



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 09:09 AM EDT

PDB ID : 7N69  
EMDB ID : EMD-24201  
Title : Pre-fusion state 2 of EEEV with localized reconstruction  
Authors : Chen, C.-L.; Kuhn, R.J.; Klose, T.  
Deposited on : 2021-06-07  
Resolution : 14.10 Å (reported)  
Based on initial model : 6MX4

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

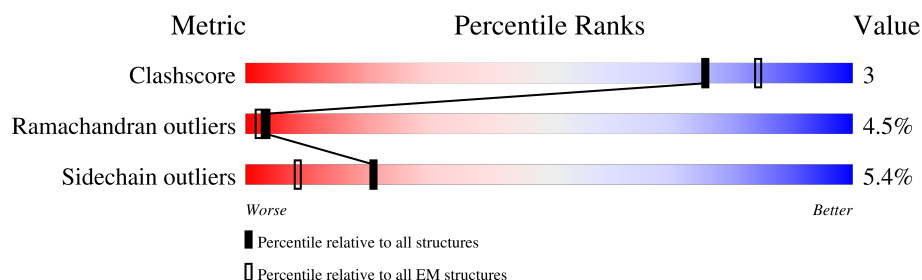
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*




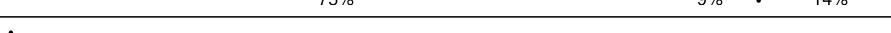




The reported resolution of this entry is 14.10 Å.

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	441	 72% 12% • 14%
1	C	441	 72% 12% • 14%
1	E	441	 75% 9% • 14%
1	G	441	 72% 12% • 14%
1	I	441	 74% 11% • 14%
1	K	441	 73% 11% • 14%
2	B	420	 44% 11% • 43%
2	D	420	 47% 9% 43%

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Mol	Chain	Length	Quality of chain
2	F	420	<div><div></div><div>48%8%43%</div></div>
2	H	420	<div><div></div><div>47%8%43%</div></div>
2	J	420	<div><div></div><div>48%8%43%</div></div>
2	L	420	<div><div></div><div>48%8%43%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28686 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 Spike glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	381	Total	C	N	O	S	0	0
			2907	1840	485	562	20		
1	C	381	Total	C	N	O	S	0	0
			2907	1840	485	562	20		
1	E	381	Total	C	N	O	S	0	0
			2907	1840	485	562	20		
1	G	381	Total	C	N	O	S	0	0
			2907	1840	485	562	20		
1	I	381	Total	C	N	O	S	0	0
			2907	1840	485	562	20		
1	K	381	Total	C	N	O	S	0	0
			2907	1840	485	562	20		

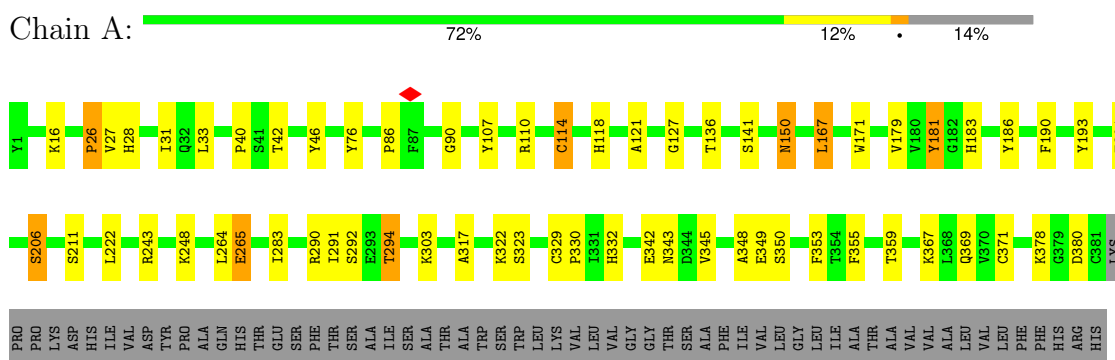
- Molecule 2 is a protein called Spike glycoprotein E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	238	Total	C	N	O	S	0	0
			1874	1179	348	336	11		
2	D	238	Total	C	N	O	S	0	0
			1874	1179	348	336	11		
2	F	238	Total	C	N	O	S	0	0
			1874	1179	348	336	11		
2	H	238	Total	C	N	O	S	0	0
			1874	1179	348	336	11		
2	J	238	Total	C	N	O	S	0	0
			1874	1179	348	336	11		
2	L	238	Total	C	N	O	S	0	0
			1874	1179	348	336	11		

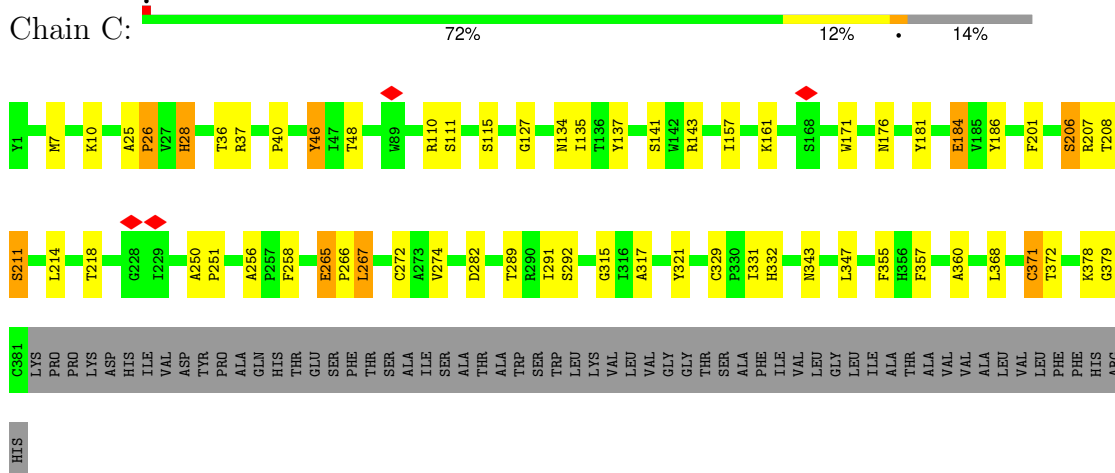
### 3 Residue-property plots [i](#)

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.

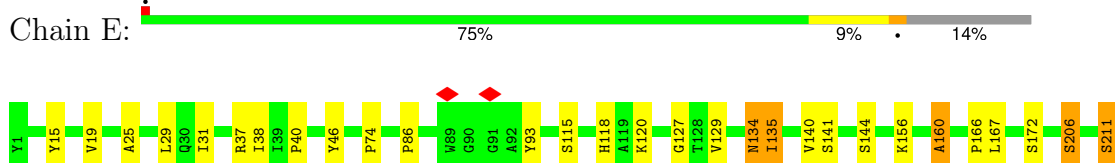
#### • Molecule 1: Spike glycoprotein E1



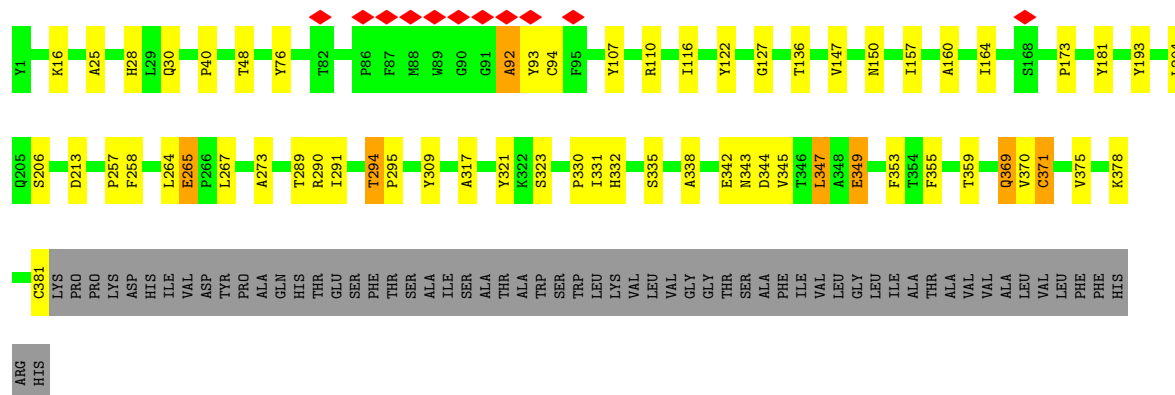
#### • Molecule 1: Spike glycoprotein E1



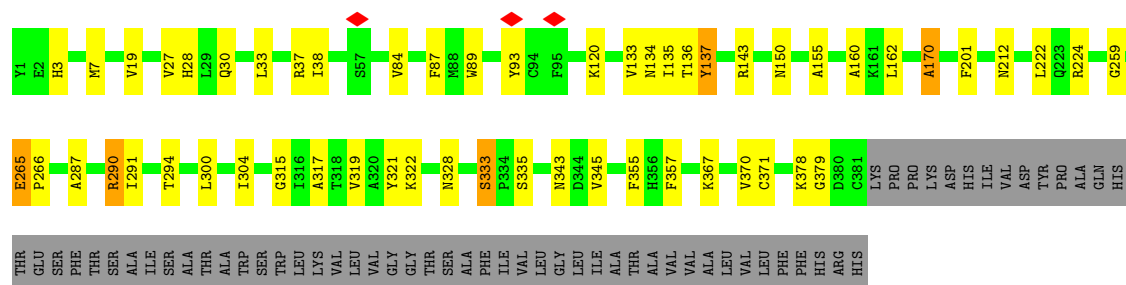
#### • Molecule 1: Spike glycoprotein E1



