1.77	98/9858 (1.0%)	1.83	407/13407 (3.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	HIS	ND1-CE1	-8.96	1.23	1.32
1	B	199	HIS	CE1-NE2	-8.91	1.23	1.32
1	A	199	HIS	ND1-CE1	-8.90	1.23	1.32
1	C	199	HIS	CE1-NE2	-8.87	1.23	1.32
1	B	140	HIS	CE1-NE2	-8.87	1.23	1.32
1	C	212	HIS	CE1-NE2	-8.86	1.23	1.32
1	C	258	HIS	ND1-CE1	-8.83	1.23	1.32
1	B	258	HIS	ND1-CE1	-8.83	1.23	1.32
1	A	140	HIS	CE1-NE2	-8.83	1.23	1.32
1	C	199	HIS	ND1-CE1	-8.82	1.23	1.32
1	B	212	HIS	CE1-NE2	-8.82	1.23	1.32
1	A	199	HIS	CE1-NE2	-8.80	1.23	1.32
1	C	140	HIS	CE1-NE2	-8.77	1.23	1.32
1	A	258	HIS	ND1-CE1	-8.75	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	HIS	CE1-NE2	-8.75	1.23	1.32
1	A	116	ARG	CZ-NH2	-8.23	1.22	1.33
1	C	140	HIS	CD2-NE2	-8.21	1.28	1.37
1	B	116	ARG	CZ-NH2	-8.18	1.22	1.33
1	C	116	ARG	CZ-NH2	-8.16	1.22	1.33
1	C	199	HIS	CD2-NE2	-8.16	1.28	1.37
1	A	199	HIS	CD2-NE2	-8.15	1.28	1.37
1	A	212	HIS	CD2-NE2	-8.15	1.28	1.37
1	B	199	HIS	CD2-NE2	-8.13	1.28	1.37
1	A	140	HIS	CD2-NE2	-8.09	1.28	1.37
1	C	212	HIS	CD2-NE2	-8.06	1.28	1.37
1	B	212	HIS	CD2-NE2	-8.05	1.28	1.37
1	B	140	HIS	CD2-NE2	-8.02	1.29	1.37
1	A	83	ARG	CZ-NH2	-7.51	1.23	1.33
1	C	83	ARG	CZ-NH2	-7.50	1.23	1.33
1	B	83	ARG	CZ-NH2	-7.50	1.23	1.33
1	C	108	ALA	CA-CB	-6.96	1.42	1.53
1	B	108	ALA	CA-CB	-6.88	1.42	1.53
1	B	245	ALA	CA-CB	-6.83	1.42	1.53
1	A	245	ALA	CA-CB	-6.83	1.42	1.53
1	C	116	ARG	CZ-NH1	-6.82	1.23	1.32
1	A	108	ALA	CA-CB	-6.81	1.42	1.53
1	C	245	ALA	CA-CB	-6.80	1.42	1.53
1	A	116	ARG	CZ-NH1	-6.72	1.23	1.32
1	B	116	ARG	CZ-NH1	-6.67	1.23	1.32
1	B	239	ALA	CA-CB	-6.67	1.42	1.53
1	A	239	ALA	CA-CB	-6.65	1.42	1.53
1	C	239	ALA	CA-CB	-6.64	1.42	1.53
1	C	198	ALA	CA-CB	-6.55	1.42	1.53
1	A	198	ALA	CA-CB	-6.52	1.42	1.53
1	A	396	ALA	CA-CB	-6.52	1.42	1.53
1	C	396	ALA	CA-CB	-6.51	1.42	1.53
1	B	198	ALA	CA-CB	-6.50	1.42	1.53
1	C	314	GLY	N-CA	-6.36	1.38	1.45
1	A	314	GLY	N-CA	-6.36	1.38	1.45
1	B	251	ALA	CA-CB	-6.23	1.42	1.53
1	A	251	ALA	CA-CB	-6.22	1.42	1.53
1	C	251	ALA	CA-CB	-6.22	1.42	1.53
1	A	83	ARG	CZ-NH1	-6.20	1.24	1.32
1	C	83	ARG	CZ-NH1	-6.18	1.24	1.32
1	B	83	ARG	CZ-NH1	-6.18	1.24	1.32
1	B	396	ALA	CA-CB	-6.14	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	GLN	CA-CB	-6.14	1.43	1.53
1	C	443	ALA	CA-CB	-6.12	1.43	1.53
1	B	443	ALA	CA-CB	-6.12	1.43	1.53
1	B	79	GLN	CA-CB	-6.11	1.43	1.53
1	C	448	GLN	CA-CB	-6.09	1.43	1.53
1	C	79	GLN	CA-CB	-6.08	1.44	1.53
1	C	446	GLY	N-CA	-6.06	1.38	1.45
1	A	443	ALA	CA-CB	-6.04	1.44	1.53
1	B	448	GLN	CA-CB	-6.03	1.43	1.53
1	B	446	GLY	N-CA	-6.00	1.38	1.45
1	A	448	GLN	CA-CB	-6.00	1.43	1.53
1	A	446	GLY	N-CA	-5.80	1.38	1.45
1	C	451	LEU	CA-CB	-5.54	1.48	1.54
1	C	193	SER	CA-CB	-5.53	1.47	1.54
1	A	116	ARG	CD-NE	-5.46	1.38	1.46
1	A	193	SER	CA-CB	-5.46	1.47	1.54
1	A	83	ARG	CD-NE	-5.45	1.38	1.46
1	C	83	ARG	CD-NE	-5.45	1.38	1.46
1	B	83	ARG	CD-NE	-5.42	1.38	1.46
1	B	193	SER	CA-CB	-5.41	1.47	1.54
1	C	116	ARG	CD-NE	-5.40	1.38	1.46
1	A	205	GLY	N-CA	-5.38	1.37	1.45
1	C	247	GLY	N-CA	-5.38	1.37	1.45
1	B	299	ASN	CA-CB	-5.36	1.47	1.53
1	A	193	SER	N-CA	-5.33	1.41	1.45
1	B	205	GLY	N-CA	-5.32	1.37	1.45
1	B	247	GLY	N-CA	-5.31	1.37	1.45
1	B	116	ARG	CD-NE	-5.29	1.38	1.46
1	A	247	GLY	N-CA	-5.29	1.37	1.45
1	A	299	ASN	CA-CB	-5.29	1.47	1.53
1	C	299	ASN	CA-CB	-5.27	1.47	1.53
1	C	205	GLY	N-CA	-5.25	1.37	1.45
1	C	189	GLY	N-CA	-5.25	1.37	1.45
1	A	189	GLY	N-CA	-5.24	1.37	1.45
1	B	193	SER	N-CA	-5.23	1.41	1.45
1	B	189	GLY	N-CA	-5.19	1.37	1.45
1	C	264	PRO	CA-CB	-5.18	1.46	1.53
1	C	193	SER	N-CA	-5.16	1.41	1.45
1	B	383	PRO	CA-CB	-5.15	1.47	1.53
1	C	383	PRO	CA-CB	-5.10	1.47	1.53
1	A	264	PRO	CA-CB	-5.08	1.46	1.53
1	B	264	PRO	CA-CB	-5.04	1.46	1.53

