



## Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 02:22 PM EDT

PDB ID : 7LGH  
EMDB ID : EMD-23324  
Title : Asymmetric unit for phage Qbeta small prolate particle  
Authors : Chang, J.Y.; Zhang, J.  
Deposited on : 2021-01-20  
Resolution : 8.90 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.dev113  
MolProbity : 4.02b-467  
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) : 2.39

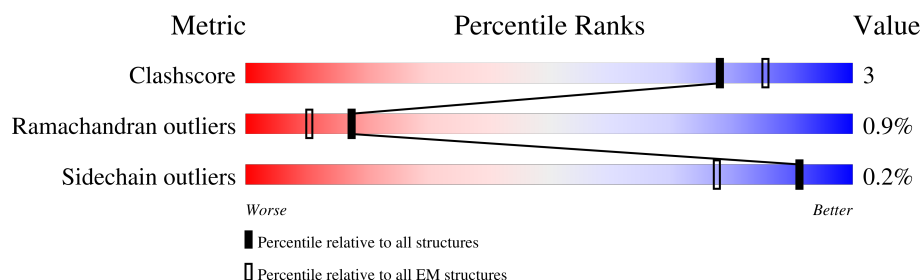
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.90 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	133	<div> <div>6%</div> <div>91%</div> <div>8%</div> <div>•</div> </div>
1	B	133	<div> <div>10%</div> <div>95%</div> <div>5%</div> <div>•</div> </div>
1	C	133	<div> <div>8%</div> <div>86%</div> <div>11%</div> <div>•••</div> </div>
1	D	133	<div> <div>•</div> <div>86%</div> <div>11%</div> <div>••</div> </div>
1	E	133	<div> <div>5%</div> <div>84%</div> <div>14%</div> <div>••</div> </div>
1	F	133	<div> <div>5%</div> <div>87%</div> <div>11%</div> <div>••</div> </div>
1	G	133	<div> <div>5%</div> <div>89%</div> <div>10%</div> <div>••</div> </div>
1	H	133	<div> <div>5%</div> <div>85%</div> <div>11%</div> <div>•••</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	133	
1	J	133	
1	K	133	
1	L	133	
1	M	133	
1	N	133	
1	O	133	
1	P	133	
1	Q	133	
1	R	133	
1	S	133	
1	T	133	
1	U	133	
1	V	133	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 21846 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	B	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	C	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	L	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	D	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	M	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	E	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	N	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	F	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	O	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	G	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	P	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	H	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	Q	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	R	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	I	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	S	132	Total 993	C 616	N 177	O 198	S 2	0	0

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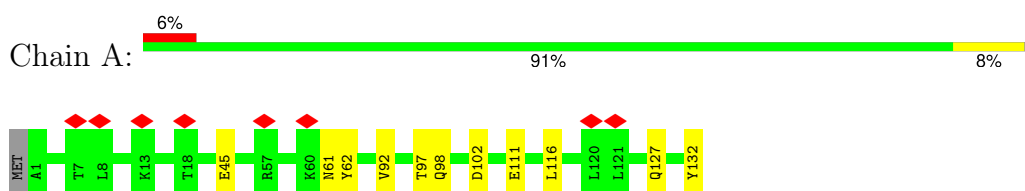
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	T	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	U	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	K	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	V	132	Total 993	C 616	N 177	O 198	S 2	0	0

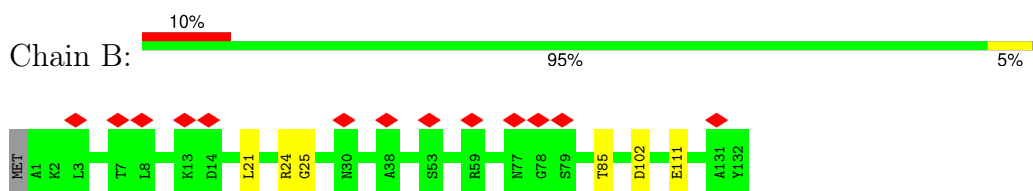
### 3 Residue-property plots [i](#)

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.

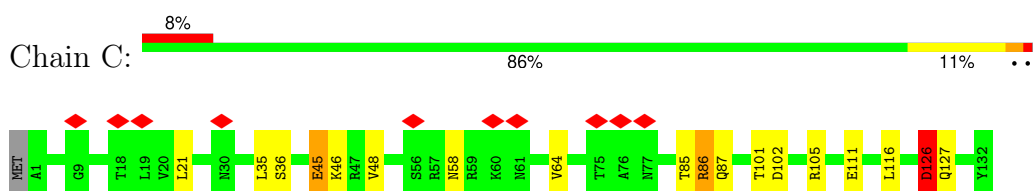
- Molecule 1: Capsid protein



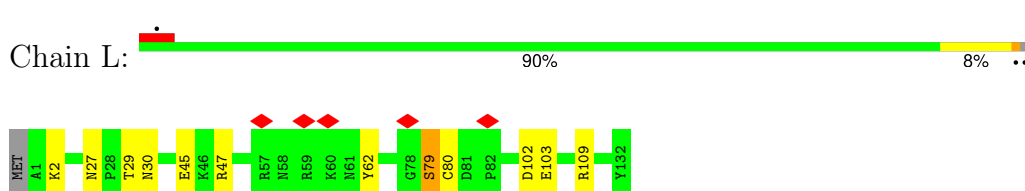
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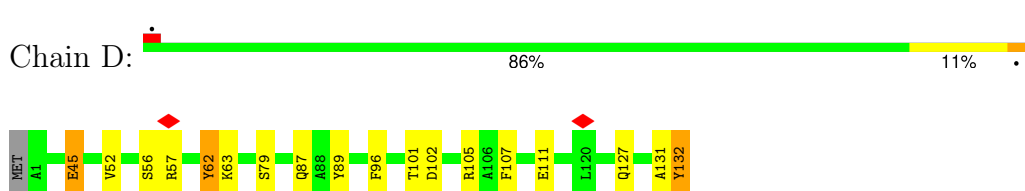
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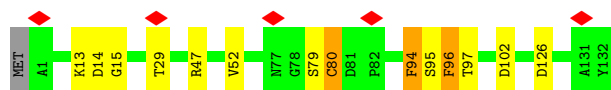
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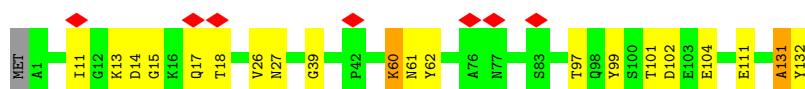
- Molecule 1: Capsid protein




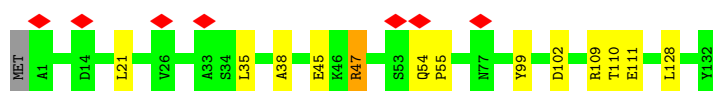
## • Molecule 1: Capsid protein

Chain M:  89% 8% ..


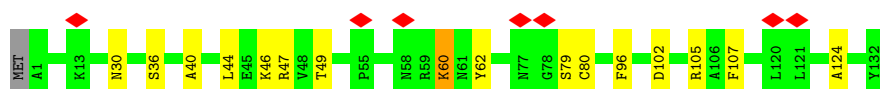
## • Molecule 1: Capsid protein

Chain E:  84% 14% ..


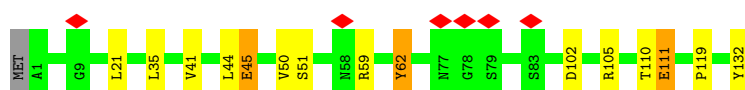
## • Molecule 1: Capsid protein

Chain N:  89% 9% ..


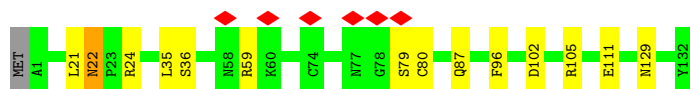
## • Molecule 1: Capsid protein

Chain F:  87% 11% ..


## • Molecule 1: Capsid protein

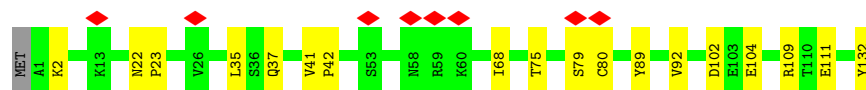
Chain O:  88% 9% ..

## • Molecule 1: Capsid protein

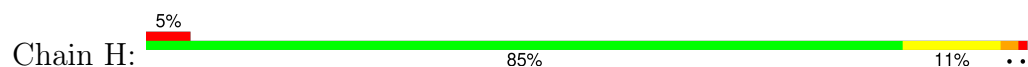
Chain G:  89% 10% ..

## • Molecule 1: Capsid protein

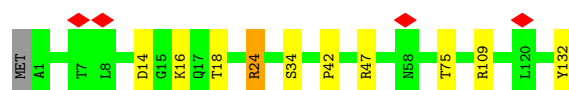
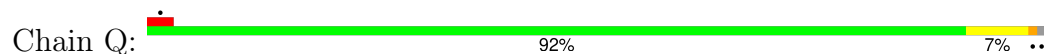
Chain P:  86% 14% ..



