



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 02:55 AM UTC

PDB ID : 8BL4 / pdb_00008bl4
EMDB ID : EMD-16101
Title : Cryo-EM structure of a contractile injection system in *Streptomyces coelicolor*, the sheath-tube module in extended state.
Authors : Casu, B.; Sallmen, J.W.; Schlimpert, S.; Pilhofer, M.
Deposited on : 2022-11-09
Resolution : 3.90 Å(reported)

This is a wwPDB EM Validation Summary 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:

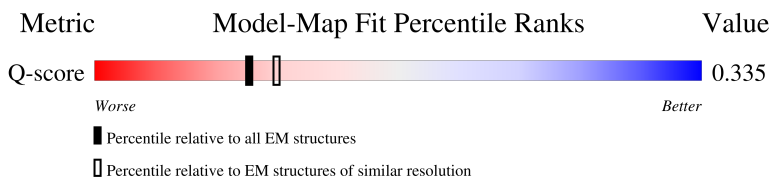
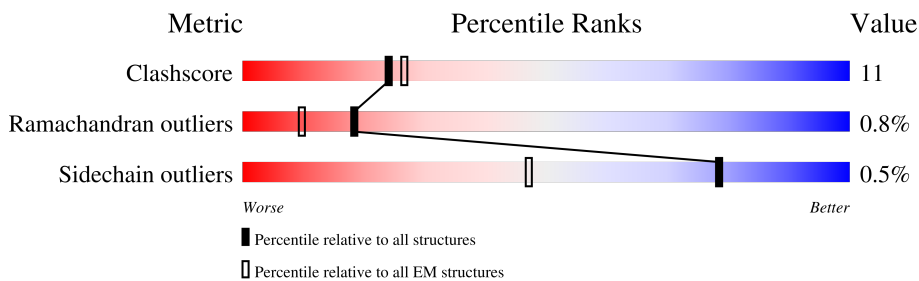
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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

Mol	Chain	Length	Quality of chain
1	A	539	5% (red), 57% (green), 11% (yellow), 31% (grey)
1	B	539	5% (red), 54% (green), 14% (yellow), 31% (grey)
1	C	539	5% (red), 56% (green), 12% (yellow), 31% (grey)
1	D	539	5% (red), 56% (green), 12% (yellow), 31% (grey)

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Mol	Chain	Length	Quality of chain	
1	E	539	56%	12%
1	F	539	57%	11%
1	G	539	55%	12%
1	H	539	56%	11%
1	I	539	57%	10%
1	J	539	57%	10%
1	K	539	55%	12%
1	L	539	55%	12%
1	M	539	56%	12%
1	N	539	58%	10%
1	O	539	57%	11%
1	P	539	56%	12%
1	Q	539	56%	12%
1	R	539	56%	12%
1	S	539	53%	14%
1	T	539	56%	12%
1	U	539	55%	13%
1	V	539	55%	13%
1	W	539	55%	12%
1	X	539	55%	13%
2	a	149	71%	26%
2	b	149	72%	24%
2	c	149	73%	24%
2	d	149	73%	25%
2	e	149	70%	28%

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Mol	Chain	Length	Quality of chain
2	f	149	 5% 74% 23% .
2	g	149	 5% 83% 15% ..
2	h	149	 6% 81% 17% ..
2	i	149	 5% 81% 18% ..
2	j	149	 0% 82% 16% ..
2	k	149	 5% 82% 16% ..
2	l	149	 5% 80% 18% ..
2	m	149	 7% 63% 34% .
2	n	149	 7% 60% 37% .
2	o	149	 8% 62% 34% .
2	p	149	 8% 60% 36% 5%
2	q	149	 7% 62% 34% .
2	r	149	 7% 60% 36% .
2	s	149	 9% 81% 17% .
2	t	149	 7% 81% 16% .
2	u	149	 9% 81% 15% .
2	v	149	 9% 81% 15% .
2	w	149	 7% 81% 15% .
2	x	149	 9% 81% 16% .

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 96456 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 Phage tail sheath family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	V	371	2867	1819	502	538	8	0	0
1	P	371	2867	1819	502	538	8	0	0
1	J	371	2867	1819	502	538	8	0	0
1	D	371	2867	1819	502	538	8	0	0
1	W	371	2867	1819	502	538	8	0	0
1	Q	371	2867	1819	502	538	8	0	0
1	K	371	2867	1819	502	538	8	0	0
1	E	371	2867	1819	502	538	8	0	0
1	X	371	2867	1819	502	538	8	0	0
1	R	371	2867	1819	502	538	8	0	0
1	L	371	2867	1819	502	538	8	0	0
1	F	371	2867	1819	502	538	8	0	0
1	S	371	2867	1819	502	538	8	0	0
1	M	371	2867	1819	502	538	8	0	0
1	G	371	2867	1819	502	538	8	0	0
1	A	371	2867	1819	502	538	8	0	0
1	T	371	2867	1819	502	538	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	371	Total 2867	C 1819	N 502	O 538	S 8	0	0
1	H	371	Total 2867	C 1819	N 502	O 538	S 8	0	0
1	B	371	Total 2867	C 1819	N 502	O 538	S 8	0	0
1	U	371	Total 2867	C 1819	N 502	O 538	S 8	0	0
1	O	371	Total 2867	C 1819	N 502	O 538	S 8	0	0
1	I	371	Total 2867	C 1819	N 502	O 538	S 8	0	0
1	C	371	Total 2867	C 1819	N 502	O 538	S 8	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	26	ILE	-	insertion	UNP Q9L0N8
V	27	GLU	-	insertion	UNP Q9L0N8
V	28	GLY	-	insertion	UNP Q9L0N8
V	29	VAL	-	insertion	UNP Q9L0N8
V	30	GLY	-	insertion	UNP Q9L0N8
P	26	ILE	-	insertion	UNP Q9L0N8
P	27	GLU	-	insertion	UNP Q9L0N8
P	28	GLY	-	insertion	UNP Q9L0N8
P	29	VAL	-	insertion	UNP Q9L0N8
P	30	GLY	-	insertion	UNP Q9L0N8
J	26	ILE	-	insertion	UNP Q9L0N8
J	27	GLU	-	insertion	UNP Q9L0N8
J	28	GLY	-	insertion	UNP Q9L0N8
J	29	VAL	-	insertion	UNP Q9L0N8
J	30	GLY	-	insertion	UNP Q9L0N8
D	26	ILE	-	insertion	UNP Q9L0N8
D	27	GLU	-	insertion	UNP Q9L0N8
D	28	GLY	-	insertion	UNP Q9L0N8
D	29	VAL	-	insertion	UNP Q9L0N8
D	30	GLY	-	insertion	UNP Q9L0N8
W	26	ILE	-	insertion	UNP Q9L0N8
W	27	GLU	-	insertion	UNP Q9L0N8
W	28	GLY	-	insertion	UNP Q9L0N8
W	29	VAL	-	insertion	UNP Q9L0N8
W	30	GLY	-	insertion	UNP Q9L0N8

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	26	ILE	-	insertion	UNP Q9L0N8
Q	27	GLU	-	insertion	UNP Q9L0N8
Q	28	GLY	-	insertion	UNP Q9L0N8
Q	29	VAL	-	insertion	UNP Q9L0N8
Q	30	GLY	-	insertion	UNP Q9L0N8
K	26	ILE	-	insertion	UNP Q9L0N8
K	27	GLU	-	insertion	UNP Q9L0N8
K	28	GLY	-	insertion	UNP Q9L0N8
K	29	VAL	-	insertion	UNP Q9L0N8
K	30	GLY	-	insertion	UNP Q9L0N8
E	26	ILE	-	insertion	UNP Q9L0N8
E	27	GLU	-	insertion	UNP Q9L0N8
E	28	GLY	-	insertion	UNP Q9L0N8
E	29	VAL	-	insertion	UNP Q9L0N8
E	30	GLY	-	insertion	UNP Q9L0N8
X	26	ILE	-	insertion	UNP Q9L0N8
X	27	GLU	-	insertion	UNP Q9L0N8
X	28	GLY	-	insertion	UNP Q9L0N8
X	29	VAL	-	insertion	UNP Q9L0N8
X	30	GLY	-	insertion	UNP Q9L0N8
R	26	ILE	-	insertion	UNP Q9L0N8
R	27	GLU	-	insertion	UNP Q9L0N8
R	28	GLY	-	insertion	UNP Q9L0N8
R	29	VAL	-	insertion	UNP Q9L0N8
R	30	GLY	-	insertion	UNP Q9L0N8
L	26	ILE	-	insertion	UNP Q9L0N8
L	27	GLU	-	insertion	UNP Q9L0N8
L	28	GLY	-	insertion	UNP Q9L0N8
L	29	VAL	-	insertion	UNP Q9L0N8
L	30	GLY	-	insertion	UNP Q9L0N8
F	26	ILE	-	insertion	UNP Q9L0N8
F	27	GLU	-	insertion	UNP Q9L0N8
F	28	GLY	-	insertion	UNP Q9L0N8
F	29	VAL	-	insertion	UNP Q9L0N8
F	30	GLY	-	insertion	UNP Q9L0N8
S	26	ILE	-	insertion	UNP Q9L0N8
S	27	GLU	-	insertion	UNP Q9L0N8
S	28	GLY	-	insertion	UNP Q9L0N8
S	29	VAL	-	insertion	UNP Q9L0N8
S	30	GLY	-	insertion	UNP Q9L0N8
M	26	ILE	-	insertion	UNP Q9L0N8
M	27	GLU	-	insertion	UNP Q9L0N8

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Chain	Residue	Modelled	Actual	Comment	Reference
M	28	GLY	-	insertion	UNP Q9L0N8
M	29	VAL	-	insertion	UNP Q9L0N8
M	30	GLY	-	insertion	UNP Q9L0N8
G	26	ILE	-	insertion	UNP Q9L0N8
G	27	GLU	-	insertion	UNP Q9L0N8
G	28	GLY	-	insertion	UNP Q9L0N8
G	29	VAL	-	insertion	UNP Q9L0N8
G	30	GLY	-	insertion	UNP Q9L0N8
A	26	ILE	-	insertion	UNP Q9L0N8
A	27	GLU	-	insertion	UNP Q9L0N8
A	28	GLY	-	insertion	UNP Q9L0N8
A	29	VAL	-	insertion	UNP Q9L0N8
A	30	GLY	-	insertion	UNP Q9L0N8
T	26	ILE	-	insertion	UNP Q9L0N8
T	27	GLU	-	insertion	UNP Q9L0N8
T	28	GLY	-	insertion	UNP Q9L0N8
T	29	VAL	-	insertion	UNP Q9L0N8
T	30	GLY	-	insertion	UNP Q9L0N8
N	26	ILE	-	insertion	UNP Q9L0N8
N	27	GLU	-	insertion	UNP Q9L0N8
N	28	GLY	-	insertion	UNP Q9L0N8
N	29	VAL	-	insertion	UNP Q9L0N8
N	30	GLY	-	insertion	UNP Q9L0N8
H	26	ILE	-	insertion	UNP Q9L0N8
H	27	GLU	-	insertion	UNP Q9L0N8
H	28	GLY	-	insertion	UNP Q9L0N8
H	29	VAL	-	insertion	UNP Q9L0N8
H	30	GLY	-	insertion	UNP Q9L0N8
B	26	ILE	-	insertion	UNP Q9L0N8
B	27	GLU	-	insertion	UNP Q9L0N8
B	28	GLY	-	insertion	UNP Q9L0N8
B	29	VAL	-	insertion	UNP Q9L0N8
B	30	GLY	-	insertion	UNP Q9L0N8
U	26	ILE	-	insertion	UNP Q9L0N8
U	27	GLU	-	insertion	UNP Q9L0N8
U	28	GLY	-	insertion	UNP Q9L0N8
U	29	VAL	-	insertion	UNP Q9L0N8
U	30	GLY	-	insertion	UNP Q9L0N8
O	26	ILE	-	insertion	UNP Q9L0N8
O	27	GLU	-	insertion	UNP Q9L0N8
O	28	GLY	-	insertion	UNP Q9L0N8
O	29	VAL	-	insertion	UNP Q9L0N8