All (407) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	262	LYS	CA-C-N	7.58	130.01	123.04
1	C	262	LYS	C-N-CA	7.58	130.01	123.04
1	A	262	LYS	CA-C-N	7.56	130.00	123.04
1	A	262	LYS	C-N-CA	7.56	130.00	123.04
1	B	196	ASP	CA-CB-CG	7.36	119.96	112.60
1	C	196	ASP	CA-CB-CG	7.33	119.93	112.60
1	C	206	ASN	CA-CB-CG	7.30	119.90	112.60
1	A	196	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	206	ASN	CA-CB-CG	7.24	119.84	112.60
1	B	206	ASN	CA-CB-CG	7.22	119.82	112.60
1	C	197	PHE	CA-CB-CG	7.16	120.96	113.80
1	B	197	PHE	CA-CB-CG	7.14	120.94	113.80
1	A	197	PHE	CA-CB-CG	7.12	120.92	113.80
1	C	267	ASP	CA-CB-CG	7.10	119.70	112.60
1	B	267	ASP	CA-CB-CG	7.10	119.70	112.60
1	A	267	ASP	CA-CB-CG	7.09	119.69	112.60
1	C	242	ASP	CA-CB-CG	6.97	119.58	112.60
1	B	242	ASP	CA-CB-CG	6.97	119.58	112.60
1	A	242	ASP	CA-CB-CG	6.97	119.57	112.60
1	B	405	ASN	CA-CB-CG	6.91	119.51	112.60
1	C	405	ASN	CA-CB-CG	6.87	119.47	112.60
1	A	175	PHE	CA-CB-CG	6.87	120.67	113.80
1	C	187	PHE	CA-CB-CG	6.87	120.67	113.80
1	A	405	ASN	CA-CB-CG	6.86	119.46	112.60
1	A	210	PHE	CA-CB-CG	6.85	120.65	113.80
1	B	211	ASN	CA-CB-CG	6.85	119.45	112.60
1	A	187	PHE	CA-CB-CG	6.84	120.64	113.80
1	A	211	ASN	CA-CB-CG	6.84	119.44	112.60
1	C	210	PHE	CA-CB-CG	6.83	120.63	113.80
1	C	211	ASN	CA-CB-CG	6.83	119.43	112.60
1	C	175	PHE	CA-CB-CG	6.83	120.63	113.80
1	C	113	ASN	CA-CB-CG	6.81	119.41	112.60
1	B	113	ASN	CA-CB-CG	6.81	119.41	112.60
1	B	175	PHE	CA-CB-CG	6.79	120.59	113.80
1	B	210	PHE	CA-CB-CG	6.78	120.58	113.80
1	B	187	PHE	CA-CB-CG	6.77	120.57	113.80
1	A	113	ASN	CA-CB-CG	6.73	119.33	112.60
1	C	243	ASN	CA-CB-CG	6.73	119.33	112.60
1	C	179	ASN	CA-CB-CG	6.68	119.28	112.60
1	B	243	ASN	CA-CB-CG	6.67	119.27	112.60
1	A	179	ASN	CA-CB-CG	6.67	119.27	112.60
1	A	243	ASN	CA-CB-CG	6.66	119.26	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	ASN	CA-CB-CG	6.62	119.22	112.60
1	B	266	PHE	CA-CB-CG	6.61	120.41	113.80
1	B	298	CYS	CA-C-N	6.58	131.12	123.15
1	B	298	CYS	C-N-CA	6.58	131.12	123.15
1	A	266	PHE	CA-CB-CG	6.58	120.38	113.80
1	A	115	ASN	CA-CB-CG	6.56	119.16	112.60
1	A	372	SER	CA-C-N	6.55	131.07	123.15
1	A	372	SER	C-N-CA	6.55	131.07	123.15
1	C	115	ASN	CA-CB-CG	6.54	119.14	112.60
1	C	266	PHE	CA-CB-CG	6.54	120.34	113.80
1	B	372	SER	CA-C-N	6.53	131.05	123.15
1	B	372	SER	C-N-CA	6.53	131.05	123.15
1	C	298	CYS	CA-C-N	6.52	131.04	123.15
1	C	298	CYS	C-N-CA	6.52	131.04	123.15
1	B	115	ASN	CA-CB-CG	6.50	119.10	112.60
1	A	208	PHE	CA-CB-CG	6.48	120.28	113.80
1	C	362	ASP	CA-CB-CG	6.47	119.07	112.60
1	A	298	CYS	CA-C-N	6.46	130.97	123.15
1	A	298	CYS	C-N-CA	6.46	130.97	123.15
1	C	208	PHE	CA-CB-CG	6.46	120.26	113.80
1	C	372	SER	CA-C-N	6.46	130.96	123.15
1	C	372	SER	C-N-CA	6.46	130.96	123.15
1	A	362	ASP	CA-CB-CG	6.45	119.05	112.60
1	B	208	PHE	CA-CB-CG	6.43	120.23	113.80
1	B	362	ASP	CA-CB-CG	6.41	119.01	112.60
1	B	184	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	184	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	199	HIS	CA-CB-CG	6.36	120.16	113.80
1	B	199	HIS	CA-CB-CG	6.34	120.14	113.80
1	C	199	HIS	CA-CB-CG	6.33	120.13	113.80
1	C	301	ASN	CA-CB-CG	6.31	118.91	112.60
1	C	184	ASP	CA-CB-CG	6.31	118.91	112.60
1	B	301	ASN	CA-CB-CG	6.26	118.86	112.60
1	B	299	ASN	CA-CB-CG	6.25	118.84	112.60
1	A	301	ASN	CA-CB-CG	6.24	118.84	112.60
1	A	299	ASN	CA-CB-CG	6.19	118.79	112.60
1	C	299	ASN	CA-CB-CG	6.19	118.79	112.60
1	C	240	PHE	CA-CB-CG	6.07	119.87	113.80
1	A	370	ASN	CA-CB-CG	6.06	118.66	112.60
1	A	240	PHE	CA-CB-CG	6.05	119.85	113.80
1	B	240	PHE	CA-CB-CG	6.03	119.83	113.80
1	C	370	ASN	CA-CB-CG	6.01	118.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	ASN	CA-CB-CG	5.98	118.58	112.60
1	C	384	ALA	CA-C-N	5.97	131.40	122.99
1	C	384	ALA	C-N-CA	5.97	131.40	122.99
1	A	117	PHE	CA-CB-CG	5.92	119.72	113.80
1	B	262	LYS	CA-C-N	5.92	129.94	123.43
1	B	262	LYS	C-N-CA	5.92	129.94	123.43
1	B	384	ALA	CA-C-N	5.92	131.33	122.99
1	B	384	ALA	C-N-CA	5.92	131.33	122.99
1	C	109	VAL	CA-C-N	5.91	131.32	122.99
1	C	109	VAL	C-N-CA	5.91	131.32	122.99
1	C	117	PHE	CA-CB-CG	5.89	119.69	113.80
1	B	114	LEU	CA-C-N	5.89	130.60	122.77
1	B	114	LEU	C-N-CA	5.89	130.60	122.77
1	B	117	PHE	CA-CB-CG	5.89	119.69	113.80
1	B	445	LEU	CA-C-N	5.80	126.42	119.98
1	B	445	LEU	C-N-CA	5.80	126.42	119.98
1	A	114	LEU	CA-C-N	5.79	130.72	122.72
1	A	114	LEU	C-N-CA	5.79	130.72	122.72
1	C	114	LEU	CA-C-N	5.79	130.70	122.72
1	C	114	LEU	C-N-CA	5.79	130.70	122.72
1	A	384	ALA	CA-C-N	5.79	131.32	122.93
1	A	384	ALA	C-N-CA	5.79	131.32	122.93
1	C	253	ILE	CA-C-N	5.77	130.34	123.19
1	C	253	ILE	C-N-CA	5.77	130.34	123.19
1	B	253	ILE	CA-C-N	5.72	130.29	123.19
1	B	253	ILE	C-N-CA	5.72	130.29	123.19
1	B	90	TRP	CB-CA-C	5.72	115.97	111.00
1	C	445	LEU	CA-C-N	5.69	126.29	119.98
1	C	445	LEU	C-N-CA	5.69	126.29	119.98
1	A	444	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	196	ASP	CA-C-N	5.67	129.95	122.30
1	A	196	ASP	C-N-CA	5.67	129.95	122.30
1	B	112	CYS	CA-C-N	5.67	129.95	122.30
1	B	112	CYS	C-N-CA	5.67	129.95	122.30
1	B	196	ASP	CA-C-N	5.65	129.93	122.30
1	B	196	ASP	C-N-CA	5.65	129.93	122.30
1	B	447	GLY	CA-C-N	5.64	128.11	120.38
1	B	447	GLY	C-N-CA	5.64	128.11	120.38
1	C	112	CYS	CA-C-N	5.64	129.91	122.30
1	C	112	CYS	C-N-CA	5.64	129.91	122.30
1	C	447	GLY	CA-C-N	5.63	128.09	120.38
1	C	447	GLY	C-N-CA	5.63	128.09	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	196	ASP	CA-C-N	5.62	129.89	122.30
1	C	196	ASP	C-N-CA	5.62	129.89	122.30
1	C	207	CYS	CA-C-N	5.62	131.02	122.65
1	C	207	CYS	C-N-CA	5.62	131.02	122.65
1	C	248	PHE	CA-CB-CG	5.61	119.41	113.80
1	B	248	PHE	CA-CB-CG	5.61	119.41	113.80
1	A	248	PHE	CA-CB-CG	5.61	119.41	113.80
1	A	379	GLU	CA-C-N	5.60	130.93	122.98
1	A	379	GLU	C-N-CA	5.60	130.93	122.98
1	B	109	VAL	CA-C-N	5.58	131.33	122.74
1	B	109	VAL	C-N-CA	5.58	131.33	122.74
1	B	207	CYS	CA-C-N	5.58	130.96	122.65
1	B	207	CYS	C-N-CA	5.58	130.96	122.65
1	B	444	ASP	CA-CB-CG	5.58	118.17	112.60
1	B	379	GLU	CA-C-N	5.57	130.89	122.98
1	B	379	GLU	C-N-CA	5.57	130.89	122.98
1	C	379	GLU	CA-C-N	5.56	130.88	122.98
1	C	379	GLU	C-N-CA	5.56	130.88	122.98
1	A	112	CYS	CA-C-N	5.56	129.78	121.72
1	A	112	CYS	C-N-CA	5.56	129.78	121.72
1	C	444	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	198	ALA	CA-C-N	5.55	130.66	123.00
1	B	198	ALA	C-N-CA	5.55	130.66	123.00
1	C	198	ALA	CA-C-N	5.54	130.65	123.00
1	C	198	ALA	C-N-CA	5.54	130.65	123.00
1	A	80	ILE	N-CA-CB	5.54	116.44	110.62
1	C	116	ARG	CA-CB-CG	5.54	125.18	114.10
1	A	76	VAL	N-CA-CB	5.54	116.66	110.51
1	B	76	VAL	N-CA-CB	5.53	116.65	110.51
1	A	198	ALA	CA-C-N	5.53	130.63	123.00
1	A	198	ALA	C-N-CA	5.53	130.63	123.00
1	C	90	TRP	CB-CA-C	5.53	115.81	111.00
1	B	116	ARG	CA-CB-CG	5.52	125.14	114.10
1	A	207	CYS	CA-C-N	5.52	130.87	122.65
1	A	207	CYS	C-N-CA	5.52	130.87	122.65
1	C	80	ILE	N-CA-CB	5.51	116.41	110.62
1	B	385	THR	CA-C-N	5.51	130.36	123.14
1	B	385	THR	C-N-CA	5.51	130.36	123.14
1	A	116	ARG	CA-CB-CG	5.51	125.11	114.10
1	B	363	LEU	CA-C-N	5.50	130.76	123.00
1	B	363	LEU	C-N-CA	5.50	130.76	123.00
1	A	181	THR	CA-C-N	5.50	130.91	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	THR	C-N-CA	5.50	130.91	122.77
1	C	363	LEU	CA-C-N	5.49	130.73	122.99
1	C	363	LEU	C-N-CA	5.49	130.73	122.99
1	B	80	ILE	N-CA-CB	5.47	116.36	110.62
1	A	363	LEU	CA-C-N	5.47	130.70	122.99
1	A	363	LEU	C-N-CA	5.47	130.70	122.99
1	A	109	VAL	CA-C-N	5.46	131.16	122.74
1	A	109	VAL	C-N-CA	5.46	131.16	122.74
1	B	181	THR	CA-C-N	5.46	130.85	122.77
1	B	181	THR	C-N-CA	5.46	130.85	122.77
1	C	181	THR	CA-C-N	5.46	130.85	122.77
1	C	181	THR	C-N-CA	5.46	130.85	122.77
1	A	447	GLY	CA-C-N	5.41	127.80	120.38
1	A	447	GLY	C-N-CA	5.41	127.80	120.38
1	C	76	VAL	N-CA-CB	5.41	116.52	110.51
1	C	258	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	A	258	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	C	371	SER	N-CA-CB	5.41	117.99	110.26
1	B	371	SER	N-CA-CB	5.41	117.99	110.26
1	B	258	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
1	C	385	THR	CA-C-N	5.39	130.20	123.14
1	C	385	THR	C-N-CA	5.39	130.20	123.14
1	A	371	SER	N-CA-CB	5.37	117.94	110.26
1	C	250	ASP	CA-C-N	5.37	130.71	122.93
1	C	250	ASP	C-N-CA	5.37	130.71	122.93
1	C	386	ILE	CA-C-N	5.36	130.98	122.62
1	C	386	ILE	C-N-CA	5.36	130.98	122.62
1	A	386	ILE	CA-C-N	5.35	130.97	122.62
1	A	386	ILE	C-N-CA	5.35	130.97	122.62
1	B	395	LYS	N-CA-CB	5.35	117.77	110.01
1	C	284	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	C	176	TYR	CA-C-N	5.33	130.86	123.07