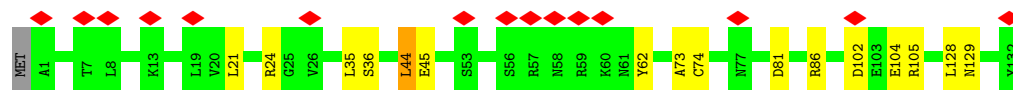
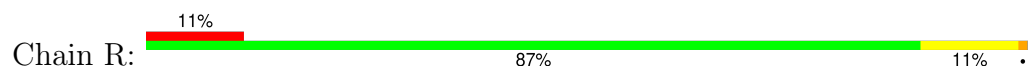
- Molecule 1: Capsid protein



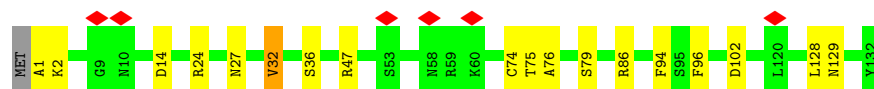
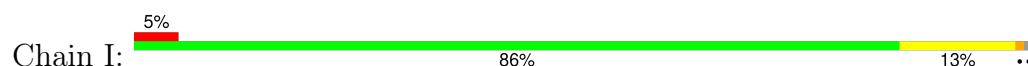
- Molecule 1: Capsid protein



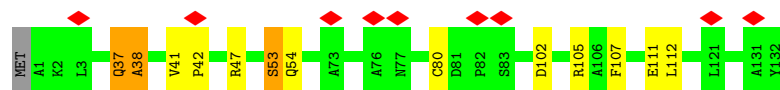
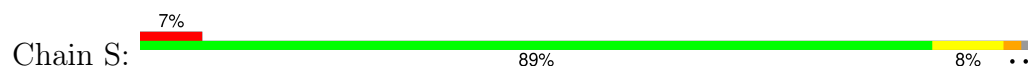
- Molecule 1: Capsid protein



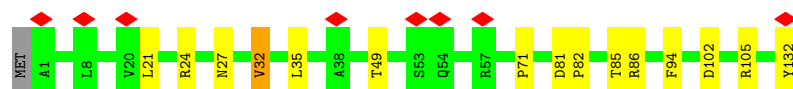
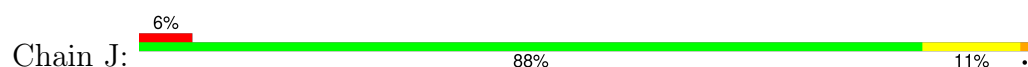
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

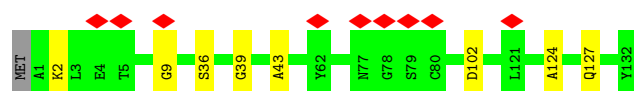
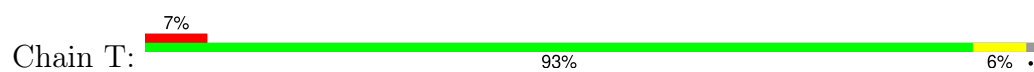


- Molecule 1: Capsid protein

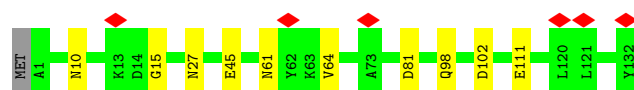
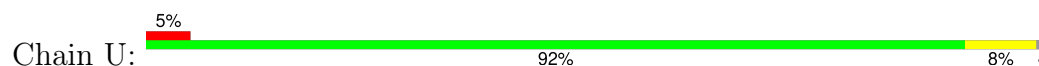


- Molecule 1: Capsid protein

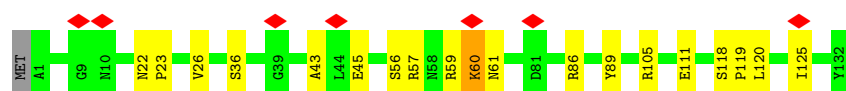
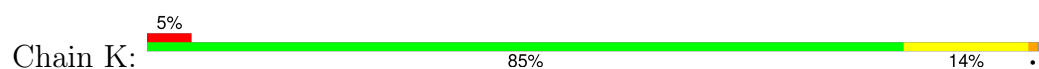




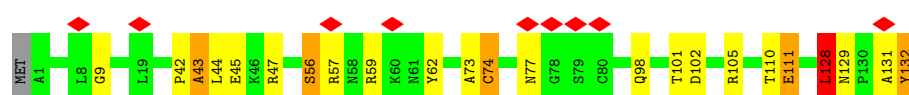
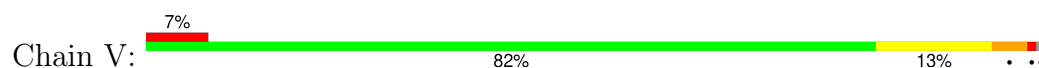
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC, FEI TECNAI F20	Depositor
Voltage (kV)	300, 200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30, 30	Depositor
Minimum defocus (nm)	Not provided, Not provided	Depositor
Maximum defocus (nm)	Not provided, Not provided	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	400.0, 400.0, 400.0	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.5, 2.5, 2.5	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	0.99	4/1007 (0.4%)	1.09	4/1371 (0.3%)
1	B	0.95	1/1007 (0.1%)	1.07	1/1371 (0.1%)
1	C	0.93	1/1007 (0.1%)	1.05	3/1371 (0.2%)
1	D	1.04	4/1007 (0.4%)	1.13	6/1371 (0.4%)
1	E	1.05	4/1007 (0.4%)	1.21	2/1371 (0.1%)
1	F	0.96	1/1007 (0.1%)	1.11	5/1371 (0.4%)
1	G	0.94	1/1007 (0.1%)	1.04	5/1371 (0.4%)
1	H	0.96	4/1007 (0.4%)	1.43	6/1371 (0.4%)
1	I	0.95	1/1007 (0.1%)	1.05	3/1371 (0.2%)
1	J	0.88	1/1007 (0.1%)	1.10	6/1371 (0.4%)
1	K	0.99	4/1007 (0.4%)	1.21	7/1371 (0.5%)
1	L	0.98	1/1007 (0.1%)	1.14	2/1371 (0.1%)
1	M	0.98	2/1007 (0.2%)	1.09	5/1371 (0.4%)
1	N	0.97	2/1007 (0.2%)	1.03	3/1371 (0.2%)
1	O	1.02	2/1007 (0.2%)	1.14	5/1371 (0.4%)
1	P	0.99	2/1007 (0.2%)	1.03	2/1371 (0.1%)
1	Q	0.94	0/1007	1.16	7/1371 (0.5%)
1	R	0.94	1/1007 (0.1%)	1.08	6/1371 (0.4%)
1	S	1.03	2/1007 (0.2%)	1.08	3/1371 (0.2%)
1	T	0.89	0/1007	1.08	1/1371 (0.1%)
1	U	0.98	5/1007 (0.5%)	1.04	2/1371 (0.1%)
1	V	0.94	2/1007 (0.2%)	1.13	5/1371 (0.4%)
All	All	0.97	45/22154 (0.2%)	1.12	89/30162 (0.3%)

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	2
1	C	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	7
1	F	0	4
1	H	0	1
1	K	0	1
1	L	0	3
1	M	0	4
1	N	0	2
1	O	0	1
1	P	0	1
1	Q	0	5
1	S	0	3
1	T	0	5
1	U	0	2
1	V	0	3
All	All	0	47