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Chain	Residue	Modelled	Actual	Comment	Reference
O	30	GLY	-	insertion	UNP Q9L0N8
I	26	ILE	-	insertion	UNP Q9L0N8
I	27	GLU	-	insertion	UNP Q9L0N8
I	28	GLY	-	insertion	UNP Q9L0N8
I	29	VAL	-	insertion	UNP Q9L0N8
I	30	GLY	-	insertion	UNP Q9L0N8
C	26	ILE	-	insertion	UNP Q9L0N8
C	27	GLU	-	insertion	UNP Q9L0N8
C	28	GLY	-	insertion	UNP Q9L0N8
C	29	VAL	-	insertion	UNP Q9L0N8
C	30	GLY	-	insertion	UNP Q9L0N8

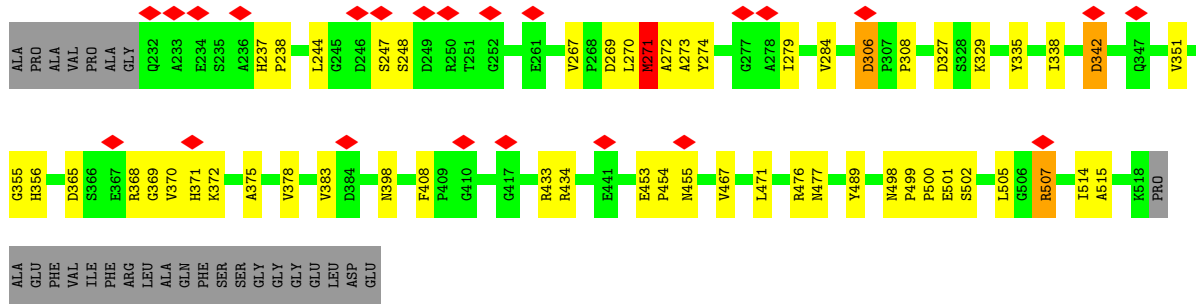
- Molecule 2 is a protein called Phage tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	v	149	1152	717	200	227	8	0	0
2	p	149	1152	717	200	227	8	0	0
2	j	149	1152	717	200	227	8	0	0
2	d	149	1152	717	200	227	8	0	0
2	w	149	1152	717	200	227	8	0	0
2	q	149	1152	717	200	227	8	0	0
2	k	149	1152	717	200	227	8	0	0
2	e	149	1152	717	200	227	8	0	0
2	x	149	1152	717	200	227	8	0	0
2	r	149	1152	717	200	227	8	0	0
2	l	149	1152	717	200	227	8	0	0
2	f	149	1152	717	200	227	8	0	0
2	s	149	1152	717	200	227	8	0	0
2	m	149	1152	717	200	227	8	0	0

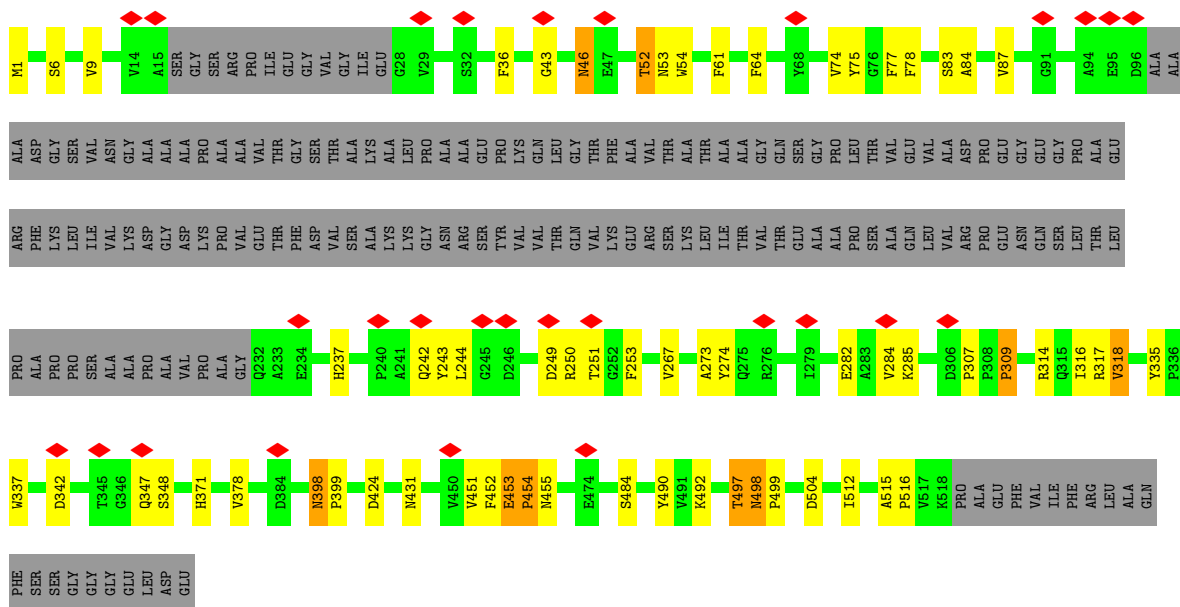
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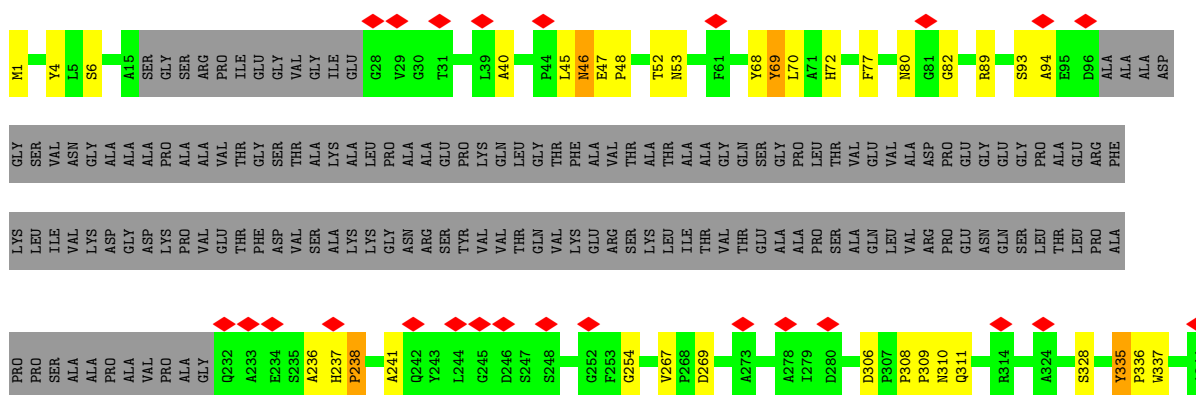
Mol	Chain	Residues	Atoms					AltConf	Trace
2	g	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	a	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	t	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	n	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	h	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	b	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	u	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	o	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	i	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	c	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		

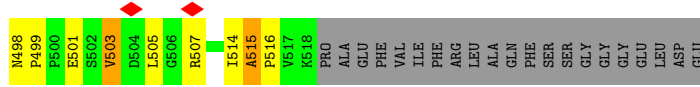


● Molecule 1: Phage tail sheath family protein

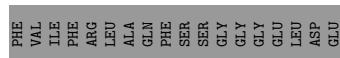
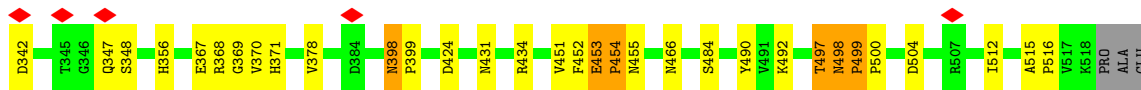
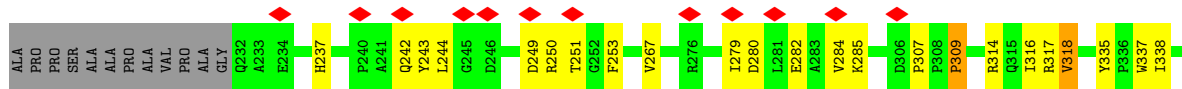
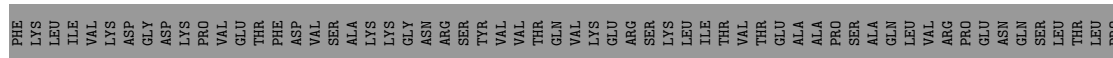
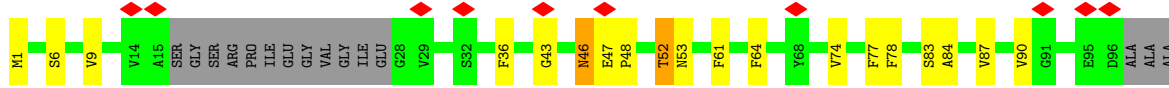


● Molecule 1: Phage tail sheath family protein

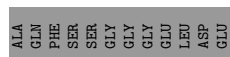
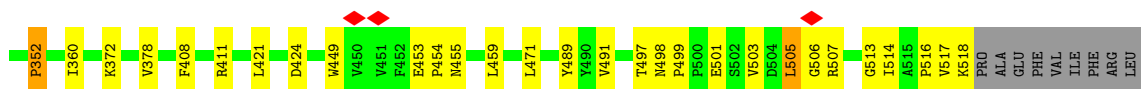
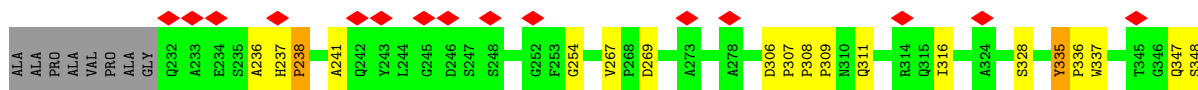
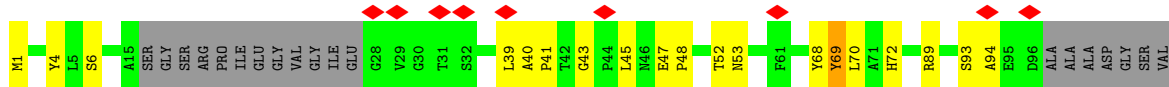




• Molecule 1: Phage tail sheath family protein



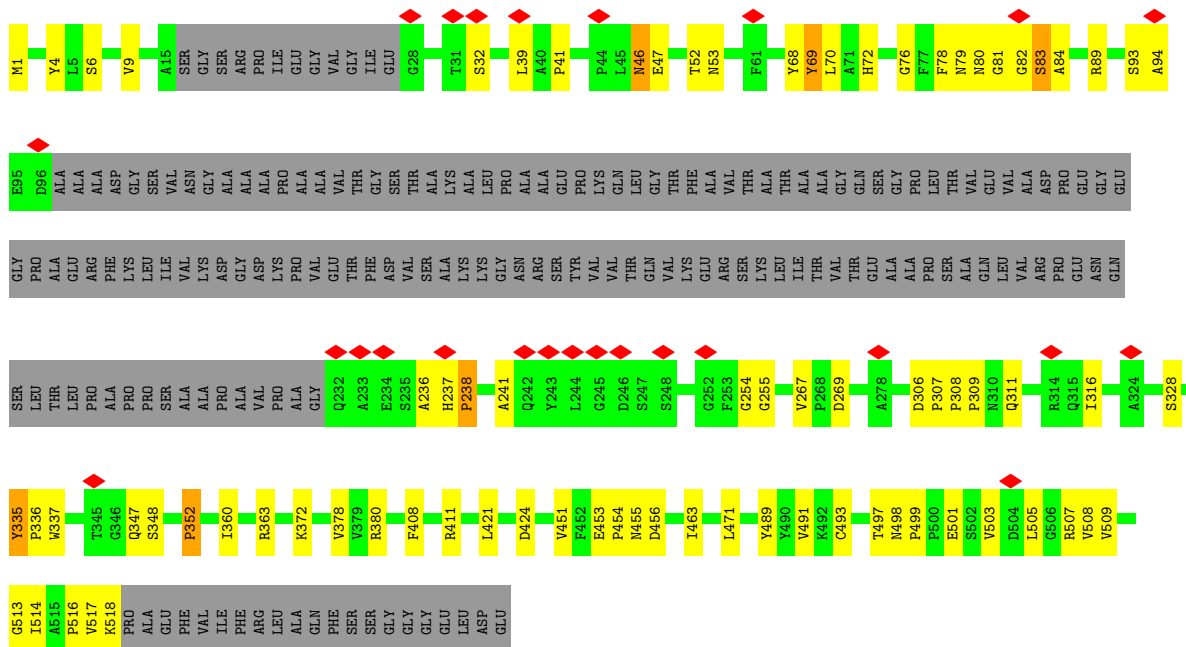
• Molecule 1: Phage tail sheath family protein