1	C	176	TYR	C-N-CA	5.33	130.86	123.07
1	B	386	ILE	CA-C-N	5.33	130.93	122.62
1	B	386	ILE	C-N-CA	5.33	130.93	122.62
1	A	250	ASP	CA-C-N	5.32	130.64	122.93
1	A	250	ASP	C-N-CA	5.32	130.64	122.93
1	A	399	TYR	N-CA-CB	5.32	117.72	110.01
1	B	399	TYR	N-CA-CB	5.32	117.72	110.01
1	A	395	LYS	N-CA-CB	5.32	117.72	110.01
1	A	385	THR	CA-C-N	5.31	130.10	123.14
1	A	385	THR	C-N-CA	5.31	130.10	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ILE	CA-C-N	5.31	129.78	123.19
1	A	253	ILE	C-N-CA	5.31	129.78	123.19
1	B	199	HIS	ND1-CG-CD2	-5.30	100.80	106.10
1	B	442	LEU	CA-C-N	5.30	127.33	120.44
1	B	442	LEU	C-N-CA	5.30	127.33	120.44
1	A	199	HIS	CA-C-N	5.30	130.35	122.71
1	A	199	HIS	C-N-CA	5.30	130.35	122.71
1	C	199	HIS	ND1-CG-CD2	-5.29	100.81	106.10
1	A	176	TYR	CA-C-N	5.29	130.80	123.07
1	A	176	TYR	C-N-CA	5.29	130.80	123.07
1	B	250	ASP	CA-C-N	5.29	130.60	122.93
1	B	250	ASP	C-N-CA	5.29	130.60	122.93
1	A	258	HIS	ND1-CG-CD2	-5.29	100.81	106.10
1	C	442	LEU	CA-C-N	5.29	127.32	120.44
1	C	442	LEU	C-N-CA	5.29	127.32	120.44
1	B	258	HIS	ND1-CG-CD2	-5.29	100.81	106.10
1	C	399	TYR	N-CA-CB	5.29	117.68	110.01
1	B	199	HIS	CA-C-N	5.28	130.31	122.71
1	B	199	HIS	C-N-CA	5.28	130.31	122.71
1	B	310	TYR	N-CA-CB	5.28	117.80	109.83
1	C	286	VAL	CA-C-N	5.27	130.84	122.94
1	C	286	VAL	C-N-CA	5.27	130.84	122.94
1	C	395	LYS	N-CA-CB	5.27	117.71	110.07
1	C	258	HIS	ND1-CG-CD2	-5.27	100.83	106.10
1	A	258	HIS	CG-CD2-NE2	5.27	112.47	107.20
1	A	310	TYR	N-CA-CB	5.27	117.78	109.83
1	B	176	TYR	CA-C-N	5.26	130.75	123.07
1	B	176	TYR	C-N-CA	5.26	130.75	123.07
1	C	199	HIS	CA-C-N	5.25	130.28	122.71
1	C	199	HIS	C-N-CA	5.25	130.28	122.71
1	C	258	HIS	CG-CD2-NE2	5.25	112.45	107.20
1	A	199	HIS	ND1-CG-CD2	-5.25	100.85	106.10
1	A	138	VAL	CA-C-N	5.25	130.44	122.56
1	A	138	VAL	C-N-CA	5.25	130.44	122.56
1	B	258	HIS	CG-CD2-NE2	5.24	112.44	107.20
1	C	310	TYR	N-CA-CB	5.24	117.74	109.83
1	B	298	CYS	N-CA-CB	5.24	117.74	109.83
1	A	117	PHE	CA-C-N	5.23	128.20	120.82
1	A	117	PHE	C-N-CA	5.23	128.20	120.82
1	A	286	VAL	CA-C-N	5.23	130.79	122.94
1	A	286	VAL	C-N-CA	5.23	130.79	122.94
1	B	138	VAL	CA-C-N	5.23	130.40	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	VAL	C-N-CA	5.23	130.40	122.56
1	C	138	VAL	CA-C-N	5.22	130.39	122.56
1	C	138	VAL	C-N-CA	5.22	130.39	122.56
1	B	284	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	B	286	VAL	CA-C-N	5.22	130.77	122.94
1	B	286	VAL	C-N-CA	5.22	130.77	122.94
1	C	117	PHE	CA-C-N	5.22	128.18	120.82
1	C	117	PHE	C-N-CA	5.22	128.18	120.82
1	C	115	ASN	CA-C-N	5.21	128.71	120.89
1	C	115	ASN	C-N-CA	5.21	128.71	120.89
1	A	115	ASN	CA-C-N	5.21	128.71	120.89
1	A	115	ASN	C-N-CA	5.21	128.71	120.89
1	C	80	ILE	CA-C-N	5.21	127.21	120.44
1	C	80	ILE	C-N-CA	5.21	127.21	120.44
1	A	441	LEU	CA-C-N	5.20	127.20	120.44
1	A	441	LEU	C-N-CA	5.20	127.20	120.44
1	B	117	PHE	CA-C-N	5.20	128.15	120.82
1	B	117	PHE	C-N-CA	5.20	128.15	120.82
1	C	438	VAL	N-CA-CB	5.20	116.28	110.51
1	A	80	ILE	CA-C-N	5.19	127.19	120.44
1	A	80	ILE	C-N-CA	5.19	127.19	120.44
1	A	298	CYS	N-CA-CB	5.18	117.66	109.83
1	A	402	LYS	CA-C-N	5.18	127.18	120.44
1	A	402	LYS	C-N-CA	5.18	127.18	120.44
1	B	438	VAL	N-CA-CB	5.18	116.26	110.51
1	A	438	VAL	N-CA-CB	5.18	116.26	110.51
1	C	401	SER	N-CA-CB	5.18	117.52	110.01
1	C	402	LYS	CA-C-N	5.18	127.17	120.44
1	C	402	LYS	C-N-CA	5.18	127.17	120.44
1	B	359	GLU	N-CA-CB	5.17	117.51	110.01
1	B	402	LYS	CA-C-N	5.17	127.16	120.44
1	B	402	LYS	C-N-CA	5.17	127.16	120.44
1	C	359	GLU	N-CA-CB	5.16	117.50	110.01
1	B	320	LYS	CA-CB-CG	5.16	124.42	114.10
1	B	313	SER	N-CA-CB	5.15	117.48	110.01
1	C	298	CYS	N-CA-CB	5.15	117.61	109.83
1	B	80	ILE	CA-C-N	5.15	127.13	120.44
1	B	80	ILE	C-N-CA	5.15	127.13	120.44
1	A	371	SER	CA-C-N	5.15	128.13	120.31
1	A	371	SER	C-N-CA	5.15	128.13	120.31
1	A	359	GLU	N-CA-CB	5.14	117.47	110.01
1	C	82	ILE	N-CA-CB	5.14	116.56	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	441	LEU	CA-C-N	5.14	127.12	120.44
1	B	441	LEU	C-N-CA	5.14	127.12	120.44
1	C	116	ARG	CD-NE-CZ	5.14	131.59	124.40
1	C	313	SER	N-CA-CB	5.14	117.46	110.01
1	B	115	ASN	CA-C-N	5.14	128.59	120.89
1	B	115	ASN	C-N-CA	5.14	128.59	120.89
1	A	262	LYS	CA-CB-CG	5.14	124.38	114.10
1	A	395	LYS	CA-C-N	5.14	127.68	120.28
1	A	395	LYS	C-N-CA	5.14	127.68	120.28
1	A	313	SER	N-CA-CB	5.13	117.45	110.01
1	C	441	LEU	CA-C-N	5.12	127.10	120.44
1	C	441	LEU	C-N-CA	5.12	127.10	120.44
1	C	76	VAL	CA-C-N	5.12	127.14	120.28
1	C	76	VAL	C-N-CA	5.12	127.14	120.28
1	B	118	GLN	CA-C-N	5.12	127.10	120.44
1	B	118	GLN	C-N-CA	5.12	127.10	120.44
1	B	76	VAL	CA-C-N	5.11	127.13	120.28
1	B	76	VAL	C-N-CA	5.11	127.13	120.28
1	A	76	VAL	CA-C-N	5.11	127.13	120.28
1	A	76	VAL	C-N-CA	5.11	127.13	120.28
1	A	118	GLN	CA-C-N	5.11	127.08	120.44
1	A	118	GLN	C-N-CA	5.11	127.08	120.44
1	A	320	LYS	CA-CB-CG	5.11	124.31	114.10
1	C	118	GLN	CA-C-N	5.10	127.08	120.44
1	C	118	GLN	C-N-CA	5.10	127.08	120.44
1	C	358	ILE	CA-C-N	5.10	127.08	120.44
1	C	358	ILE	C-N-CA	5.10	127.08	120.44
1	B	116	ARG	CD-NE-CZ	5.10	131.54	124.40
1	C	320	LYS	CA-CB-CG	5.10	124.30	114.10
1	C	371	SER	CA-C-N	5.09	128.05	120.31
1	C	371	SER	C-N-CA	5.09	128.05	120.31
1	A	401	SER	CA-C-N	5.08	127.05	120.44
1	A	401	SER	C-N-CA	5.08	127.05	120.44
1	A	116	ARG	CD-NE-CZ	5.08	131.51	124.40
1	A	82	ILE	N-CA-CB	5.08	116.49	110.55
1	C	395	LYS	CA-C-N	5.07	127.59	120.28
1	C	395	LYS	C-N-CA	5.07	127.59	120.28
1	B	82	ILE	N-CA-CB	5.07	116.48	110.55
1	B	371	SER	CA-C-N	5.07	128.02	120.31
1	B	371	SER	C-N-CA	5.07	128.02	120.31
1	C	440	GLU	CA-C-N	5.07	127.03	120.44
1	C	440	GLU	C-N-CA	5.07	127.03	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	ILE	CA-C-N	5.07	127.03	120.44
1	B	358	ILE	C-N-CA	5.07	127.03	120.44
1	A	302	ILE	N-CA-CB	5.07	116.62	110.95
1	B	174	GLY	CA-C-N	5.06	127.90	120.71
1	B	174	GLY	C-N-CA	5.06	127.90	120.71
1	A	401	SER	N-CA-CB	5.06	117.48	109.94
1	A	78	TRP	CA-C-N	5.06	127.01	120.44
1	A	78	TRP	C-N-CA	5.06	127.01	120.44
1	A	79	GLN	CA-C-N	5.06	127.40	120.77
1	A	79	GLN	C-N-CA	5.06	127.40	120.77
1	A	358	ILE	CA-C-N	5.06	127.01	120.44
1	A	358	ILE	C-N-CA	5.06	127.01	120.44
1	C	75	LEU	CA-C-N	5.05	127.12	120.60
1	C	75	LEU	C-N-CA	5.05	127.12	120.60
1	C	78	TRP	CA-C-N	5.05	127.01	120.44
1	C	78	TRP	C-N-CA	5.05	127.01	120.44
1	C	174	GLY	CA-C-N	5.05	127.88	120.71
1	C	174	GLY	C-N-CA	5.05	127.88	120.71
1	B	185	CYS	CA-C-N	5.05	130.52	122.74
1	B	185	CYS	C-N-CA	5.05	130.52	122.74
1	C	312	THR	CA-C-N	5.05	127.00	120.44
1	C	312	THR	C-N-CA	5.05	127.00	120.44
1	C	401	SER	CA-C-N	5.04	127.00	120.44
1	C	401	SER	C-N-CA	5.04	127.00	120.44
1	B	116	ARG	CG-CD-NE	5.04	123.10	112.00
1	A	284	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	B	78	TRP	CA-C-N	5.04	127.00	120.44
1	B	78	TRP	C-N-CA	5.04	127.00	120.44
1	B	402	LYS	CA-CB-CG	5.04	124.18	114.10
1	B	405	ASN	CA-C-N	5.04	130.99	122.87
1	B	405	ASN	C-N-CA	5.04	130.99	122.87
1	B	401	SER	N-CA-CB	5.04	117.45	109.94
1	A	405	ASN	CA-C-N	5.04	130.98	122.87
1	A	405	ASN	C-N-CA	5.04	130.98	122.87
1	B	302	ILE	N-CA-CB	5.03	116.59	110.95
1	A	403	LYS	N-CA-CB	5.03	117.31	110.01
1	B	440	GLU	CA-C-N	5.03	127.02	120.28
1	B	440	GLU	C-N-CA	5.03	127.02	120.28
1	C	116	ARG	CG-CD-NE	5.03	123.07	112.00
1	B	377	CYS	CA-C-N	5.03	130.47	122.62
1	B	377	CYS	C-N-CA	5.03	130.47	122.62
1	A	75	LEU	CA-C-N	5.03	127.09	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	LEU	C-N-CA	5.03	127.09	120.60
1	B	401	SER	CA-C-N	5.03	126.97	120.44
1	B	401	SER	C-N-CA	5.03	126.97	120.44
1	C	262	LYS	CA-CB-CG	5.03	124.15	114.10
1	C	302	ILE	N-CA-CB	5.03	116.58	110.95
1	B	403	LYS	N-CA-CB	5.02	117.29	110.01
1	A	174	GLY	CA-C-N	5.02	127.90	120.82
1	A	174	GLY	C-N-CA	5.02	127.90	120.82
1	C	403	LYS	N-CA-CB	5.02	117.29	110.01
1	C	438	VAL	CA-C-N	5.02	126.97	120.44
1	C	438	VAL	C-N-CA	5.02	126.97	120.44
1	A	443	ALA	CA-C-N	5.02	127.94	120.31
1	A	443	ALA	C-N-CA	5.02	127.94	120.31
1	C	185	CYS	CA-C-N	5.01	130.46	122.74
1	C	185	CYS	C-N-CA	5.01	130.46	122.74
1	A	402	LYS	CA-CB-CG	5.01	124.12	114.10
1	B	119	THR	CA-C-N	5.01	126.95	120.44
1	B	119	THR	C-N-CA	5.01	126.95	120.44
1	C	79	GLN	CA-C-N	5.01	127.33	120.77
1	C	79	GLN	C-N-CA	5.01	127.33	120.77
1	B	75	LEU	CA-C-N	5.01	127.06	120.60
1	B	75	LEU	C-N-CA	5.01	127.06	120.60
1	B	262	LYS	CA-CB-CG	5.01	124.11	114.10
1	C	119	THR	CA-C-N	5.01	126.95	120.44
1	C	119	THR	C-N-CA	5.01	126.95	120.44
1	A	119	THR	CA-C-N	5.00	126.95	120.44
1	A	119	THR	C-N-CA	5.00	126.95	120.44
1	B	79	GLN	CA-C-N	5.00	127.32	120.77
1	B	79	GLN	C-N-CA	5.00	127.32	120.77