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	111	GLU	CG-CD	-8.82	1.38	1.51
1	M	96	PHE	CG-CD1	-8.27	1.26	1.38
1	S	107	PHE	CB-CG	-7.80	1.38	1.51
1	K	26	VAL	CB-CG1	-6.94	1.38	1.52
1	O	132	TYR	CG-CD2	-6.20	1.31	1.39
1	D	62	TYR	CD2-CE2	-6.14	1.30	1.39
1	D	111	GLU	CD-OE1	-6.14	1.18	1.25
1	V	56	SER	CB-OG	-6.12	1.34	1.42
1	A	111	GLU	CG-CD	-5.87	1.43	1.51
1	H	45	GLU	CD-OE2	-5.85	1.19	1.25
1	M	94	PHE	CB-CG	-5.78	1.41	1.51
1	J	32	VAL	CB-CG1	-5.75	1.40	1.52
1	P	104	GLU	CD-OE2	-5.71	1.19	1.25
1	U	45	GLU	CD-OE2	-5.67	1.19	1.25
1	I	32	VAL	CB-CG2	-5.60	1.41	1.52
1	U	111	GLU	CD-OE1	-5.60	1.19	1.25
1	G	111	GLU	CD-OE2	-5.59	1.19	1.25
1	O	111	GLU	CD-OE1	-5.59	1.19	1.25
1	A	111	GLU	CD-OE1	-5.55	1.19	1.25
1	N	45	GLU	CD-OE1	-5.49	1.19	1.25
1	H	111	GLU	CD-OE1	-5.44	1.19	1.25
1	H	111	GLU	CG-CD	-5.35	1.44	1.51
1	H	111	GLU	CD-OE2	-5.32	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	111	GLU	CD-OE2	-5.32	1.19	1.25
1	N	111	GLU	CD-OE2	-5.31	1.19	1.25
1	F	62	TYR	CG-CD1	-5.31	1.32	1.39
1	E	104	GLU	CG-CD	-5.26	1.44	1.51
1	K	89	TYR	CB-CG	-5.24	1.43	1.51
1	K	111	GLU	CD-OE2	-5.24	1.19	1.25
1	U	111	GLU	CD-OE2	-5.24	1.19	1.25
1	U	45	GLU	CD-OE1	-5.21	1.20	1.25
1	U	64	VAL	CB-CG2	-5.19	1.42	1.52
1	K	45	GLU	CD-OE2	-5.15	1.20	1.25
1	R	104	GLU	CD-OE2	-5.14	1.20	1.25
1	V	111	GLU	CD-OE2	-5.14	1.20	1.25
1	A	45	GLU	CD-OE2	-5.13	1.20	1.25
1	E	132	TYR	CD1-CE1	-5.11	1.31	1.39
1	D	63	LYS	CE-NZ	-5.10	1.36	1.49
1	S	111	GLU	CD-OE2	-5.06	1.20	1.25
1	C	111	GLU	CG-CD	-5.05	1.44	1.51
1	A	62	TYR	CD2-CE2	-5.05	1.31	1.39
1	D	45	GLU	CD-OE2	-5.05	1.20	1.25
1	B	111	GLU	CD-OE1	-5.02	1.20	1.25
1	P	111	GLU	CD-OE1	-5.01	1.20	1.25
1	L	45	GLU	CG-CD	-5.00	1.44	1.51

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	56	SER	O-C-N	23.57	160.41	122.70
1	H	56	SER	CA-C-N	-18.00	77.61	117.20
1	H	56	SER	CA-C-O	-17.70	82.92	120.10
1	A	61	ASN	C-N-CA	13.18	154.65	121.70
1	B	21	LEU	C-N-CA	13.14	154.54	121.70
1	E	131	ALA	C-N-CA	12.96	154.10	121.70
1	T	2	LYS	C-N-CA	12.74	153.54	121.70
1	C	116	LEU	C-N-CA	12.54	153.04	121.70
1	V	128	LEU	C-N-CA	12.11	151.97	121.70
1	H	37	GLN	C-N-CA	11.96	151.60	121.70
1	L	62	TYR	CB-CG-CD2	-9.61	115.23	121.00
1	I	86	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	K	86	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	L	109	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	O	132	TYR	CB-CG-CD2	-8.51	115.89	121.00
1	S	47	ARG	NE-CZ-NH2	-8.47	116.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	60	LYS	C-N-CA	8.18	142.15	121.70
1	O	62	TYR	CB-CG-CD2	-8.12	116.13	121.00
1	Q	109	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	Q	24	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	K	59	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	D	62	TYR	CB-CG-CD2	-7.64	116.42	121.00
1	V	47	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	N	99	TYR	CB-CG-CD2	-7.58	116.45	121.00
1	D	96	PHE	CB-CG-CD1	7.53	126.07	120.80
1	F	60	LYS	C-N-CA	7.50	140.46	121.70
1	D	96	PHE	CB-CG-CD2	-7.36	115.65	120.80
1	R	105	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	M	96	PHE	CA-CB-CG	7.25	131.30	113.90
1	G	59	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	J	24	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	G	59	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	O	50	VAL	C-N-CA	6.92	138.99	121.70
1	D	132	TYR	CB-CG-CD1	-6.90	116.86	121.00
1	M	47	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	O	132	TYR	CB-CG-CD1	6.73	125.04	121.00
1	J	132	TYR	CB-CG-CD1	-6.71	116.97	121.00
1	G	24	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	N	109	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	M	96	PHE	CB-CG-CD2	-6.58	116.20	120.80
1	V	62	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	F	102	ASP	CB-CG-OD1	6.56	124.21	118.30
1	R	86	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	C	126	ASP	N-CA-C	-6.46	93.57	111.00
1	N	47	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	J	94	PHE	CB-CG-CD2	-6.35	116.36	120.80
1	S	37	GLN	C-N-CA	6.31	137.47	121.70
1	Q	75	THR	N-CA-C	-6.29	94.03	111.00
1	M	96	PHE	C-N-CA	6.23	137.27	121.70
1	A	62	TYR	CB-CG-CD2	-6.19	117.28	121.00
1	I	86	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	M	96	PHE	CB-CG-CD1	6.12	125.08	120.80
1	J	94	PHE	CB-CG-CD1	6.01	125.01	120.80
1	E	60	LYS	C-N-CA	5.94	136.54	121.70
1	Q	132	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	O	59	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	K	60	LYS	CA-C-N	5.84	130.04	117.20
1	P	132	TYR	CB-CG-CD2	-5.75	117.55	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	99	TYR	CB-CG-CD1	-5.71	117.57	121.00
1	H	47	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	R	44	LEU	C-N-CA	5.67	135.89	121.70
1	J	105	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	Q	47	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	R	81	ASP	N-CA-C	5.59	126.11	111.00
1	K	105	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	K	86	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	R	105	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	Q	109	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	J	86	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	F	60	LYS	N-CA-C	5.45	125.72	111.00
1	K	60	LYS	N-CA-C	5.45	125.71	111.00
1	U	81	ASP	CB-CG-OD1	5.44	123.19	118.30
1	I	24	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	S	53	SER	C-N-CA	5.40	135.19	121.70
1	F	102	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	G	87	GLN	C-N-CA	5.34	135.06	121.70
1	A	132	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	V	132	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	C	86	ARG	C-N-CA	5.27	134.88	121.70
1	F	60	LYS	CA-C-N	5.22	128.69	117.20
1	D	89	TYR	CA-CB-CG	5.22	123.31	113.40
1	R	62	TYR	CB-CG-CD2	-5.19	117.88	121.00
1	P	92	VAL	CB-CA-C	-5.17	101.57	111.40
1	D	52	VAL	C-N-CA	5.16	134.60	121.70
1	Q	24	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	V	56	SER	CB-CA-C	5.04	119.68	110.10
1	U	81	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	G	129	ASN	N-CA-C	5.03	124.58	111.00
1	A	92	VAL	CB-CA-C	-5.03	101.85	111.40

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	GLN	Mainchain
1	B	24	ARG	Mainchain
1	B	85	THR	Mainchain
1	C	21	LEU	Mainchain
1	C	45	GLU	Mainchain
1	D	127	GLN	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
1	D	131	ALA	Mainchain
1	D	45	GLU	Mainchain
1	D	79	SER	Mainchain,Peptide
1	D	87	GLN	Mainchain
1	F	107	PHE	Mainchain
1	F	30	ASN	Mainchain,Peptide
1	F	36	SER	Mainchain
1	H	101	THR	Mainchain
1	K	120	LEU	Mainchain
1	L	103	GLU	Mainchain,Peptide
1	L	2	LYS	Mainchain
1	M	29	THR	Mainchain,Peptide
1	M	52	VAL	Mainchain,Peptide
1	N	38	ALA	Mainchain,Peptide
1	O	119	PRO	Mainchain
1	P	109	ARG	Mainchain
1	Q	18	THR	Mainchain,Peptide
1	Q	34	SER	Mainchain,Peptide
1	Q	42	PRO	Mainchain
1	S	105	ARG	Mainchain
1	S	112	LEU	Mainchain
1	S	80	CYS	Mainchain
1	T	124	ALA	Mainchain
1	T	127	GLN	Mainchain
1	T	36	SER	Mainchain
1	T	9	GLY	Mainchain,Peptide
1	U	61	ASN	Mainchain,Peptide
1	V	9	GLY	Mainchain,Peptide
1	V	98	GLN	Mainchain