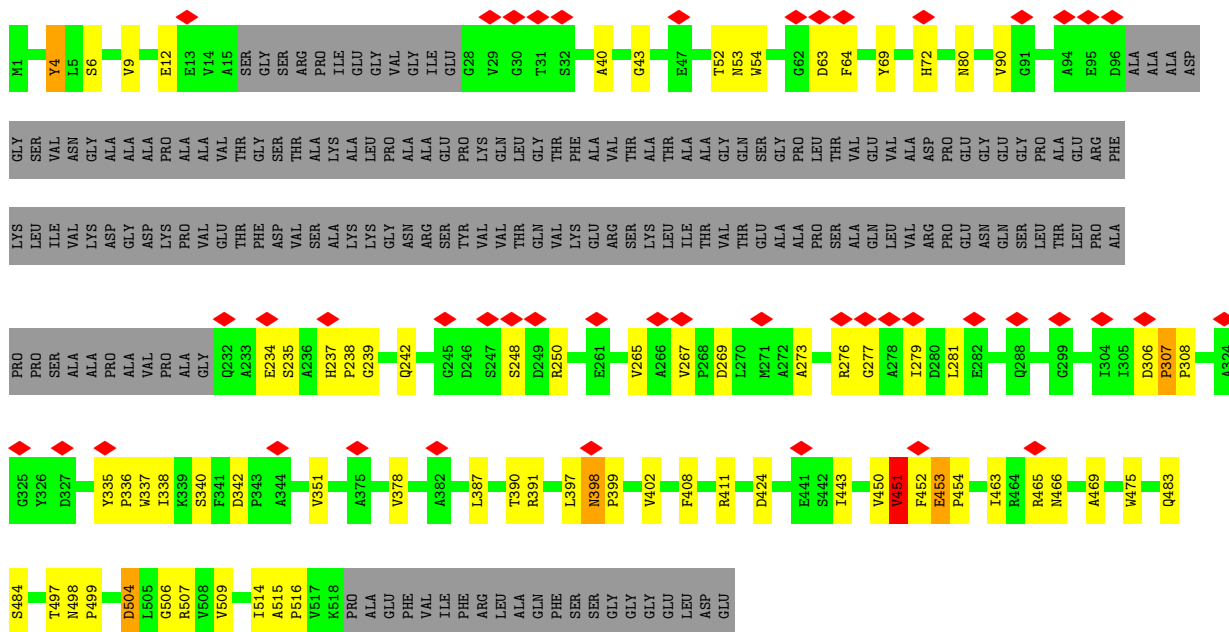
• Molecule 1: Phage tail sheath family protein

V517
 K518
 PRO
 ALA
 GLU
 PHE
 VAL
 ILE
 PHE
 ARG
 LEU
 ALA
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 SER
 SER
 SER
 GLY
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 LEU
 ASP
 GLU

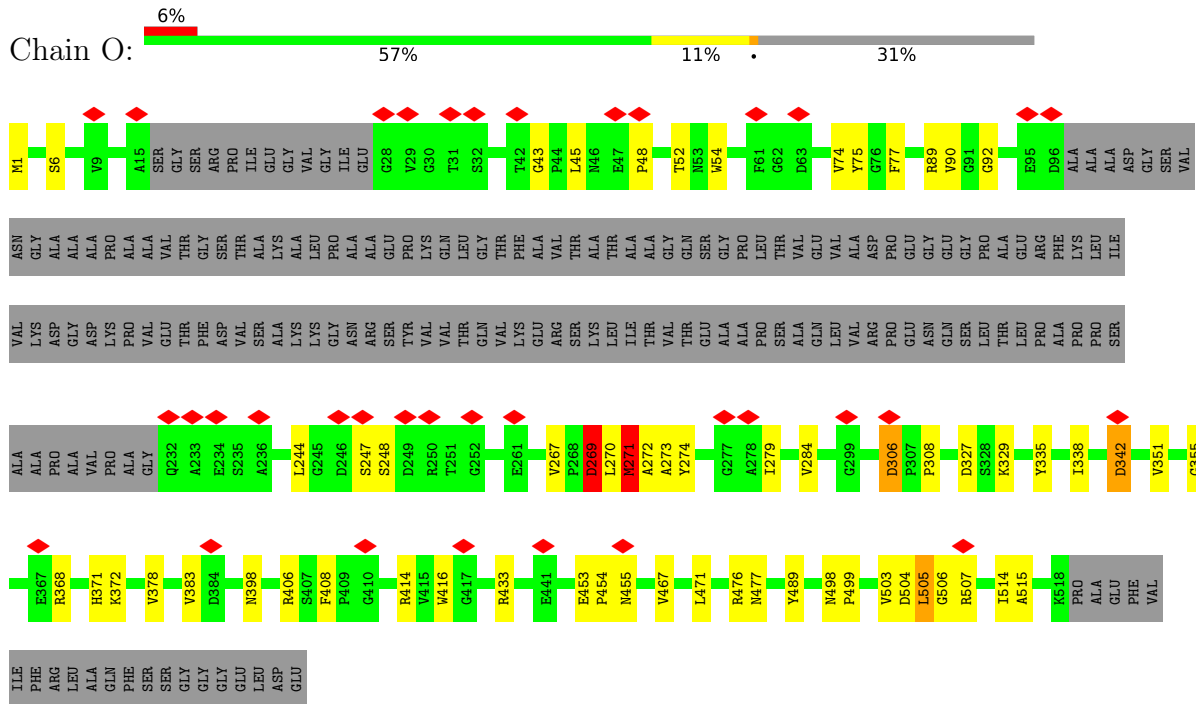
• Molecule 1: Phage tail sheath family protein



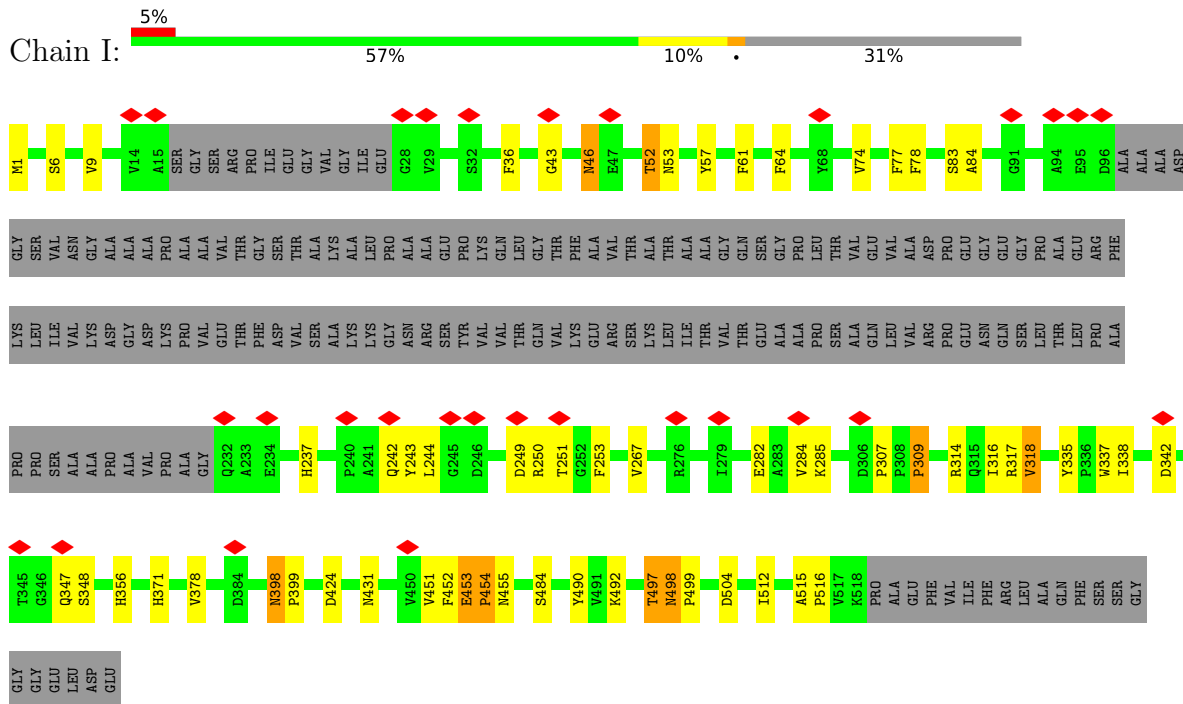
• Molecule 1: Phage tail sheath family protein



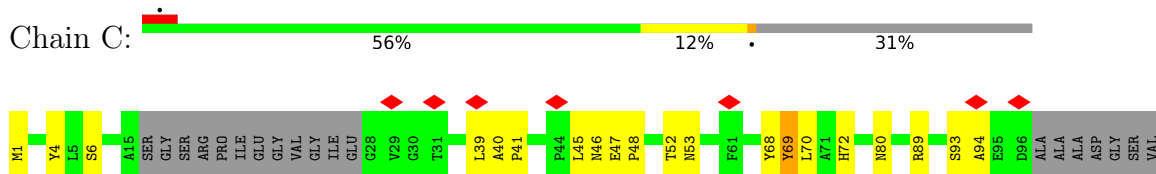
• Molecule 1: Phage tail sheath family protein

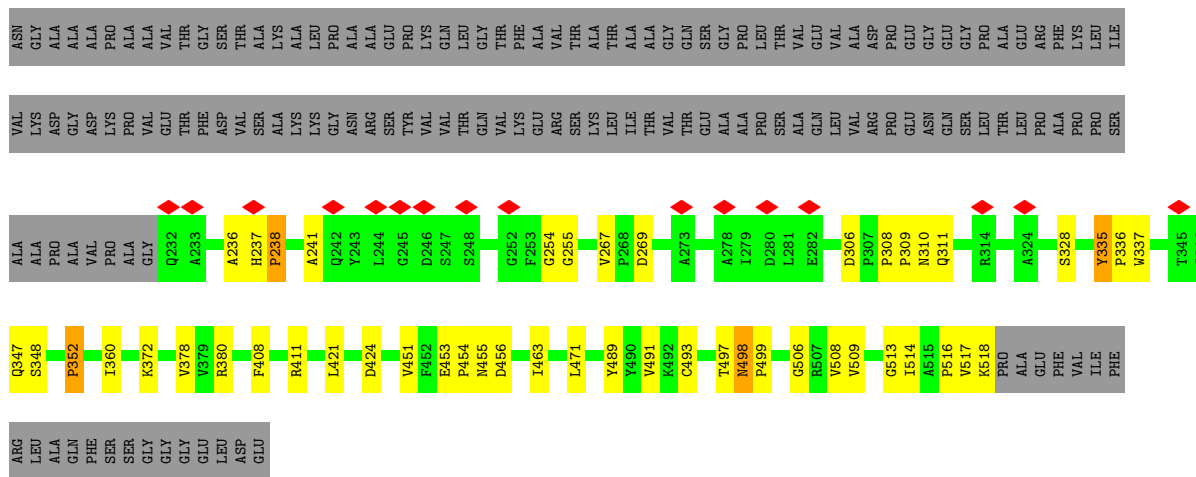


• Molecule 1: Phage tail sheath family protein

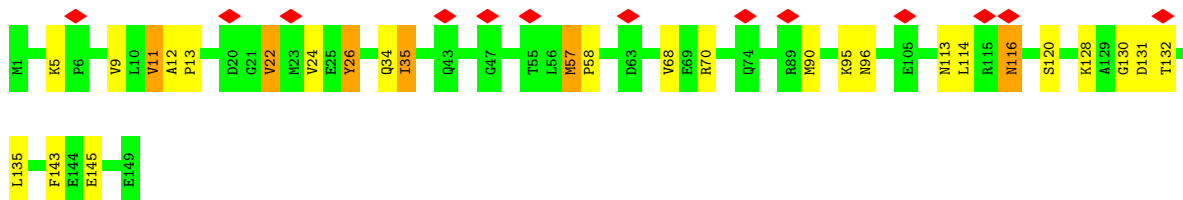
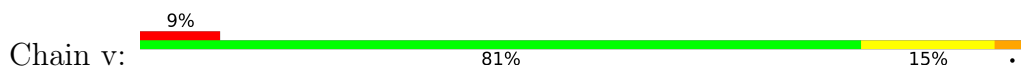