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	ARG	Sidechain
1	B	227	ARG	Sidechain
1	C	227	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3209	3075	3002	16	0
1	B	3209	3075	3002	17	0
1	C	3209	3075	3002	17	0
All	All	9627	9225	9006	50	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 3.

All (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:THR:OG1	1:B:207:CYS:SG	2.43	0.76
1:A:202:THR:OG1	1:A:207:CYS:SG	2.44	0.76
1:C:202:THR:OG1	1:C:207:CYS:SG	2.48	0.71
1:B:343:ASP:OD1	1:B:344:LEU:N	2.24	0.71
1:B:292:GLU:N	1:B:292:GLU:OE1	2.23	0.71
1:C:292:GLU:N	1:C:292:GLU:OE1	2.23	0.71
1:C:343:ASP:OD1	1:C:344:LEU:N	2.24	0.71
1:A:343:ASP:OD1	1:A:344:LEU:N	2.24	0.70
1:A:292:GLU:N	1:A:292:GLU:OE1	2.23	0.70
1:B:341:GLU:OE1	1:B:341:GLU:N	2.27	0.68
1:A:341:GLU:N	1:A:341:GLU:OE1	2.27	0.68
1:B:242:ASP:OD1	1:B:243:ASN:N	2.28	0.67
1:C:341:GLU:N	1:C:341:GLU:OE1	2.26	0.66
1:C:381:GLU:N	1:C:381:GLU:OE1	2.28	0.66
1:B:381:GLU:OE1	1:B:381:GLU:N	2.28	0.66
1:C:242:ASP:OD1	1:C:243:ASN:N	2.28	0.66
1:A:242:ASP:OD1	1:A:243:ASN:N	2.28	0.66
1:A:381:GLU:N	1:A:381:GLU:OE1	2.28	0.66
1:A:326:LYS:O	1:A:326:LYS:NZ	2.29	0.63
1:B:326:LYS:O	1:B:326:LYS:NZ	2.29	0.63
1:C:326:LYS:O	1:C:326:LYS:NZ	2.30	0.59
1:C:184:ASP:OD1	1:C:185:CYS:N	2.40	0.54
1:A:184:ASP:OD1	1:A:185:CYS:N	2.40	0.54
1:C:69:VAL:O	1:C:73:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASP:OD1	1:B:185:CYS:N	2.41	0.53
1:B:69:VAL:O	1:B:73:VAL:HG23	2.09	0.53
1:C:120:ASP:OD1	1:C:121:ALA:N	2.42	0.53
1:A:120:ASP:OD1	1:A:121:ALA:N	2.42	0.53
1:B:120:ASP:OD1	1:B:121:ALA:N	2.43	0.52
1:A:69:VAL:O	1:A:73:VAL:HG23	2.09	0.52
1:C:318:GLU:OE2	1:C:322:GLN:NE2	2.41	0.51
1:A:318:GLU:OE2	1:A:322:GLN:NE2	2.41	0.51
1:A:325:LYS:O	1:A:329:GLY:N	2.43	0.48
1:C:310:TYR:OH	1:C:374:PRO:O	2.25	0.46
1:C:325:LYS:O	1:C:329:GLY:N	2.44	0.45
1:B:310:TYR:OH	1:B:374:PRO:O	2.24	0.44
1:B:318:GLU:OE2	1:B:322:GLN:NE2	2.41	0.44
1:B:325:LYS:O	1:B:329:GLY:N	2.42	0.43
1:C:125:PHE:O	1:C:128:ILE:HG22	2.19	0.43
1:A:125:PHE:O	1:A:128:ILE:HG22	2.19	0.42
1:C:119:THR:HG23	1:C:120:ASP:N	2.35	0.41
1:A:119:THR:HG23	1:A:120:ASP:N	2.35	0.41
1:A:119:THR:HG22	1:A:239:ALA:O	2.21	0.41
1:B:125:PHE:O	1:B:128:ILE:HG22	2.20	0.41
1:B:119:THR:HG22	1:B:239:ALA:O	2.21	0.41
1:C:352:SER:HB3	1:C:353:PRO:HD3	2.03	0.40
1:B:119:THR:HG23	1:B:120:ASP:N	2.35	0.40
1:A:352:SER:HB3	1:A:353:PRO:HD3	2.04	0.40
1:C:119:THR:HG22	1:C:239:ALA:O	2.21	0.40
1:B:352:SER:HB3	1:B:353:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	420/435 (97%)	401 (96%)	19 (4%)	0	100	100
1	B	420/435 (97%)	400 (95%)	20 (5%)	0	100	100
1	C	420/435 (97%)	399 (95%)	21 (5%)	0	100	100
All	All	1260/1305 (97%)	1200 (95%)	60 (5%)	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	328/390 (84%)	326 (99%)	2 (1%)	84	91
1	B	328/390 (84%)	325 (99%)	3 (1%)	75	85
1	C	328/390 (84%)	327 (100%)	1 (0%)	91	96
All	All	984/1170 (84%)	978 (99%)	6 (1%)	82	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	422	TYR
1	B	413	GLU
1	B	422	TYR
1	B	451	LEU
1	A	422	TYR
1	A	451	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	99	GLN
1	C	133	HIS
1	B	99	GLN
1	B	133	HIS

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Mol	Chain	Res	Type
1	B	234	ASN
1	B	426	ASN
1	A	99	GLN
1	A	133	HIS
1	A	234	ASN

### 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](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

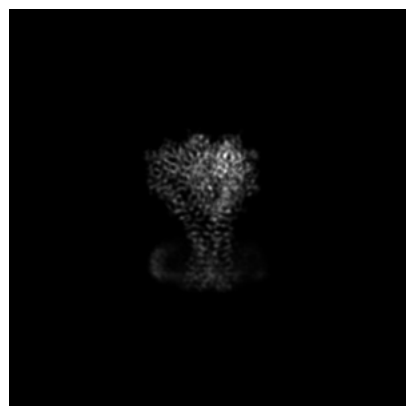
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48343. These allow visual inspection of the internal detail of the map and identification of artifacts.