## 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	993	0	1006	2	0
1	B	993	0	1007	1	0
1	C	993	0	1006	8	0
1	D	993	0	1006	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	993	0	1006	10	0
1	F	993	0	1006	5	0
1	G	993	0	1006	6	0
1	H	993	0	1005	8	0
1	I	993	0	1007	9	0
1	J	993	0	1007	8	0
1	K	993	0	1007	5	0
1	L	993	0	1006	3	0
1	M	993	0	1006	7	0
1	N	993	0	1007	5	0
1	O	993	0	1006	8	0
1	P	993	0	1006	7	0
1	Q	993	0	1007	1	0
1	R	993	0	1006	7	0
1	S	993	0	1006	4	0
1	T	993	0	1006	2	0
1	U	993	0	1008	4	0
1	V	993	0	1006	12	0
All	All	21846	0	22139	119	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 (119) 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:R:44:LEU:H	1:R:45:GLU:HB2	1.62	0.63
1:G:79:SER:OG	1:G:80:CYS:N	2.33	0.62
1:B:102:ASP:N	1:B:102:ASP:OD1	2.34	0.60
1:M:96:PHE:HB3	1:M:97:THR:C	2.22	0.60
1:M:13:LYS:NZ	1:M:126:ASP:OD2	2.35	0.59
1:V:102:ASP:N	1:V:102:ASP:OD1	2.36	0.58
1:F:47:ARG:NH1	1:F:49:THR:OG1	2.38	0.57
1:L:79:SER:OG	1:L:80:CYS:N	2.36	0.56
1:L:102:ASP:N	1:L:102:ASP:OD1	2.39	0.55
1:R:102:ASP:N	1:R:102:ASP:OD1	2.39	0.55
1:J:102:ASP:N	1:J:102:ASP:OD1	2.38	0.55
1:E:13:LYS:NZ	1:N:102:ASP:OD2	2.36	0.55
1:M:102:ASP:OD1	1:M:102:ASP:N	2.39	0.54
1:T:102:ASP:OD1	1:T:102:ASP:N	2.40	0.54
1:R:24:ARG:NE	1:R:36:SER:OG	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASP:OD1	1:A:102:ASP:N	2.41	0.53
1:O:102:ASP:N	1:O:102:ASP:OD1	2.41	0.53
1:H:101:THR:OG1	1:H:102:ASP:N	2.42	0.53
1:G:102:ASP:N	1:G:102:ASP:OD1	2.38	0.53
1:H:51:SER:OG	1:H:65:GLN:N	2.42	0.52
1:J:21:LEU:HB3	1:J:35:LEU:HB3	1.91	0.51
1:C:86:ARG:HA	1:C:87:GLN:HB2	1.93	0.51
1:V:42:PRO:O	1:V:43:ALA:C	2.50	0.51
1:V:56:SER:OG	1:V:59:ARG:N	2.45	0.50
1:P:22:ASN:HB3	1:P:37:GLN:HB2	1.93	0.50
1:R:73:ALA:O	1:R:74:CYS:C	2.46	0.50
1:I:36:SER:HA	1:I:47:ARG:HB3	1.93	0.50
1:D:62:TYR:OH	1:D:105:ARG:NH1	2.45	0.50
1:H:21:LEU:HB3	1:H:35:LEU:HB3	1.94	0.49
1:C:35:LEU:HB3	1:C:36:SER:HA	1.94	0.49
1:R:128:LEU:O	1:R:129:ASN:C	2.51	0.49
1:O:110:THR:O	1:O:111:GLU:C	2.51	0.49
1:J:81:ASP:N	1:J:82:PRO:HD3	2.27	0.49
1:K:118:SER:HB3	1:K:119:PRO:HD2	1.95	0.48
1:H:101:THR:HG23	1:H:104:GLU:H	1.78	0.48
1:E:14:ASP:OD1	1:E:15:GLY:N	2.46	0.48
1:S:102:ASP:OD1	1:S:102:ASP:N	2.47	0.48
1:F:124:ALA:O	1:O:62:TYR:OH	2.24	0.48
1:S:53:SER:HA	1:S:54:GLN:HB2	1.96	0.48
1:C:64:VAL:HG23	1:C:105:ARG:HH22	1.79	0.48
1:V:56:SER:HB2	1:V:57:ARG:HB2	1.96	0.47
1:K:118:SER:HB3	1:K:119:PRO:CD	2.43	0.47
1:G:21:LEU:O	1:G:22:ASN:C	2.52	0.47
1:D:56:SER:OG	1:D:57:ARG:N	2.49	0.46
1:H:45:GLU:O	1:H:71:PRO:HD2	2.16	0.46
1:P:102:ASP:N	1:P:102:ASP:OD1	2.47	0.46
1:I:27:ASN:HB3	1:I:32:VAL:HB	1.98	0.46
1:M:14:ASP:OD1	1:M:15:GLY:N	2.48	0.46
1:E:26:VAL:O	1:E:27:ASN:C	2.53	0.46
1:O:44:LEU:O	1:O:45:GLU:HB2	2.16	0.46
1:E:97:THR:HG22	1:E:99:TYR:H	1.80	0.45
1:N:54:GLN:HB2	1:N:55:PRO:HD2	1.96	0.45
1:F:79:SER:OG	1:F:80:CYS:N	2.49	0.45
1:O:41:VAL:HA	1:O:44:LEU:O	2.15	0.45
1:P:68:ILE:O	1:P:89:TYR:HB2	2.16	0.45
1:R:44:LEU:N	1:R:45:GLU:HB2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1:ALA:O	1:I:2:LYS:C	2.53	0.45
1:I:14:ASP:OD1	1:I:14:ASP:N	2.47	0.45
1:R:21:LEU:HB3	1:R:35:LEU:HB3	1.99	0.45
1:G:21:LEU:HB3	1:G:35:LEU:HB3	1.99	0.44
1:S:37:GLN:HA	1:S:38:ALA:HB3	1.97	0.44
1:J:27:ASN:ND2	1:U:27:ASN:O	2.50	0.44
1:E:39:GLY:O	1:O:105:ARG:NH2	2.49	0.44
1:I:128:LEU:HB3	1:I:129:ASN:HA	1.99	0.44
1:H:27:ASN:N	1:H:28:PRO:CD	2.81	0.44
1:H:62:TYR:O	1:H:63:LYS:HB2	2.18	0.44
1:K:22:ASN:HA	1:K:23:PRO:HD3	1.86	0.43
1:M:94:PHE:CG	1:M:95:SER:N	2.87	0.43
1:F:40:ALA:O	1:F:44:LEU:HG	2.18	0.43
1:A:97:THR:OG1	1:A:98:GLN:N	2.45	0.43
1:V:128:LEU:HB2	1:V:129:ASN:CA	2.48	0.43
1:I:102:ASP:OD1	1:I:102:ASP:N	2.51	0.43
1:U:102:ASP:OD1	1:U:102:ASP:N	2.46	0.43
1:S:41:VAL:N	1:S:42:PRO:HD2	2.34	0.43
1:V:43:ALA:O	1:V:45:GLU:N	2.51	0.43
1:M:96:PHE:HB3	1:M:97:THR:CA	2.47	0.43
1:L:29:THR:OG1	1:L:30:ASN:N	2.50	0.43
1:E:17:GLN:HB3	1:E:18:THR:HB	2.01	0.43
1:J:32:VAL:CG1	1:J:49:THR:HB	2.48	0.43
1:J:81:ASP:N	1:J:82:PRO:CD	2.82	0.42
1:V:77:ASN:OD1	1:V:77:ASN:N	2.50	0.42
1:I:74:CYS:O	1:I:75:THR:OG1	2.30	0.42
1:I:94:PHE:HB3	1:I:96:PHE:CZ	2.55	0.42
1:P:79:SER:OG	1:P:80:CYS:N	2.52	0.42
1:D:132:TYR:OXT	1:P:2:LYS:NZ	2.53	0.42
1:E:101:THR:OG1	1:E:102:ASP:N	2.52	0.42
1:V:101:THR:O	1:V:105:ARG:HD3	2.20	0.42
1:D:101:THR:OG1	1:D:102:ASP:N	2.52	0.42
1:G:96:PHE:CD2	1:G:105:ARG:HG2	2.55	0.42
1:Q:14:ASP:OD2	1:Q:16:LYS:NZ	2.50	0.42
1:I:76:ALA:H	1:I:79:SER:HG	1.67	0.42
1:C:126:ASP:O	1:C:127:GLN:C	2.55	0.42
1:O:110:THR:O	1:O:110:THR:HG22	2.20	0.42
1:P:23:PRO:HA	1:P:35:LEU:HA	2.02	0.42
1:J:71:PRO:HB2	1:J:85:THR:CG2	2.50	0.42
1:V:73:ALA:O	1:V:74:CYS:C	2.58	0.42
1:M:79:SER:OG	1:M:80:CYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:TYR:CD2	1:N:128:LEU:HD22	2.55	0.41
1:U:10:ASN:HB3	1:U:15:GLY:O	2.20	0.41
1:U:98:GLN:OE1	1:U:98:GLN:N	2.52	0.41
1:E:60:LYS:HB3	1:E:61:ASN:HA	2.02	0.41
1:P:41:VAL:HA	1:P:42:PRO:HD3	1.87	0.41
1:N:21:LEU:HB3	1:N:35:LEU:HB3	2.02	0.41
1:F:96:PHE:CG	1:F:105:ARG:HG2	2.55	0.41
1:V:110:THR:O	1:V:111:GLU:C	2.57	0.41
1:J:81:ASP:N	1:J:81:ASP:OD1	2.47	0.41
1:K:56:SER:OG	1:K:57:ARG:N	2.54	0.41
1:V:131:ALA:O	1:V:132:TYR:HB2	2.21	0.41
1:E:11:ILE:O	1:N:110:THR:OG1	2.37	0.41
1:C:35:LEU:HD22	1:C:48:VAL:H	1.86	0.40
1:O:21:LEU:HB3	1:O:35:LEU:HB3	2.03	0.40
1:C:45:GLU:OE1	1:C:46:LYS:NZ	2.49	0.40
1:D:107:PHE:CD1	1:D:107:PHE:C	2.94	0.40
1:C:85:THR:OG1	1:C:86:ARG:N	2.54	0.40
1:C:101:THR:OG1	1:C:102:ASP:N	2.54	0.40
1:H:100:SER:O	1:H:101:THR:C	2.59	0.40
1:V:128:LEU:HB2	1:V:129:ASN:HA	2.03	0.40
1:K:36:SER:OG	1:K:43:ALA:O	2.33	0.40
1:G:105:ARG:NH2	1:T:39:GLY:O	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	130/133 (98%)	121 (93%)	8 (6%)	1 (1%)	16	55
1	B	130/133 (98%)	125 (96%)	4 (3%)	1 (1%)	16	55
1	C	130/133 (98%)	118 (91%)	10 (8%)	2 (2%)	8	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	130/133 (98%)	120 (92%)	10 (8%)	0	100	100
1	E	130/133 (98%)	125 (96%)	4 (3%)	1 (1%)	16	55
1	F	130/133 (98%)	126 (97%)	3 (2%)	1 (1%)	16	55
1	G	130/133 (98%)	121 (93%)	7 (5%)	2 (2%)	8	40
1	H	130/133 (98%)	124 (95%)	3 (2%)	3 (2%)	5	28
1	I	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	J	130/133 (98%)	124 (95%)	6 (5%)	0	100	100
1	K	130/133 (98%)	124 (95%)	3 (2%)	3 (2%)	5	28
1	L	130/133 (98%)	121 (93%)	7 (5%)	2 (2%)	8	40
1	M	130/133 (98%)	124 (95%)	5 (4%)	1 (1%)	16	55
1	N	130/133 (98%)	124 (95%)	6 (5%)	0	100	100
1	O	130/133 (98%)	121 (93%)	7 (5%)	2 (2%)	8	40
1	P	130/133 (98%)	121 (93%)	8 (6%)	1 (1%)	16	55
1	Q	130/133 (98%)	117 (90%)	13 (10%)	0	100	100
1	R	130/133 (98%)	124 (95%)	6 (5%)	0	100	100
1	S	130/133 (98%)	126 (97%)	3 (2%)	1 (1%)	16	55
1	T	130/133 (98%)	126 (97%)	3 (2%)	1 (1%)	16	55
1	U	130/133 (98%)	124 (95%)	6 (5%)	0	100	100
1	V	130/133 (98%)	121 (93%)	5 (4%)	4 (3%)	3	22
All	All	2860/2926 (98%)	2699 (94%)	135 (5%)	26 (1%)	17	52