• Molecule 1: Phage tail sheath family protein

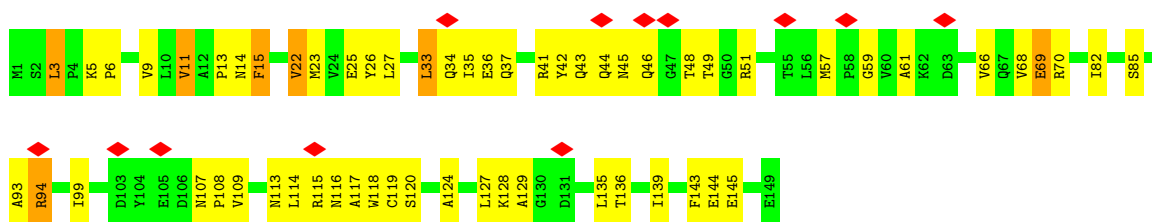




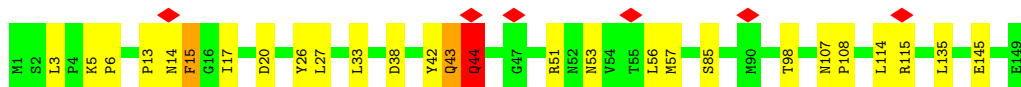
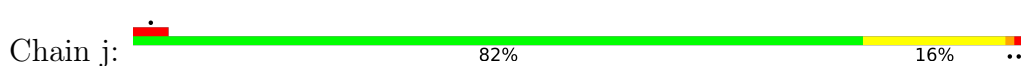
• Molecule 2: Phage tail protein



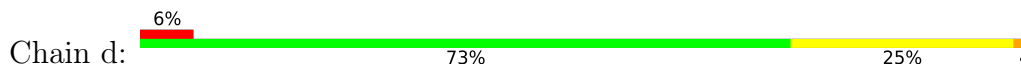
• Molecule 2: Phage tail protein

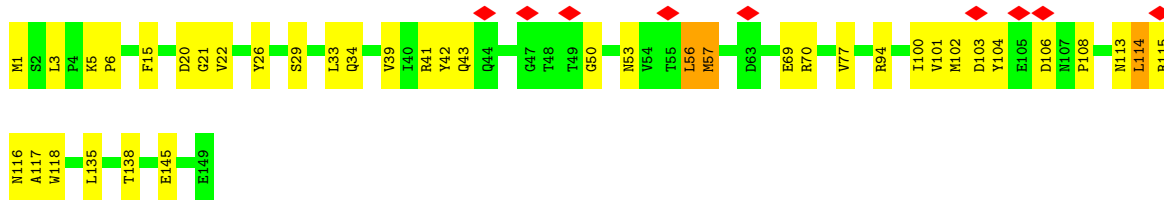


• Molecule 2: Phage tail protein

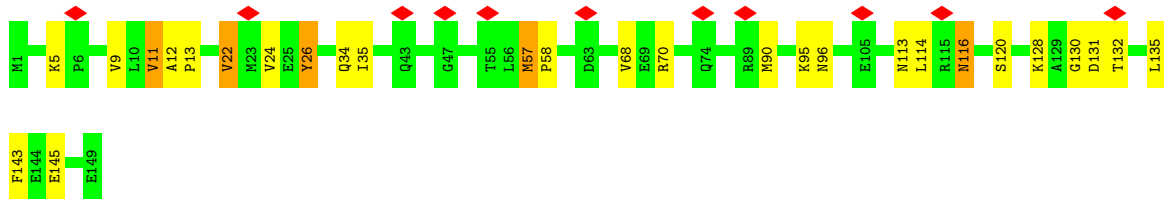
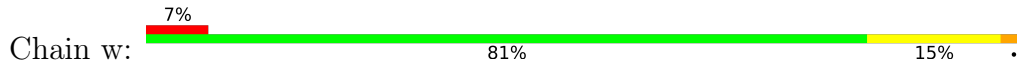


• Molecule 2: Phage tail protein

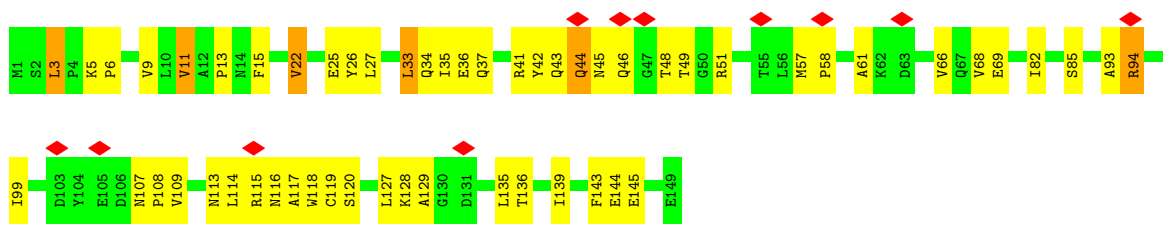




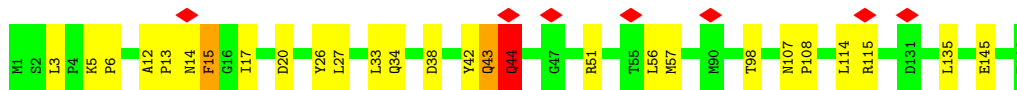
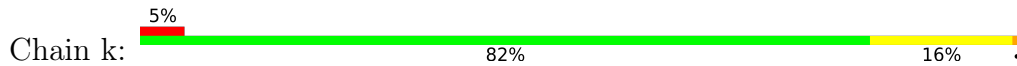
• Molecule 2: Phage tail protein