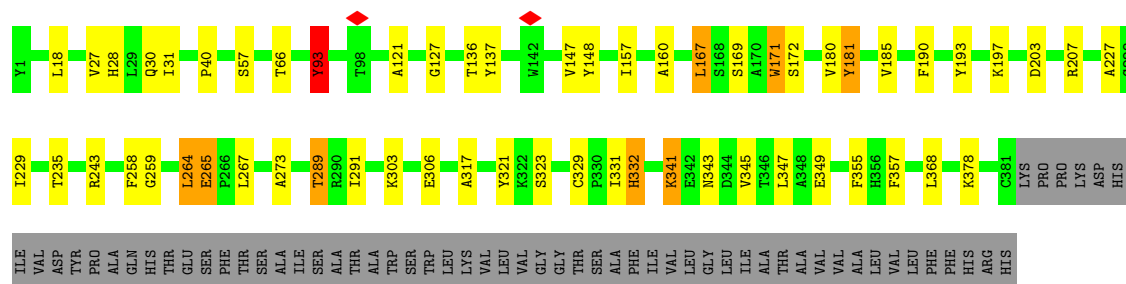
- Molecule 1: Spike glycoprotein E1



- Molecule 1: Spike glycoprotein E1



- Molecule 1: Spike glycoprotein E1



- Molecule 2: Spike glycoprotein E2

Category	Percentage
Very good	44%
Good	11%
Not good	43%
Very bad	1%



Response	Percentage
Yes	47%
No	9%
Don't know	43%

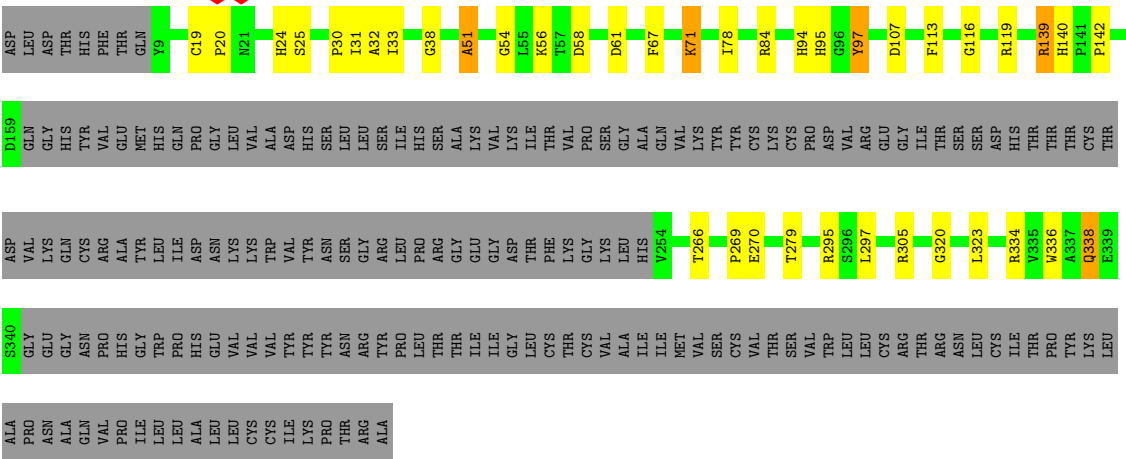


Response	Percentage
U.S. is responsible	48%
U.S. is not responsible	8%
U.S. is not responsible	43%

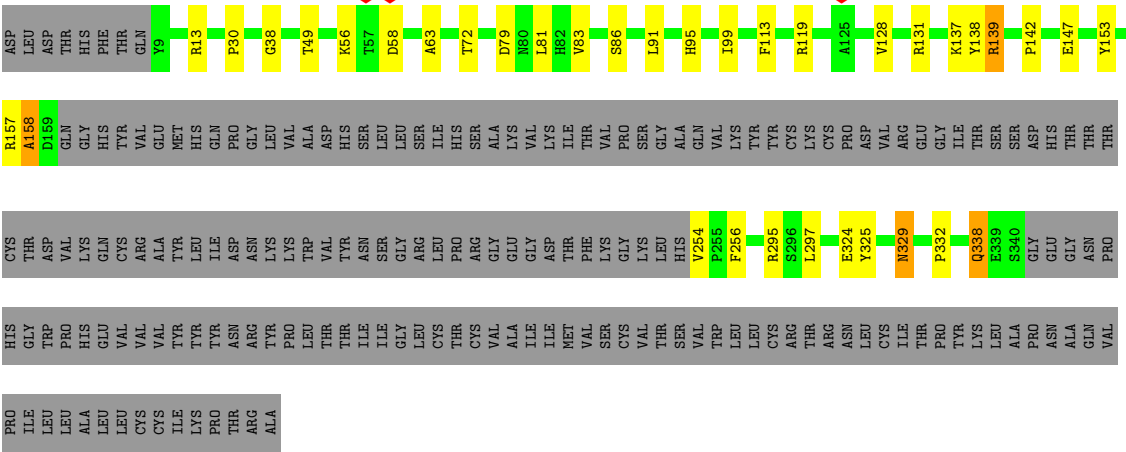


ASN  
ALA  
GLN  
ASP  
VAL  
HIS  
PRO  
PHE  
ILE  
LEU  
LEU  
ALA  
LEU  
CYS  
CYS  
ILE  
LYS  
PRO  
THR  
ARG  
ALA

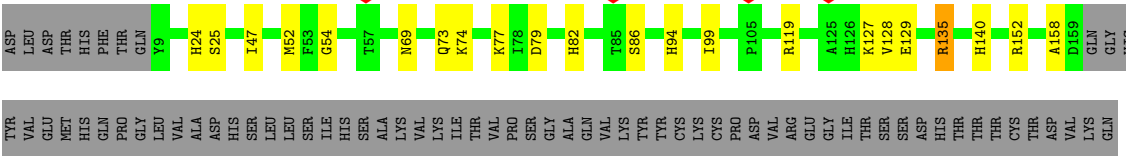
• Molecule 2: Spike glycoprotein E2



• Molecule 2: Spike glycoprotein E2



• Molecule 2: Spike glycoprotein E2





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

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	192060	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.010	Depositor
Minimum map value	-3.203	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	503.424, 503.424, 503.424	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.496, 3.496, 3.496	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	0.92	0/2984	1.15	4/4070 (0.1%)
1	C	0.92	0/2984	1.14	2/4070 (0.0%)
1	E	0.92	0/2984	1.18	7/4070 (0.2%)
1	G	0.90	0/2984	1.14	1/4070 (0.0%)
1	I	0.91	0/2984	1.14	2/4070 (0.0%)
1	K	0.90	0/2984	1.16	8/4070 (0.2%)
2	B	0.92	0/1930	1.25	5/2630 (0.2%)
2	D	0.93	0/1930	1.23	1/2630 (0.0%)
2	F	0.92	0/1930	1.18	1/2630 (0.0%)
2	H	0.93	0/1930	1.16	4/2630 (0.2%)
2	J	0.92	0/1930	1.18	1/2630 (0.0%)
2	L	0.93	0/1930	1.19	2/2630 (0.1%)
All	All	0.92	0/29484	1.17	38/40200 (0.1%)

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	2
1	C	0	4
1	E	0	4
1	G	0	4
1	I	0	2
1	K	0	3
2	D	0	2
2	F	0	3
2	H	0	1
2	J	0	3
2	L	0	2
All	All	0	30

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	67	PHE	CB-CG-CD1	8.02	126.42	120.80
1	K	93	TYR	CB-CG-CD2	7.40	125.44	121.00
1	A	181	TYR	CB-CG-CD2	-7.08	116.75	121.00
2	B	67	PHE	CB-CG-CD2	-7.00	115.90	120.80
1	K	181	TYR	CB-CG-CD2	-7.00	116.80	121.00
1	K	93	TYR	CB-CG-CD1	-6.86	116.88	121.00
2	H	51	ALA	N-CA-CB	6.78	119.59	110.10
1	C	211	SER	N-CA-CB	6.57	120.36	110.50
2	F	119	ARG	N-CA-C	-6.33	93.91	111.00
2	B	51	ALA	N-CA-C	-5.98	94.85	111.00
1	A	181	TYR	CB-CG-CD1	5.93	124.56	121.00
2	H	97	TYR	CB-CG-CD1	-5.92	117.44	121.00
1	E	160	ALA	N-CA-CB	5.92	118.39	110.10
1	K	181	TYR	CB-CG-CD1	5.86	124.52	121.00
1	E	211	SER	N-CA-CB	5.70	119.05	110.50
1	E	93	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	E	215	TYR	N-CA-C	-5.58	95.93	111.00
1	K	148	TYR	CB-CG-CD1	-5.53	117.68	121.00
2	D	327	TRP	N-CA-C	-5.49	96.19	111.00
1	E	93	TYR	CB-CG-CD2	5.47	124.28	121.00
1	A	186	TYR	N-CA-C	-5.44	96.31	111.00
1	E	296	THR	N-CA-C	-5.40	96.43	111.00
1	C	181	TYR	CB-CG-CD1	-5.37	117.78	121.00
2	B	325	TYR	N-CA-C	-5.29	96.72	111.00
2	H	51	ALA	N-CA-C	-5.29	96.72	111.00
1	K	258	PHE	CB-CG-CD2	5.27	124.49	120.80
1	K	258	PHE	CB-CG-CD1	-5.26	117.12	120.80
1	G	92	ALA	N-CA-CB	5.23	117.43	110.10
1	K	148	TYR	CB-CG-CD2	5.21	124.12	121.00
2	H	97	TYR	CB-CG-CD2	5.18	124.11	121.00
2	B	296	SER	N-CA-CB	5.18	118.27	110.50
1	E	19	VAL	N-CA-C	-5.15	97.09	111.00
1	I	345	VAL	N-CA-C	-5.14	97.13	111.00
2	J	329	ASN	N-CA-CB	5.13	119.83	110.60
2	L	52	MET	CG-SD-CE	-5.09	92.06	100.20
2	L	278	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	A	243	ARG	NE-CZ-NH2	5.05	122.82	120.30
1	I	333	SER	N-CA-CB	5.02	118.03	110.50

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	264	LEU	Peptide
1	A	265	GLU	Peptide
1	C	256	ALA	Peptide
1	C	265	GLU	Peptide
1	C	321	TYR	Sidechain
1	C	46	TYR	Sidechain
2	D	138	TYR	Sidechain
2	D	139	ARG	Sidechain
1	E	15	TYR	Sidechain
1	E	264	LEU	Peptide
1	E	265	GLU	Peptide
1	E	321	TYR	Sidechain
2	F	138	TYR	Sidechain
2	F	256	PHE	Sidechain
2	F	46	ARG	Sidechain
1	G	122	TYR	Sidechain
1	G	264	LEU	Peptide
1	G	265	GLU	Peptide
1	G	321	TYR	Sidechain
2	H	305	ARG	Sidechain
1	I	137	TYR	Sidechain
1	I	265	GLU	Peptide
2	J	153	TYR	Sidechain
2	J	256	PHE	Sidechain
2	J	325	TYR	Sidechain
1	K	193	TYR	Sidechain
1	K	264	LEU	Peptide
1	K	265	GLU	Peptide
2	L	278	ARG	Sidechain
2	L	295	ARG	Sidechain