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	GLY
1	C	126	ASP
1	H	101	THR
1	V	43	ALA
1	V	44	LEU
1	A	116	LEU
1	C	58	ASN
1	E	131	ALA
1	O	51	SER
1	P	75	THR
1	V	74	CYS

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Mol	Chain	Res	Type
1	F	60	LYS
1	K	60	LYS
1	K	125	ILE
1	M	80	CYS
1	O	45	GLU
1	G	36	SER
1	S	38	ALA
1	V	128	LEU
1	L	79	SER
1	H	63	LYS
1	T	43	ALA
1	K	61	ASN
1	G	22	ASN
1	H	27	ASN
1	L	27	ASN

### 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	110/111 (99%)	110 (100%)	0	100	100
1	B	110/111 (99%)	110 (100%)	0	100	100
1	C	110/111 (99%)	110 (100%)	0	100	100
1	D	110/111 (99%)	110 (100%)	0	100	100
1	E	110/111 (99%)	110 (100%)	0	100	100
1	F	110/111 (99%)	109 (99%)	1 (1%)	75	83
1	G	110/111 (99%)	110 (100%)	0	100	100
1	H	110/111 (99%)	110 (100%)	0	100	100
1	I	110/111 (99%)	110 (100%)	0	100	100
1	J	110/111 (99%)	110 (100%)	0	100	100
1	K	110/111 (99%)	110 (100%)	0	100	100
1	L	110/111 (99%)	109 (99%)	1 (1%)	75	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	110/111 (99%)	110 (100%)	0	100	100
1	N	110/111 (99%)	109 (99%)	1 (1%)	75	83
1	O	110/111 (99%)	110 (100%)	0	100	100
1	P	110/111 (99%)	110 (100%)	0	100	100
1	Q	110/111 (99%)	109 (99%)	1 (1%)	75	83
1	R	110/111 (99%)	110 (100%)	0	100	100
1	S	110/111 (99%)	110 (100%)	0	100	100
1	T	110/111 (99%)	110 (100%)	0	100	100
1	U	110/111 (99%)	110 (100%)	0	100	100
1	V	110/111 (99%)	110 (100%)	0	100	100
All	All	2420/2442 (99%)	2416 (100%)	4 (0%)	91	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	47	ARG
1	N	47	ARG
1	F	46	LYS
1	Q	24	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	I	30	ASN

### 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 [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.



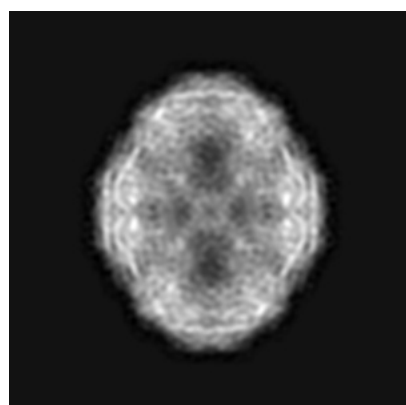
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23324. These allow visual inspection of the internal detail of the map and identification of artifacts.

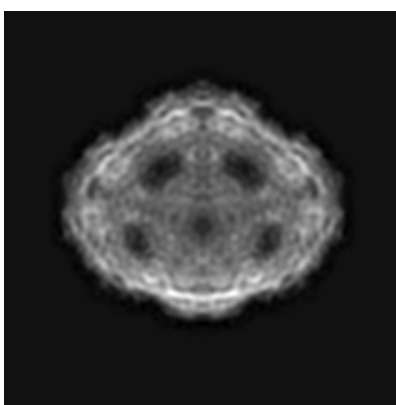
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

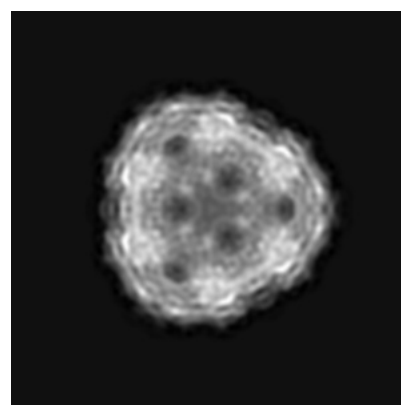
#### 6.1.1 Primary map



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: 80



Y Index: 80

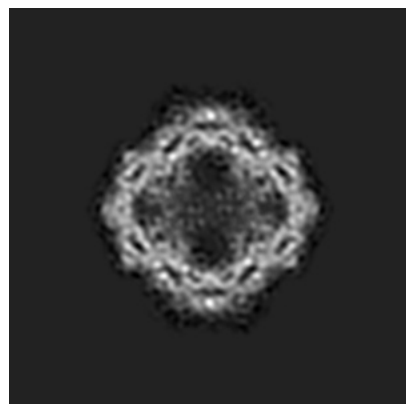


Z Index: 80

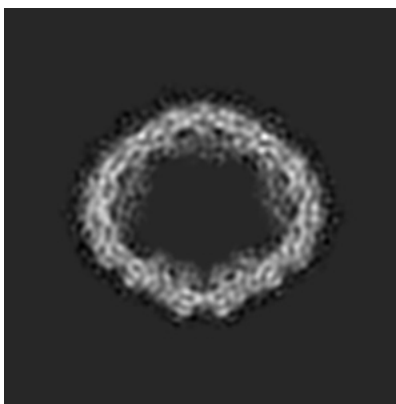
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 52



Y Index: 100

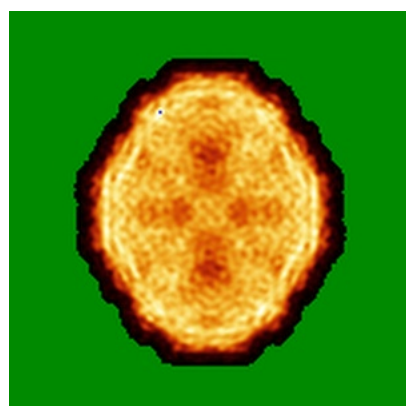


Z Index: 87

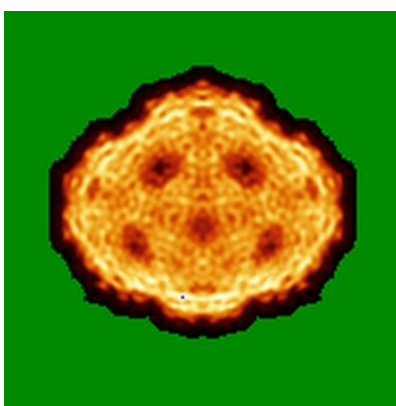
The images above show the largest variance slices of the map in three orthogonal directions.

