



Full wwPDB EM Validation Report ⓘ

Dec 3, 2024 – 03:34 AM JST

PDB ID : 9JZ0
EMDB ID : EMD-61911
Title : portal-tail complex of DNA-ejected T7
Authors : Liu, H.R.; Chen, W.Y.
Deposited on : 2024-10-13
Resolution : 3.50 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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) : 2.40

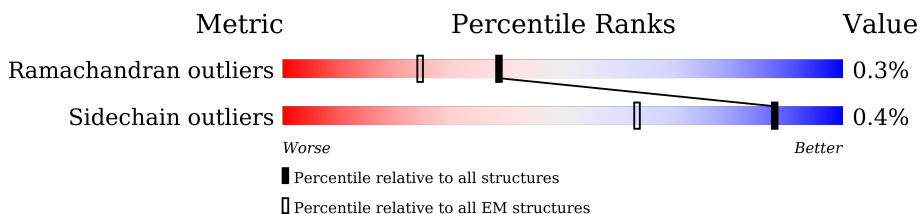
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	0	196	61%	39%
1	1	196	61%	39%
1	Y	196	61%	39%
1	Z	196	61%	39%
1	y	196	61%	39%
1	z	196	61%	39%
2	2	88	9% (red), 35% (green)	65% (grey)
2	3	88	13% (red), 35% (green)	65% (grey)
2	4	88	9% (red), 35% (green)	65% (grey)

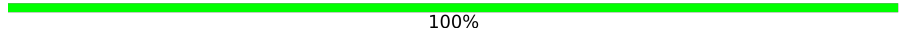
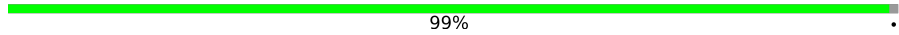
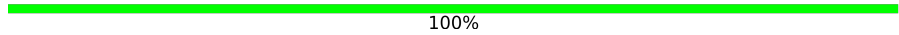
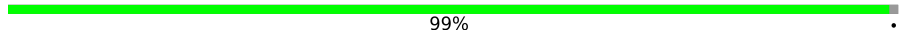
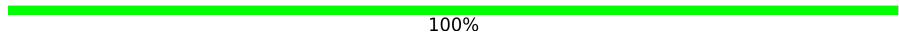
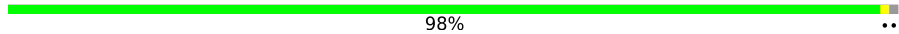
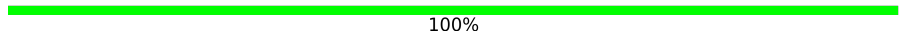
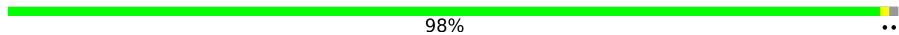

















Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	5	88	
2	6	88	
2	7	88	
2	8	88	
2	9	88	
2	AA	88	
2	AB	88	
2	AC	88	
2	AD	88	
3	A	536	
3	B	536	
3	C	536	
3	D	536	
3	E	536	
3	F	536	
3	G	536	
3	H	536	
3	I	536	
3	J	536	
3	K	536	
3	L	536	
4	M	196	
4	N	196	
4	O	196	
4	P	196	


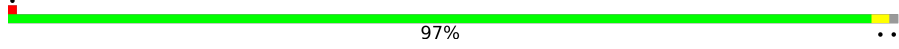
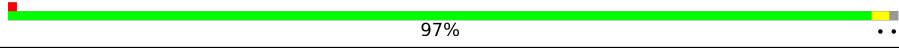
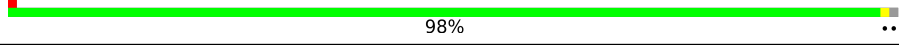
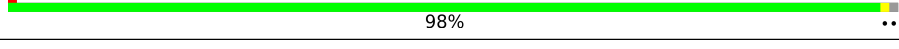
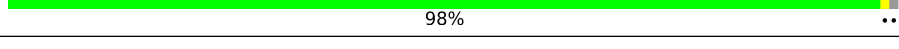
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	Q	196	 100%
4	R	196	 99%
4	S	196	 100%
4	T	196	 99%
4	U	196	 100%
4	V	196	 98%
4	W	196	 100%
4	X	196	 98%
5	a	553	 21% 79%
5	b	553	 20% 80%
5	c	553	 20% 80%
5	d	553	 21% 79%
5	e	553	 20% 80%
5	f	553	 20% 80%
5	g	553	 21% 79%
5	h	553	 20% 80%
5	i	553	 20% 80%
5	j	553	 21% 79%
5	k	553	 20% 80%
5	l	553	 20% 80%
5	m	553	 21% 79%
5	n	553	 20% 80%
5	o	553	 20% 80%
5	p	553	 21% 79%
5	q	553	 20% 80%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	r	553	 20% 80%
6	s	794	 97%
6	t	794	 97%
6	u	794	 98%
6	v	794	 98%
6	w	794	 98%
6	x	794	 98%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 122376 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 Internal virion protein gp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	119	920	556	172	185	7	0	0
1	1	119	920	556	172	185	7	0	0
1	Y	119	920	556	172	185	7	0	0
1	Z	119	920	556	172	185	7	0	0
1	y	119	920	556	172	185	7	0	0
1	z	119	920	556	172	185	7	0	0

- Molecule 2 is a protein called Protein 6.7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	31	231	139	38	53	1	0	0
2	3	31	231	139	38	53	1	0	0
2	4	31	231	139	38	53	1	0	0
2	5	31	231	139	38	53	1	0	0
2	6	31	231	139	38	53	1	0	0
2	7	31	231	139	38	53	1	0	0
2	8	49	368	219	64	84	1	0	0
2	9	49	368	219	64	84	1	0	0
2	AA	49	368	219	64	84	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	49	Total	C	N	O	S	0	0
			368	219	64	84	1		
2	AC	49	Total	C	N	O	S	0	0
			368	219	64	84	1		
2	AD	49	Total	C	N	O	S	0	0
			368	219	64	84	1		

- Molecule 3 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	429	Total	C	N	O	S	0	0
			3363	2120	562	667	14		
3	B	431	Total	C	N	O	S	0	0
			3378	2128	567	669	14		
3	C	429	Total	C	N	O	S	0	0
			3363	2120	562	667	14		
3	D	431	Total	C	N	O	S	0	0
			3378	2128	567	669	14		
3	E	429	Total	C	N	O	S	0	0
			3363	2120	562	667	14		
3	F	431	Total	C	N	O	S	0	0
			3378	2128	567	669	14		
3	G	429	Total	C	N	O	S	0	0
			3363	2120	562	667	14		
3	H	431	Total	C	N	O	S	0	0
			3378	2128	567	669	14		
3	I	429	Total	C	N	O	S	0	0
			3363	2120	562	667	14		
3	J	431	Total	C	N	O	S	0	0
			3378	2128	567	669	14		
3	K	429	Total	C	N	O	S	0	0
			3363	2120	562	667	14		
3	L	431	Total	C	N	O	S	0	0
			3378	2128	567	669	14		

- Molecule 4 is a protein called Tail tubular protein gp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
4	N	194	Total	C	N	O	S	0	0
			1546	960	262	316	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
4	P	194	Total	C	N	O	S	0	0
			1546	960	262	316	8		
4	Q	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
4	R	194	Total	C	N	O	S	0	0
			1546	960	262	316	8		
4	S	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
4	T	194	Total	C	N	O	S	0	0
			1546	960	262	316	8		
4	U	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
4	V	194	Total	C	N	O	S	0	0
			1546	960	262	316	8		
4	W	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
4	X	194	Total	C	N	O	S	0	0
			1546	960	262	316	8		

- Molecule 5 is a protein called Tail fiber protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
5	b	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	c	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	d	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
5	e	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	f	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	g	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
5	h	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	i	113	Total	C	N	O	S	0	0
			907	575	157	174	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	j	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
5	k	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	l	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	m	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
5	n	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	o	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	p	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
5	q	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	r	113	Total	C	N	O	S	0	0
			907	575	157	174	1		

- Molecule 6 is a protein called Tail tubular protein gp12.

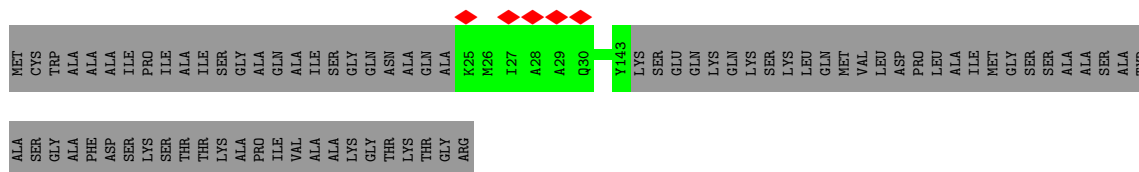
Mol	Chain	Residues	Atoms					AltConf	Trace
6	s	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		
6	t	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		
6	u	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		
6	v	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		
6	w	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		
6	x	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		

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.

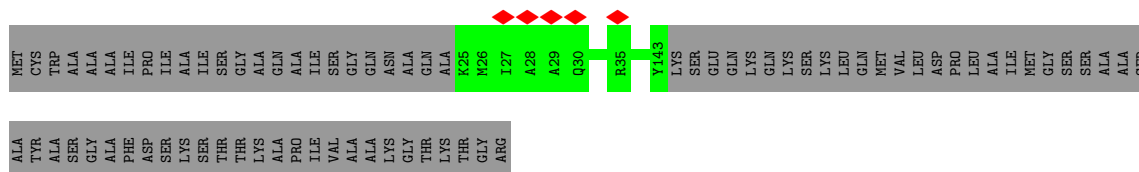
- Molecule 1: Internal virion protein gp14

Chain 0: 



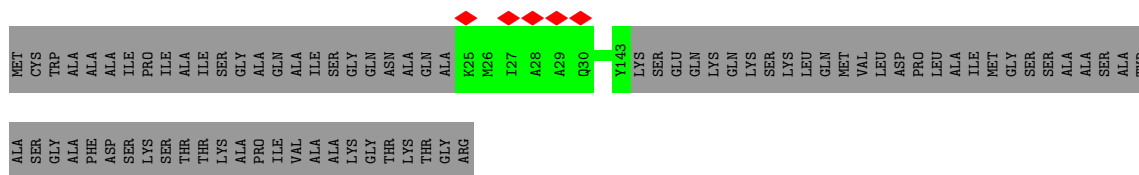
- Molecule 1: Internal virion protein gp14

Chain 1: 



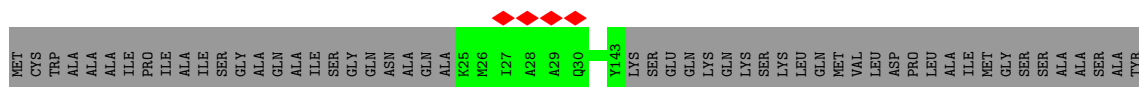
- Molecule 1: Internal virion protein gp14

Chain Y: 



- Molecule 1: Internal virion protein gp14

Chain Z: 



ALA
SER
GLY
ALA
PHE
ASP
SER
LYS
THR
THR
LYS
LYS
ALA
PRO
ILE
VAL
ALA
ALA
GLY
LYS
THR
THR
GLY
ARG

• Molecule 1: Internal virion protein gp14



MET CYS TRP ALA SER ALA PHE ASP SER LYS THR THR LYS LYS ALA PRO ILE VAL ALA ALA GLY LYS THR THR GLY ARG
K25 K26 I27 A28 A29 Q30 E141 I142 Y143 LYS SER GLU GLN LYS LYS LYS LEU LEU MET VAL ASP PRO LEU LEU MET MET GLY SER SER ALA ALA SER