## 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	2907	0	2805	22	0
1	C	2907	0	2805	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2907	0	2805	15	0
1	G	2907	0	2805	22	0
1	I	2907	0	2805	18	0
1	K	2907	0	2805	15	0
2	B	1874	0	1831	15	0
2	D	1874	0	1831	7	0
2	F	1874	0	1831	10	0
2	H	1874	0	1831	7	0
2	J	1874	0	1831	9	0
2	L	1874	0	1831	14	0
All	All	28686	0	27816	164	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 (164) 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:317:ALA:HB3	1:A:355:PHE:CZ	2.33	0.63
1:C:360:ALA:HA	2:D:278:ARG:HE	1.68	0.57
1:A:28:HIS:CD2	1:A:343:ASN:HB2	2.40	0.56
1:K:180:VAL:HG13	1:K:264:LEU:HD21	1.86	0.56
1:I:38:ILE:HD11	1:I:170:ALA:HB1	1.88	0.56
1:A:110:ARG:H	1:A:211:SER:HB3	1.70	0.56
1:I:137:TYR:H	1:I:143:ARG:HH22	1.54	0.56
2:L:268:ALA:HB3	2:L:327:TRP:CH2	2.41	0.55
1:C:46:TYR:HB2	1:C:206:SER:H	1.71	0.55
1:A:136:THR:HG23	1:A:141:SER:HA	1.87	0.55
1:K:18:LEU:HG	1:K:332:HIS:CG	2.42	0.54
2:L:278:ARG:HA	2:L:278:ARG:HE	1.73	0.54
2:L:24:HIS:CG	2:L:25:SER:H	2.26	0.53
2:B:267:LEU:HA	2:B:288:HIS:CE1	2.43	0.53
2:B:139:ARG:HE	2:B:139:ARG:H	1.57	0.53
2:L:268:ALA:HB1	2:L:286:PRO:HA	1.91	0.53
1:C:331:ILE:HG12	1:C:368:LEU:HD11	1.91	0.52
1:I:28:HIS:CE1	1:I:328:ASN:HB3	2.45	0.52
1:K:317:ALA:HB3	1:K:355:PHE:CZ	2.46	0.51
2:L:135:ARG:HE	2:L:291:LEU:HD23	1.76	0.51
2:B:127:LYS:H	2:B:127:LYS:HD2	1.75	0.51
1:E:273:ALA:HB1	2:F:298:GLY:H	1.74	0.51
1:G:317:ALA:HB3	1:G:355:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:81:LEU:HD11	2:F:111:VAL:HG12	1.93	0.50
1:K:185:VAL:HB	1:K:264:LEU:HD22	1.92	0.50
1:A:28:HIS:CE1	1:A:136:THR:HG21	2.46	0.50
1:A:329:CYS:HB3	1:A:371:CYS:H	1.76	0.50
1:E:317:ALA:HB3	1:E:355:PHE:CZ	2.46	0.50
2:H:320:GLY:HA2	2:H:338:GLN:HB3	1.93	0.50
1:E:134:ASN:HA	1:E:144:SER:HA	1.94	0.50
1:I:155:ALA:HB3	1:I:162:LEU:HB2	1.94	0.50
2:H:297:LEU:H	2:H:323:LEU:HA	1.77	0.49
1:A:330:PRO:HA	1:A:343:ASN:O	2.12	0.49
1:C:40:PRO:HA	1:C:127:GLY:HA3	1.94	0.49
1:C:272:CYS:HB3	1:C:274:VAL:HG12	1.94	0.49
2:B:267:LEU:HD22	2:B:330:HIS:CE1	2.48	0.49
2:H:54:GLY:CA	2:H:94:HIS:HB3	2.43	0.49
2:B:278:ARG:HH21	2:B:320:GLY:HA3	1.78	0.48
1:G:48:THR:HG23	1:G:204:LEU:H	1.76	0.48
1:G:294:THR:H	1:G:295:PRO:HD2	1.78	0.48
2:J:157:ARG:HD2	2:J:157:ARG:H	1.79	0.48
1:G:317:ALA:HB3	1:G:355:PHE:CE2	2.48	0.48
2:H:24:HIS:CG	2:H:25:SER:H	2.31	0.48
1:E:38:ILE:HG23	1:E:129:VAL:HG22	1.95	0.48
2:H:56:LYS:HG3	2:H:58:ASP:H	1.79	0.48
2:J:95:HIS:CE1	2:J:158:ALA:H	2.32	0.47
2:H:119:ARG:HH22	2:J:63:ALA:HB1	1.79	0.47
1:C:317:ALA:HB3	1:C:355:PHE:CZ	2.48	0.47
2:B:320:GLY:HA2	2:B:340:SER:H	1.80	0.47
1:A:27:VAL:HG11	1:A:283:ILE:HG21	1.97	0.47
2:B:54:GLY:CA	2:B:94:HIS:HB3	2.44	0.47
2:L:54:GLY:HA3	2:L:94:HIS:CG	2.50	0.47
1:C:48:THR:HG21	1:C:201:PHE:CE1	2.49	0.47
2:F:267:LEU:HD22	2:F:330:HIS:CE1	2.50	0.47
1:C:329:CYS:HB3	1:C:371:CYS:H	1.80	0.46
1:G:16:LYS:HB2	1:G:332:HIS:CE1	2.50	0.46
2:J:119:ARG:HE	2:L:82:HIS:CD2	2.33	0.46
2:F:295:ARG:HA	2:F:302:ASN:O	2.16	0.46
1:I:317:ALA:HB3	1:I:355:PHE:CZ	2.50	0.46
2:D:56:LYS:HG3	2:D:58:ASP:H	1.81	0.46
1:C:315:GLY:HA3	1:C:357:PHE:CZ	2.51	0.46
1:G:345:VAL:HG23	1:G:353:PHE:CD1	2.51	0.46
1:I:38:ILE:HD12	1:I:38:ILE:N	2.31	0.46
2:D:322:GLY:HA3	2:D:336:TRP:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:VAL:HG11	1:G:164:ILE:H	1.81	0.45
2:L:94:HIS:CE1	2:L:99:ILE:HG23	2.51	0.45
1:A:222:LEU:HD22	1:A:222:LEU:H	1.80	0.45
2:B:91:LEU:HA	2:B:101:ALA:HA	1.98	0.45
1:C:315:GLY:HA3	1:C:357:PHE:CE1	2.52	0.45
1:C:331:ILE:CG1	1:C:368:LEU:HD11	2.47	0.45
1:E:38:ILE:HG21	1:E:172:SER:N	2.30	0.45
2:F:273:VAL:HG13	2:F:280:LEU:HD21	1.98	0.45
1:A:179:VAL:HG13	1:A:201:PHE:CZ	2.51	0.45
1:G:25:ALA:H	1:G:289:THR:HG23	1.82	0.45
1:G:347:LEU:HD13	1:G:349:GLU:H	1.80	0.45
1:I:27:VAL:HA	1:I:287:ALA:HB3	1.98	0.45
1:E:329:CYS:HB3	1:E:371:CYS:H	1.81	0.45
1:G:323:SER:HB3	1:G:347:LEU:HD11	1.99	0.45
1:I:38:ILE:HD11	1:I:170:ALA:CB	2.47	0.45
1:I:222:LEU:HD22	1:I:222:LEU:H	1.81	0.45
2:J:38:GLY:H	2:J:128:VAL:HG21	1.82	0.45
1:K:259:GLY:HA3	2:L:297:LEU:HA	1.98	0.45
1:K:40:PRO:HA	1:K:127:GLY:HA3	1.98	0.45
1:G:258:PHE:HB3	1:G:273:ALA:H	1.81	0.45
1:A:76:TYR:HA	1:A:107:TYR:HB3	1.99	0.45
1:G:28:HIS:CE1	1:G:342:GLU:HA	2.51	0.45
1:K:323:SER:H	1:K:349:GLU:HG2	1.82	0.45
1:A:40:PRO:HA	1:A:127:GLY:HA3	1.98	0.44
1:A:121:ALA:HB1	1:A:190:PHE:CE1	2.52	0.44
1:A:28:HIS:CE1	1:A:342:GLU:HA	2.52	0.44
1:C:28:HIS:CD2	1:C:343:ASN:HB3	2.51	0.44
2:F:31:ILE:HD13	2:F:111:VAL:HB	1.99	0.44
1:I:136:THR:HG21	1:I:343:ASN:HB3	1.98	0.44
2:B:56:LYS:HG3	2:B:58:ASP:H	1.82	0.44
1:I:304:ILE:H	1:I:379:GLY:HA3	1.81	0.44
1:E:264:LEU:H	1:E:264:LEU:HD22	1.82	0.44
2:J:56:LYS:HG3	2:J:58:ASP:H	1.82	0.44
1:K:28:HIS:NE2	1:K:136:THR:HG21	2.33	0.44
1:A:345:VAL:HG23	1:A:353:PHE:CG	2.52	0.44
1:C:161:LYS:H	1:C:282:ASP:HB3	1.82	0.44
2:J:81:LEU:HD12	2:J:113:PHE:CE1	2.52	0.44
1:K:121:ALA:HB1	1:K:190:PHE:CE1	2.52	0.44
1:A:323:SER:H	1:A:349:GLU:HG2	1.82	0.44
2:F:114:HIS:CE1	2:F:119:ARG:HE	2.36	0.44
1:G:309:TYR:HA	1:G:381:CYS:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:PRO:HA	1:G:127:GLY:HA3	1.98	0.43
1:G:370:VAL:HG12	1:G:371:CYS:H	1.83	0.43
1:I:3:HIS:HB2	1:I:19:VAL:HG13	1.99	0.43
2:B:10:LYS:H	2:B:10:LYS:HZ2	1.66	0.43
1:A:150:ASN:HA	1:A:167:LEU:H	1.84	0.43
2:F:81:LEU:HD13	2:F:113:PHE:CE2	2.53	0.43
1:C:171:TRP:H	1:C:274:VAL:HG11	1.83	0.43
2:B:143:GLU:O	2:B:144:HIS:CG	2.71	0.43
1:E:29:LEU:C	1:E:343:ASN:HD21	2.21	0.43
1:G:330:PRO:HG2	1:G:369:GLN:HE22	1.84	0.43
2:B:54:GLY:HA3	2:B:94:HIS:HB3	2.00	0.43
1:I:259:GLY:HA2	2:J:297:LEU:HD23	2.00	0.43
1:K:331:ILE:HD12	1:K:368:LEU:HD12	2.00	0.43
1:C:137:TYR:H	1:C:143:ARG:HH22	1.67	0.42
1:K:329:CYS:SG	1:K:347:LEU:HD11	2.59	0.42
1:C:184:GLU:HB3	1:C:186:TYR:CE2	2.55	0.42
1:G:28:HIS:CE1	1:G:136:THR:HG22	2.54	0.42
1:G:338:ALA:HB2	1:G:359:THR:HG22	2.02	0.42
2:F:56:LYS:HG3	2:F:58:ASP:H	1.83	0.42
2:F:95:HIS:HB2	2:F:256:PHE:CE1	2.55	0.42
2:H:95:HIS:O	2:H:95:HIS:CG	2.72	0.42
1:I:7:MET:SD	1:I:133:VAL:HG13	2.59	0.42
2:B:60:VAL:HG21	2:B:159:ASP:HB2	2.01	0.42
1:C:10:LYS:HA	2:D:336:TRP:CH2	2.55	0.42
1:E:368:LEU:HD23	1:E:377:CYS:SG	2.60	0.42
1:A:16:LYS:HB2	1:A:332:HIS:CE1	2.55	0.42
2:B:98:TYR:C	2:B:99:ILE:HD12	2.40	0.42
1:E:40:PRO:HA	1:E:127:GLY:HA3	2.02	0.42
1:I:300:LEU:HD21	1:I:370:VAL:HG21	2.01	0.42
1:E:31:ILE:HA	1:E:134:ASN:O	2.20	0.42
1:G:28:HIS:HA	1:G:343:ASN:HB2	2.02	0.42
1:I:133:VAL:HG12	1:I:135:ILE:HG13	2.02	0.42
2:D:10:LYS:HB2	2:D:96:GLY:HA3	2.02	0.42
2:D:135:ARG:HE	2:D:332:PRO:HD3	1.84	0.42
1:K:27:VAL:HG22	1:K:289:THR:H	1.85	0.42
1:E:46:TYR:HB2	1:E:206:SER:H	1.85	0.41
1:K:341:LYS:H	1:K:357:PHE:HA	1.85	0.41
2:L:268:ALA:HB1	2:L:269:PRO:HD2	2.02	0.41
1:I:315:GLY:HA3	1:I:357:PHE:CZ	2.55	0.41
1:A:121:ALA:HB1	1:A:190:PHE:CZ	2.55	0.41
2:L:54:GLY:HA3	2:L:94:HIS:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:268:ALA:HB3	2:L:327:TRP:CZ2	2.55	0.41
1:A:46:TYR:CB	1:A:206:SER:H	2.33	0.41
1:G:76:TYR:HA	1:G:107:TYR:HB3	2.02	0.41
2:D:295:ARG:HA	2:D:302:ASN:H	1.85	0.41
2:J:83:VAL:HG21	2:J:91:LEU:HD21	2.02	0.41
1:A:46:TYR:CE1	1:A:121:ALA:HB2	2.55	0.41
2:B:318:VAL:HG11	2:B:340:SER:HB2	2.03	0.41
1:E:135:ILE:HD12	1:E:135:ILE:H	1.85	0.41
1:G:294:THR:H	1:G:295:PRO:CD	2.34	0.41
1:E:38:ILE:HD12	1:E:38:ILE:N	2.35	0.40
1:G:28:HIS:HB2	1:G:344:ASP:CB	2.51	0.40
1:I:84:VAL:HA	1:I:224:ARG:HH22	1.86	0.40
2:L:24:HIS:CG	2:L:25:SER:N	2.89	0.40
1:K:167:LEU:HG	1:K:169:SER:H	1.86	0.40
1:A:46:TYR:HB2	1:A:206:SER:H	1.87	0.40
1:C:25:ALA:H	1:C:291:ILE:H	1.70	0.40
1:E:315:GLY:HA3	1:E:357:PHE:CE1	2.57	0.40
1:K:273:ALA:HB2	2:L:336:TRP:CZ3	2.56	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	379/441 (86%)	325 (86%)	38 (10%)	16 (4%)	2	17
1	C	379/441 (86%)	324 (86%)	36 (10%)	19 (5%)	1	16
1	E	379/441 (86%)	333 (88%)	33 (9%)	13 (3%)	3	21
1	G	379/441 (86%)	332 (88%)	29 (8%)	18 (5%)	2	16
1	I	379/441 (86%)	320 (84%)	44 (12%)	15 (4%)	2	18
1	K	379/441 (86%)	332 (88%)	35 (9%)	12 (3%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	234/420 (56%)	193 (82%)	27 (12%)	14 (6%)	1	13
2	D	234/420 (56%)	195 (83%)	29 (12%)	10 (4%)	2	17
2	F	234/420 (56%)	197 (84%)	27 (12%)	10 (4%)	2	17
2	H	234/420 (56%)	197 (84%)	21 (9%)	16 (7%)	1	12
2	J	234/420 (56%)	195 (83%)	27 (12%)	12 (5%)	1	15
2	L	234/420 (56%)	193 (82%)	30 (13%)	11 (5%)	2	16
All	All	3678/5166 (71%)	3136 (85%)	376 (10%)	166 (4%)	3	17