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

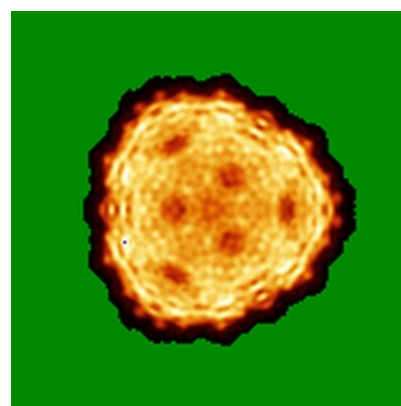
### 6.4.1 Primary map



X



Y

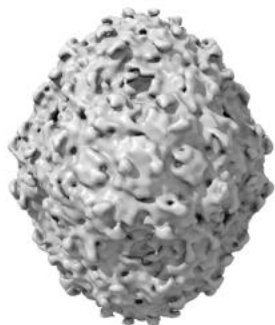


Z

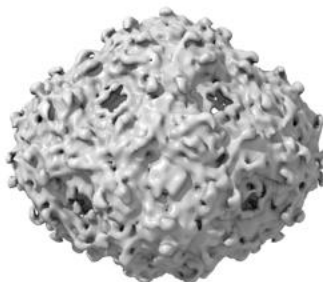
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

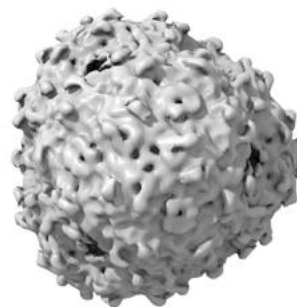
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

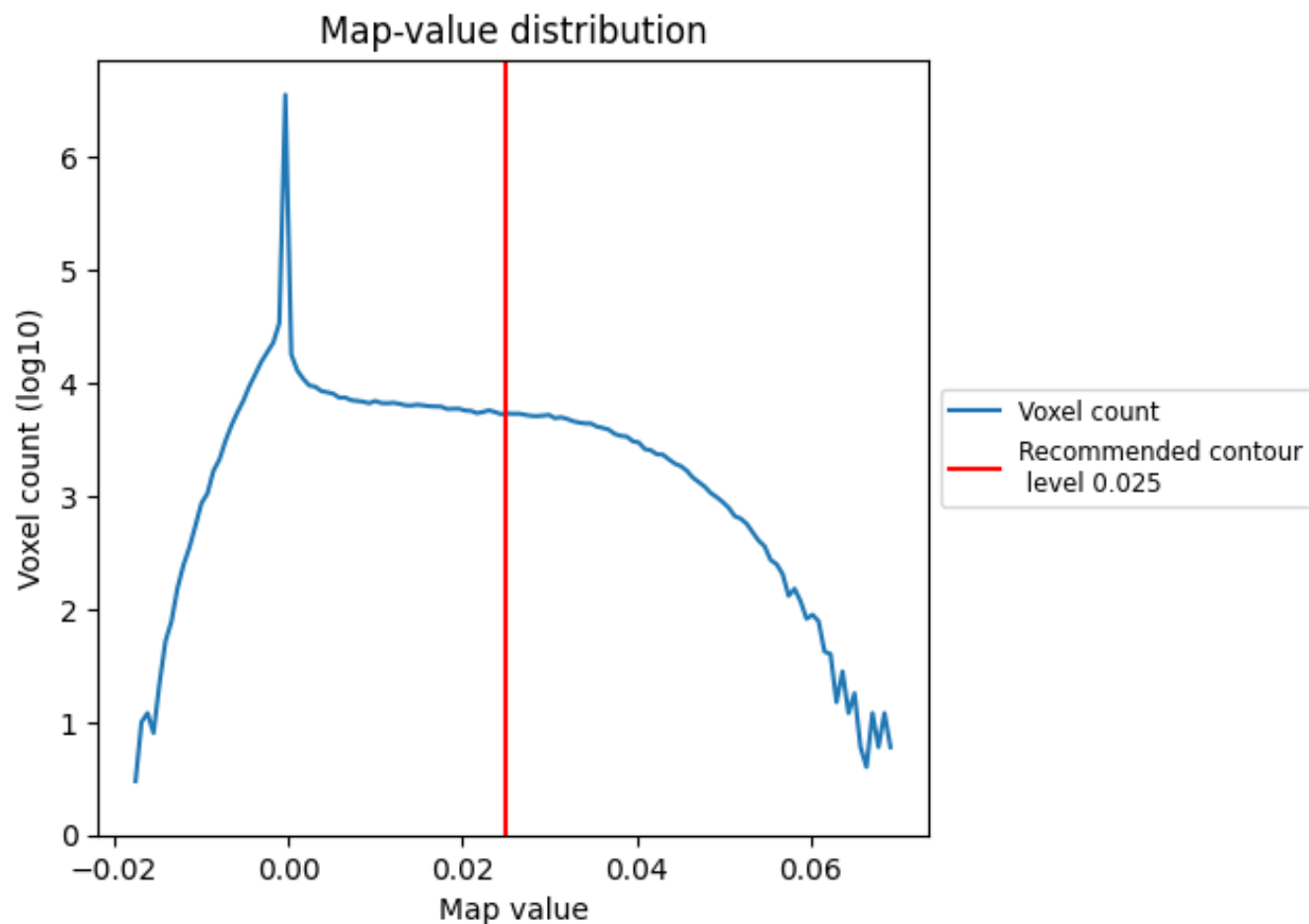
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

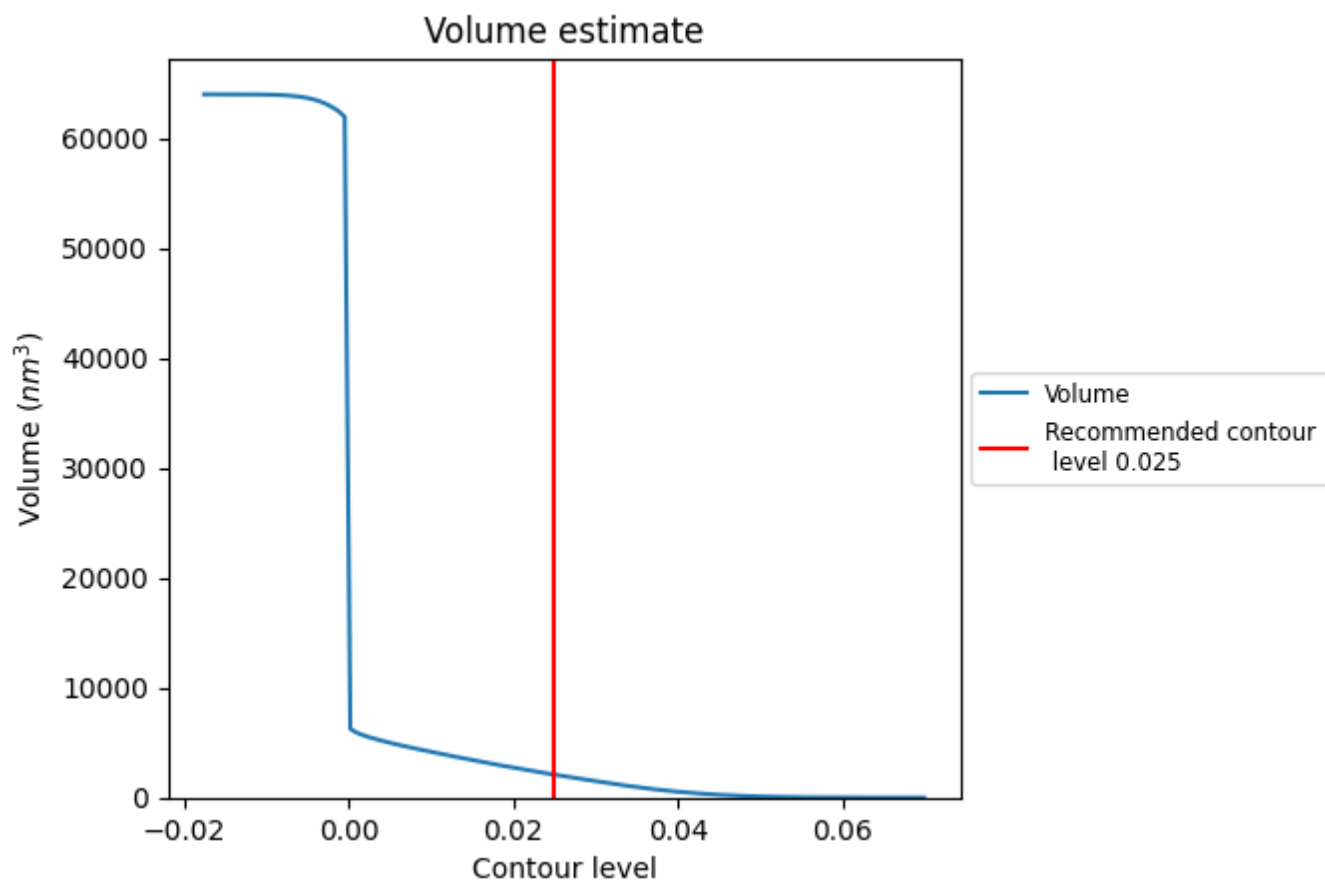
This section contains the results of statistical analysis of the map.