ALA
THR
ALA
SER
GLY
ALA
PHE
ASP
SER
SER
LYS
SER
THR
THR
LYS
ALA
PRO
ILE
VAL
ALA
ALA
GLY
LYS
THR
THR
GLY
ARG

• Molecule 1: Internal virion protein gp14



MET CYS TRP ALA SER ALA PHE ASP SER LYS THR THR LYS LYS ALA PRO ILE VAL ALA ALA GLY LYS THR THR GLY ARG
K25 K26 I27 A28 A29 Q30 R35 Y143 LYS SER GLU GLN LYS LYS LYS LEU LEU MET VAL ASP PRO LEU LEU MET MET GLY SER SER ALA ALA SER

ALA
THR
ALA
SER
GLY
ALA
PHE
ASP
SER
SER
LYS
SER
THR
THR
LYS
ALA
PRO
ILE
VAL
ALA
ALA
GLY
LYS
THR
THR
GLY
ARG

• Molecule 2: Protein 6.7



MET CYS PHE SER PRO LYS ILE LYS THR PRO K11 V29 S30 S31 V32 E33 S37 S38 D39 E40 T41 ASP THR GLU GLY THR GLU VAL SER GLY ARG LYS GLY LEU VAL VAL ARG ASP ASP VAL ALA LYS SER LYS ALA ALA GLY ASN SER SER ARG MET LYS SER SER

ILE
ARG
LYS
SER
ALA
PHE
GLY
LYS

• Molecule 2: Protein 6.7



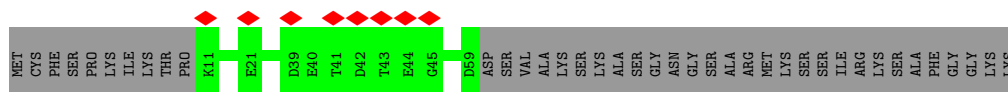
MET CYS PHE SER PRO LYS ILE LYS THR PRO K11 A23 V29 S30 S31 V32 E33 S37 S38 D39 E40 T41 ASP THR GLU GLY THR GLU VAL SER GLY ARG LYS GLY LEU VAL VAL ARG ASP ASP VAL ALA LYS SER LYS ALA ALA GLY ASN SER SER ARG MET LYS SER SER

SER
SER
ILE
LYS
ARG
SER
ALA
PHE
GLY
LYS

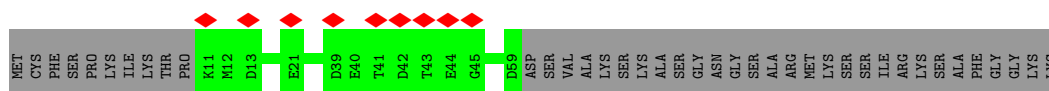
• Molecule 2: Protein 6.7



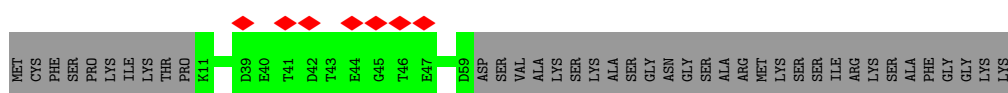
MET CYS PHE SER PRO LYS ILE LYS THR PRO K11 V29 S30 S31 V32 E33 S37 S38 D39 E40 T41 ASP THR GLU GLY THR GLU VAL SER GLY ARG LYS GLY LEU VAL VAL ARG ASP ASP VAL ALA LYS SER LYS ALA ALA GLY ASN SER SER ARG MET LYS SER SER



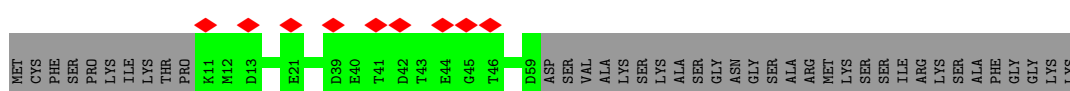
• Molecule 2: Protein 6.7



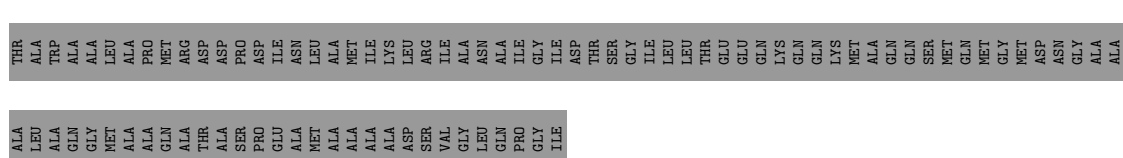
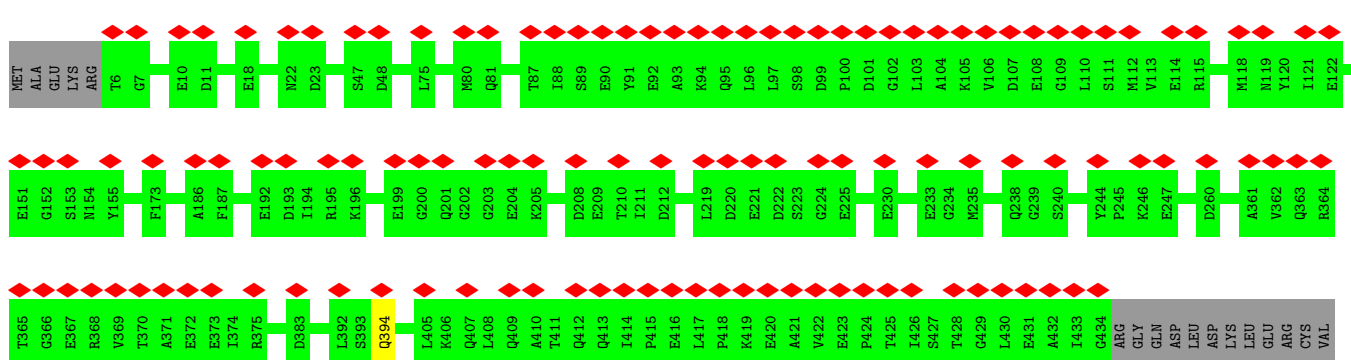
• Molecule 2: Protein 6.7



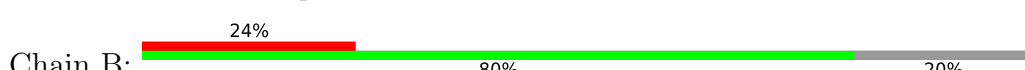
• Molecule 2: Protein 6.7

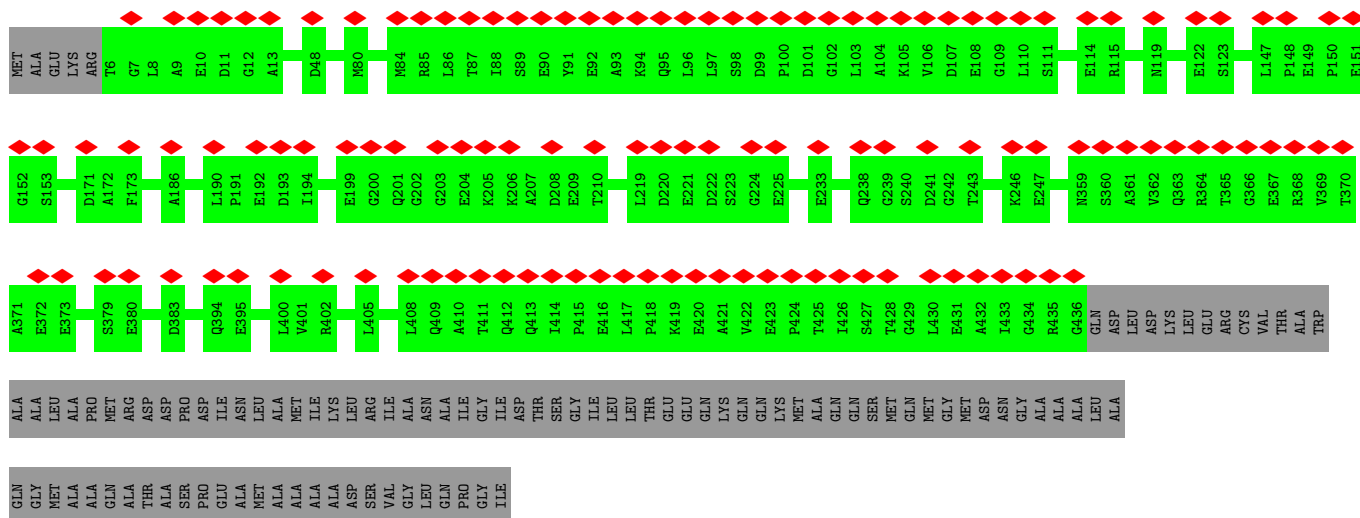


• Molecule 3: Portal protein



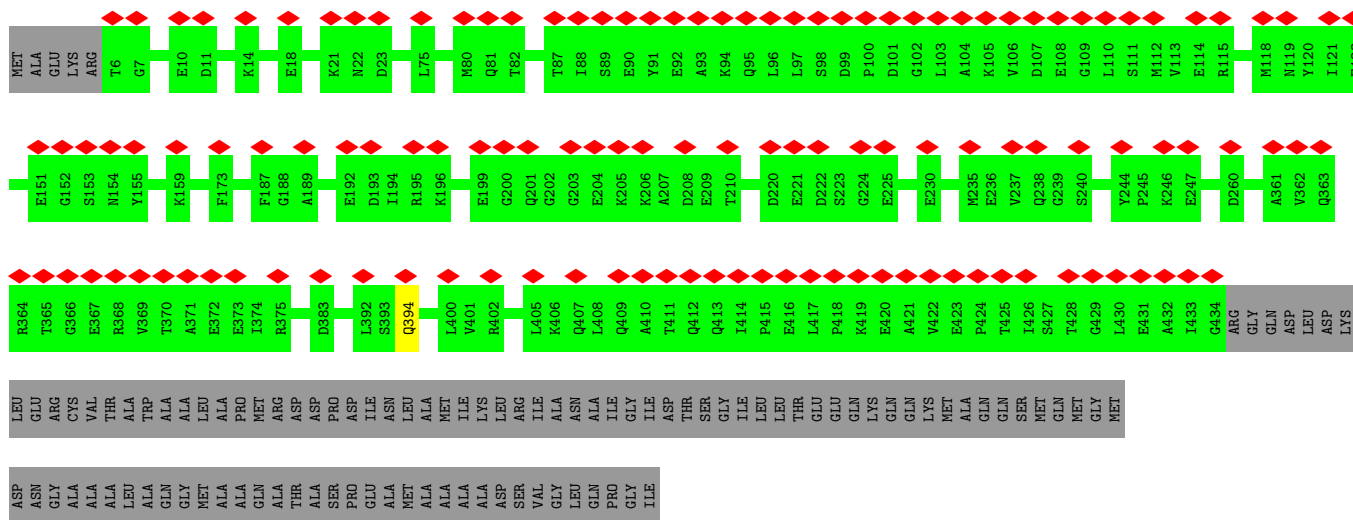
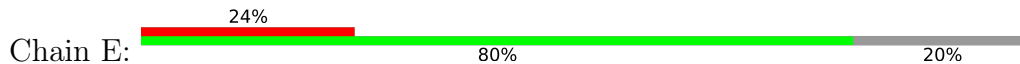
• Molecule 3: Portal protein