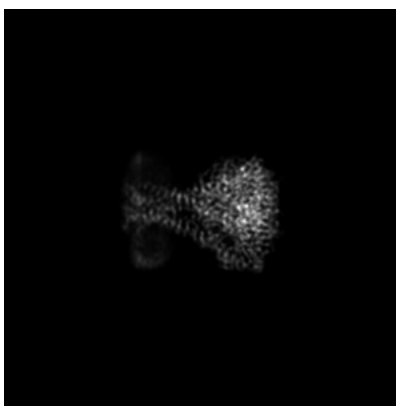
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

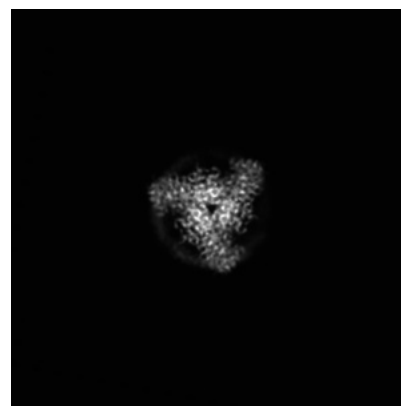
#### 6.1.1 Primary map



X

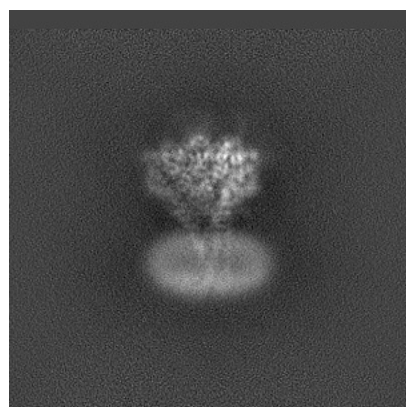


Y

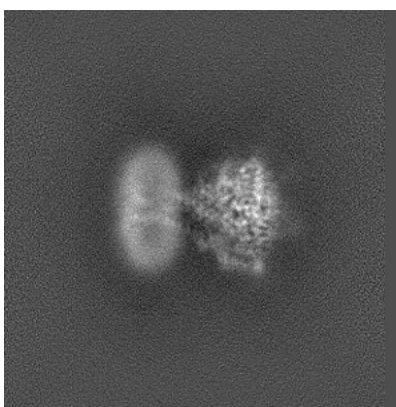


Z

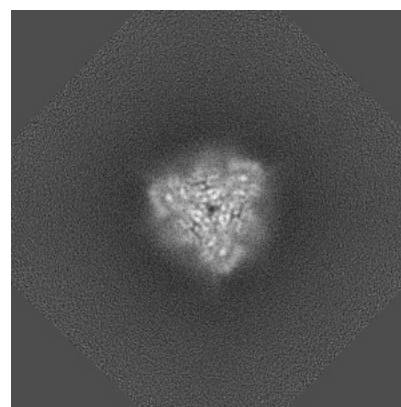
#### 6.1.2 Raw map



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: 168

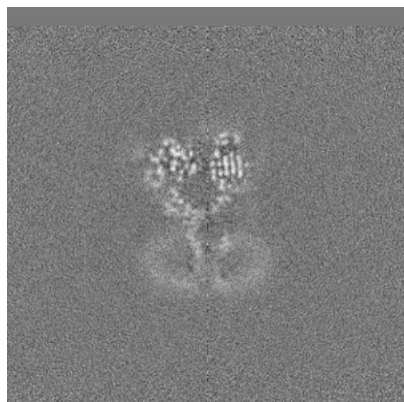


Y Index: 168

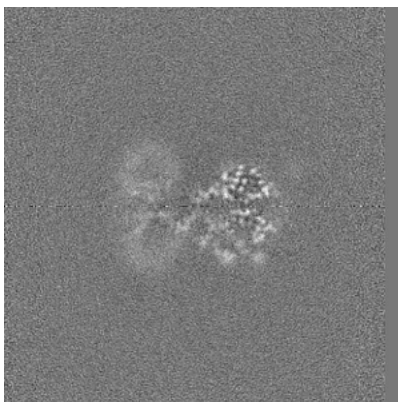


Z Index: 168

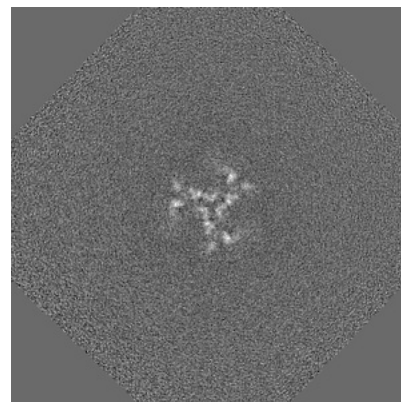
### 6.2.2 Raw map



X Index: 168



Y Index: 168



Z Index: 168

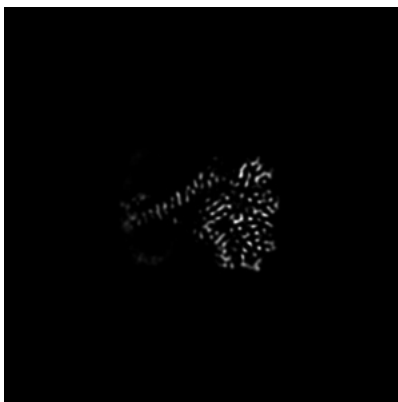
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 158

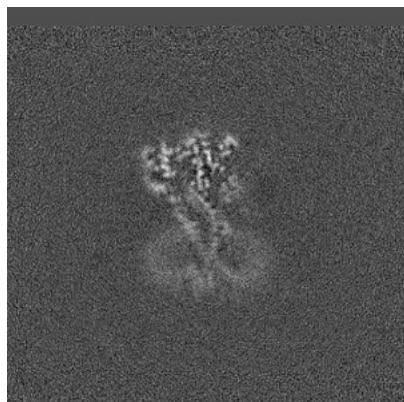


Y Index: 181

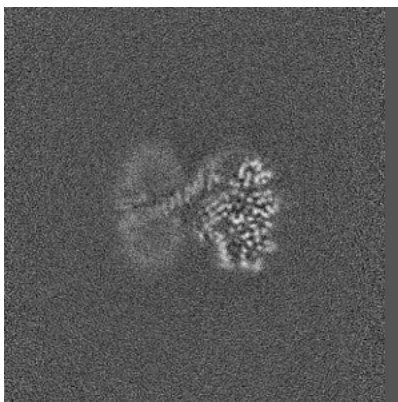


Z Index: 202

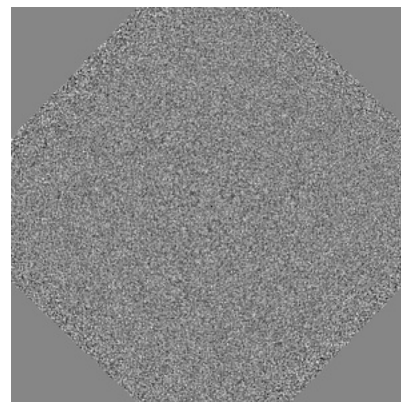
### 6.3.2 Raw map



X Index: 177



Y Index: 181

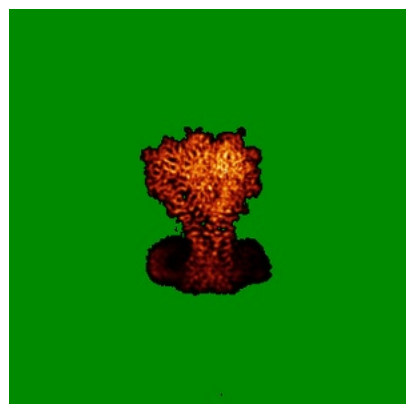


Z Index: 0

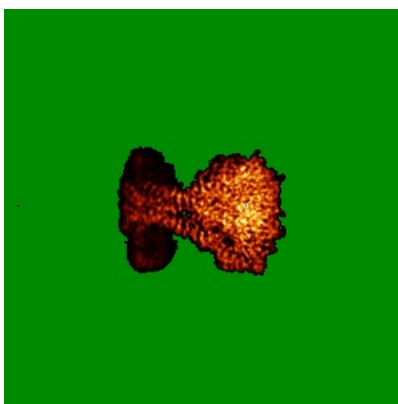
The images above show the largest variance slices of the map in three orthogonal directions.