### 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.

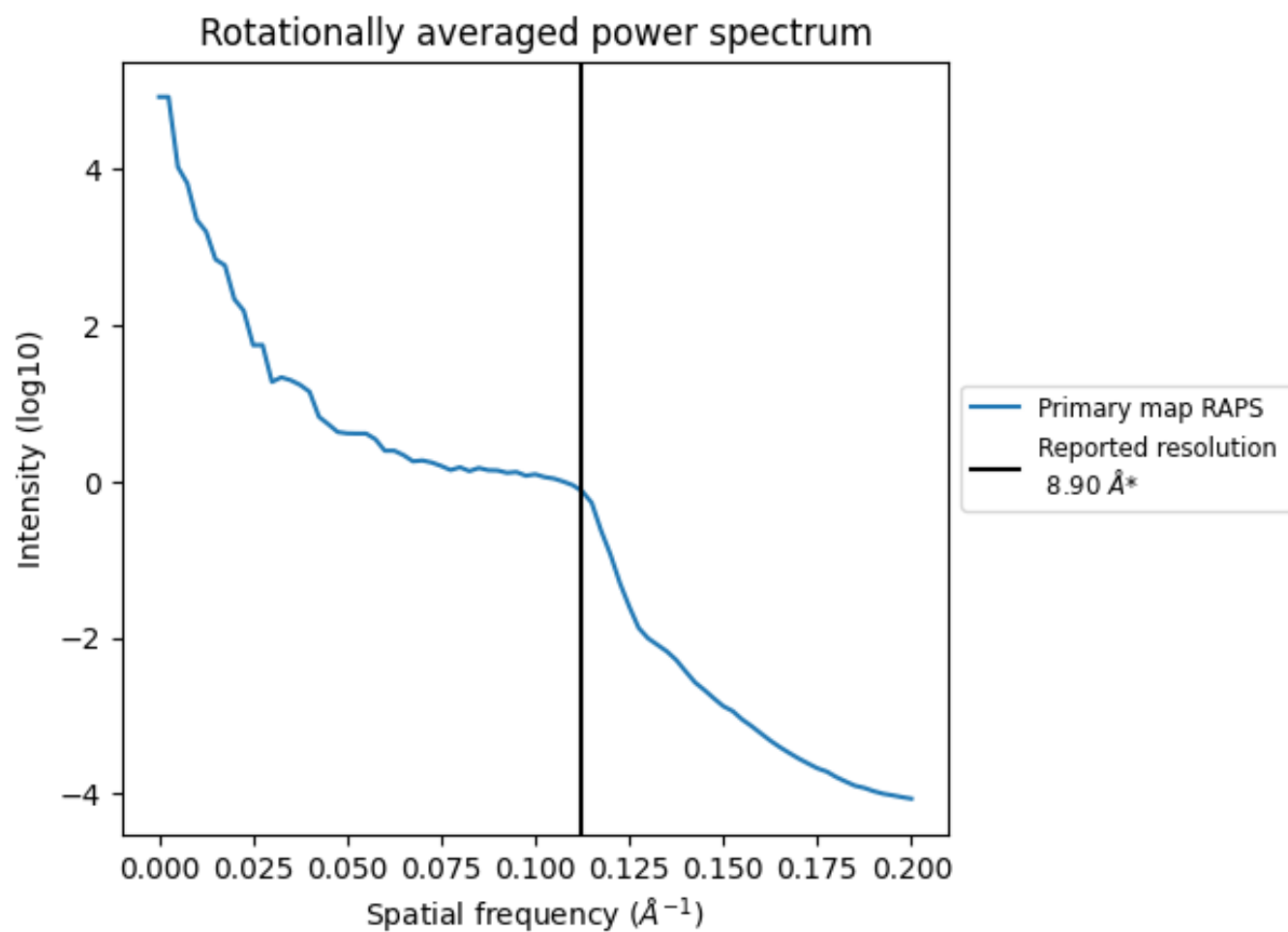
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2084 nm<sup>3</sup>; this corresponds to an approximate mass of 1882 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 ⓘ

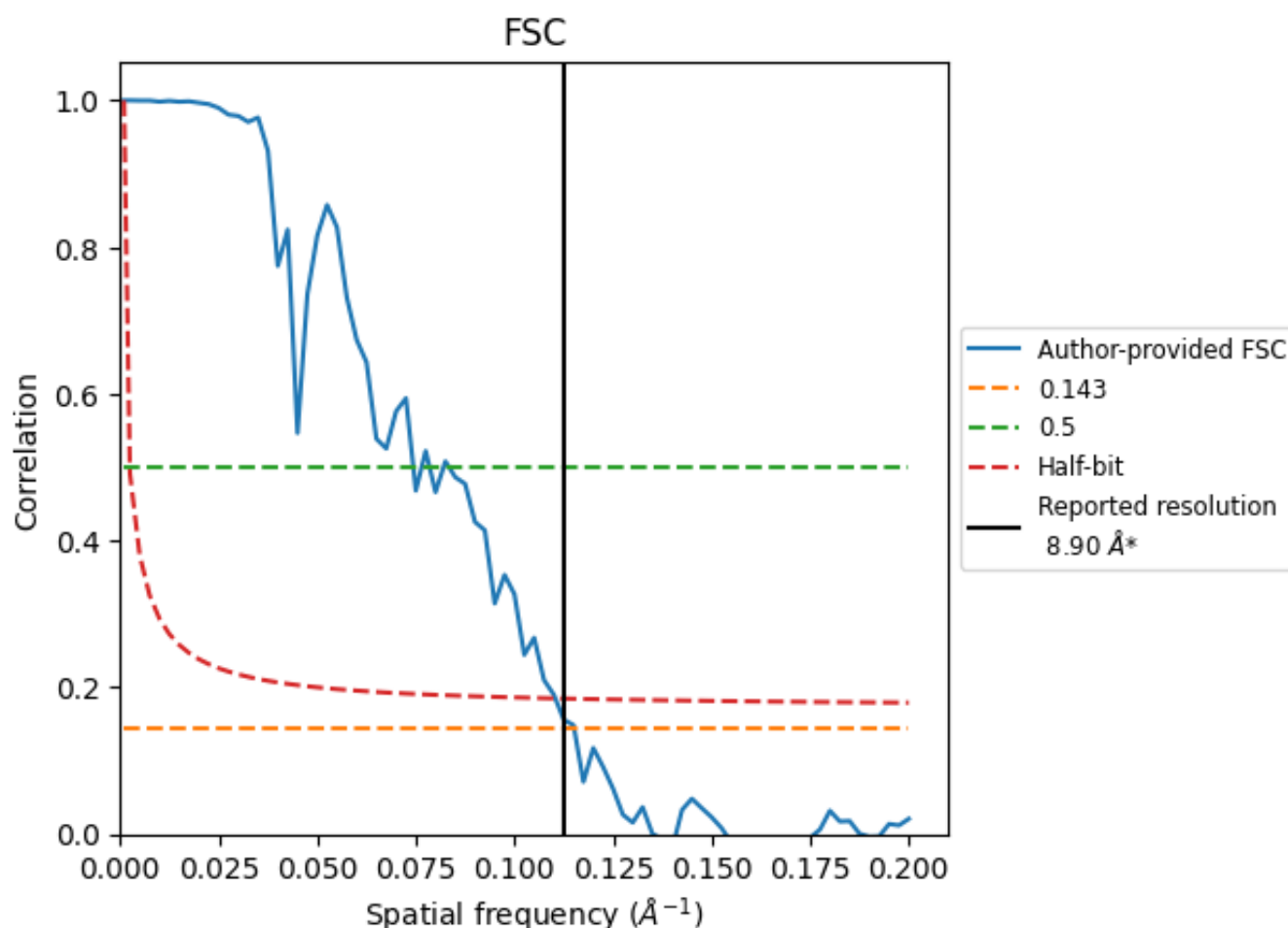


\*Reported resolution corresponds to spatial frequency of 0.112 Å<sup>-1</sup>

## 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 0.112 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.90	-	-
Author-provided FSC curve	8.68	13.44	9.06
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

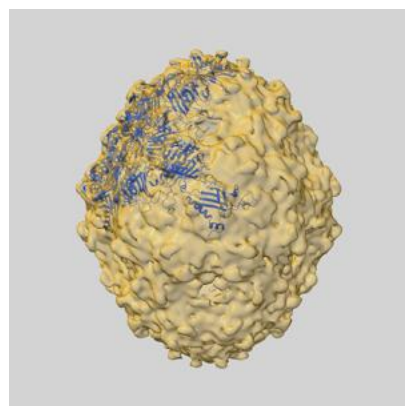


## 9 Map-model fit [i](#)

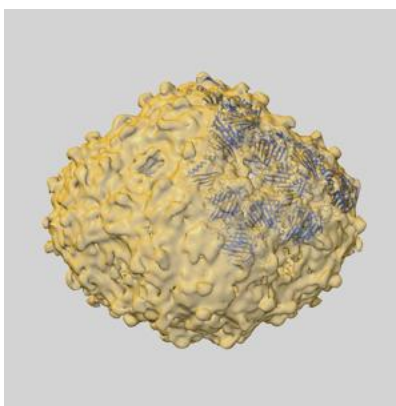
This section contains information regarding the fit between EMDB map EMD-23324 and PDB model 7LGH. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlays