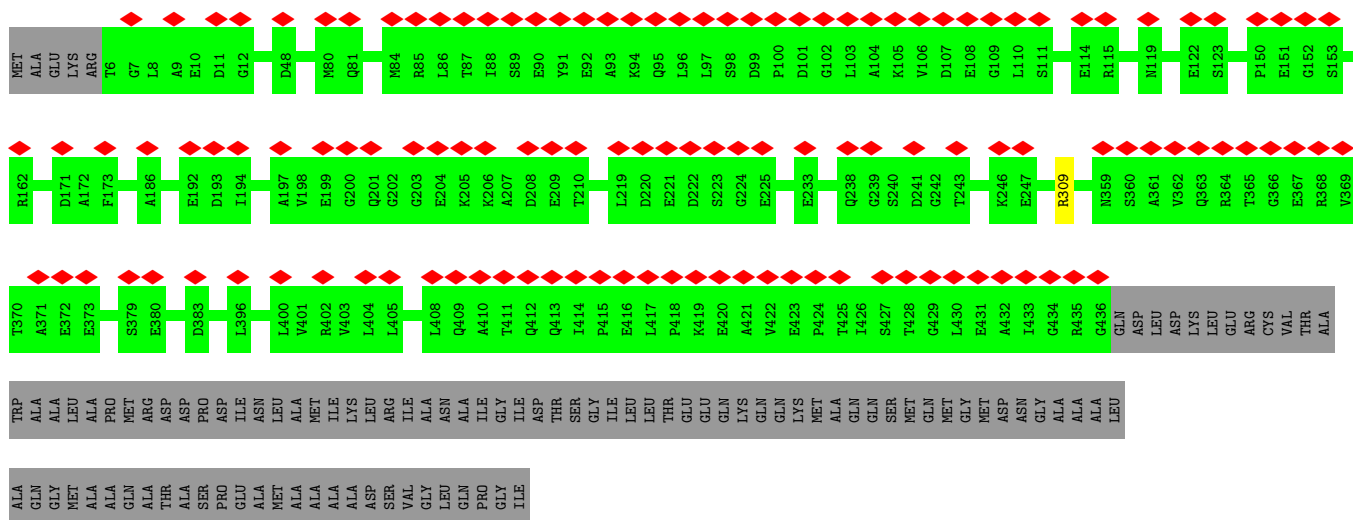
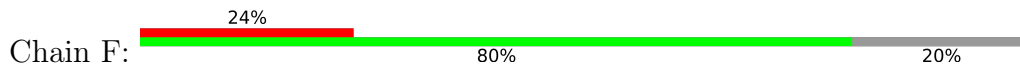


ALA ALA ALA
LEU LEU LEU
ALA ALA ALA
PRO PRO PRO
MET MET MET
ARG ARG ARG
ASP ASP ASP
ASP ASP ASP
PRO PRO PRO
SER SER SER
ILE ILE ILE
GLN GLN GLN
LEU LEU LEU
ALA ALA ALA
MET MET MET
ILE ILE ILE
LYS LYS LYS
LEU LEU LEU
ASP ASP ASP
ARG ARG ARG
ILE ILE ILE
ALA ALA ALA
ASN ASN ASN
LEU LEU LEU
GLY GLY GLY
PRO PRO PRO
ILE ILE ILE

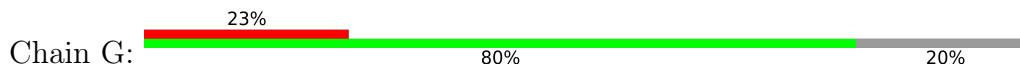
• Molecule 3: Portal protein

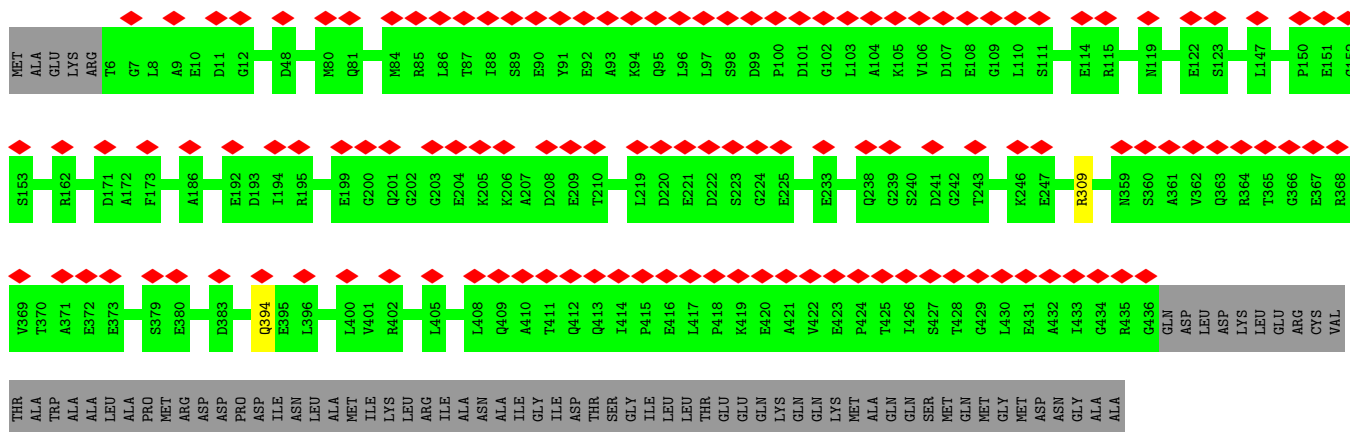


• Molecule 3: Portal protein



• Molecule 3: Portal protein







- Molecule 4: Tail tubular protein gp11



There are no outlier residues recorded for this chain.

- Molecule 4: Tail tubular protein gp11

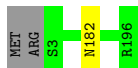


- Molecule 4: Tail tubular protein gp11



There are no outlier residues recorded for this chain.

- Molecule 4: Tail tubular protein gp11

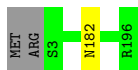


- Molecule 4: Tail tubular protein gp11

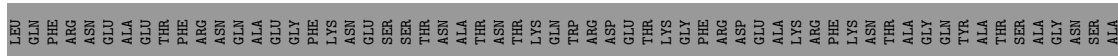
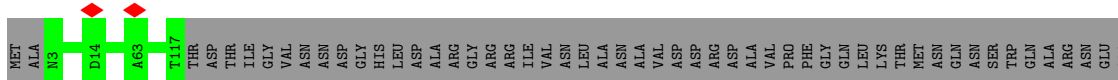


There are no outlier residues recorded for this chain.

- Molecule 4: Tail tubular protein gp11



- Molecule 5: Tail fiber protein





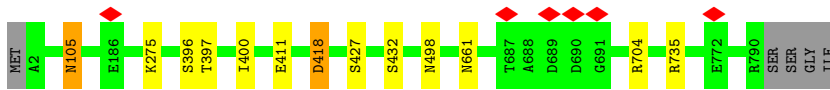
- Molecule 6: Tail tubular protein gp12

Chain u: 98%



- Molecule 6: Tail tubular protein gp12

Chain v: 98%



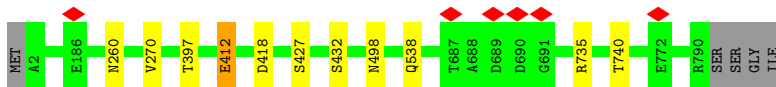
- Molecule 6: Tail tubular protein gp12

Chain w: 98%



- Molecule 6: Tail tubular protein gp12

Chain x: 98%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23461	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	30.188	Depositor
Minimum map value	-18.529	Depositor
Average map value	0.012	Depositor
Map value standard deviation	1.377	Depositor
Recommended contour level	3.9	Depositor
Map size (\AA)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0	0.25	0/924	0.50	0/1235
1	1	0.25	0/924	0.49	0/1235
1	Y	0.26	0/924	0.50	0/1235
1	Z	0.25	0/924	0.49	0/1235
1	y	0.25	0/924	0.50	0/1235
1	z	0.25	0/924	0.48	0/1235
2	2	0.24	0/233	0.47	0/315
2	3	0.24	0/233	0.47	0/315
2	4	0.24	0/233	0.47	0/315
2	5	0.24	0/233	0.47	0/315
2	6	0.24	0/233	0.47	0/315
2	7	0.24	0/233	0.47	0/315
2	8	0.29	0/370	0.53	0/497
2	9	0.28	0/370	0.54	0/497
2	AA	0.27	0/370	0.52	0/497
2	AB	0.27	0/370	0.54	0/497
2	AC	0.24	0/370	0.53	0/497
2	AD	0.25	0/370	0.51	0/497
3	A	0.26	0/3419	0.49	0/4632
3	B	0.27	0/3434	0.49	0/4651
3	C	0.26	0/3419	0.49	1/4632 (0.0%)
3	D	0.27	0/3434	0.49	1/4651 (0.0%)
3	E	0.26	0/3419	0.49	0/4632
3	F	0.26	0/3434	0.48	0/4651
3	G	0.26	0/3419	0.49	0/4632
3	H	0.27	0/3434	0.48	0/4651
3	I	0.26	0/3419	0.49	1/4632 (0.0%)
3	J	0.27	0/3434	0.48	0/4651
3	K	0.26	0/3419	0.49	0/4632
3	L	0.26	0/3434	0.48	0/4651
4	M	0.30	0/1592	0.51	0/2153
4	N	0.29	0/1573	0.50	0/2129
4	O	0.30	0/1592	0.51	0/2153
4	P	0.29	0/1573	0.50	0/2129