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

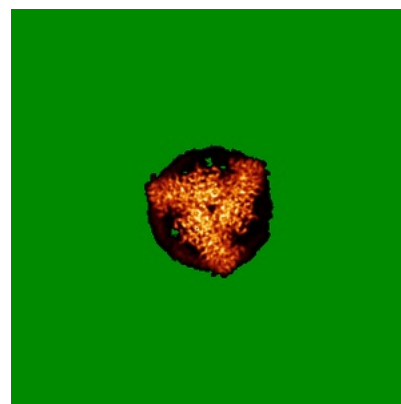
### 6.4.1 Primary map



X

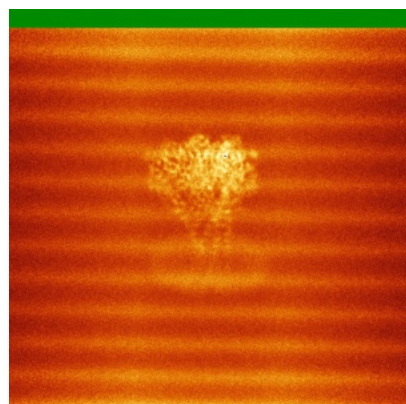


Y

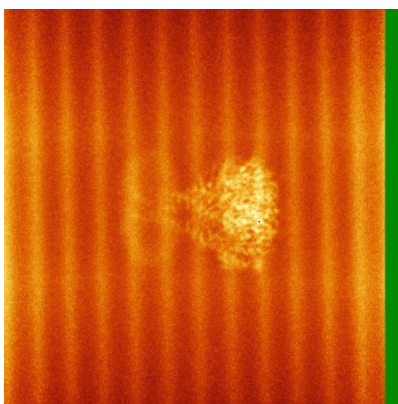


Z

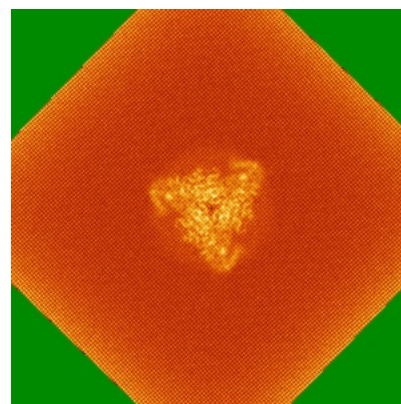
### 6.4.2 Raw map



X



Y

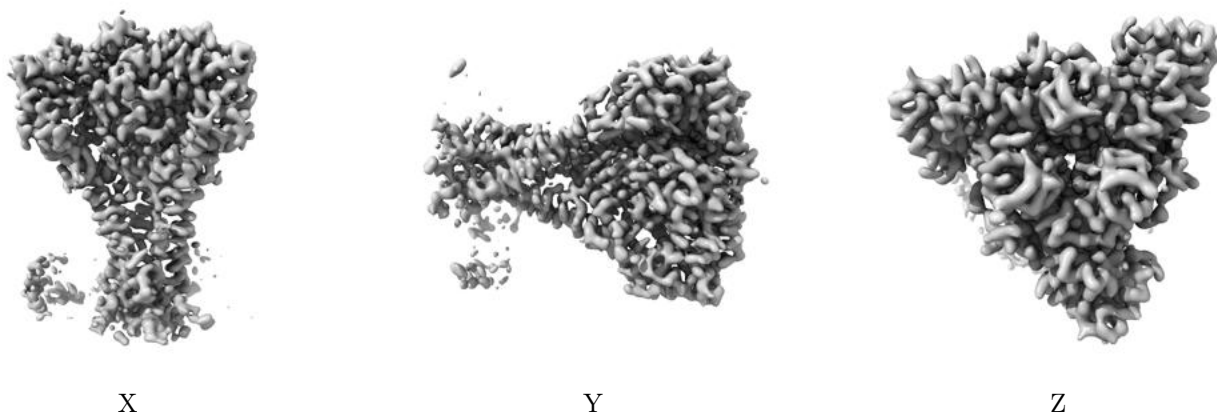


Z

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.

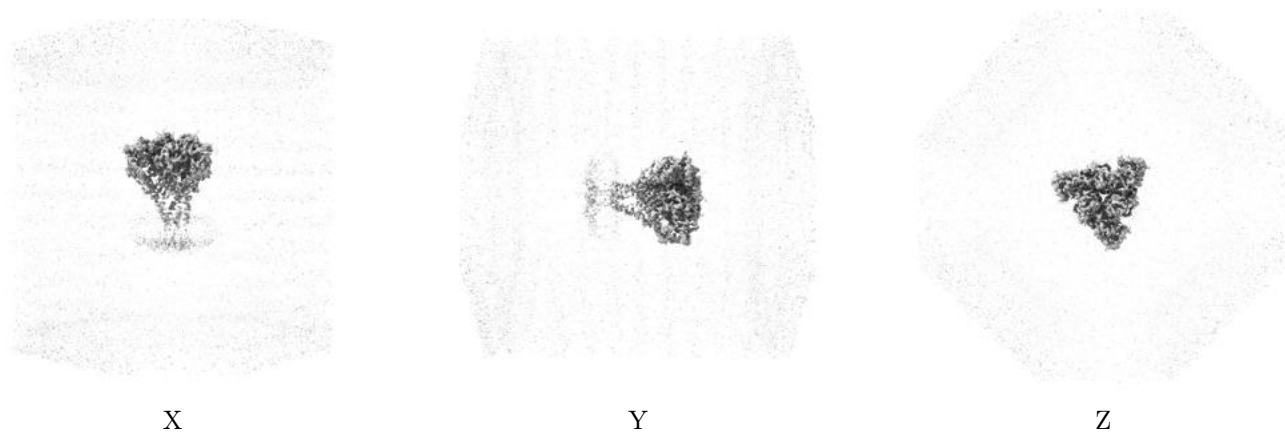
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

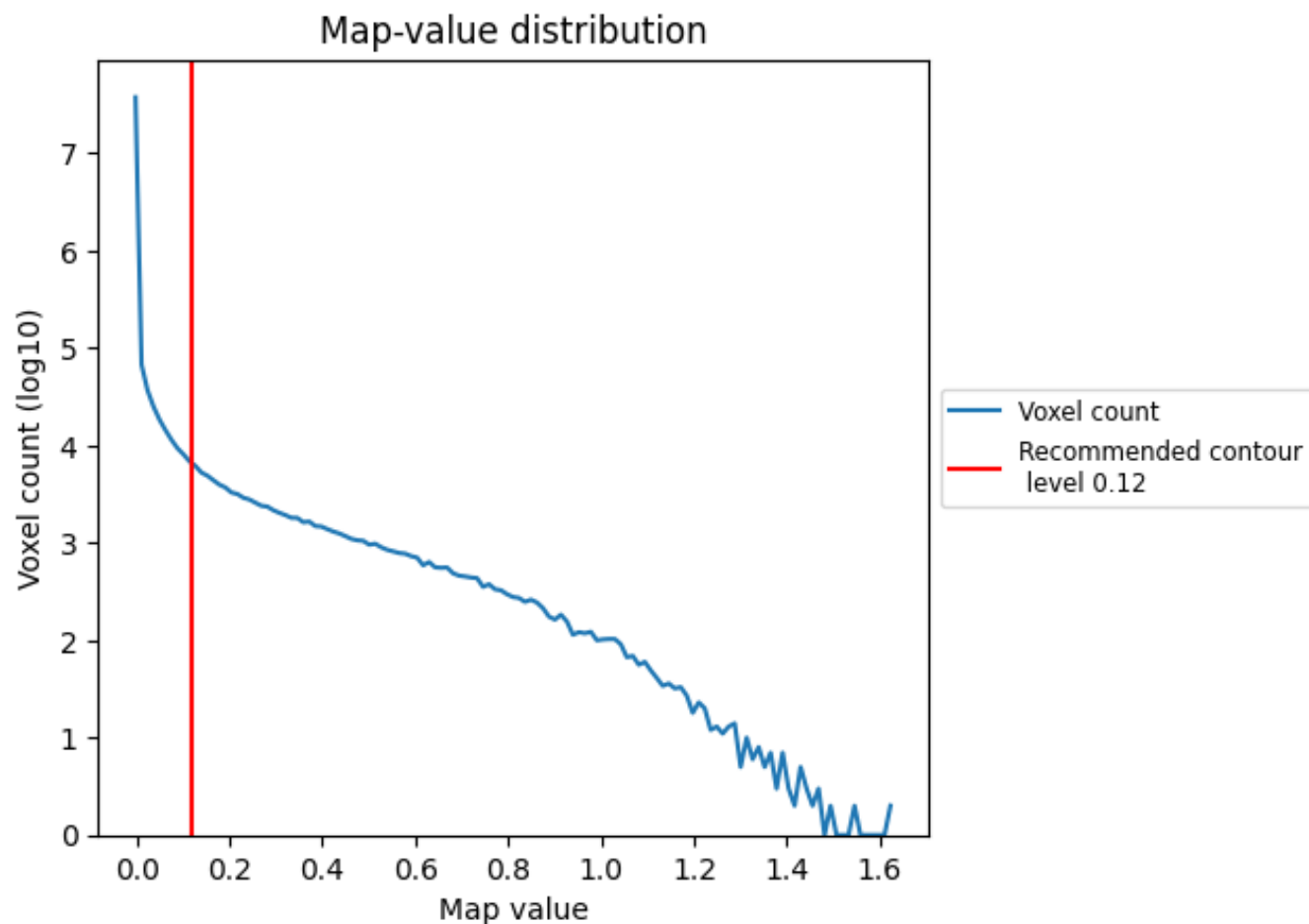
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