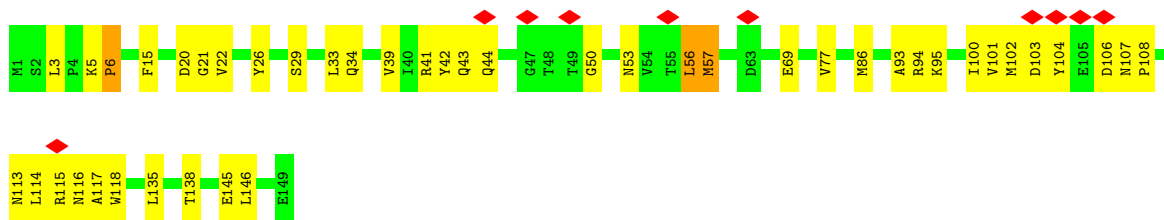
• Molecule 2: Phage tail protein



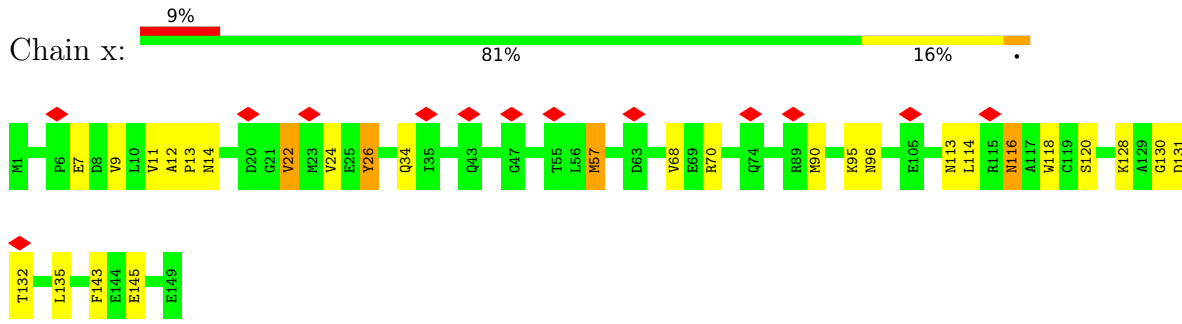
• Molecule 2: Phage tail protein



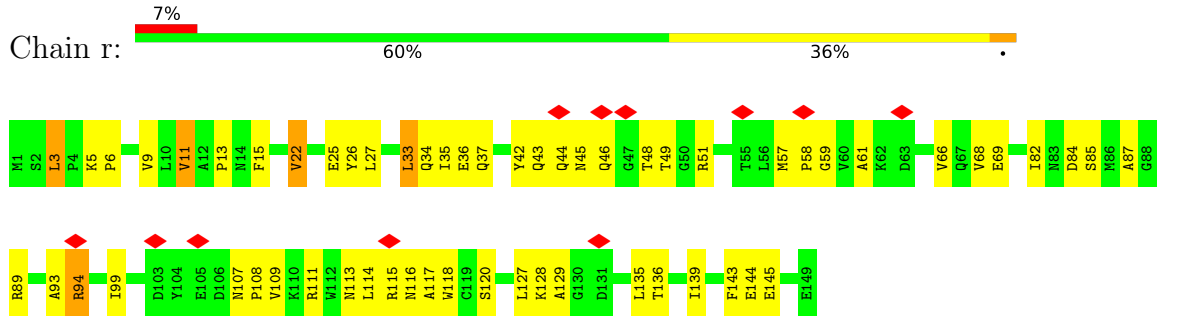
• Molecule 2: Phage tail protein



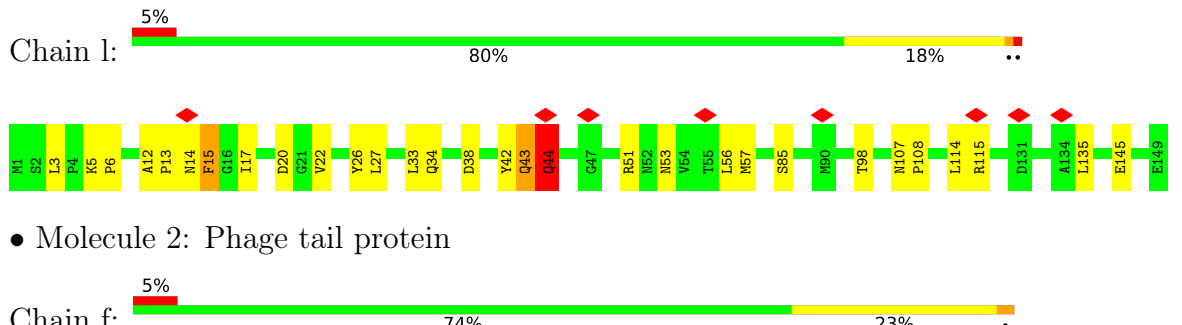
• Molecule 2: Phage tail protein



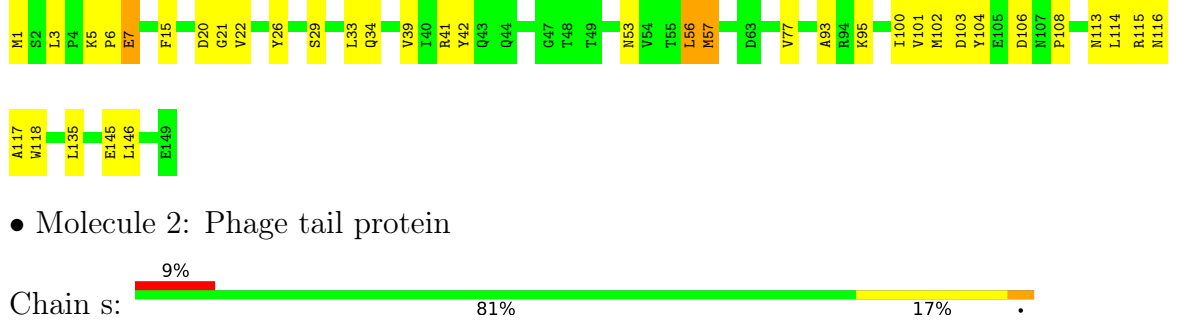
• Molecule 2: Phage tail protein



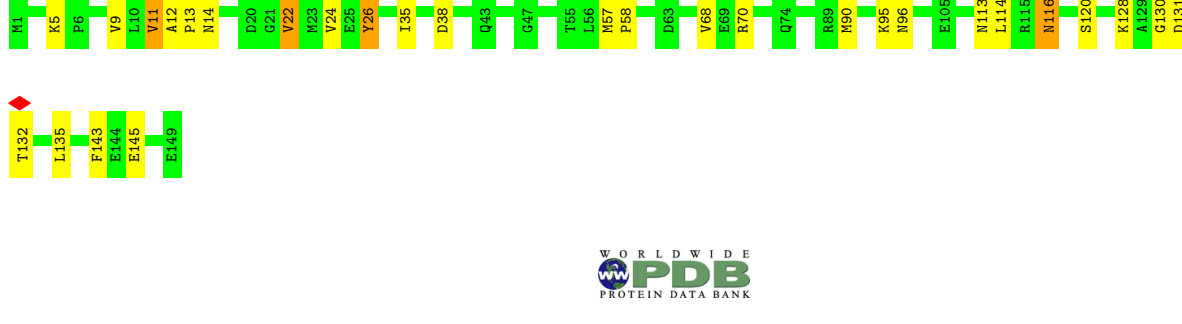
• Molecule 2: Phage tail protein



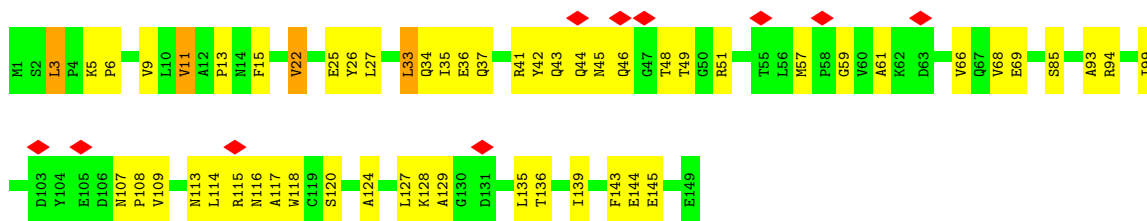
• Molecule 2: Phage tail protein



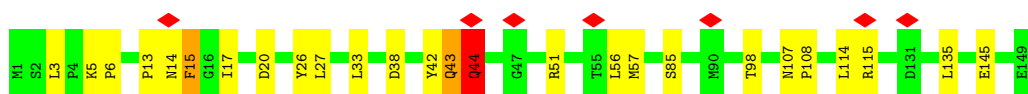
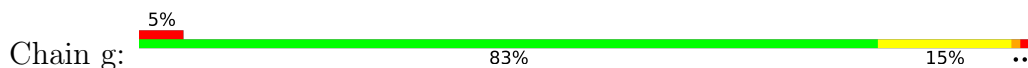
• Molecule 2: Phage tail protein



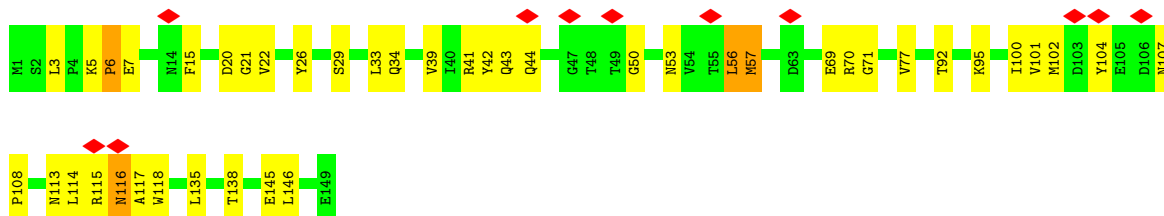
• Molecule 2: Phage tail protein



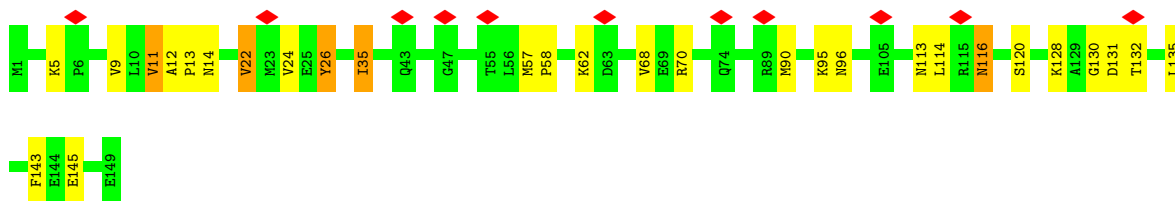
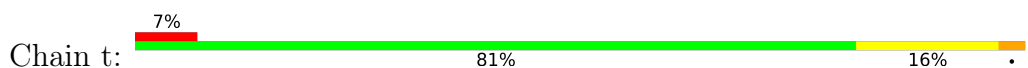
• Molecule 2: Phage tail protein



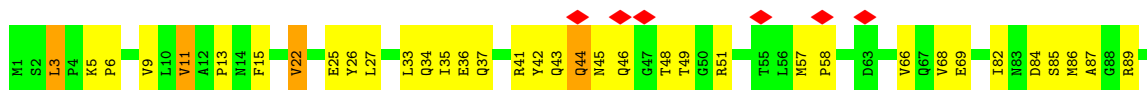
• Molecule 2: Phage tail protein

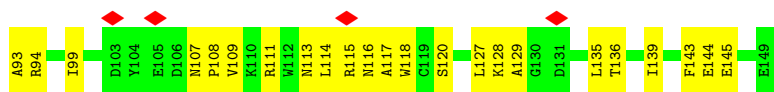


• Molecule 2: Phage tail protein

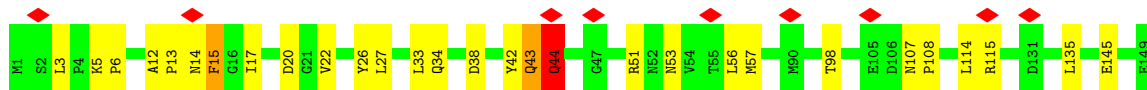
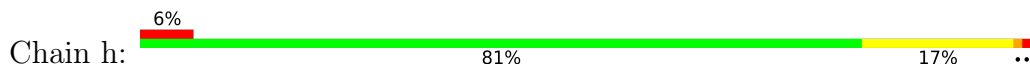


• Molecule 2: Phage tail protein

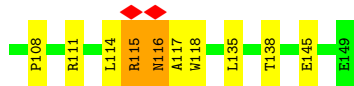
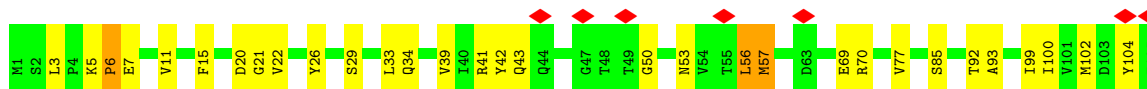




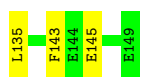
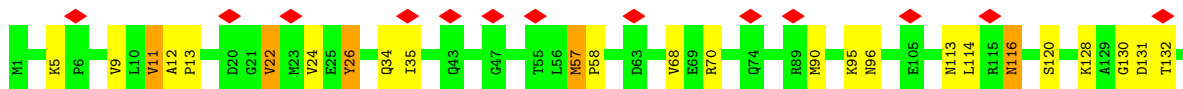
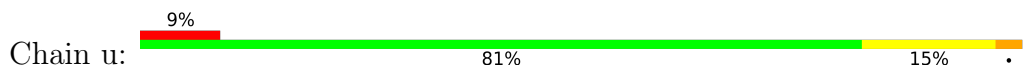
• Molecule 2: Phage tail protein



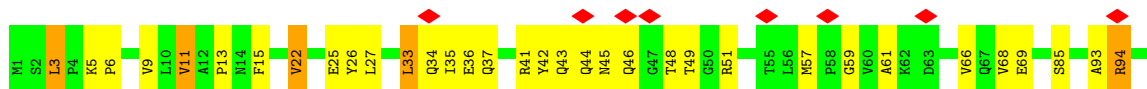
• Molecule 2: Phage tail protein



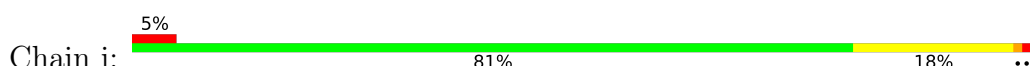
• Molecule 2: Phage tail protein

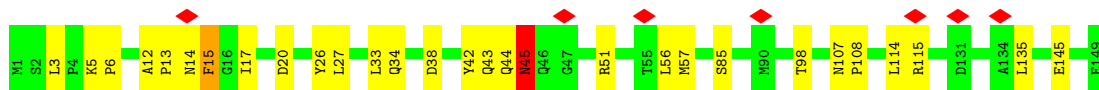


• Molecule 2: Phage tail protein

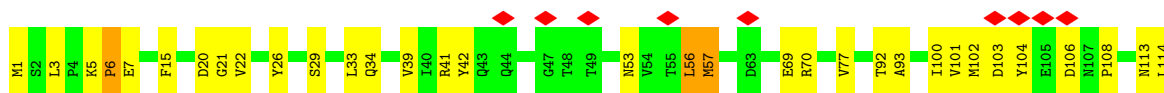
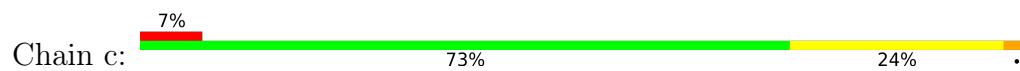


• Molecule 2: Phage tail protein





- Molecule 2: Phage tail protein



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=23.10°, rise=38.50 Å, axial sym=C6	Depositor
Number of segments used	18822	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 ($e^-/\text{Å}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.183	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	448.0, 448.0, 448.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.01	1/2942 (0.0%)	1.34	32/4014 (0.8%)
1	B	1.01	1/2942 (0.0%)	1.34	32/4014 (0.8%)
1	C	1.01	1/2942 (0.0%)	1.34	31/4014 (0.8%)
1	D	1.02	1/2942 (0.0%)	1.34	33/4014 (0.8%)
1	E	1.02	1/2942 (0.0%)	1.34	30/4014 (0.7%)
1	F	1.02	1/2942 (0.0%)	1.34	31/4014 (0.8%)
1	G	0.99	0/2942	1.36	39/4014 (1.0%)
1	H	0.99	0/2942	1.36	37/4014 (0.9%)
1	I	0.99	0/2942	1.37	38/4014 (0.9%)
1	J	0.99	0/2942	1.37	38/4014 (0.9%)
1	K	0.99	0/2942	1.37	37/4014 (0.9%)
1	L	0.99	0/2942	1.37	38/4014 (0.9%)
1	M	1.01	2/2942 (0.1%)	1.30	31/4014 (0.8%)
1	N	1.02	2/2942 (0.1%)	1.29	30/4014 (0.7%)
1	O	1.02	2/2942 (0.1%)	1.30	30/4014 (0.7%)
1	P	1.01	1/2942 (0.0%)	1.30	30/4014 (0.7%)
1	Q	1.02	2/2942 (0.1%)	1.30	30/4014 (0.7%)
1	R	1.01	2/2942 (0.1%)	1.29	30/4014 (0.7%)
1	S	0.98	0/2942	1.36	39/4014 (1.0%)
1	T	0.99	1/2942 (0.0%)	1.39	43/4014 (1.1%)
1	U	0.99	0/2942	1.39	42/4014 (1.0%)
1	V	0.99	0/2942	1.39	43/4014 (1.1%)
1	W	0.98	0/2942	1.39	43/4014 (1.1%)
1	X	0.98	0/2942	1.39	42/4014 (1.0%)
2	a	1.04	0/1168	1.48	22/1586 (1.4%)
2	b	1.05	0/1168	1.46	20/1586 (1.3%)
2	c	1.04	0/1168	1.45	20/1586 (1.3%)
2	d	1.08	0/1168	1.45	19/1586 (1.2%)
2	e	1.04	0/1168	1.48	22/1586 (1.4%)
2	f	1.05	0/1168	1.44	19/1586 (1.2%)
2	g	1.03	0/1168	1.45	17/1586 (1.1%)
2	h	1.03	0/1168	1.45	17/1586 (1.1%)
2	i	1.03	0/1168	1.44	16/1586 (1.0%)
2	j	1.03	0/1168	1.45	17/1586 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	k	1.03	0/1168	1.45	17/1586 (1.1%)
2	l	1.03	0/1168	1.45	16/1586 (1.0%)
2	m	0.98	0/1168	1.43	14/1586 (0.9%)
2	n	0.98	0/1168	1.43	14/1586 (0.9%)
2	o	0.99	0/1168	1.43	14/1586 (0.9%)
2	p	0.99	0/1168	1.43	14/1586 (0.9%)
2	q	0.99	0/1168	1.43	14/1586 (0.9%)
2	r	0.98	0/1168	1.43	14/1586 (0.9%)
2	s	0.98	0/1168	1.45	11/1586 (0.7%)
2	t	0.98	0/1168	1.45	12/1586 (0.8%)
2	u	0.98	0/1168	1.44	11/1586 (0.7%)
2	v	0.98	0/1168	1.44	12/1586 (0.8%)
2	w	0.98	0/1168	1.44	11/1586 (0.7%)
2	x	0.98	0/1168	1.45	11/1586 (0.7%)
All	All	1.00	18/98640 (0.0%)	1.38	1223/134400 (0.9%)