All (166) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	TRP
1	A	206	SER
1	A	291	ILE
1	A	292	SER
1	A	294	THR
2	B	51	ALA
1	C	111	SER
1	C	115	SER
1	C	157	ILE
1	C	207	ARG
1	C	266	PRO
1	C	292	SER
2	D	69	ASN
2	D	142	PRO
1	E	74	PRO
1	E	115	SER
1	E	160	ALA
1	E	211	SER
1	E	265	GLU
1	G	150	ASN
1	G	193	TYR
1	G	206	SER
1	G	265	GLU
2	H	51	ALA
1	I	265	GLU
1	I	333	SER
2	J	147	GLU
1	K	57	SER
2	L	74	LYS

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Mol	Chain	Res	Type
2	L	128	VAL
1	A	348	ALA
2	B	133	VAL
2	B	142	PRO
2	B	144	HIS
2	B	328	GLY
1	C	208	THR
1	C	371	CYS
2	D	139	ARG
2	D	329	ASN
1	E	141	SER
2	F	39	ASP
2	F	86	SER
2	F	328	GLY
1	G	92	ALA
1	G	160	ALA
1	G	291	ILE
1	G	294	THR
1	G	349	GLU
2	H	31	ILE
2	H	71	LYS
1	I	150	ASN
1	I	160	ALA
1	I	170	ALA
1	I	291	ILE
1	I	335	SER
2	J	79	ASP
2	J	86	SER
2	J	139	ARG
2	J	338	GLN
1	K	157	ILE
1	K	171	TRP
1	K	229	ILE
2	L	338	GLN
1	A	90	GLY
1	A	114	CYS
1	A	265	GLU
1	A	350	SER
2	B	26	ARG
2	B	31	ILE
2	B	79	ASP
2	B	86	SER

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Mol	Chain	Res	Type
2	B	299	SER
2	B	337	ALA
1	C	176	ASN
1	C	184	GLU
1	C	206	SER
1	C	211	SER
1	C	267	LEU
2	D	73	GLN
2	D	105	PRO
1	E	140	VAL
1	E	206	SER
2	F	27	CYS
2	F	79	ASP
2	F	115	ASP
1	G	335	SER
2	H	107	ASP
2	H	139	ARG
1	I	89	TRP
1	I	93	TYR
2	J	30	PRO
2	J	72	THR
2	J	158	ALA
1	K	93	TYR
1	K	160	ALA
1	K	207	ARG
1	K	227	ALA
1	K	265	GLU
2	L	79	ASP
2	L	86	SER
2	L	129	GLU
2	L	152	ARG
1	A	86	PRO
1	A	183	HIS
1	A	193	TYR
1	A	380	ASP
1	C	141	SER
1	C	379	GLY
2	D	133	VAL
1	E	371	CYS
2	F	105	PRO
1	G	94	CYS
1	G	213	ASP

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Mol	Chain	Res	Type
2	H	19	CYS
2	H	32	ALA
2	H	33	ILE
2	H	142	PRO
2	H	266	THR
1	I	201	PHE
1	I	290	ARG
2	J	137	LYS
2	J	138	TYR
1	K	203	ASP
2	L	158	ALA
1	A	26	PRO
1	A	167	LEU
2	B	78	ILE
1	C	250	ALA
1	E	86	PRO
1	E	310	ALA
2	F	310	ARG
1	I	87	PHE
1	I	212	ASN
1	I	371	CYS
2	J	329	ASN
2	L	69	ASN
2	L	140	HIS
2	B	264	ILE
2	F	142	PRO
1	G	93	TYR
1	G	181	TYR
1	G	267	LEU
1	K	291	ILE
1	C	26	PRO
1	G	257	PRO
2	H	116	GLY
2	J	142	PRO
2	D	30	PRO
1	E	166	PRO
1	G	173	PRO
2	H	20	PRO
2	B	141	PRO
1	C	251	PRO
1	C	265	GLU
2	D	31	ILE

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Mol	Chain	Res	Type
2	H	30	PRO
1	K	172	SER
2	D	303	PRO
1	E	25	ALA
2	F	103	CYS
1	G	116	ILE
2	H	38	GLY
2	H	140	HIS
2	H	269	PRO
1	I	266	PRO
2	L	310	ARG