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	Q	0.30	0/1592	0.51	0/2153
4	R	0.29	0/1573	0.50	0/2129
4	S	0.30	0/1592	0.52	0/2153
4	T	0.30	0/1573	0.52	0/2129
4	U	0.30	0/1592	0.51	0/2153
4	V	0.29	0/1573	0.51	0/2129
4	W	0.30	0/1592	0.50	0/2153
4	X	0.29	0/1573	0.49	0/2129
5	a	0.27	0/936	0.55	0/1274
5	b	0.27	0/921	0.57	0/1253
5	c	0.27	0/921	0.60	0/1253
5	d	0.27	0/936	0.55	0/1274
5	e	0.29	0/921	0.58	0/1253
5	f	0.27	0/921	0.59	0/1253
5	g	0.28	0/936	0.55	0/1274
5	h	0.26	0/921	0.56	0/1253
5	i	0.27	0/921	0.55	0/1253
5	j	0.28	0/936	0.54	0/1274
5	k	0.28	0/921	0.58	0/1253
5	l	0.26	0/921	0.56	0/1253
5	m	0.28	0/936	0.54	0/1274
5	n	0.28	0/921	0.60	0/1253
5	o	0.27	0/921	0.58	0/1253
5	p	0.29	0/936	0.55	0/1274
5	q	0.27	0/921	0.54	0/1253
5	r	0.27	0/921	0.60	0/1253
6	s	0.34	0/6449	0.58	0/8772
6	t	0.34	0/6449	0.57	0/8772
6	u	0.33	0/6449	0.57	0/8772
6	v	0.34	0/6449	0.58	1/8772 (0.0%)
6	w	0.34	0/6449	0.58	0/8772
6	x	0.34	0/6449	0.58	0/8772
All	All	0.30	0/124632	0.53	4/168984 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	157	PRO	CA-N-CD	-5.71	103.50	111.50
6	v	105	ASN	N-CA-C	-5.32	96.63	111.00
3	I	385	LEU	CA-CB-CG	5.16	127.17	115.30
3	C	385	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	0	117/196 (60%)	115 (98%)	2 (2%)	0	100	100
1	1	117/196 (60%)	116 (99%)	1 (1%)	0	100	100
1	Y	117/196 (60%)	115 (98%)	2 (2%)	0	100	100
1	Z	117/196 (60%)	115 (98%)	2 (2%)	0	100	100
1	y	117/196 (60%)	115 (98%)	2 (2%)	0	100	100
1	z	117/196 (60%)	116 (99%)	1 (1%)	0	100	100
2	2	29/88 (33%)	25 (86%)	4 (14%)	0	100	100
2	3	29/88 (33%)	26 (90%)	3 (10%)	0	100	100
2	4	29/88 (33%)	23 (79%)	6 (21%)	0	100	100
2	5	29/88 (33%)	25 (86%)	4 (14%)	0	100	100
2	6	29/88 (33%)	23 (79%)	6 (21%)	0	100	100
2	7	29/88 (33%)	24 (83%)	5 (17%)	0	100	100
2	8	47/88 (53%)	45 (96%)	2 (4%)	0	100	100
2	9	47/88 (53%)	45 (96%)	2 (4%)	0	100	100
2	AA	47/88 (53%)	45 (96%)	2 (4%)	0	100	100
2	AB	47/88 (53%)	45 (96%)	2 (4%)	0	100	100
2	AC	47/88 (53%)	44 (94%)	3 (6%)	0	100	100
2	AD	47/88 (53%)	44 (94%)	3 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	427/536 (80%)	419 (98%)	8 (2%)	0	100	100
3	B	429/536 (80%)	422 (98%)	7 (2%)	0	100	100
3	C	427/536 (80%)	416 (97%)	11 (3%)	0	100	100
3	D	429/536 (80%)	422 (98%)	7 (2%)	0	100	100
3	E	427/536 (80%)	417 (98%)	10 (2%)	0	100	100
3	F	429/536 (80%)	422 (98%)	7 (2%)	0	100	100
3	G	427/536 (80%)	418 (98%)	9 (2%)	0	100	100
3	H	429/536 (80%)	423 (99%)	6 (1%)	0	100	100
3	I	427/536 (80%)	414 (97%)	13 (3%)	0	100	100
3	J	429/536 (80%)	425 (99%)	4 (1%)	0	100	100
3	K	427/536 (80%)	417 (98%)	10 (2%)	0	100	100
3	L	429/536 (80%)	423 (99%)	6 (1%)	0	100	100
4	M	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
4	N	192/196 (98%)	185 (96%)	7 (4%)	0	100	100
4	O	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
4	P	192/196 (98%)	185 (96%)	7 (4%)	0	100	100
4	Q	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
4	R	192/196 (98%)	187 (97%)	5 (3%)	0	100	100
4	S	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
4	T	192/196 (98%)	185 (96%)	7 (4%)	0	100	100
4	U	194/196 (99%)	191 (98%)	3 (2%)	0	100	100
4	V	192/196 (98%)	184 (96%)	8 (4%)	0	100	100
4	W	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
4	X	192/196 (98%)	186 (97%)	6 (3%)	0	100	100
5	a	113/553 (20%)	107 (95%)	6 (5%)	0	100	100
5	b	111/553 (20%)	106 (96%)	5 (4%)	0	100	100
5	c	111/553 (20%)	105 (95%)	5 (4%)	1 (1%)	14	49
5	d	113/553 (20%)	108 (96%)	5 (4%)	0	100	100
5	e	111/553 (20%)	103 (93%)	7 (6%)	1 (1%)	14	49
5	f	111/553 (20%)	106 (96%)	5 (4%)	0	100	100
5	g	113/553 (20%)	110 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	h	111/553 (20%)	105 (95%)	4 (4%)	2 (2%)	7	35
5	i	111/553 (20%)	107 (96%)	4 (4%)	0	100	100
5	j	113/553 (20%)	109 (96%)	4 (4%)	0	100	100
5	k	111/553 (20%)	104 (94%)	5 (4%)	2 (2%)	7	35
5	l	111/553 (20%)	107 (96%)	4 (4%)	0	100	100
5	m	113/553 (20%)	109 (96%)	4 (4%)	0	100	100
5	n	111/553 (20%)	103 (93%)	8 (7%)	0	100	100
5	o	111/553 (20%)	108 (97%)	3 (3%)	0	100	100
5	p	113/553 (20%)	107 (95%)	5 (4%)	1 (1%)	14	49
5	q	111/553 (20%)	106 (96%)	5 (4%)	0	100	100
5	r	111/553 (20%)	106 (96%)	5 (4%)	0	100	100
6	s	787/794 (99%)	701 (89%)	80 (10%)	6 (1%)	16	51
6	t	787/794 (99%)	702 (89%)	78 (10%)	7 (1%)	14	49
6	u	787/794 (99%)	699 (89%)	80 (10%)	8 (1%)	13	46
6	v	787/794 (99%)	699 (89%)	79 (10%)	9 (1%)	12	45
6	w	787/794 (99%)	699 (89%)	83 (10%)	5 (1%)	22	56
6	x	787/794 (99%)	702 (89%)	80 (10%)	5 (1%)	22	56
All	All	15342/25734 (60%)	14513 (95%)	782 (5%)	47 (0%)	38	68

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	c	68	ASP
6	s	432	SER
6	s	498	ASN
6	s	735	ARG
6	t	498	ASN
6	t	735	ARG
6	u	432	SER
6	u	498	ASN
6	v	432	SER
6	v	498	ASN
6	v	735	ARG
6	w	432	SER
6	w	498	ASN
6	w	735	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	x	432	SER
6	x	498	ASN
6	x	735	ARG
5	e	66	PRO
5	h	66	PRO
5	k	63	ALA
5	p	64	TRP
6	t	739	ASN
6	u	273	ALA
6	v	396	SER
6	v	411	GLU
6	v	418	ASP
6	w	396	SER
5	h	68	ASP
6	s	105	ASN
6	t	105	ASN
6	t	398	ASN
6	t	410	SER
6	u	105	ASN
6	u	398	ASN
6	u	410	SER
6	v	105	ASN
6	x	412	GLU
5	k	71	THR
6	u	735	ARG
6	v	427	SER
6	x	427	SER
6	s	13	GLY
6	s	427	SER
6	t	427	SER
6	u	427	SER
6	w	427	SER
6	v	400	ILE

5.3.2 Protein sidechains [i](#)

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	0	95/149 (64%)	95 (100%)	0	100	100
1	1	95/149 (64%)	95 (100%)	0	100	100
1	Y	95/149 (64%)	95 (100%)	0	100	100
1	Z	95/149 (64%)	95 (100%)	0	100	100
1	y	95/149 (64%)	95 (100%)	0	100	100
1	z	95/149 (64%)	95 (100%)	0	100	100
2	2	27/73 (37%)	27 (100%)	0	100	100
2	3	27/73 (37%)	27 (100%)	0	100	100
2	4	27/73 (37%)	27 (100%)	0	100	100
2	5	27/73 (37%)	27 (100%)	0	100	100
2	6	27/73 (37%)	27 (100%)	0	100	100
2	7	27/73 (37%)	27 (100%)	0	100	100
2	8	42/73 (58%)	42 (100%)	0	100	100
2	9	42/73 (58%)	42 (100%)	0	100	100
2	AA	42/73 (58%)	42 (100%)	0	100	100
2	AB	42/73 (58%)	42 (100%)	0	100	100
2	AC	42/73 (58%)	42 (100%)	0	100	100
2	AD	42/73 (58%)	42 (100%)	0	100	100
3	A	365/442 (83%)	364 (100%)	1 (0%)	91	96
3	B	366/442 (83%)	366 (100%)	0	100	100
3	C	365/442 (83%)	364 (100%)	1 (0%)	91	96
3	D	366/442 (83%)	366 (100%)	0	100	100
3	E	365/442 (83%)	364 (100%)	1 (0%)	91	96
3	F	366/442 (83%)	365 (100%)	1 (0%)	91	96
3	G	365/442 (83%)	365 (100%)	0	100	100
3	H	366/442 (83%)	366 (100%)	0	100	100
3	I	365/442 (83%)	363 (100%)	2 (0%)	86	93
3	J	366/442 (83%)	366 (100%)	0	100	100
3	K	365/442 (83%)	364 (100%)	1 (0%)	91	96
3	L	366/442 (83%)	364 (100%)	2 (0%)	86	93
4	M	169/169 (100%)	169 (100%)	0	100	100
4	N	167/169 (99%)	167 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	O	169/169 (100%)	169 (100%)	0	100	100
4	P	167/169 (99%)	167 (100%)	0	100	100
4	Q	169/169 (100%)	169 (100%)	0	100	100
4	R	167/169 (99%)	167 (100%)	0	100	100
4	S	169/169 (100%)	169 (100%)	0	100	100
4	T	167/169 (99%)	167 (100%)	0	100	100
4	U	169/169 (100%)	169 (100%)	0	100	100
4	V	167/169 (99%)	166 (99%)	1 (1%)	84	91
4	W	169/169 (100%)	169 (100%)	0	100	100
4	X	167/169 (99%)	166 (99%)	1 (1%)	84	91
5	a	102/451 (23%)	102 (100%)	0	100	100
5	b	100/451 (22%)	99 (99%)	1 (1%)	73	84
5	c	100/451 (22%)	99 (99%)	1 (1%)	73	84
5	d	102/451 (23%)	102 (100%)	0	100	100
5	e	100/451 (22%)	100 (100%)	0	100	100
5	f	100/451 (22%)	98 (98%)	2 (2%)	50	72
5	g	102/451 (23%)	102 (100%)	0	100	100
5	h	100/451 (22%)	99 (99%)	1 (1%)	73	84
5	i	100/451 (22%)	100 (100%)	0	100	100
5	j	102/451 (23%)	102 (100%)	0	100	100
5	k	100/451 (22%)	99 (99%)	1 (1%)	73	84
5	l	100/451 (22%)	99 (99%)	1 (1%)	73	84
5	m	102/451 (23%)	102 (100%)	0	100	100
5	n	100/451 (22%)	99 (99%)	1 (1%)	73	84
5	o	100/451 (22%)	99 (99%)	1 (1%)	73	84
5	p	102/451 (23%)	102 (100%)	0	100	100
5	q	100/451 (22%)	100 (100%)	0	100	100
5	r	100/451 (22%)	99 (99%)	1 (1%)	73	84
6	s	684/688 (99%)	675 (99%)	9 (1%)	65	81
6	t	684/688 (99%)	676 (99%)	8 (1%)	67	82
6	u	684/688 (99%)	682 (100%)	2 (0%)	91	96

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	v	684/688 (99%)	679 (99%)	5 (1%)	81	89
6	w	684/688 (99%)	678 (99%)	6 (1%)	75	86
6	x	684/688 (99%)	677 (99%)	7 (1%)	73	84
All	All	13302/21348 (62%)	13244 (100%)	58 (0%)	88	95