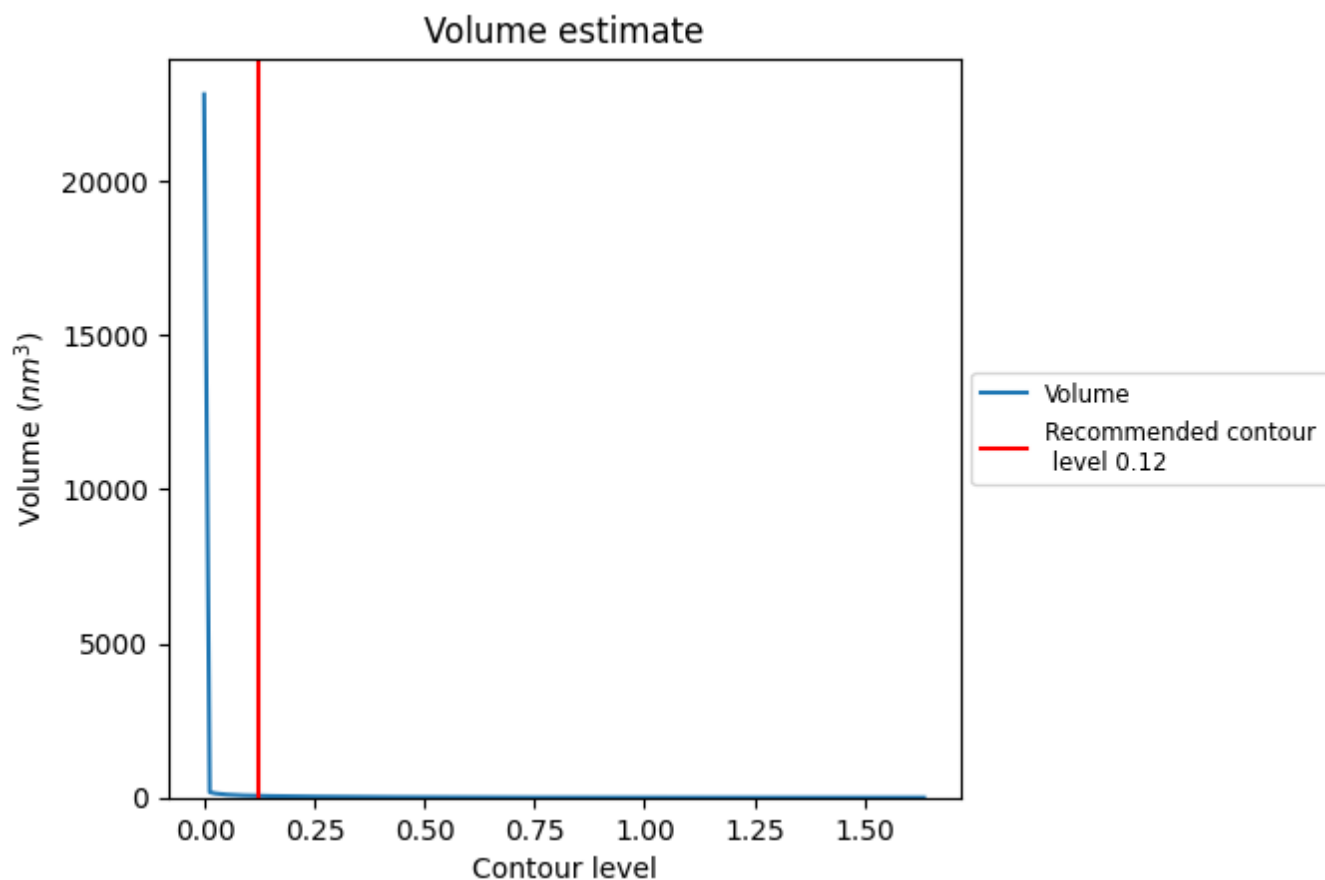
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

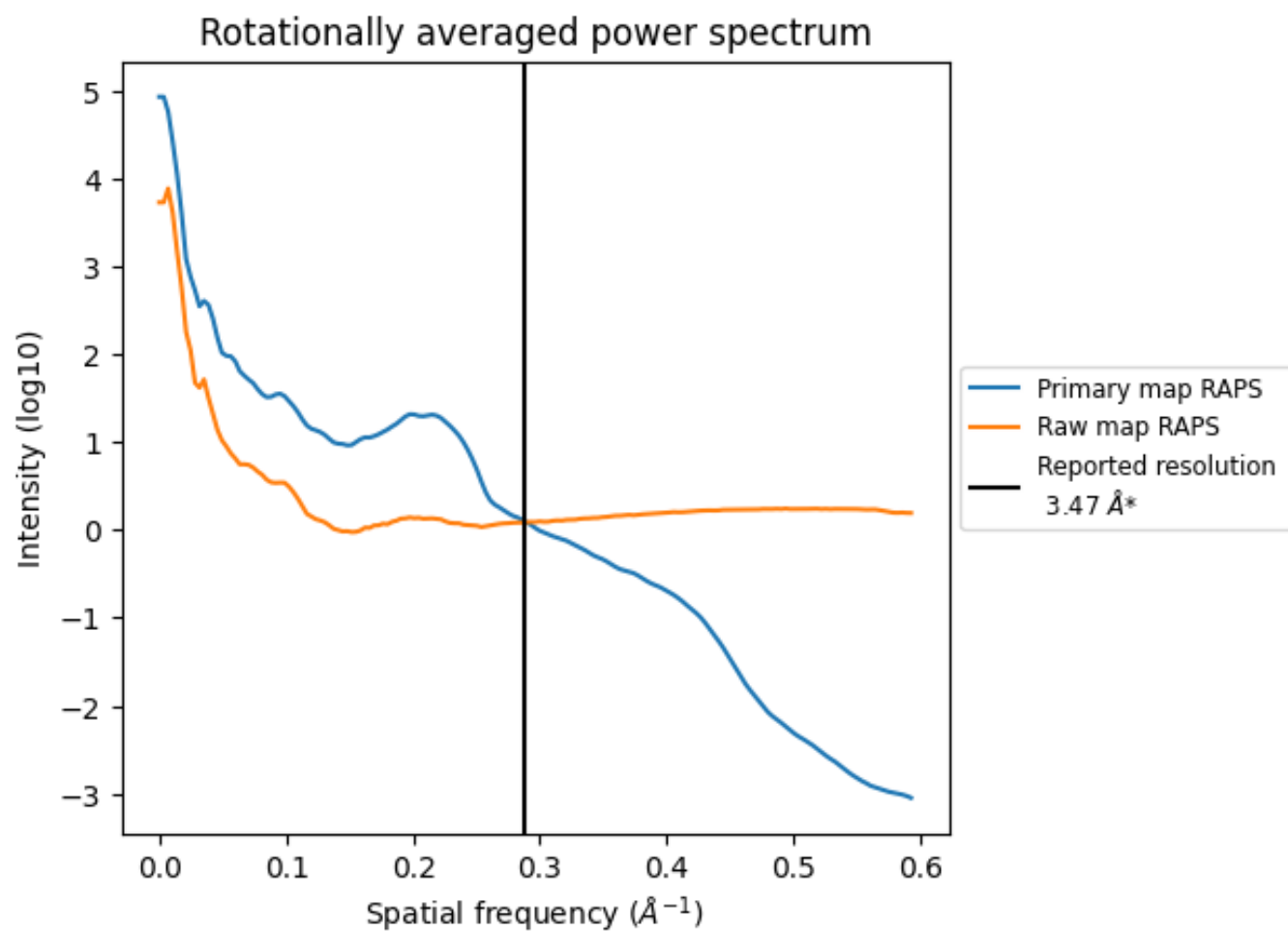
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 57  $\text{nm}^3$ ; this corresponds to an approximate mass of 51 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 ⓘ



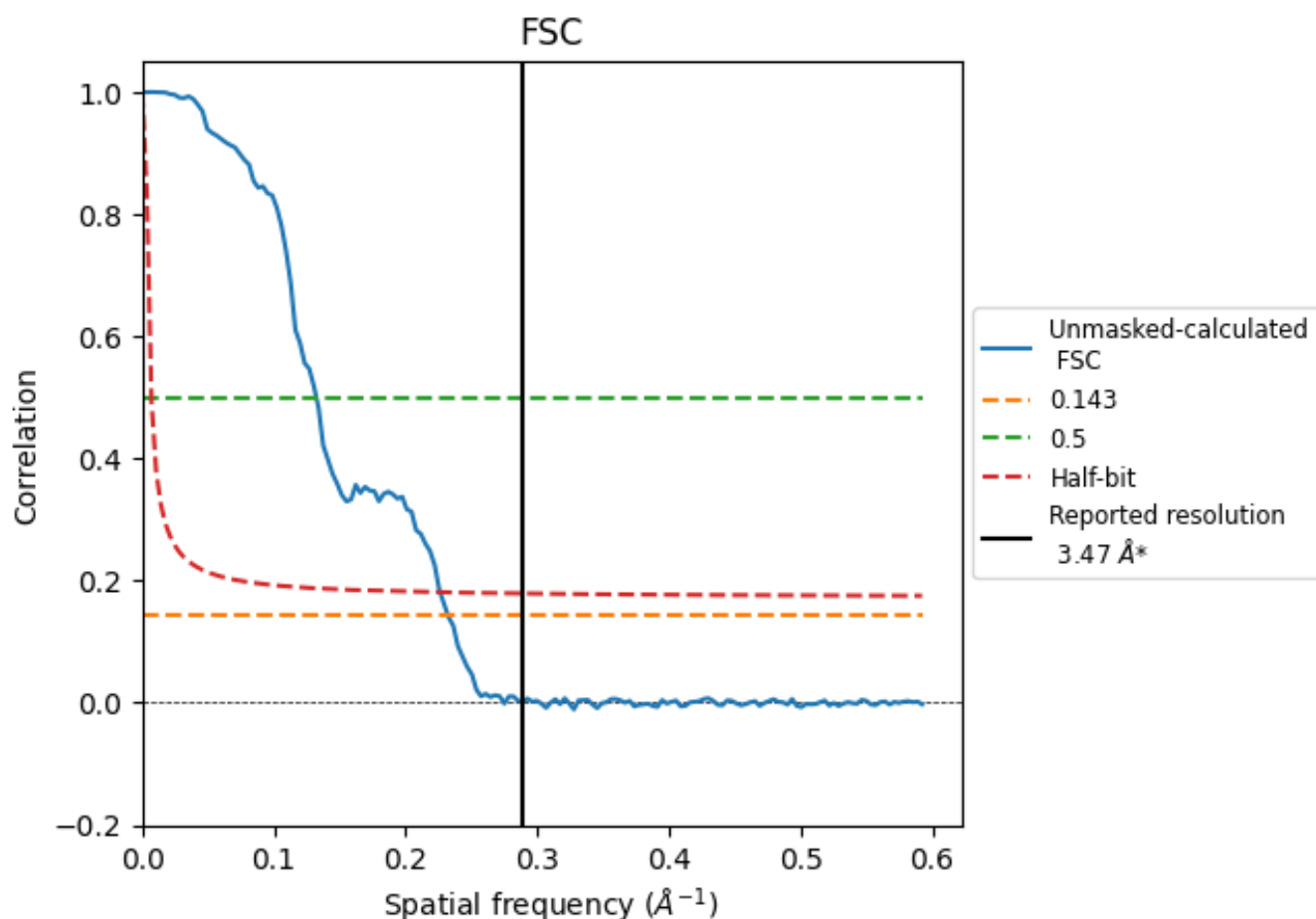
\*Reported resolution corresponds to spatial frequency of 0.288  $\text{\AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.288 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