### 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	321/370 (87%)	304 (95%)	17 (5%)	19	40
1	C	321/370 (87%)	304 (95%)	17 (5%)	19	40
1	E	321/370 (87%)	310 (97%)	11 (3%)	32	51
1	G	321/370 (87%)	311 (97%)	10 (3%)	35	54
1	I	321/370 (87%)	309 (96%)	12 (4%)	29	49
1	K	321/370 (87%)	299 (93%)	22 (7%)	13	33
2	B	206/367 (56%)	186 (90%)	20 (10%)	6	22
2	D	206/367 (56%)	187 (91%)	19 (9%)	7	23
2	F	206/367 (56%)	195 (95%)	11 (5%)	19	40
2	H	206/367 (56%)	192 (93%)	14 (7%)	13	34
2	J	206/367 (56%)	196 (95%)	10 (5%)	21	42
2	L	206/367 (56%)	197 (96%)	9 (4%)	24	45
All	All	3162/4422 (72%)	2990 (95%)	172 (5%)	21	40

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	PRO
1	A	31	ILE
1	A	33	LEU
1	A	42	THR
1	A	114	CYS
1	A	118	HIS
1	A	150	ASN
1	A	181	TYR
1	A	248	LYS
1	A	290	ARG
1	A	294	THR
1	A	303	LYS
1	A	322	LYS
1	A	359	THR
1	A	367	LYS
1	A	369	GLN
1	A	378	LYS
2	B	10	LYS
2	B	26	ARG
2	B	45	ILE
2	B	49	THR
2	B	64	TYR
2	B	65	MET
2	B	67	PHE
2	B	74	LYS
2	B	77	LYS
2	B	81	LEU
2	B	83	VAL
2	B	119	ARG
2	B	127	LYS
2	B	135	ARG
2	B	139	ARG
2	B	157	ARG
2	B	266	THR
2	B	275	HIS
2	B	324	GLU
2	B	335	VAL
1	C	7	MET
1	C	26	PRO
1	C	28	HIS
1	C	36	THR
1	C	37	ARG
1	C	110	ARG

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Mol	Chain	Res	Type
1	C	134	ASN
1	C	135	ILE
1	C	214	LEU
1	C	218	THR
1	C	258	PHE
1	C	267	LEU
1	C	289	THR
1	C	332	HIS
1	C	347	LEU
1	C	372	THR
1	C	378	LYS
2	D	10	LYS
2	D	45	ILE
2	D	46	ARG
2	D	49	THR
2	D	67	PHE
2	D	71	LYS
2	D	99	ILE
2	D	127	LYS
2	D	131	ARG
2	D	137	LYS
2	D	139	ARG
2	D	153	TYR
2	D	157	ARG
2	D	284	LEU
2	D	290	THR
2	D	293	THR
2	D	309	GLU
2	D	318	VAL
2	D	336	TRP
1	E	37	ARG
1	E	118	HIS
1	E	120	LYS
1	E	134	ASN
1	E	135	ILE
1	E	156	LYS
1	E	167	LEU
1	E	243	ARG
1	E	288	PHE
1	E	319	VAL
1	E	332	HIS
2	F	49	THR

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Mol	Chain	Res	Type
2	F	99	ILE
2	F	102	GLN
2	F	119	ARG
2	F	127	LYS
2	F	293	THR
2	F	294	THR
2	F	295	ARG
2	F	305	ARG
2	F	319	THR
2	F	324	GLU
1	G	30	GLN
1	G	110	ARG
1	G	157	ILE
1	G	290	ARG
1	G	331	ILE
1	G	347	LEU
1	G	369	GLN
1	G	371	CYS
1	G	375	VAL
1	G	378	LYS
2	H	61	ASP
2	H	67	PHE
2	H	71	LYS
2	H	78	ILE
2	H	84	ARG
2	H	97	TYR
2	H	113	PHE
2	H	139	ARG
2	H	270	GLU
2	H	279	THR
2	H	295	ARG
2	H	334	ARG
2	H	336	TRP
2	H	338	GLN
1	I	30	GLN
1	I	33	LEU
1	I	37	ARG
1	I	120	LYS
1	I	134	ASN
1	I	290	ARG
1	I	294	THR
1	I	319	VAL

*Continued on next page...*

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Mol	Chain	Res	Type
1	I	321	TYR
1	I	322	LYS
1	I	367	LYS
1	I	378	LYS
2	J	13	ARG
2	J	49	THR
2	J	99	ILE
2	J	131	ARG
2	J	139	ARG
2	J	254	VAL
2	J	295	ARG
2	J	324	GLU
2	J	332	PRO
2	J	338	GLN
1	K	30	GLN
1	K	31	ILE
1	K	66	THR
1	K	93	TYR
1	K	137	TYR
1	K	147	VAL
1	K	167	LEU
1	K	171	TRP
1	K	181	TYR
1	K	197	LYS
1	K	235	THR
1	K	243	ARG
1	K	267	LEU
1	K	289	THR
1	K	303	LYS
1	K	306	GLU
1	K	321	TYR
1	K	332	HIS
1	K	341	LYS
1	K	343	ASN
1	K	345	VAL
1	K	378	LYS
2	L	47	ILE
2	L	73	GLN
2	L	77	LYS
2	L	119	ARG
2	L	127	LYS
2	L	135	ARG

*Continued on next page...*

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Mol	Chain	Res	Type
2	L	279	THR
2	L	295	ARG
2	L	332	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	134	ASN
1	A	183	HIS
2	B	94	HIS
2	B	126	HIS
2	B	155	HIS
2	B	275	HIS
1	C	187	ASN
2	D	94	HIS
2	D	95	HIS
2	D	315	ASN
1	E	28	HIS
1	E	30	GLN
1	E	73	HIS
1	E	102	GLN
1	E	187	ASN
1	E	343	ASN
2	F	24	HIS
2	F	114	HIS
2	F	126	HIS
2	F	283	HIS
2	F	330	HIS
1	G	30	GLN
1	G	212	ASN
1	G	361	ASN
2	H	82	HIS
2	H	94	HIS
2	H	277	HIS
2	H	288	HIS
1	I	3	HIS
1	I	32	GLN
1	I	100	ASN
1	I	231	HIS
1	I	343	ASN
2	J	82	HIS

*Continued on next page...*

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Mol	Chain	Res	Type
2	J	94	HIS
2	J	95	HIS
2	J	114	HIS
2	J	144	HIS
2	J	330	HIS
1	K	187	ASN
1	K	236	GLN
2	L	82	HIS
2	L	120	HIS
2	L	288	HIS
2	L	330	HIS

### 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.

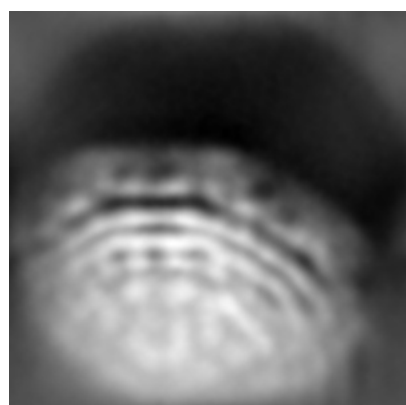
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24201. These allow visual inspection of the internal detail of the map and identification of artifacts.

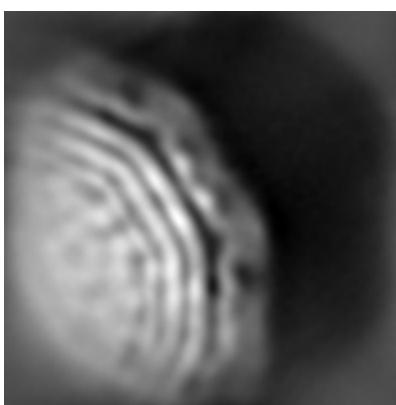
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

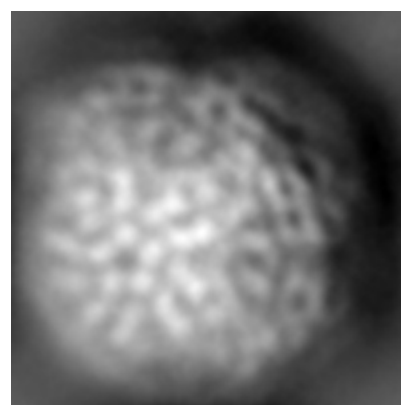
#### 6.1.1 Primary map



X



Y

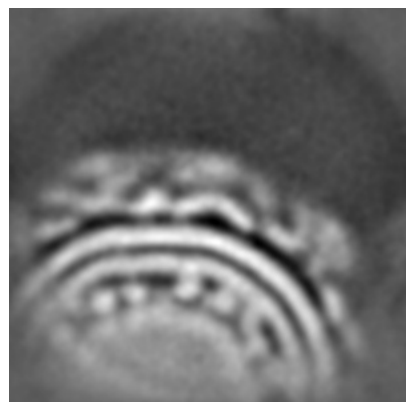


Z

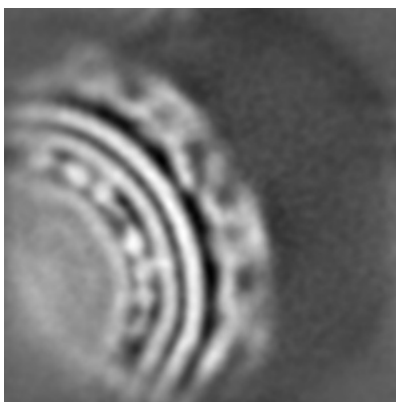
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

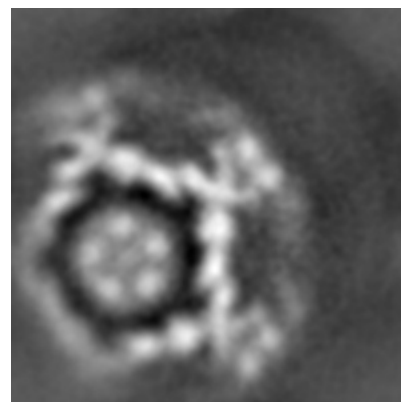
#### 6.2.1 Primary map



X Index: 72



Y Index: 72

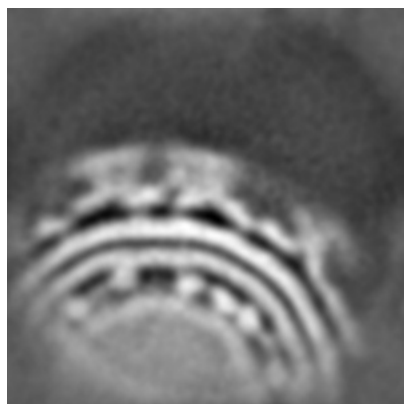


Z Index: 72

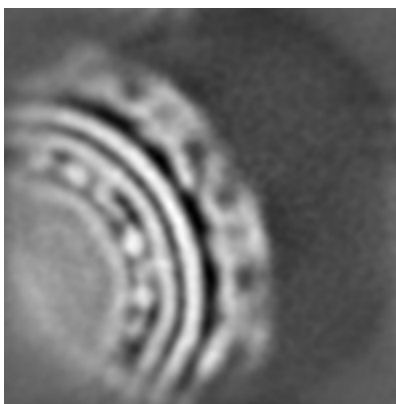
The images above show central slices of the map in three orthogonal directions.