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	394	GLN
3	C	309	ARG
3	E	394	GLN
3	F	309	ARG
3	I	309	ARG
3	I	394	GLN
3	K	309	ARG
3	L	309	ARG
3	L	394	GLN
4	V	182	ASN
4	X	182	ASN
5	b	68	ASP
5	c	64	TRP
5	f	45	THR
5	f	64	TRP
5	h	64	TRP
5	k	68	ASP
5	l	68	ASP
5	n	68	ASP
5	o	68	ASP
5	r	48	THR
6	s	78	TYR
6	s	80	VAL
6	s	260	ASN
6	s	275	LYS
6	s	279	GLN
6	s	338	ASN
6	s	397	THR
6	s	417	SER
6	s	661	ASN
6	t	78	TYR
6	t	260	ASN
6	t	275	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	t	396	SER
6	t	417	SER
6	t	431	THR
6	t	433	LYS
6	t	478	ASP
6	u	194	GLN
6	u	260	ASN
6	v	275	LYS
6	v	397	THR
6	v	418	ASP
6	v	661	ASN
6	v	704	ARG
6	w	78	TYR
6	w	260	ASN
6	w	397	THR
6	w	417	SER
6	w	433	LYS
6	w	735	ARG
6	x	260	ASN
6	x	270	VAL
6	x	397	THR
6	x	412	GLU
6	x	418	ASP
6	x	538	GLN
6	x	740	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	71	ASN
1	0	128	GLN
2	2	16	GLN
2	4	16	GLN
2	6	16	GLN
3	B	142	ASN
3	E	283	GLN
3	I	68	ASN
3	I	394	GLN
3	J	216	HIS
3	J	331	GLN
3	L	394	GLN
4	O	120	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	P	53	GLN
4	R	62	ASN
4	X	62	ASN
1	Y	111	ASN
5	g	21	ASN
5	q	100	ASN
6	s	187	HIS
6	s	279	GLN
6	s	421	GLN
6	s	570	ASN
6	s	617	HIS
6	s	645	GLN
6	t	338	ASN
6	t	538	GLN
6	t	570	ASN
6	t	661	ASN
6	u	338	ASN
6	u	538	GLN
6	u	570	ASN
6	u	617	HIS
6	u	645	GLN
6	v	102	ASN
6	v	187	HIS
6	v	260	ASN
6	v	279	GLN
6	v	338	ASN
6	v	570	ASN
6	v	617	HIS
6	v	645	GLN
6	v	661	ASN
6	w	102	ASN
6	w	338	ASN
6	w	538	GLN
6	w	570	ASN
6	x	338	ASN
6	x	570	ASN
6	x	617	HIS
6	x	645	GLN

5.3.3 RNA ⓘ

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.

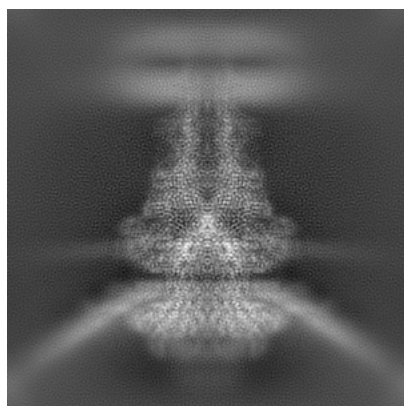
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61911. These allow visual inspection of the internal detail of the map and identification of artifacts.

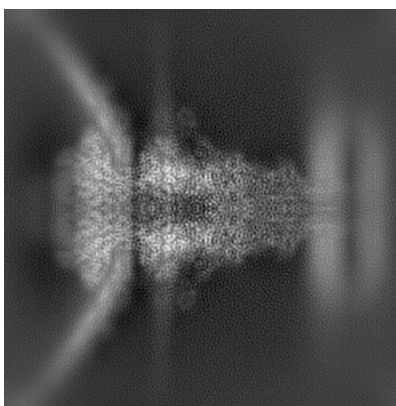
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

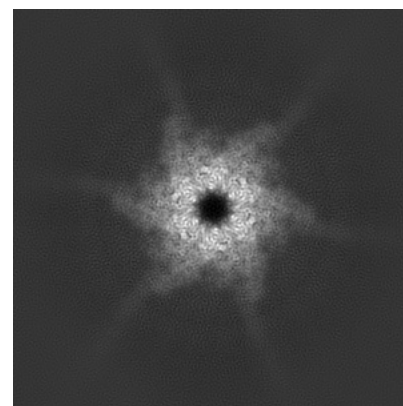
6.1.1 Primary map



X

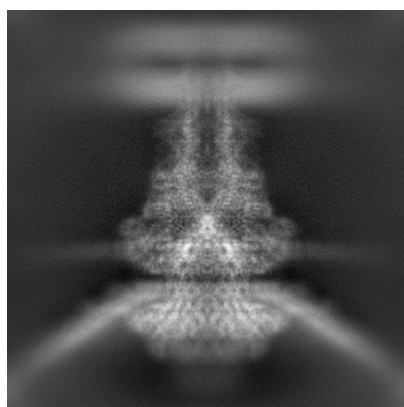


Y

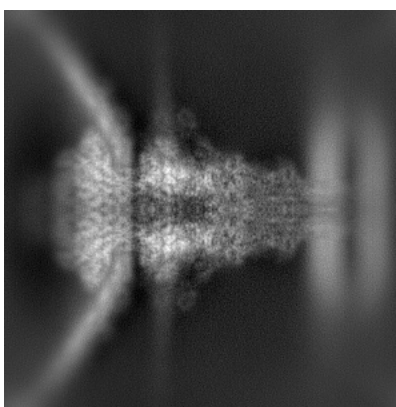


Z

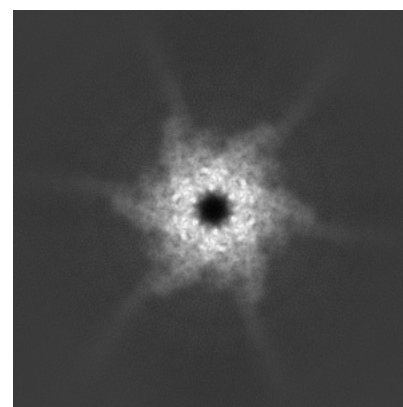
6.1.2 Raw map



X



Y

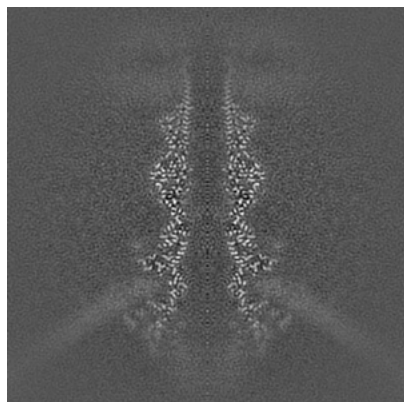


Z

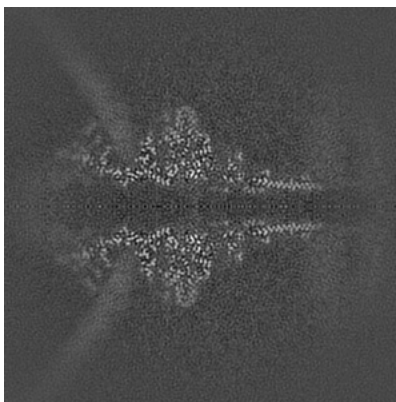
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

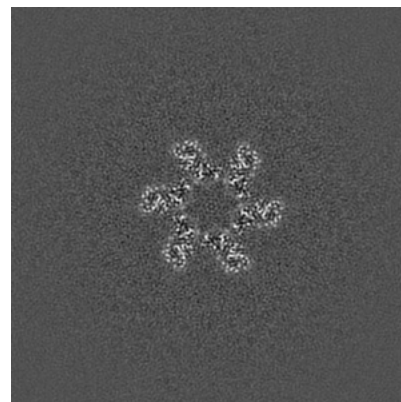
6.2.1 Primary map



X Index: 200

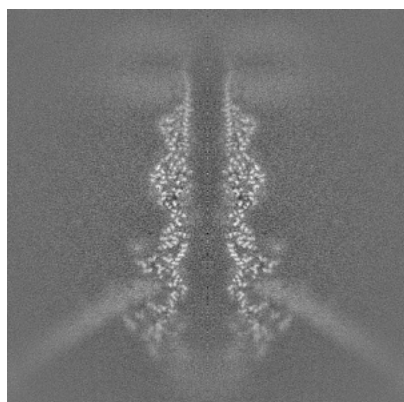


Y Index: 200

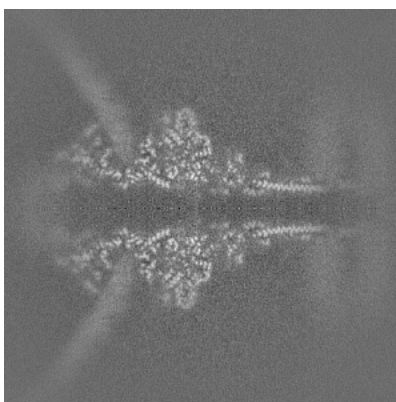


Z Index: 200

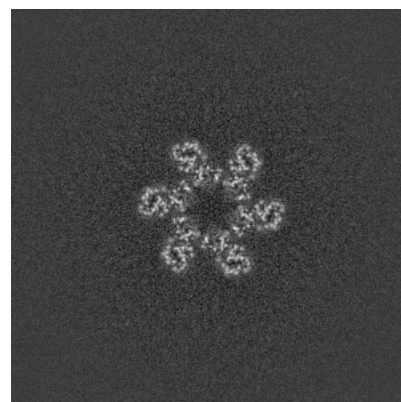
6.2.2 Raw map



X Index: 200



Y Index: 200

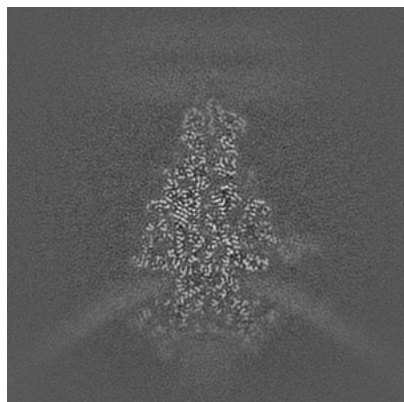


Z Index: 200

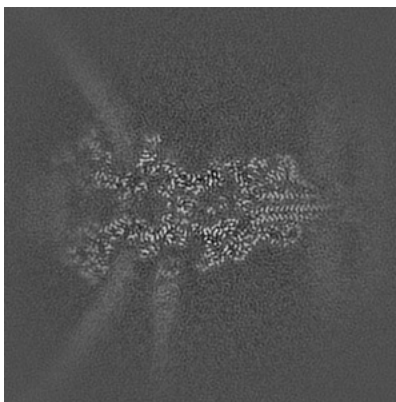
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