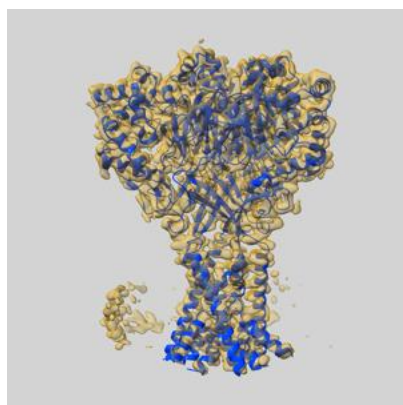
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.30	7.56	4.42

\*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 4.30 differs from the reported value 3.47 by more than 10 %

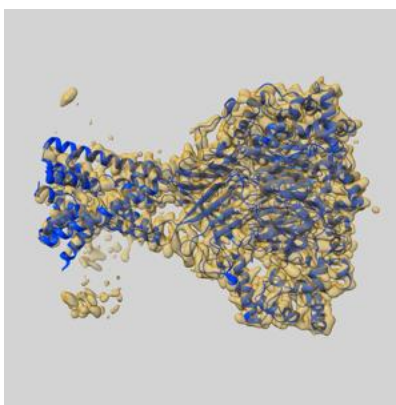
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48343 and PDB model 9MKZ. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

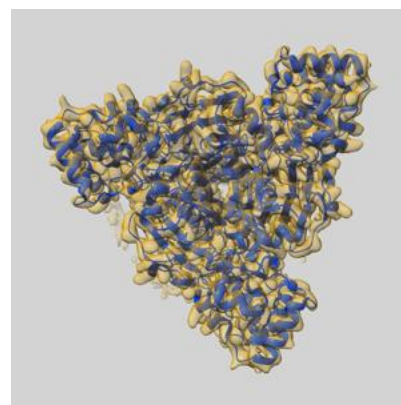
### 9.1 Map-model overlay [i](#)



X



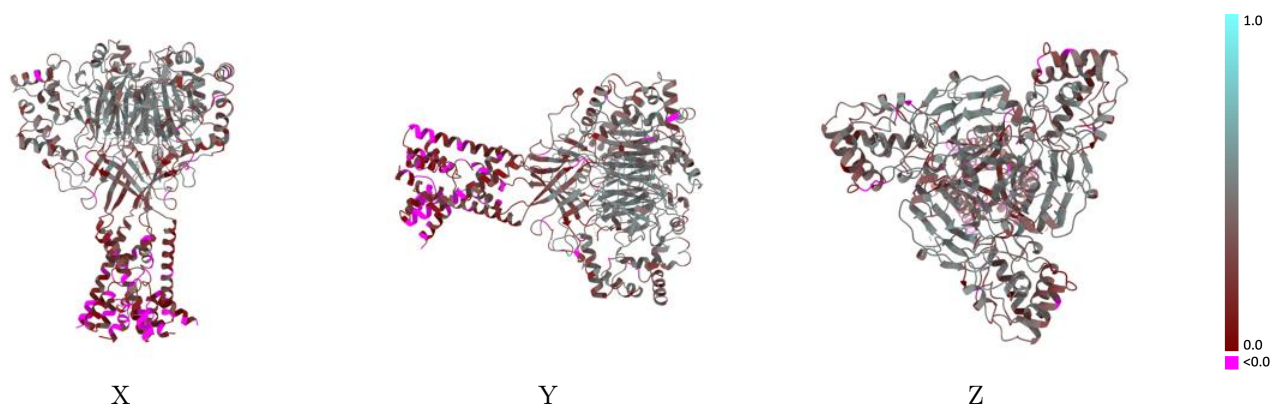
Y



Z

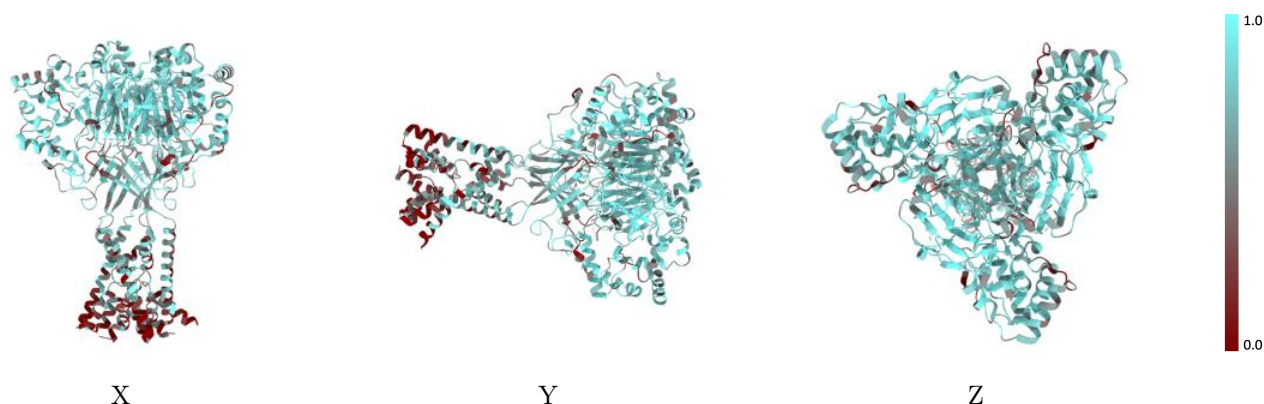
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



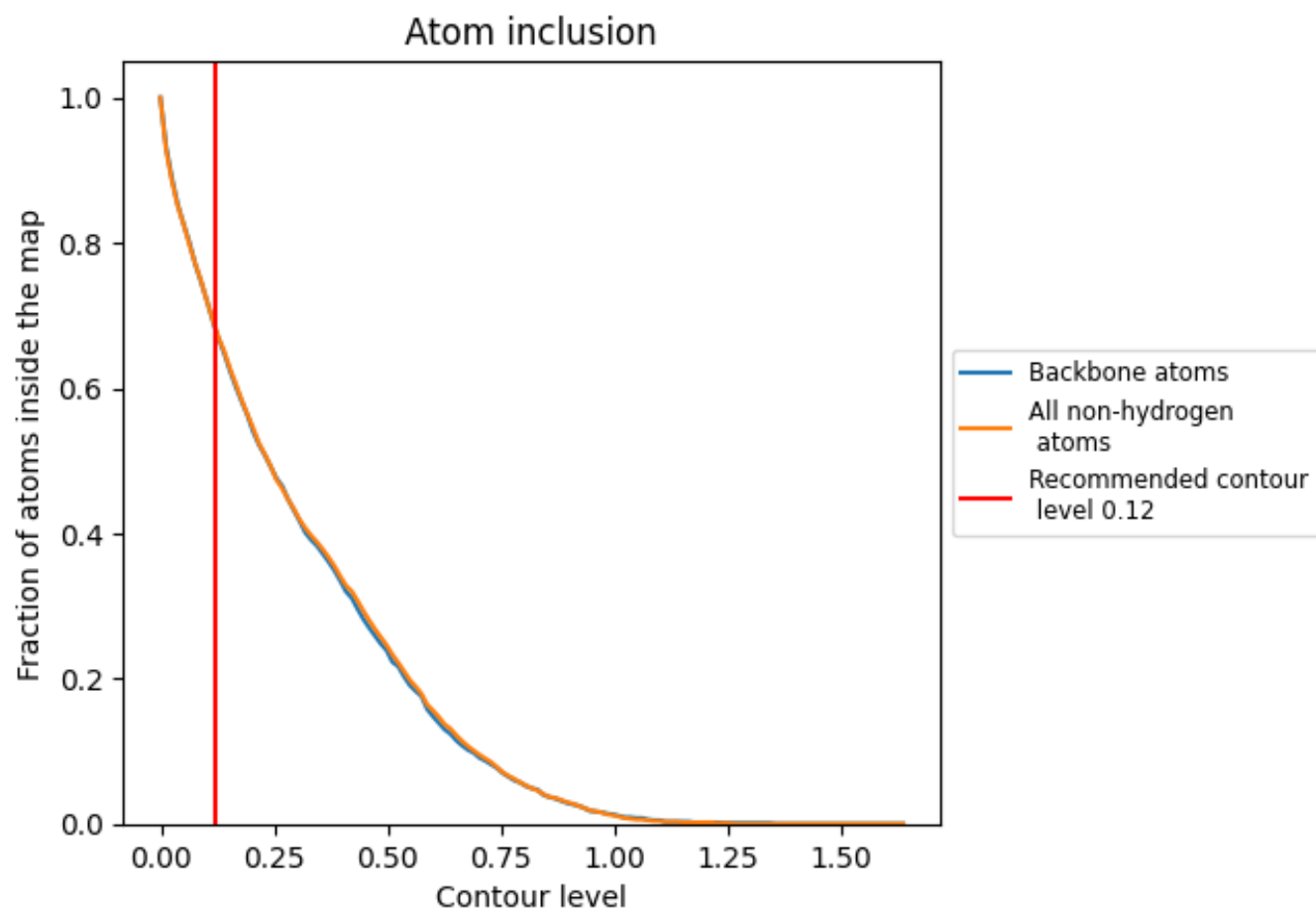
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 68% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6820	<div></div> 0.3490
A	<div></div> 0.7010	<div></div> 0.3490
B	<div></div> 0.6810	<div></div> 0.3450
C	<div></div> 0.6940	<div></div> 0.3510