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	80	ASN	N-CA	5.96	1.50	1.46
1	Q	269	ASP	C-O	5.86	1.31	1.24
1	M	269	ASP	C-O	5.64	1.31	1.24
1	N	269	ASP	C-O	5.60	1.31	1.24
1	R	269	ASP	C-O	5.26	1.30	1.24

The worst 5 of 1223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	498	ASN	CA-C-N	9.73	126.76	119.66
1	C	498	ASN	C-N-CA	9.73	126.76	119.66
1	F	498	ASN	CA-C-N	9.70	126.74	119.66
1	F	498	ASN	C-N-CA	9.70	126.74	119.66
1	E	498	ASN	CA-C-N	9.70	126.74	119.66

There are no chirality outliers.

There are no planarity outliers.

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	2867	0	2761	46	0
1	B	2867	0	2761	63	0
1	C	2867	0	2761	47	0
1	D	2867	0	2761	45	0
1	E	2867	0	2761	49	0
1	F	2867	0	2761	47	0
1	G	2867	0	2761	59	0
1	H	2867	0	2761	49	0
1	I	2867	0	2761	47	0
1	J	2867	0	2761	48	0
1	K	2867	0	2761	54	0
1	L	2867	0	2761	53	0
1	M	2867	0	2761	46	0
1	N	2867	0	2761	41	0
1	O	2867	0	2761	41	0
1	P	2867	0	2761	37	0
1	Q	2867	0	2761	53	0
1	R	2867	0	2761	49	0
1	S	2867	0	2761	83	0
1	T	2867	0	2761	60	0
1	U	2867	0	2761	65	0
1	V	2867	0	2761	72	0
1	W	2867	0	2761	64	0
1	X	2867	0	2761	61	0
2	a	1152	0	1150	55	0
2	b	1152	0	1149	57	0
2	c	1152	0	1149	32	0
2	d	1152	0	1149	41	0
2	e	1152	0	1149	49	0
2	f	1152	0	1149	36	0
2	g	1152	0	1150	33	0
2	h	1152	0	1150	52	0
2	i	1152	0	1146	64	0
2	j	1152	0	1150	34	0
2	k	1152	0	1150	40	0
2	l	1152	0	1150	52	0
2	m	1152	0	1150	94	0
2	n	1152	0	1150	78	0
2	o	1152	0	1150	99	0
2	p	1152	0	1150	120	0
2	q	1152	0	1150	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	r	1152	0	1150	100	0
2	s	1152	0	1150	35	0
2	t	1152	0	1150	31	0
2	u	1152	0	1150	30	0
2	v	1152	0	1150	31	0
2	w	1152	0	1150	34	0
2	x	1152	0	1150	32	0
All	All	96456	0	93855	2060	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 11.

The worst 5 of 2060 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:W:452:PHE:CZ	1:W:507:ARG:HD3	1.32	1.63
1:U:452:PHE:CZ	1:U:507:ARG:HD3	1.31	1.62
1:T:452:PHE:CZ	1:T:507:ARG:HD3	1.33	1.60
1:X:452:PHE:CZ	1:X:507:ARG:HD3	1.34	1.60
1:S:452:PHE:CZ	1:S:507:ARG:HD3	1.31	1.57

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	365/539 (68%)	343 (94%)	20 (6%)	2 (0%)	24 59
1	B	365/539 (68%)	341 (93%)	21 (6%)	3 (1%)	16 50
1	C	365/539 (68%)	344 (94%)	19 (5%)	2 (0%)	24 59
1	D	365/539 (68%)	343 (94%)	20 (6%)	2 (0%)	24 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	365/539 (68%)	345 (94%)	20 (6%)	0	100	100
1	F	365/539 (68%)	344 (94%)	19 (5%)	2 (0%)	24	59
1	G	365/539 (68%)	339 (93%)	23 (6%)	3 (1%)	16	50
1	H	365/539 (68%)	335 (92%)	26 (7%)	4 (1%)	11	43
1	I	365/539 (68%)	340 (93%)	22 (6%)	3 (1%)	16	50
1	J	365/539 (68%)	340 (93%)	22 (6%)	3 (1%)	16	50
1	K	365/539 (68%)	341 (93%)	21 (6%)	3 (1%)	16	50
1	L	365/539 (68%)	339 (93%)	23 (6%)	3 (1%)	16	50
1	M	365/539 (68%)	339 (93%)	22 (6%)	4 (1%)	11	43
1	N	365/539 (68%)	342 (94%)	19 (5%)	4 (1%)	11	43
1	O	365/539 (68%)	339 (93%)	22 (6%)	4 (1%)	11	43
1	P	365/539 (68%)	339 (93%)	22 (6%)	4 (1%)	11	43
1	Q	365/539 (68%)	340 (93%)	21 (6%)	4 (1%)	11	43
1	R	365/539 (68%)	342 (94%)	20 (6%)	3 (1%)	16	50
1	S	365/539 (68%)	328 (90%)	35 (10%)	2 (0%)	24	59
1	T	365/539 (68%)	331 (91%)	29 (8%)	5 (1%)	9	38
1	U	365/539 (68%)	331 (91%)	27 (7%)	7 (2%)	6	33
1	V	365/539 (68%)	331 (91%)	29 (8%)	5 (1%)	9	38
1	W	365/539 (68%)	331 (91%)	28 (8%)	6 (2%)	7	36
1	X	365/539 (68%)	331 (91%)	29 (8%)	5 (1%)	9	38
2	a	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	18	53
2	b	147/149 (99%)	133 (90%)	13 (9%)	1 (1%)	18	53
2	c	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	18	53
2	d	147/149 (99%)	134 (91%)	12 (8%)	1 (1%)	18	53
2	e	147/149 (99%)	135 (92%)	12 (8%)	0	100	100
2	f	147/149 (99%)	135 (92%)	12 (8%)	0	100	100
2	g	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	18	53
2	h	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	18	53
2	i	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	18	53
2	j	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	18	53
2	k	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	18	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	l	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	18	53
2	m	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	18	53
2	n	147/149 (99%)	138 (94%)	7 (5%)	2 (1%)	9	38
2	o	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	18	53
2	p	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	18	53
2	q	147/149 (99%)	138 (94%)	7 (5%)	2 (1%)	9	38
2	r	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	18	53
2	s	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
2	t	147/149 (99%)	142 (97%)	5 (3%)	0	100	100
2	u	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
2	v	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
2	w	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
2	x	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
All	All	12288/16512 (74%)	11462 (93%)	725 (6%)	101 (1%)	18	50

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	4	TYR
1	P	515	ALA
2	p	45	ASN
1	J	453	GLU
2	j	44	GLN

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	A	295/417 (71%)	295 (100%)	0	100	100
1	B	295/417 (71%)	294 (100%)	1 (0%)	86	85
1	C	295/417 (71%)	295 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	295/417 (71%)	295 (100%)	0	100	100
1	E	295/417 (71%)	294 (100%)	1 (0%)	86	85
1	F	295/417 (71%)	295 (100%)	0	100	100
1	G	295/417 (71%)	295 (100%)	0	100	100
1	H	295/417 (71%)	294 (100%)	1 (0%)	86	85
1	I	295/417 (71%)	295 (100%)	0	100	100
1	J	295/417 (71%)	295 (100%)	0	100	100
1	K	295/417 (71%)	295 (100%)	0	100	100
1	L	295/417 (71%)	295 (100%)	0	100	100
1	M	295/417 (71%)	291 (99%)	4 (1%)	59	71
1	N	295/417 (71%)	291 (99%)	4 (1%)	59	71
1	O	295/417 (71%)	292 (99%)	3 (1%)	68	75
1	P	295/417 (71%)	290 (98%)	5 (2%)	53	68
1	Q	295/417 (71%)	291 (99%)	4 (1%)	59	71
1	R	295/417 (71%)	291 (99%)	4 (1%)	59	71
1	S	295/417 (71%)	292 (99%)	3 (1%)	68	75
1	T	295/417 (71%)	293 (99%)	2 (1%)	76	78
1	U	295/417 (71%)	293 (99%)	2 (1%)	76	78
1	V	295/417 (71%)	293 (99%)	2 (1%)	76	78
1	W	295/417 (71%)	293 (99%)	2 (1%)	76	78
1	X	295/417 (71%)	293 (99%)	2 (1%)	76	78
2	a	129/129 (100%)	129 (100%)	0	100	100
2	b	129/129 (100%)	128 (99%)	1 (1%)	73	77
2	c	129/129 (100%)	129 (100%)	0	100	100
2	d	129/129 (100%)	129 (100%)	0	100	100
2	e	129/129 (100%)	129 (100%)	0	100	100
2	f	129/129 (100%)	128 (99%)	1 (1%)	73	77
2	g	129/129 (100%)	129 (100%)	0	100	100
2	h	129/129 (100%)	129 (100%)	0	100	100
2	i	129/129 (100%)	129 (100%)	0	100	100
2	j	129/129 (100%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	k	129/129 (100%)	129 (100%)	0	100	100
2	l	129/129 (100%)	129 (100%)	0	100	100
2	m	129/129 (100%)	129 (100%)	0	100	100
2	n	129/129 (100%)	129 (100%)	0	100	100
2	o	129/129 (100%)	128 (99%)	1 (1%)	73	77
2	p	129/129 (100%)	128 (99%)	1 (1%)	73	77
2	q	129/129 (100%)	128 (99%)	1 (1%)	73	77
2	r	129/129 (100%)	128 (99%)	1 (1%)	73	77
2	s	129/129 (100%)	129 (100%)	0	100	100
2	t	129/129 (100%)	129 (100%)	0	100	100
2	u	129/129 (100%)	129 (100%)	0	100	100
2	v	129/129 (100%)	129 (100%)	0	100	100
2	w	129/129 (100%)	129 (100%)	0	100	100
2	x	129/129 (100%)	129 (100%)	0	100	100
All	All	10176/13104 (78%)	10130 (100%)	46 (0%)	78	82

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	271	MET
1	N	271	MET
1	M	471	LEU
1	T	475	TRP
1	H	370	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	311	GLN
2	o	34	GLN
2	c	116	ASN
1	R	371	HIS
1	R	311	GLN

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.