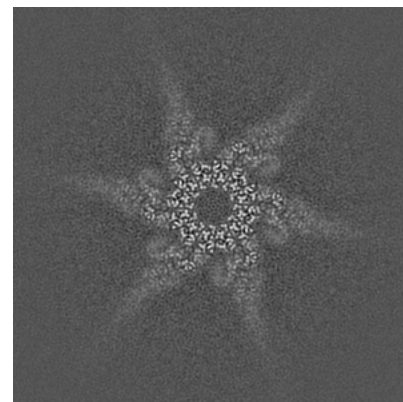
6.3.1 Primary map



X Index: 171

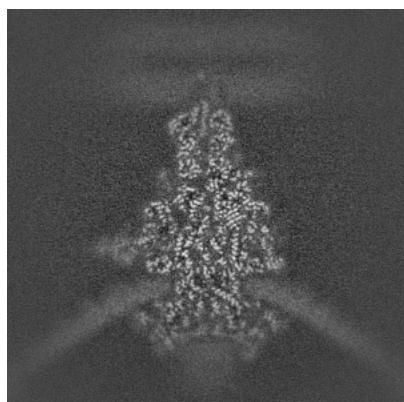


Y Index: 220

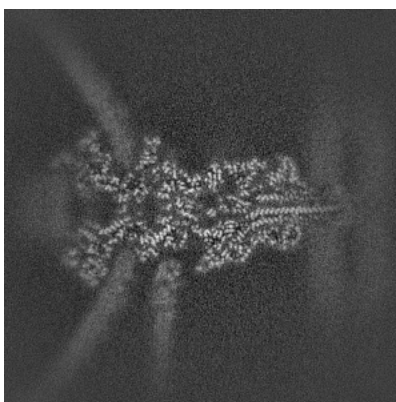


Z Index: 164

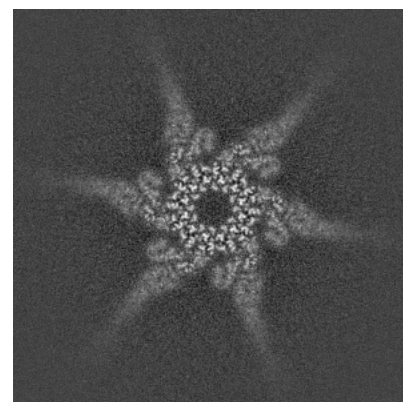
6.3.2 Raw map



X Index: 229



Y Index: 221

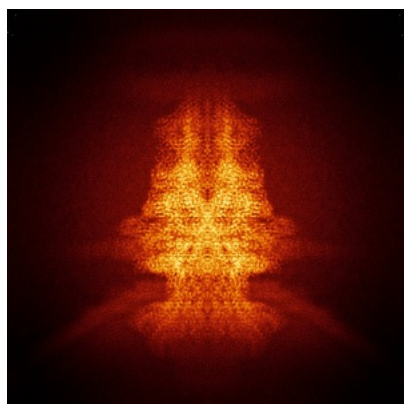


Z Index: 164

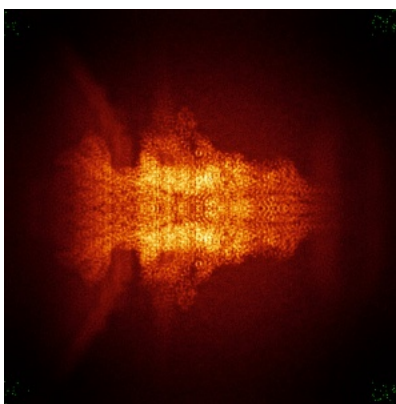
The images above show the largest variance slices of the map in three orthogonal directions.

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

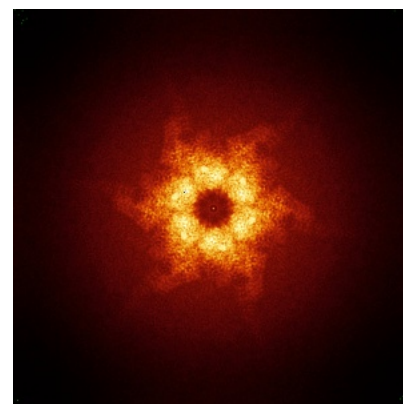
6.4.1 Primary map



X

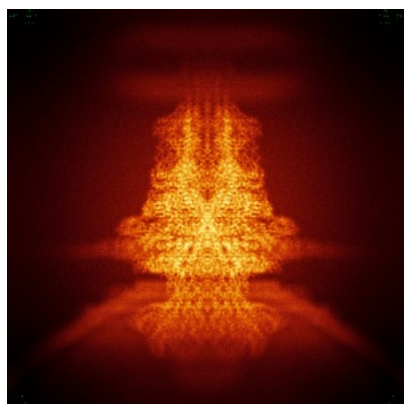


Y

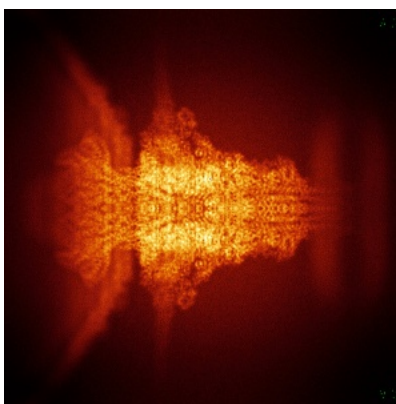


Z

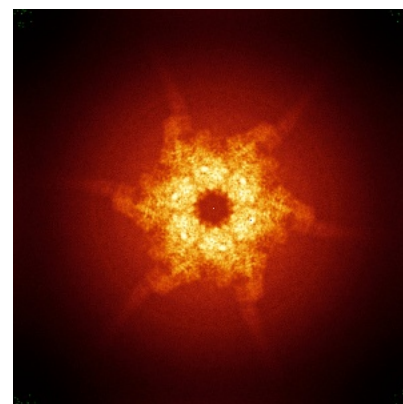
6.4.2 Raw map



X



Y

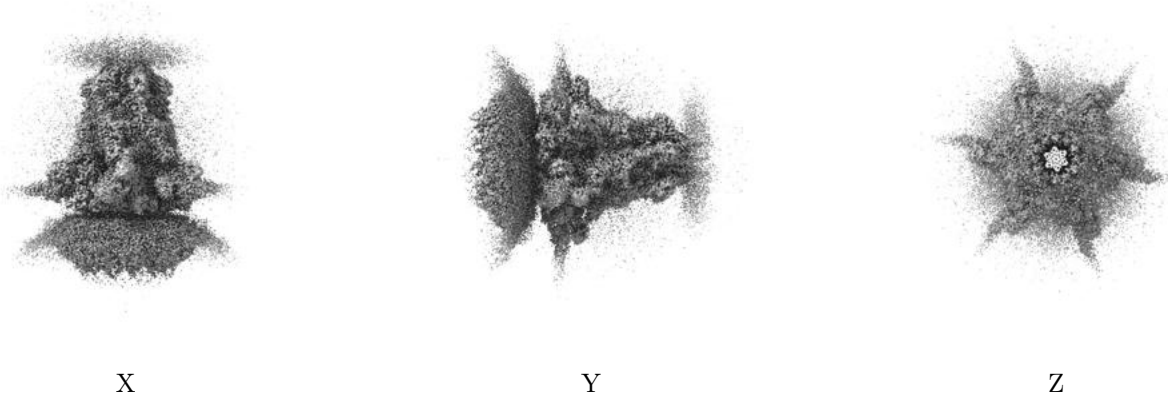


Z

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.

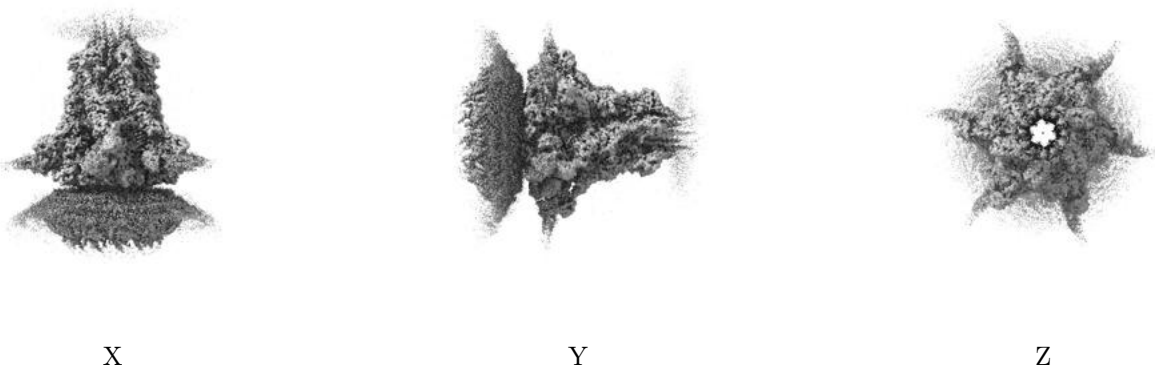
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.9. 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.

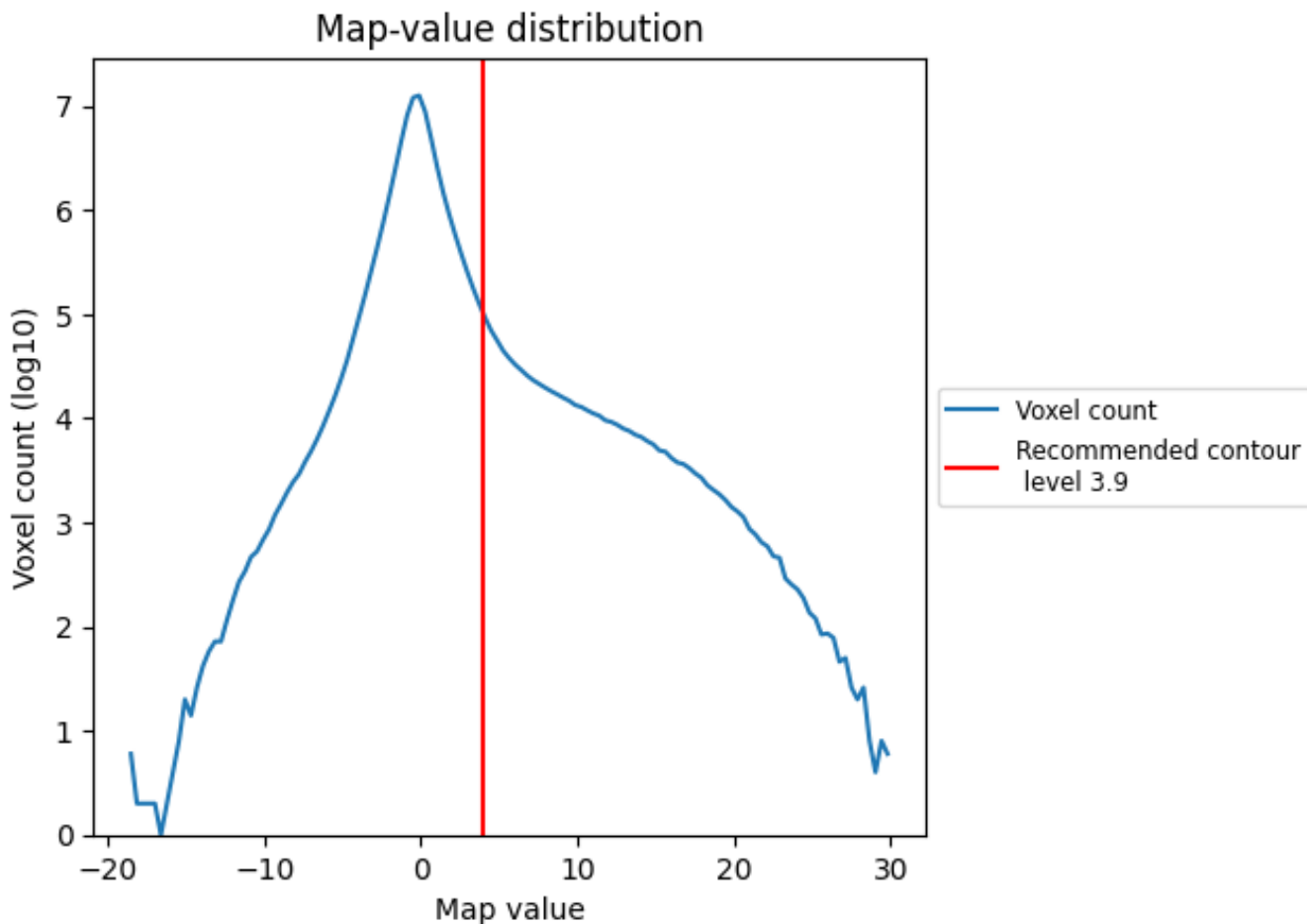
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