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

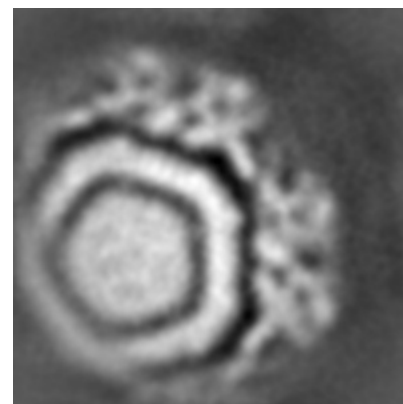
### 6.3.1 Primary map



X Index: 68



Y Index: 73

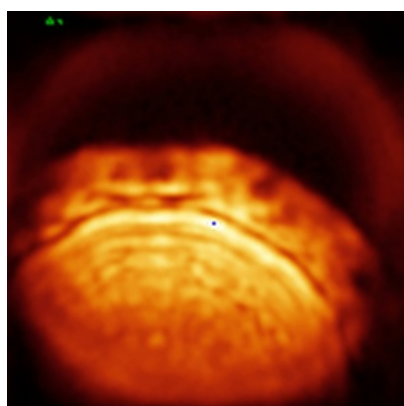


Z Index: 60

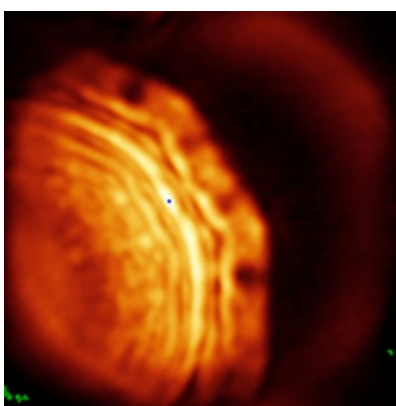
The images above show the largest variance slices of the map in three orthogonal directions.

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

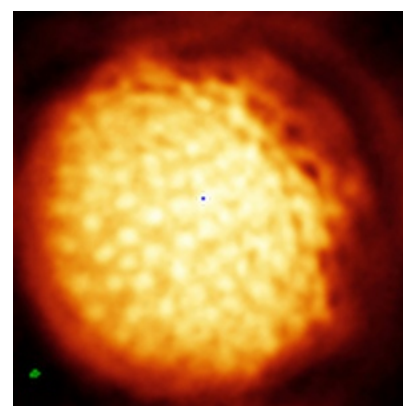
### 6.4.1 Primary map



X



Y

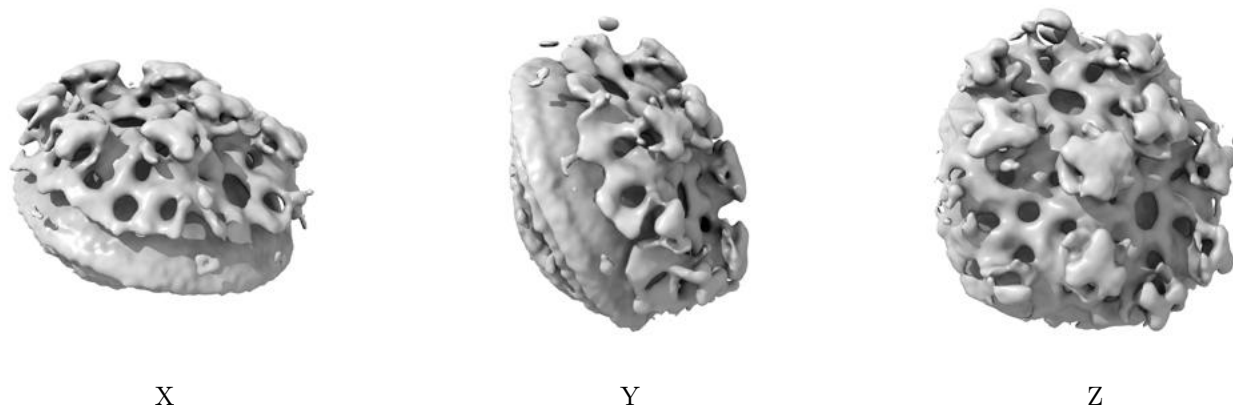


Z

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



The images above show the 3D surface view of the map at the recommended contour level 1.5. 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](#)

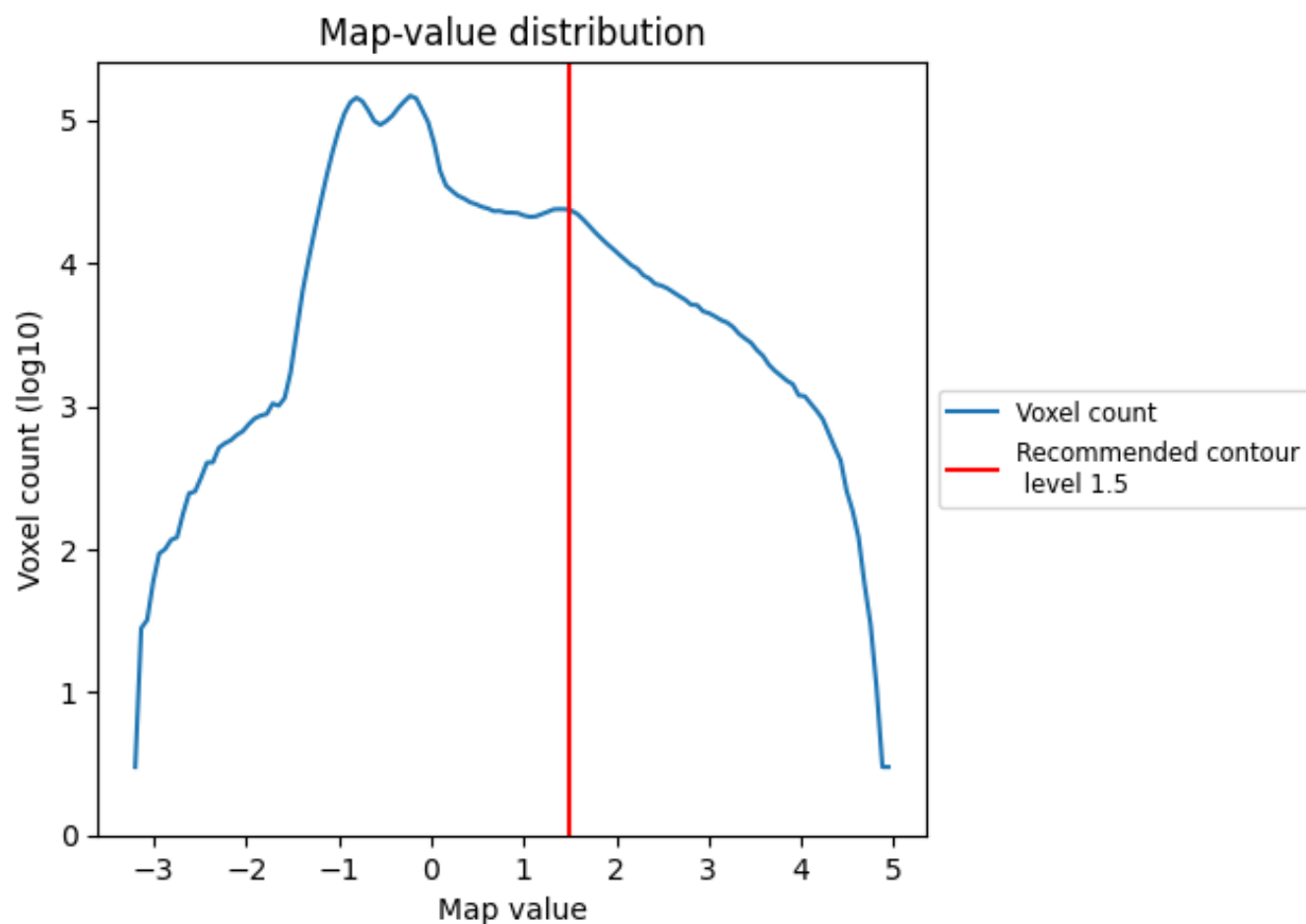
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