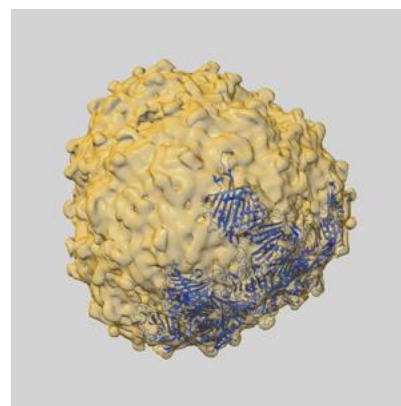
#### 9.1.1 Map-model overlay [i](#)



X

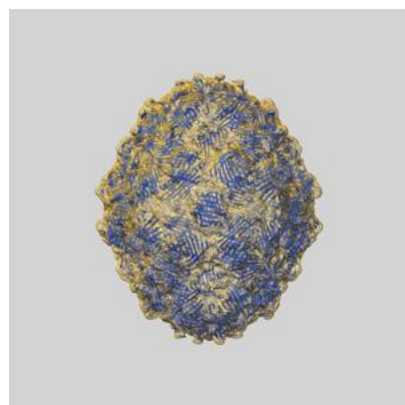


Y

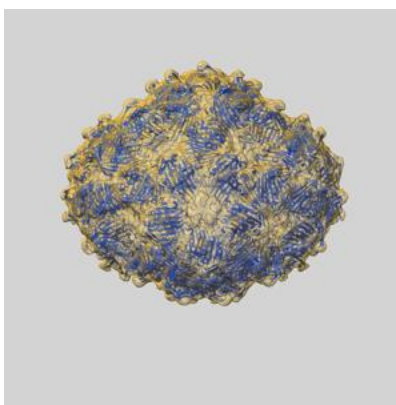


Z

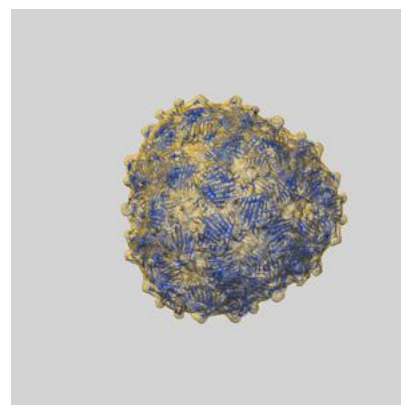
#### 9.1.2 Map-model assembly overlay [i](#)



X



Y



Z

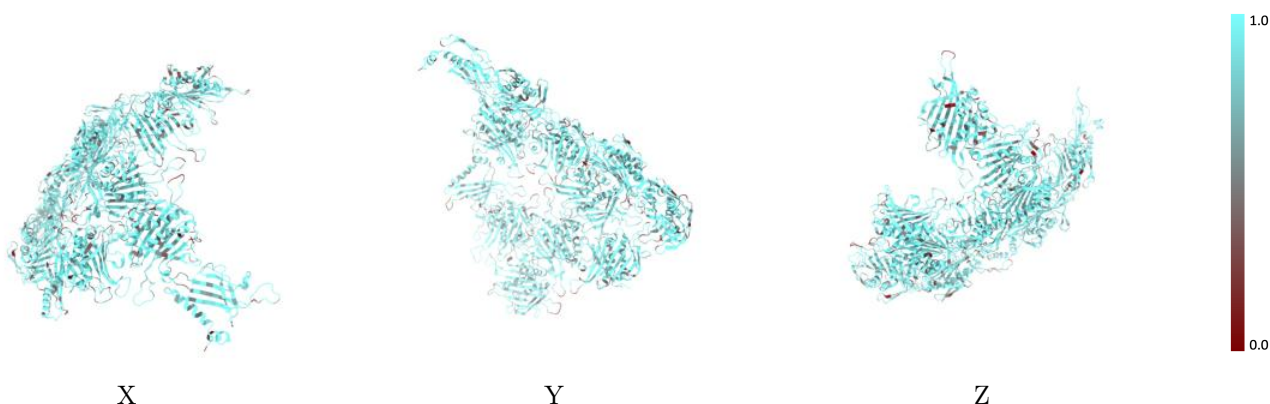
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



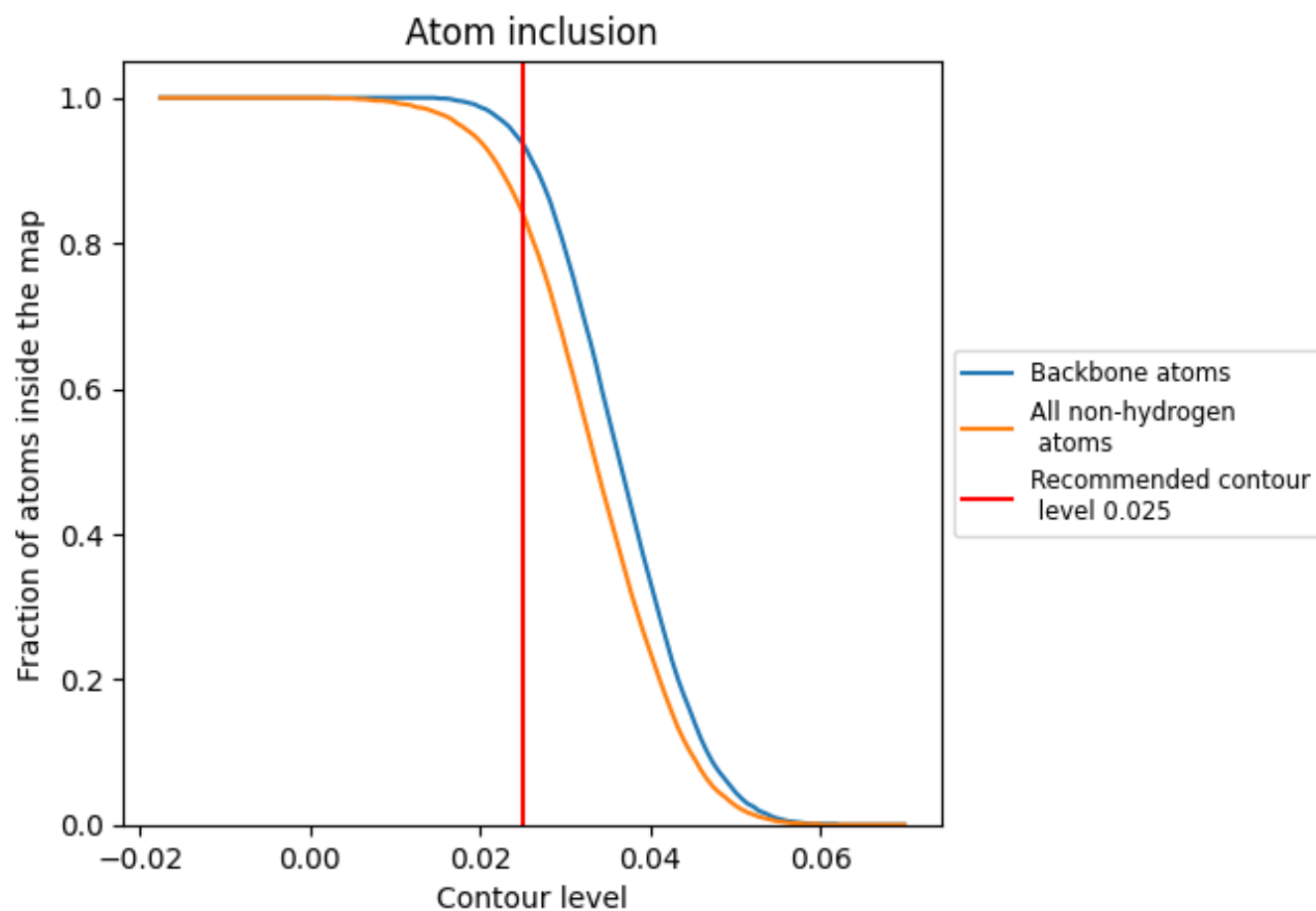
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 84% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.1140
A	 0.8460	 0.1130
B	 0.7850	 0.1070
C	 0.8300	 0.1180
D	 0.8800	 0.1240
E	 0.8550	 0.1270
F	 0.8660	 0.1140
G	 0.8520	 0.1280
H	 0.8570	 0.1250
I	 0.8430	 0.1150
J	 0.8310	 0.1060
K	 0.8460	 0.1170
L	 0.8400	 0.1020
M	 0.8570	 0.1250
N	 0.8610	 0.0960
O	 0.8430	 0.1180
P	 0.8350	 0.1070
Q	 0.8660	 0.1340
R	 0.7860	 0.0950
S	 0.8470	 0.1220
T	 0.8250	 0.0970
U	 0.8430	 0.0980
V	 0.8110	 0.1220