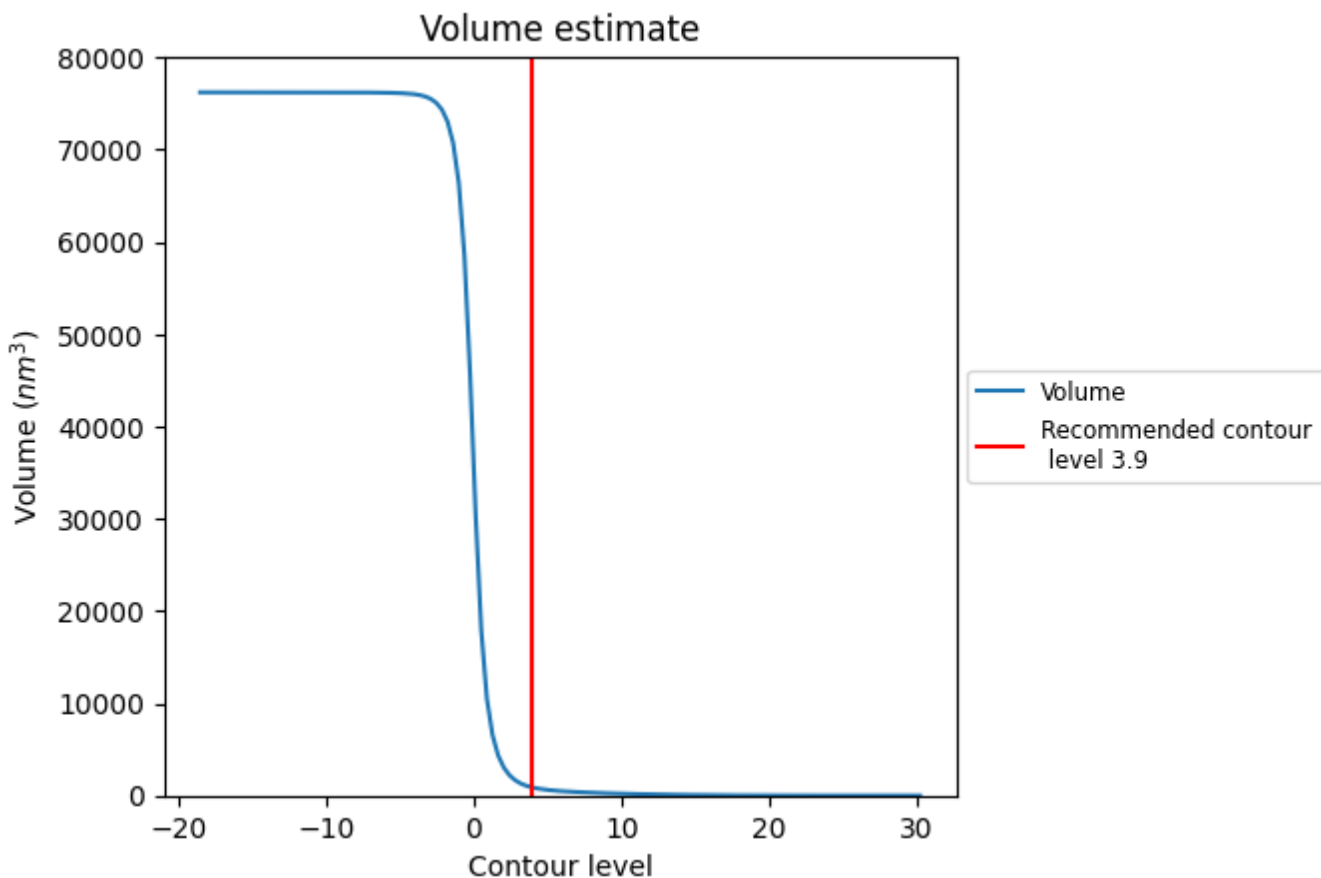
This section contains the results of statistical analysis of the map.

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.

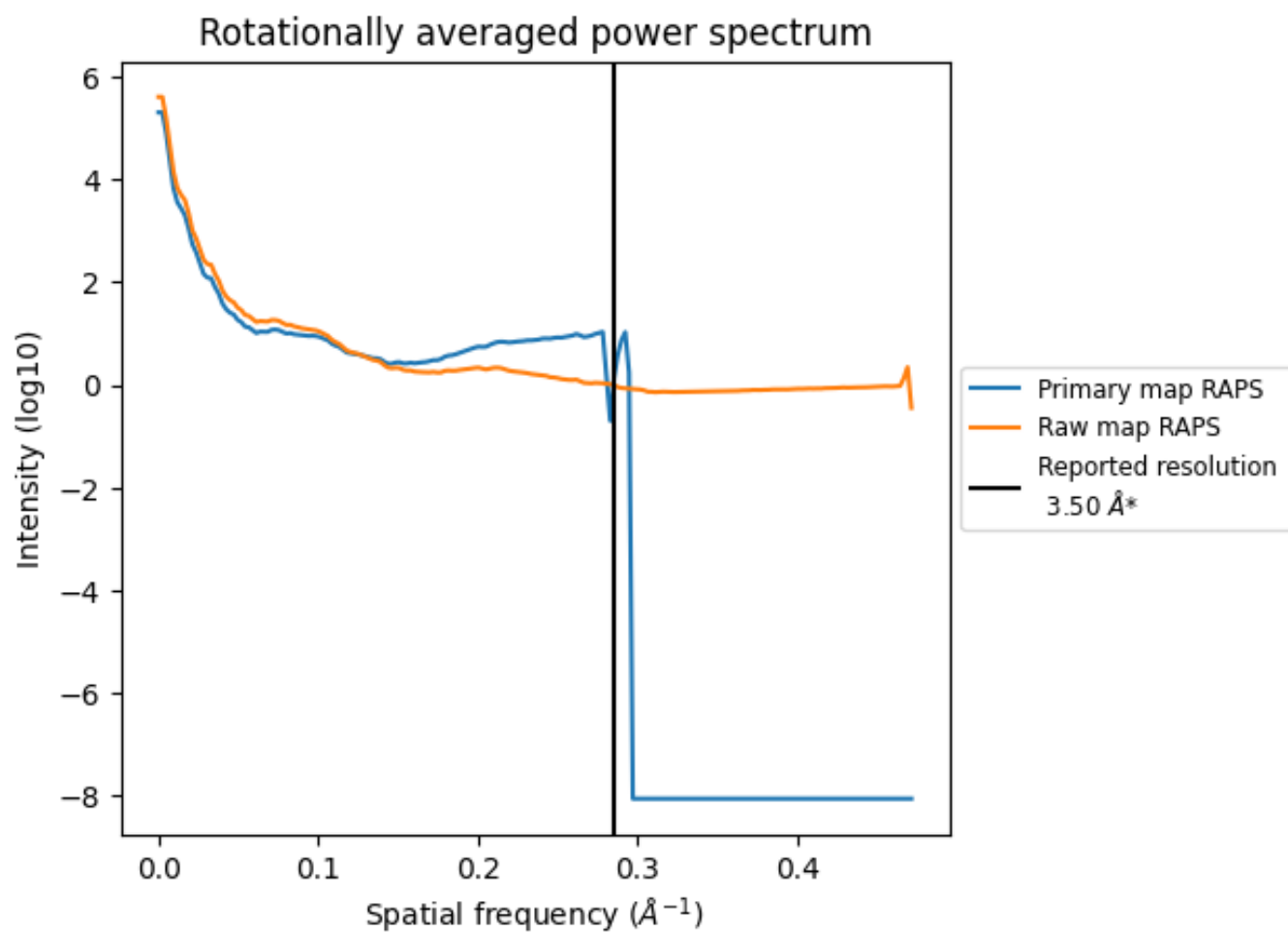
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 902 nm³; this corresponds to an approximate mass of 815 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 i