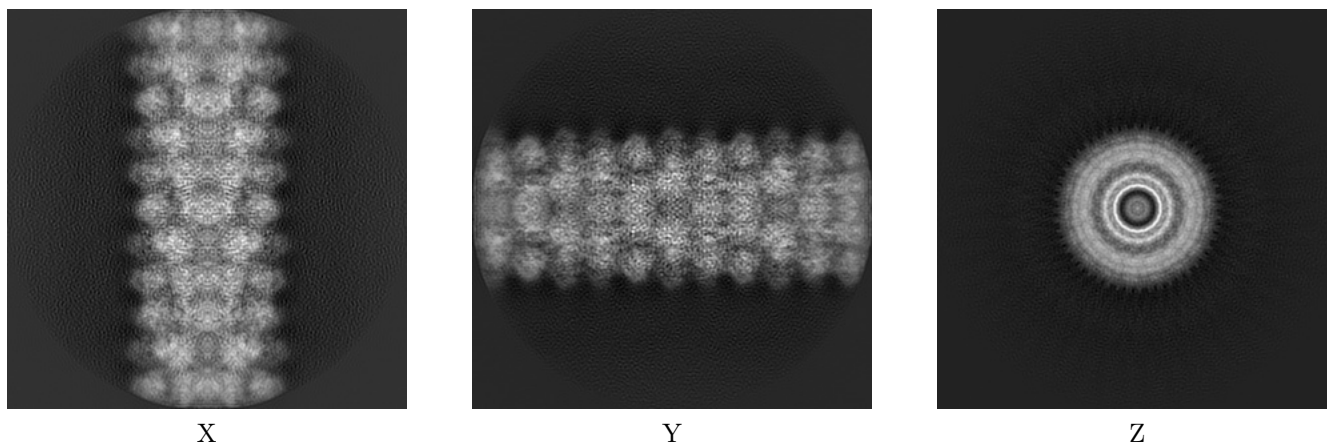
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16101. These allow visual inspection of the internal detail of the map and identification of artifacts.

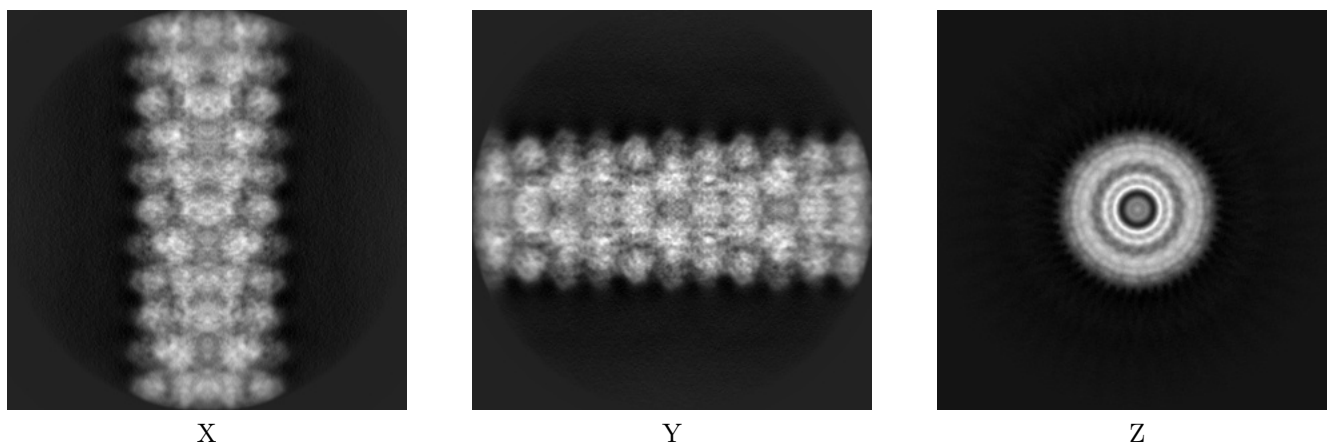
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



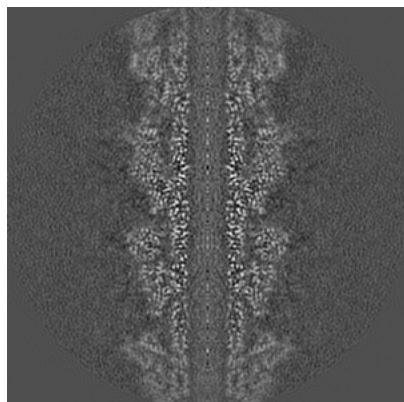
6.1.2 Raw map



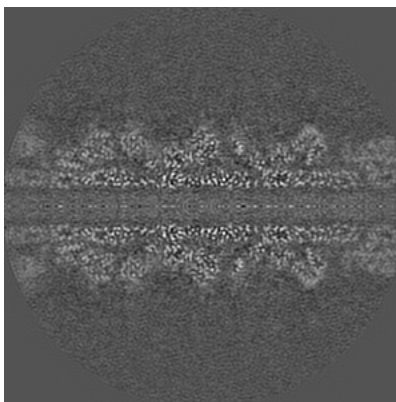
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

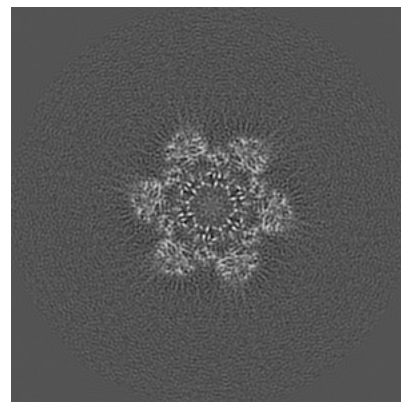
6.2.1 Primary map



X Index: 160

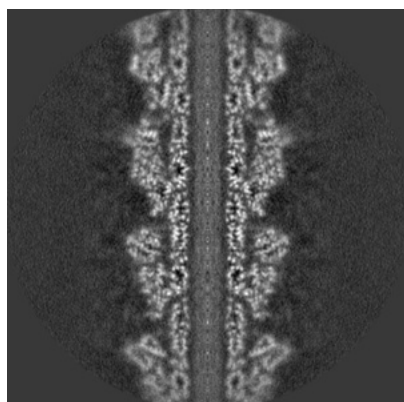


Y Index: 160

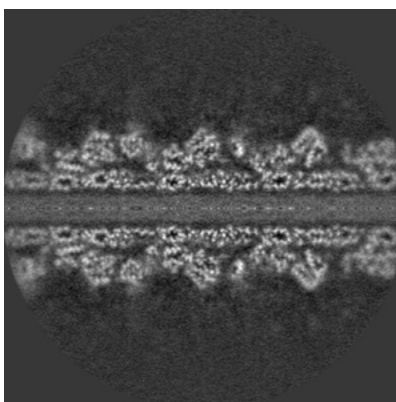


Z Index: 160

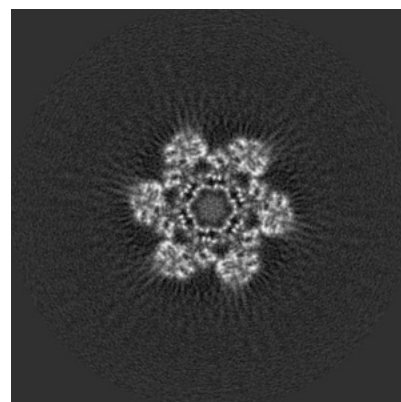
6.2.2 Raw map



X Index: 160



Y Index: 160

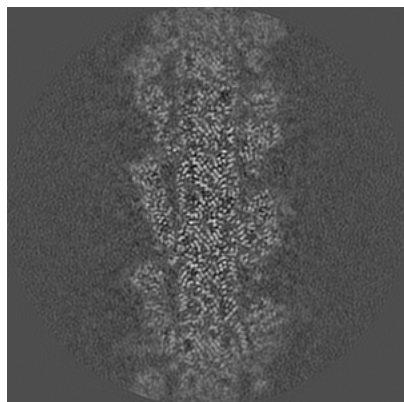


Z Index: 160

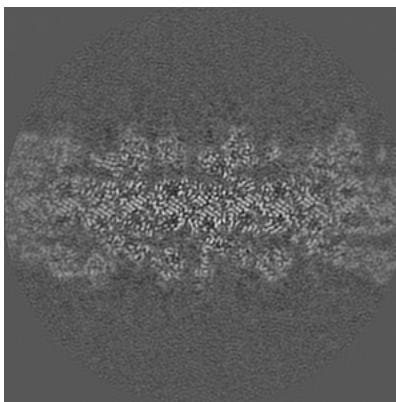
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

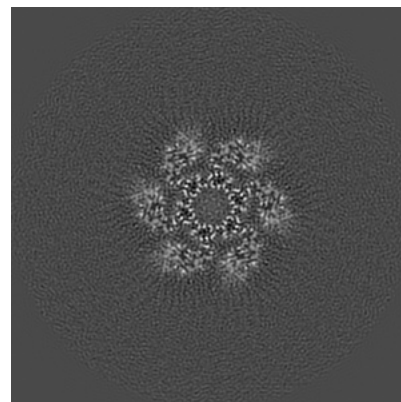
6.3.1 Primary map



X Index: 143

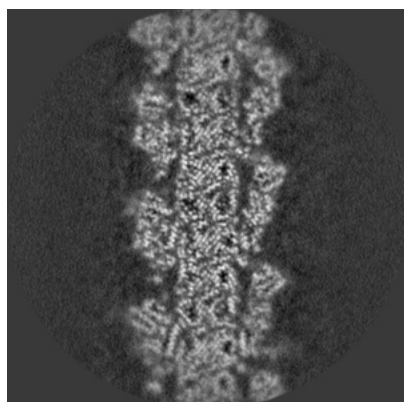


Y Index: 178

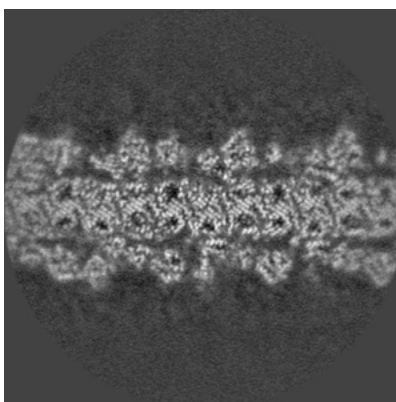


Z Index: 163

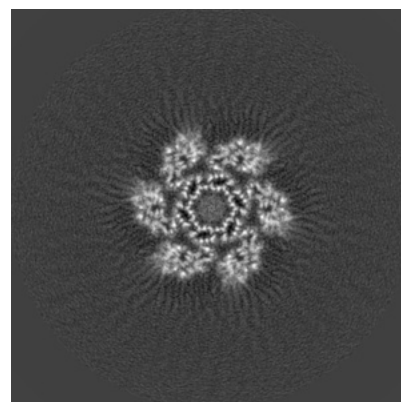
6.3.2 Raw map



X Index: 177



Y Index: 178

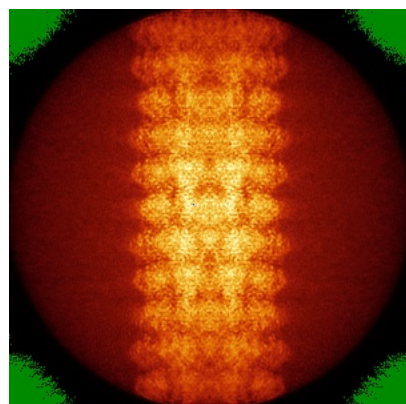


Z Index: 163

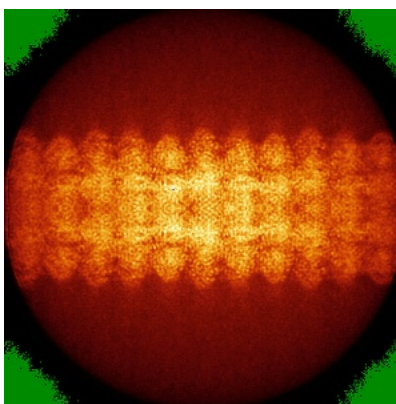
The images above show the largest variance slices of the map in three orthogonal directions.