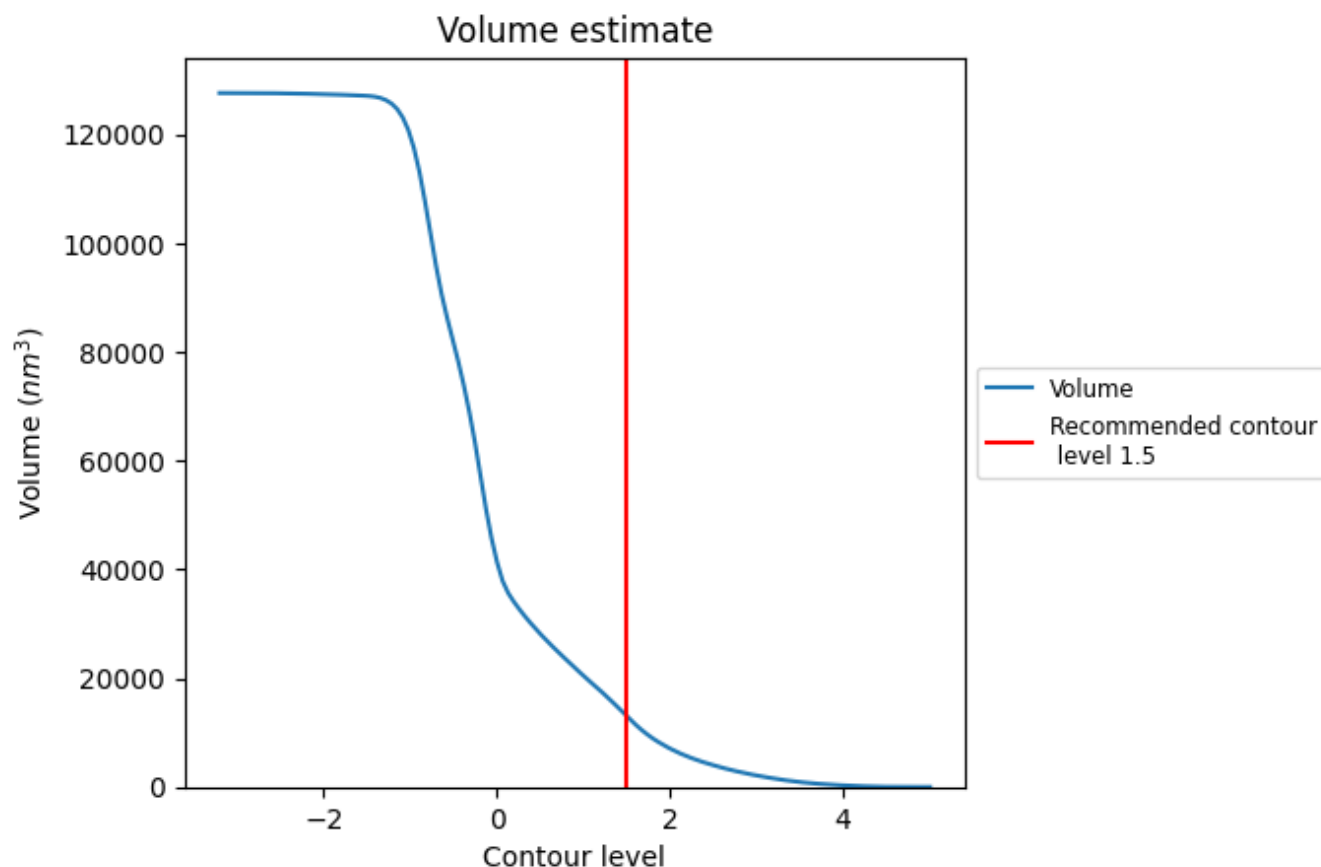
This section contains the results of statistical analysis of the map.

### 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.

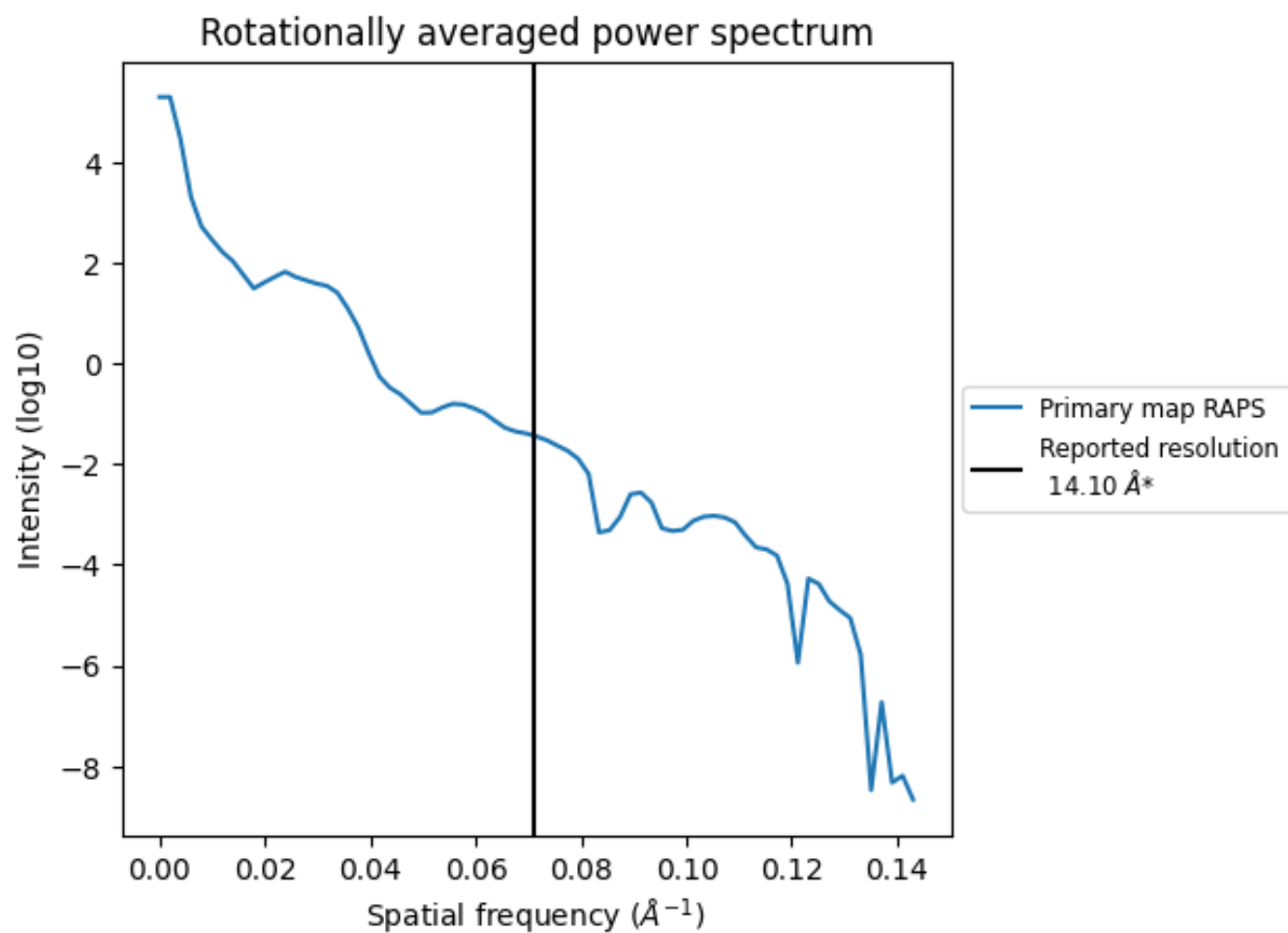
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 13083  $\text{nm}^3$ ; this corresponds to an approximate mass of 11818 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 ⓘ

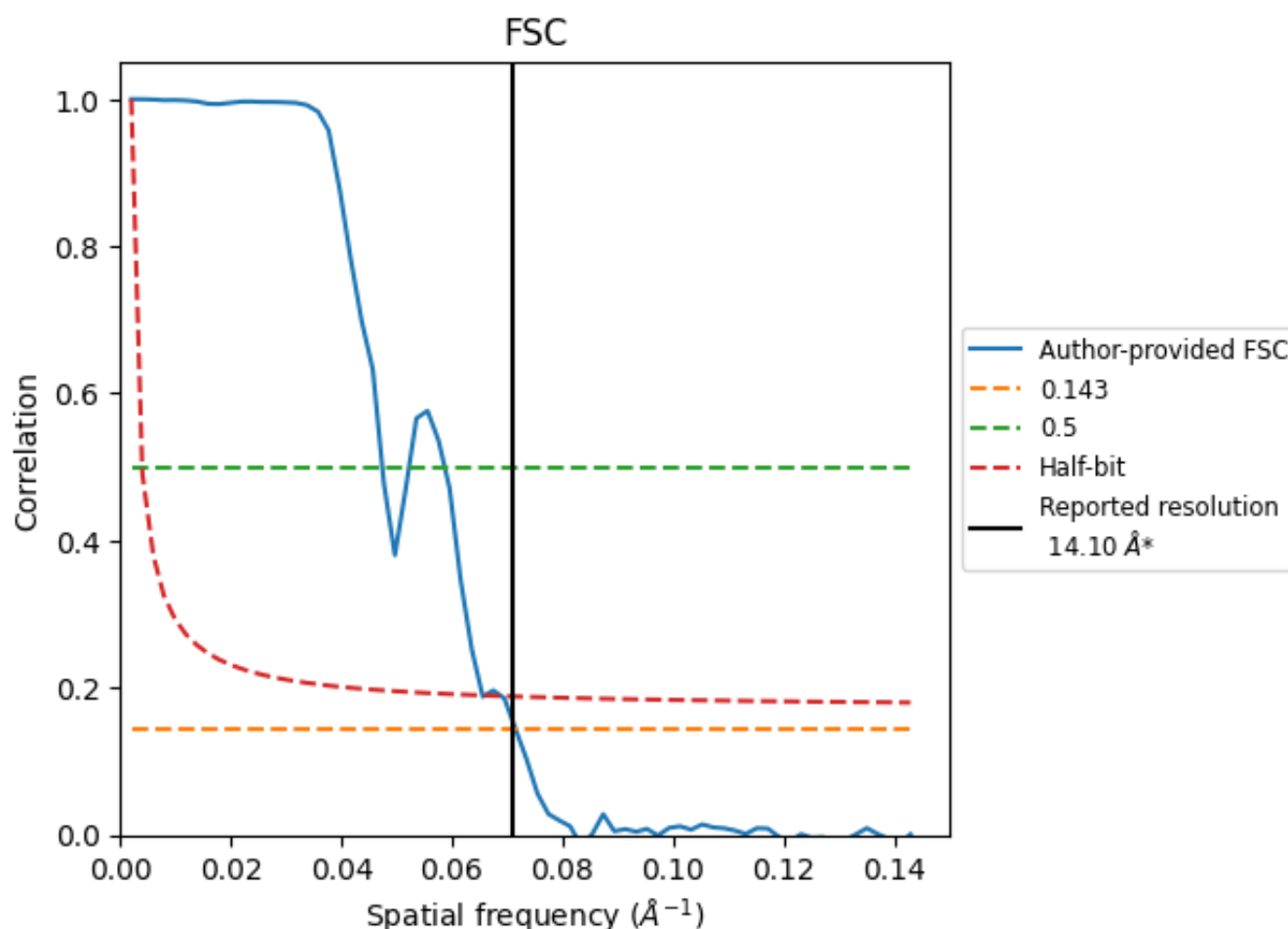


\*Reported resolution corresponds to spatial frequency of 0.071 Å<sup>-1</sup>

## 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 0.071  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

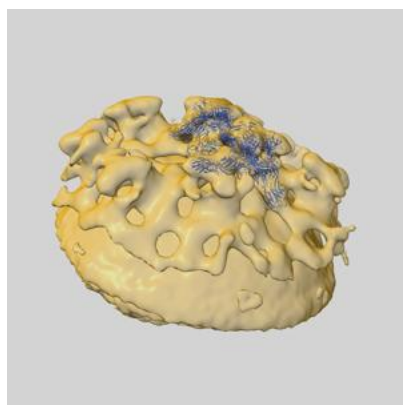
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	14.10	-	-
Author-provided FSC curve	13.97	21.10	15.27
Unmasked-calculated*	-	-	-

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

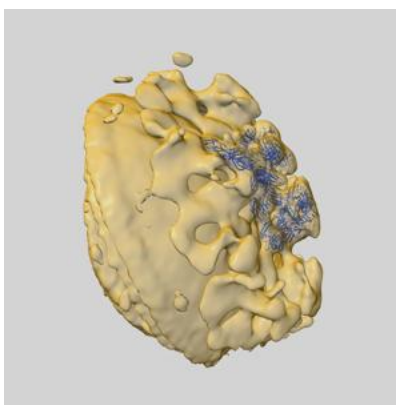
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24201 and PDB model 7N69. Per-residue inclusion information can be found in section [3](#) on page [5](#).