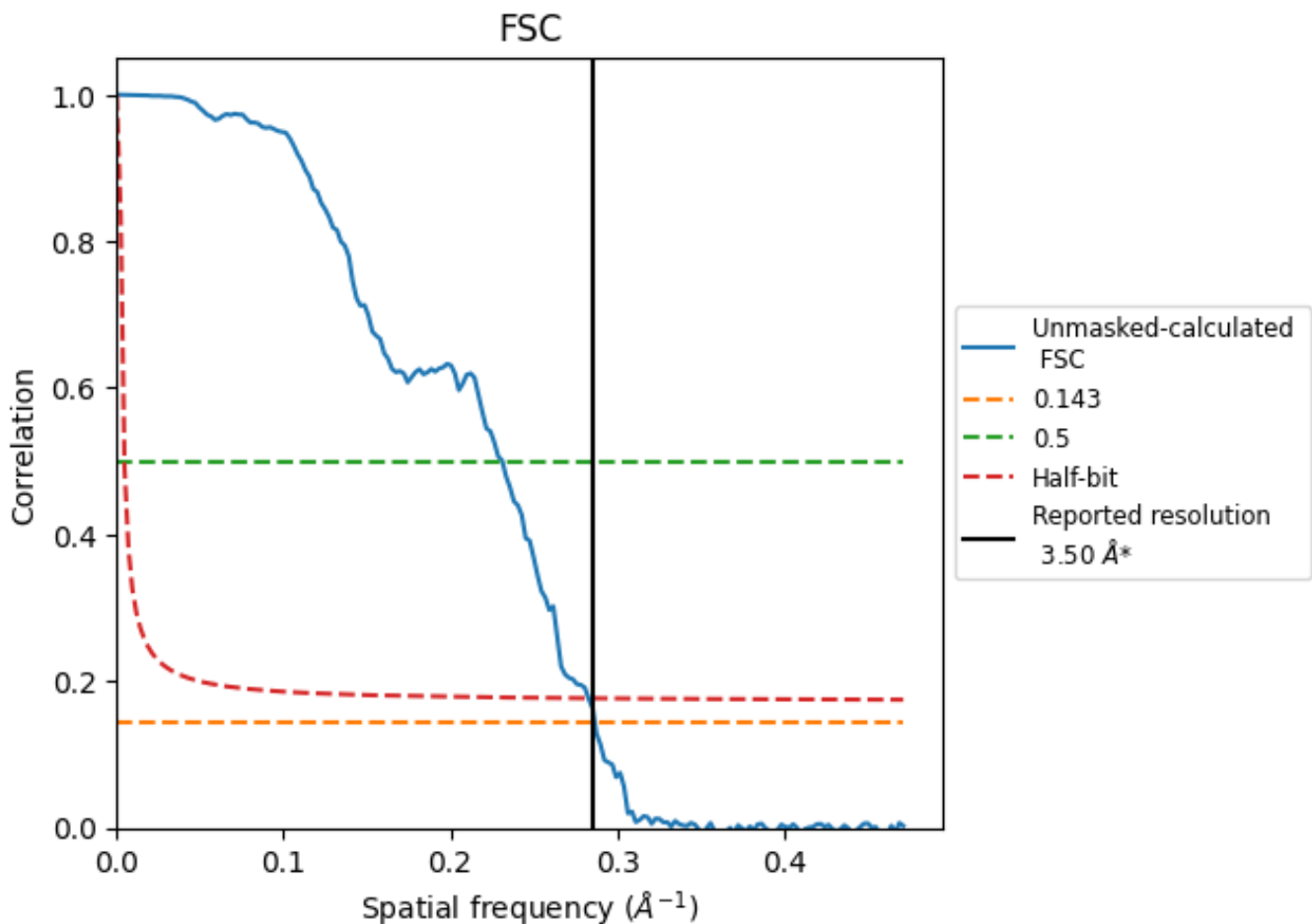


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

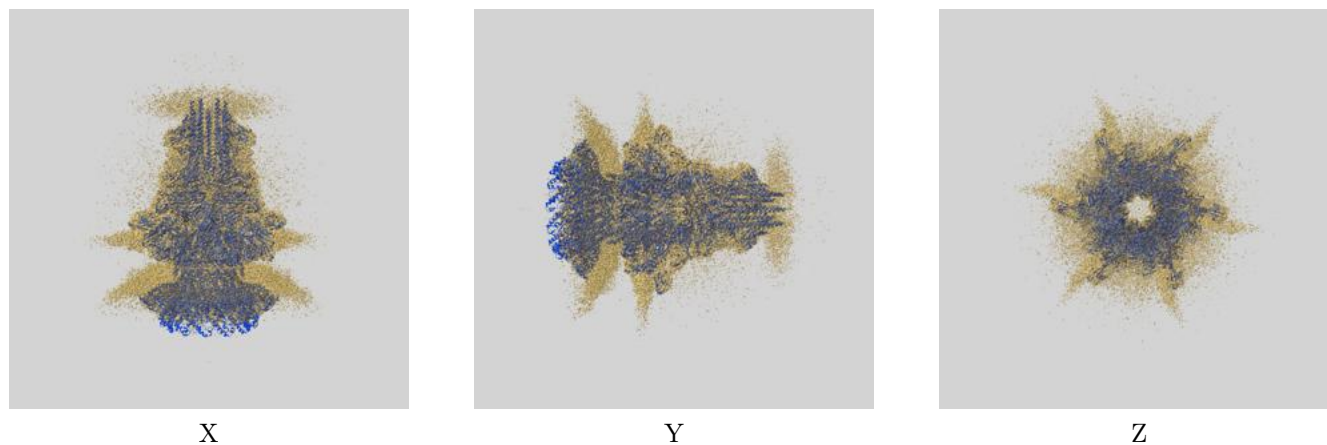
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.49	4.33	3.53

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

9 Map-model fit [i](#)

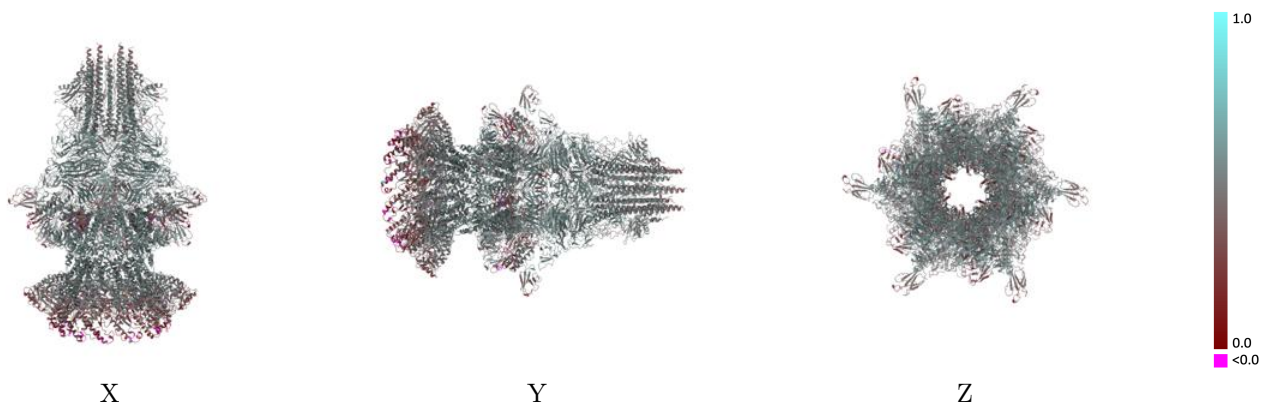
This section contains information regarding the fit between EMDB map EMD-61911 and PDB model 9JZ0. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



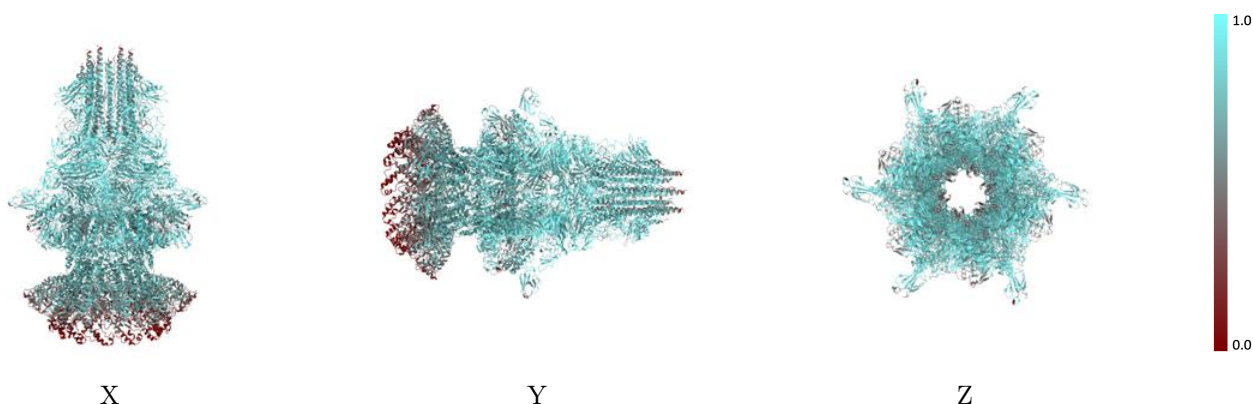
The images above show the 3D surface view of the map at the recommended contour level 3.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



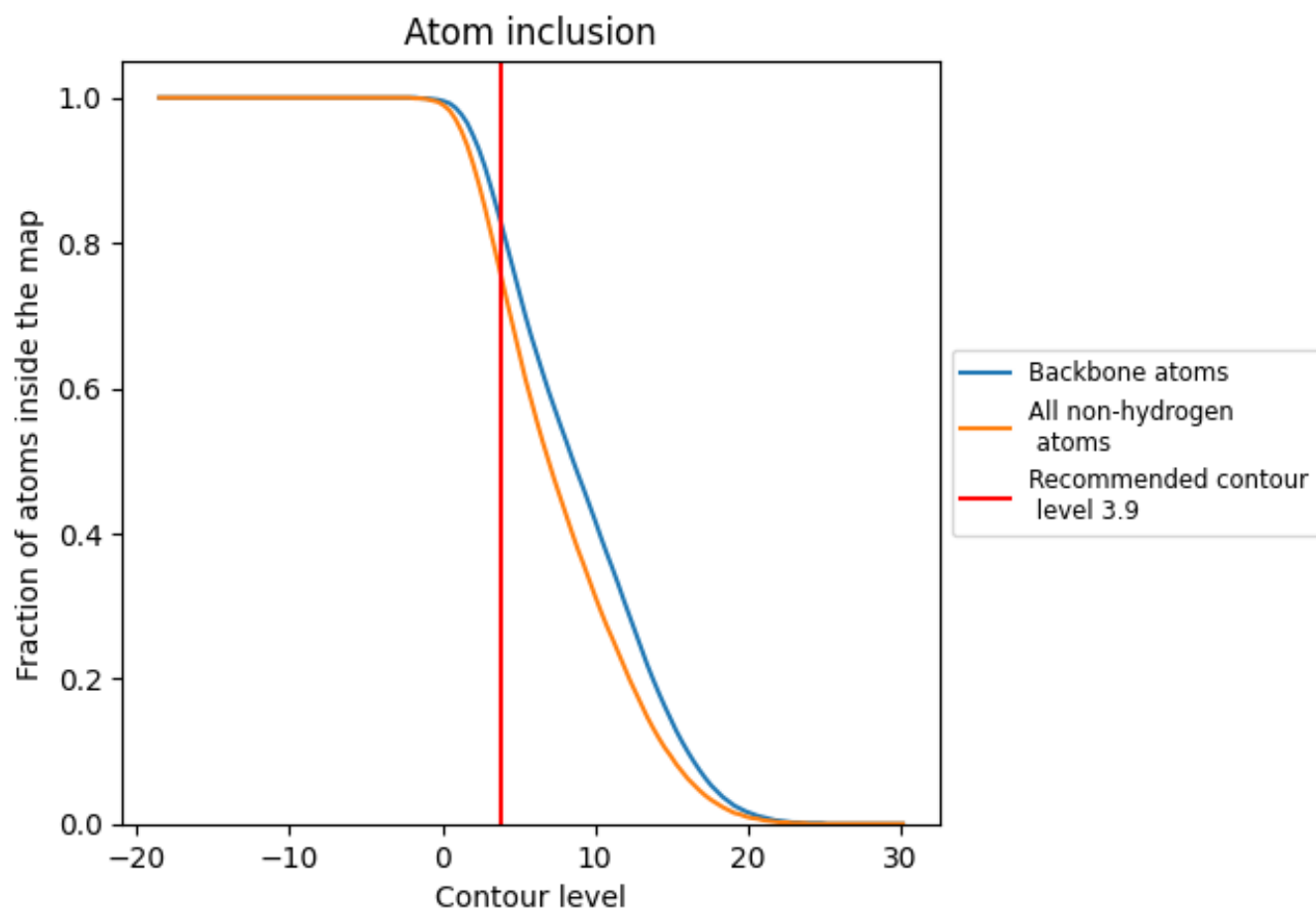
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.9).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 75% 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 (3.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7500	 0.4750
0	 0.7900	 0.4990
1	 0.7810	 0.4970
2	 0.4850	 0.3780
3	 0.4500	 0.3820
4	 0.4800	 0.3770
5	 0.4540	 0.3820
6	 0.4670	 0.3770
7	 0.4630	 0.3880
8	 0.6770	 0.4550
9	 0.6770	 0.4620
A	 0.5730	 0.4250
AA	 0.6490	 0.4660
AB	 0.6680	 0.4580
AC	 0.6740	 0.4610
AD	 0.6570	 0.4600
B	 0.5680	 0.4180
C	 0.5720	 0.4250
D	 0.5680	 0.4160
E	 0.5760	 0.4260
F	 0.5670	 0.4170
G	 0.5700	 0.4240
H	 0.5710	 0.4180
I	 0.5720	 0.4240
J	 0.5650	 0.4190
K	 0.5780	 0.4270
L	 0.5670	 0.4170
M	 0.8780	 0.5370
N	 0.8640	 0.5310
O	 0.8870	 0.5370
P	 0.8650	 0.5280
Q	 0.8780	 0.5370
R	 0.8580	 0.5310
S	 0.8740	 0.5350
T	 0.8650	 0.5310



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
U	 0.8820	 0.5360
V	 0.8660	 0.5310
W	 0.8760	 0.5350
X	 0.8580	 0.5310
Y	 0.7900	 0.4970
Z	 0.7860	 0.5030
a	 0.8100	 0.4750
b	 0.6720	 0.3580
c	 0.8090	 0.4520
d	 0.8110	 0.4780
e	 0.6690	 0.3690
f	 0.7950	 0.4460
g	 0.8270	 0.4800
h	 0.6670	 0.3680
i	 0.7980	 0.4510
j	 0.8160	 0.4790
k	 0.6760	 0.3670
l	 0.8060	 0.4540
m	 0.8140	 0.4780
n	 0.6740	 0.3610
o	 0.8000	 0.4490
p	 0.8350	 0.4820
q	 0.6700	 0.3670
r	 0.7890	 0.4440
s	 0.8880	 0.5250
t	 0.8910	 0.5240
u	 0.8850	 0.5250
v	 0.8860	 0.5230
w	 0.8890	 0.5220
x	 0.8870	 0.5240
y	 0.7870	 0.4990
z	 0.7770	 0.4970