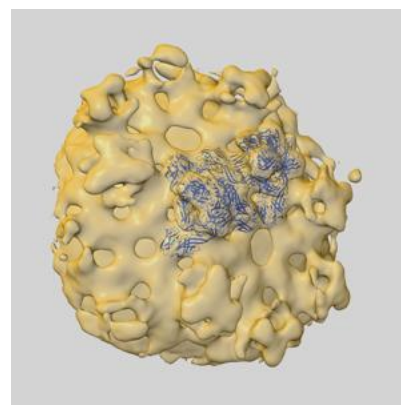
### 9.1 Map-model overlay [i](#)



X



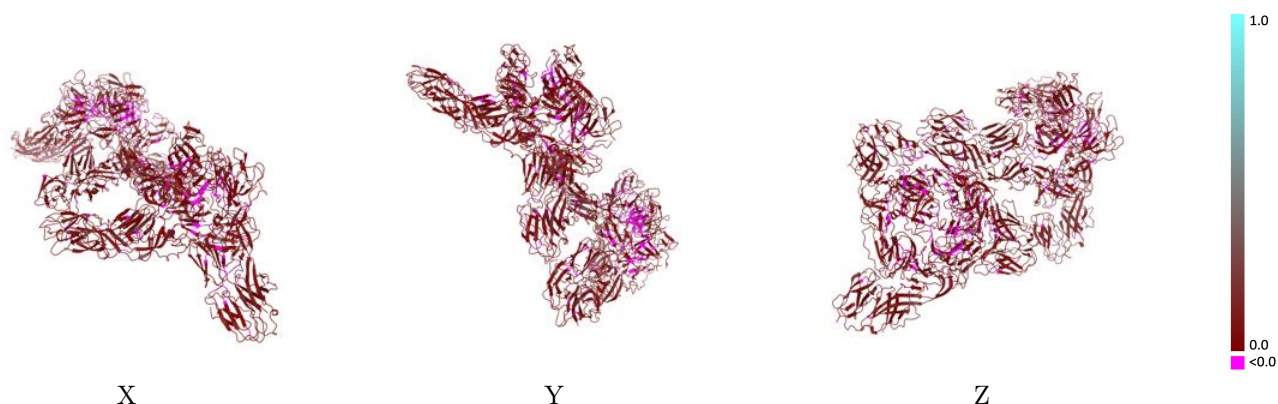
Y



Z

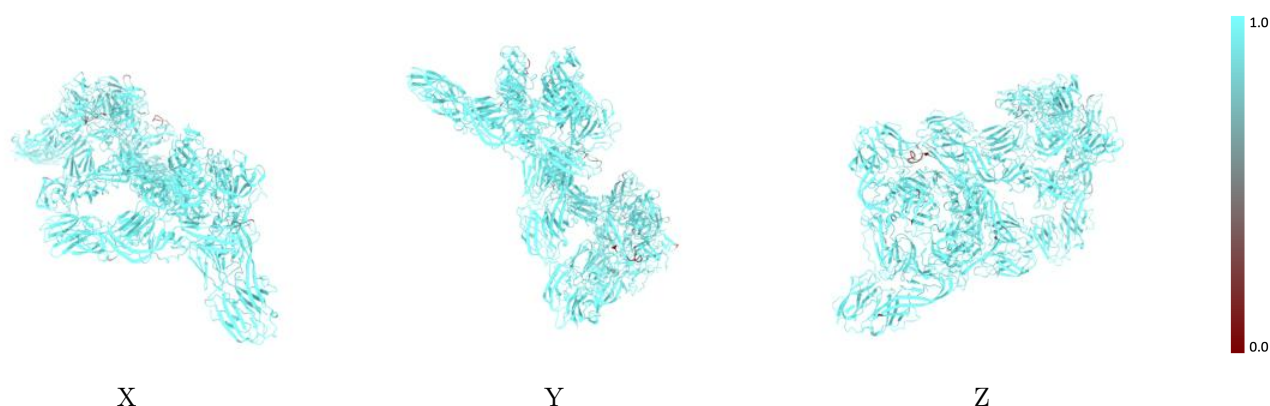
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



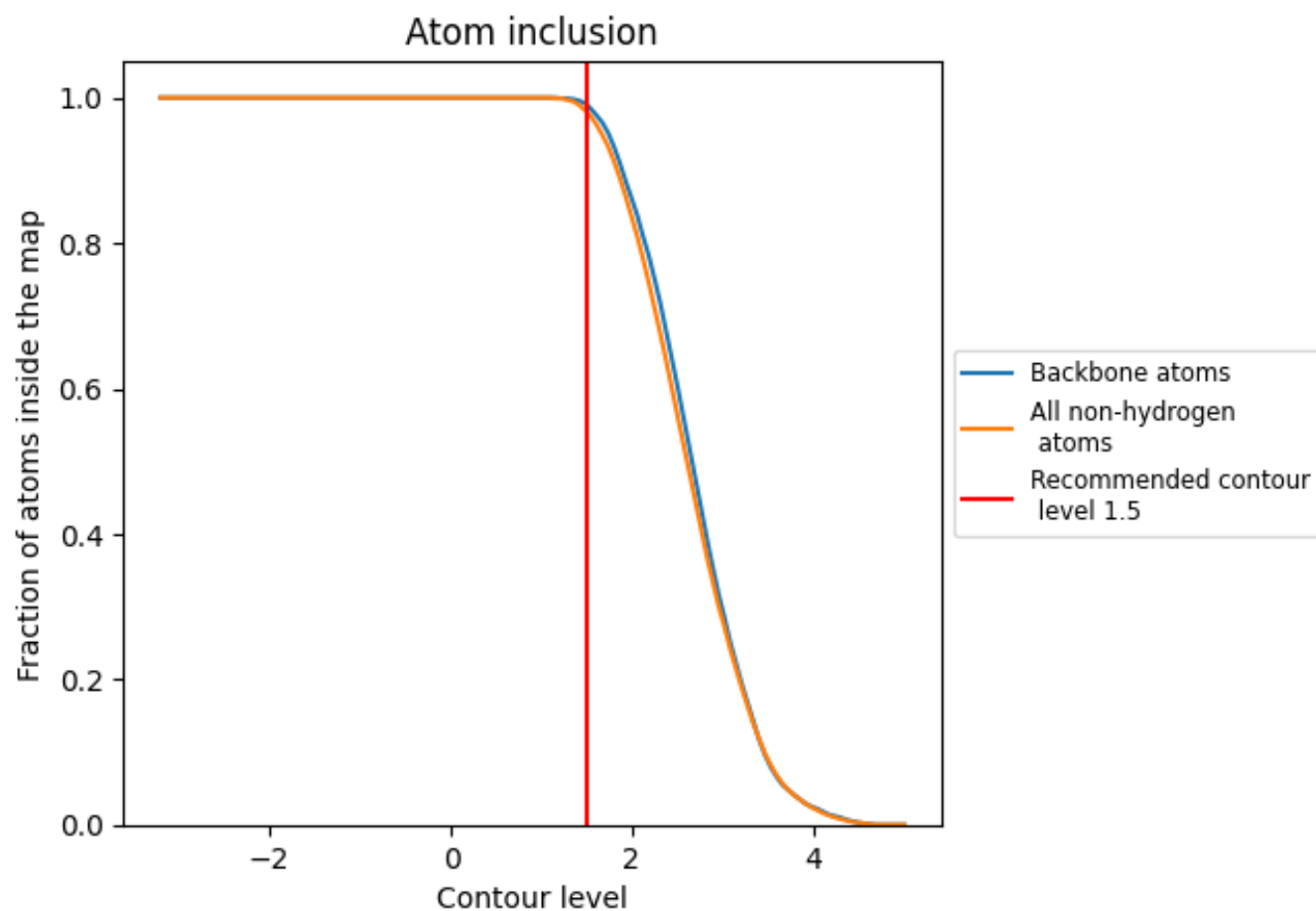
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9810</div>	<div><div></div>0.0810</div>
A	<div><div></div>0.9880</div>	<div><div></div>0.0930</div>
B	<div><div></div>0.9950</div>	<div><div></div>0.0730</div>
C	<div><div></div>0.9790</div>	<div><div></div>0.0910</div>
D	<div><div></div>0.9910</div>	<div><div></div>0.0780</div>
E	<div><div></div>0.9730</div>	<div><div></div>0.0870</div>
F	<div><div></div>0.9910</div>	<div><div></div>0.0750</div>
G	<div><div></div>0.9590</div>	<div><div></div>0.0910</div>
H	<div><div></div>0.9830</div>	<div><div></div>0.0680</div>
I	<div><div></div>0.9830</div>	<div><div></div>0.0860</div>
J	<div><div></div>0.9790</div>	<div><div></div>0.0680</div>
K	<div><div></div>0.9850</div>	<div><div></div>0.0830</div>
L	<div><div></div>0.9780</div>	<div><div></div>0.0580</div>

1.0

0.0

<0.0