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

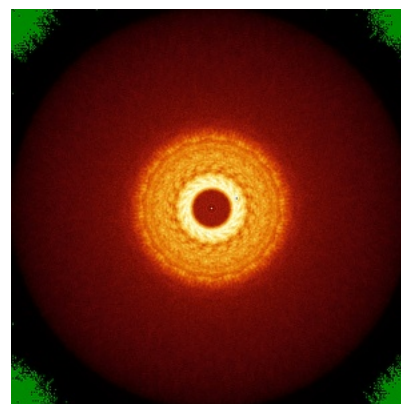
6.4.1 Primary map



X

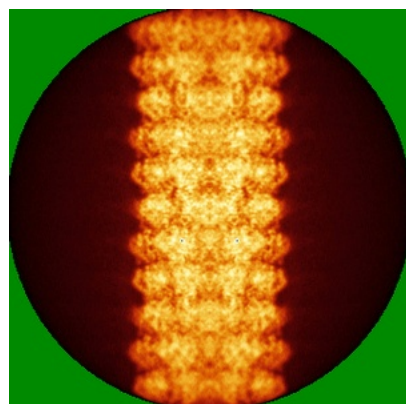


Y

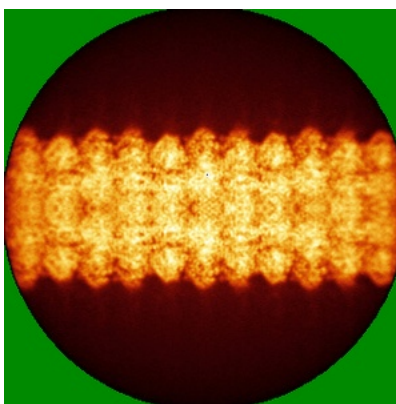


Z

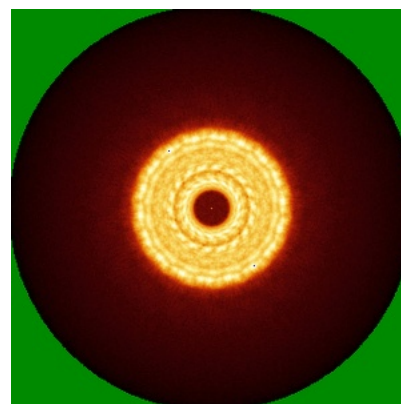
6.4.2 Raw map



X



Y

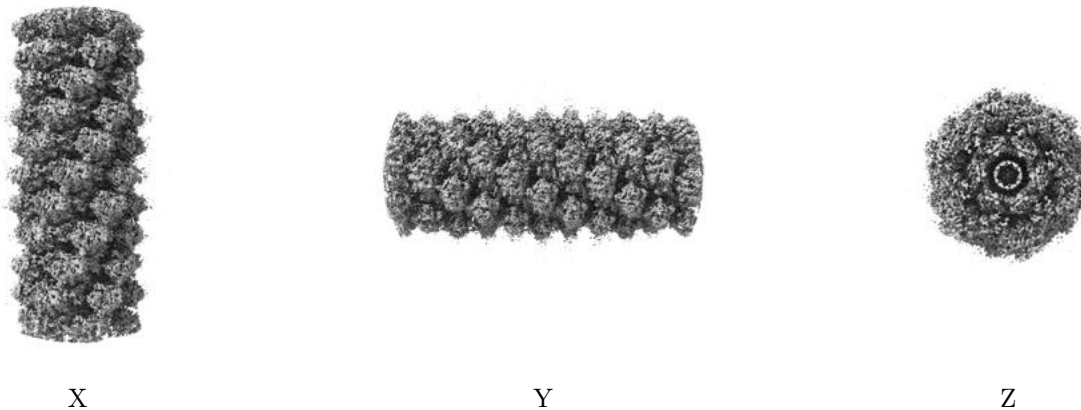


Z

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

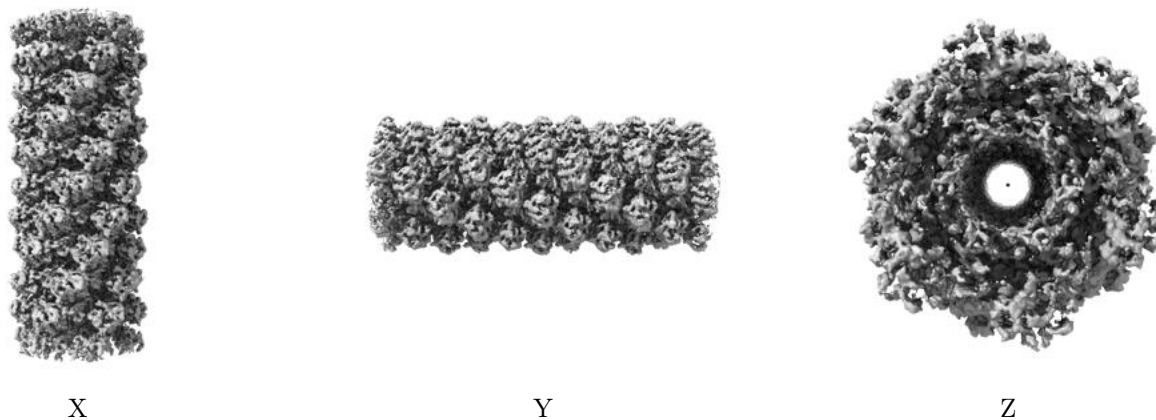
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

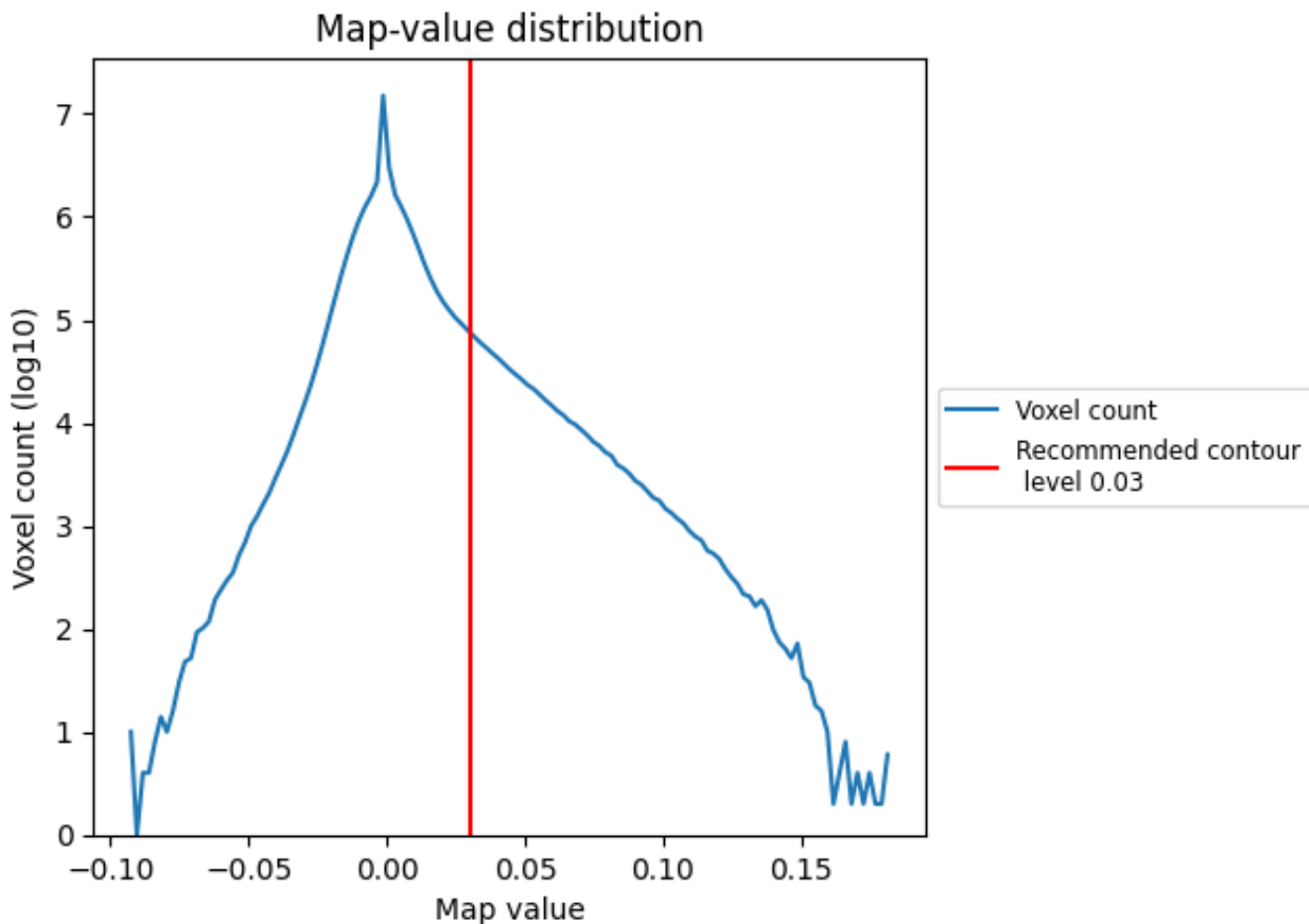
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

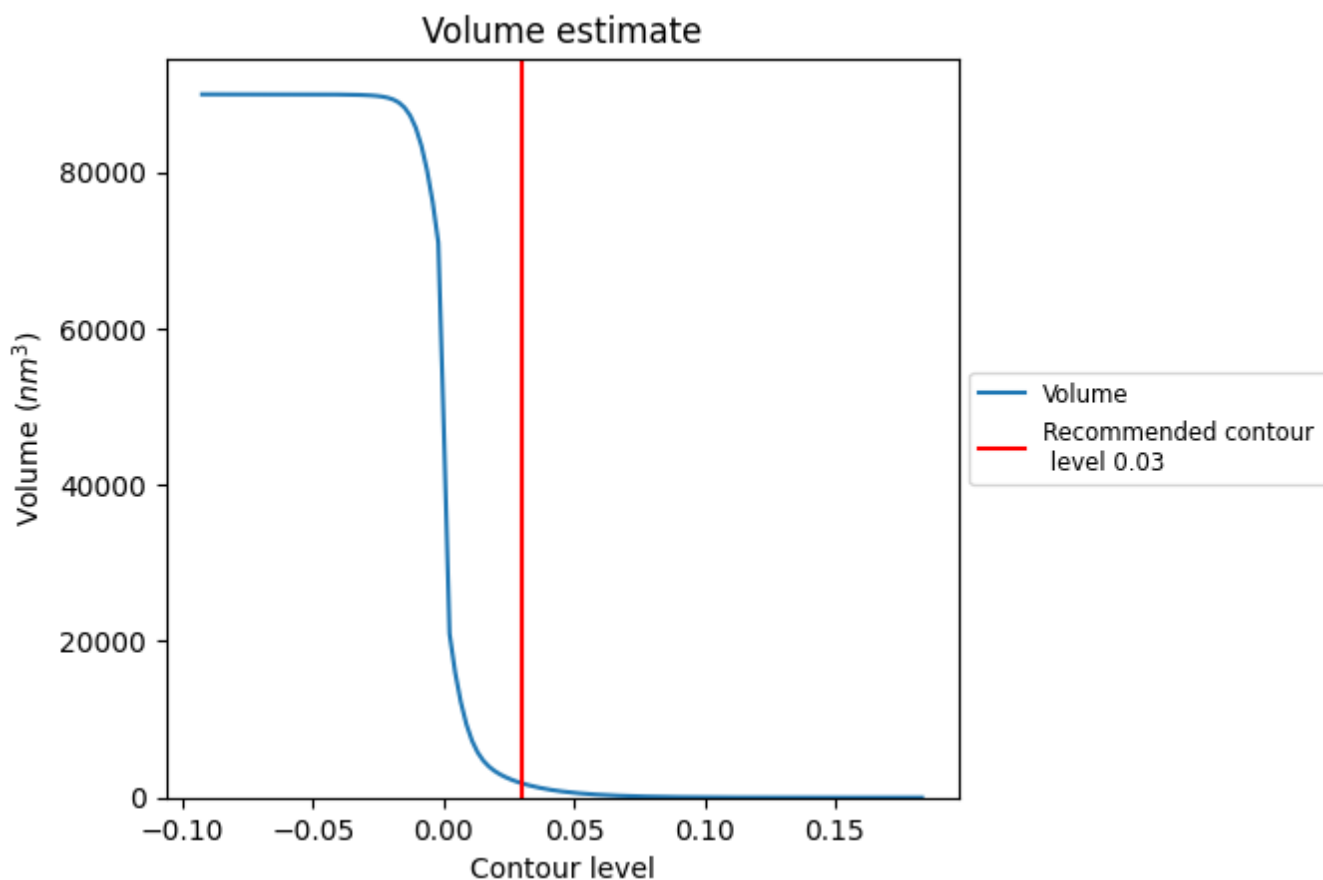
This section contains the results of statistical analysis of the map.

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.

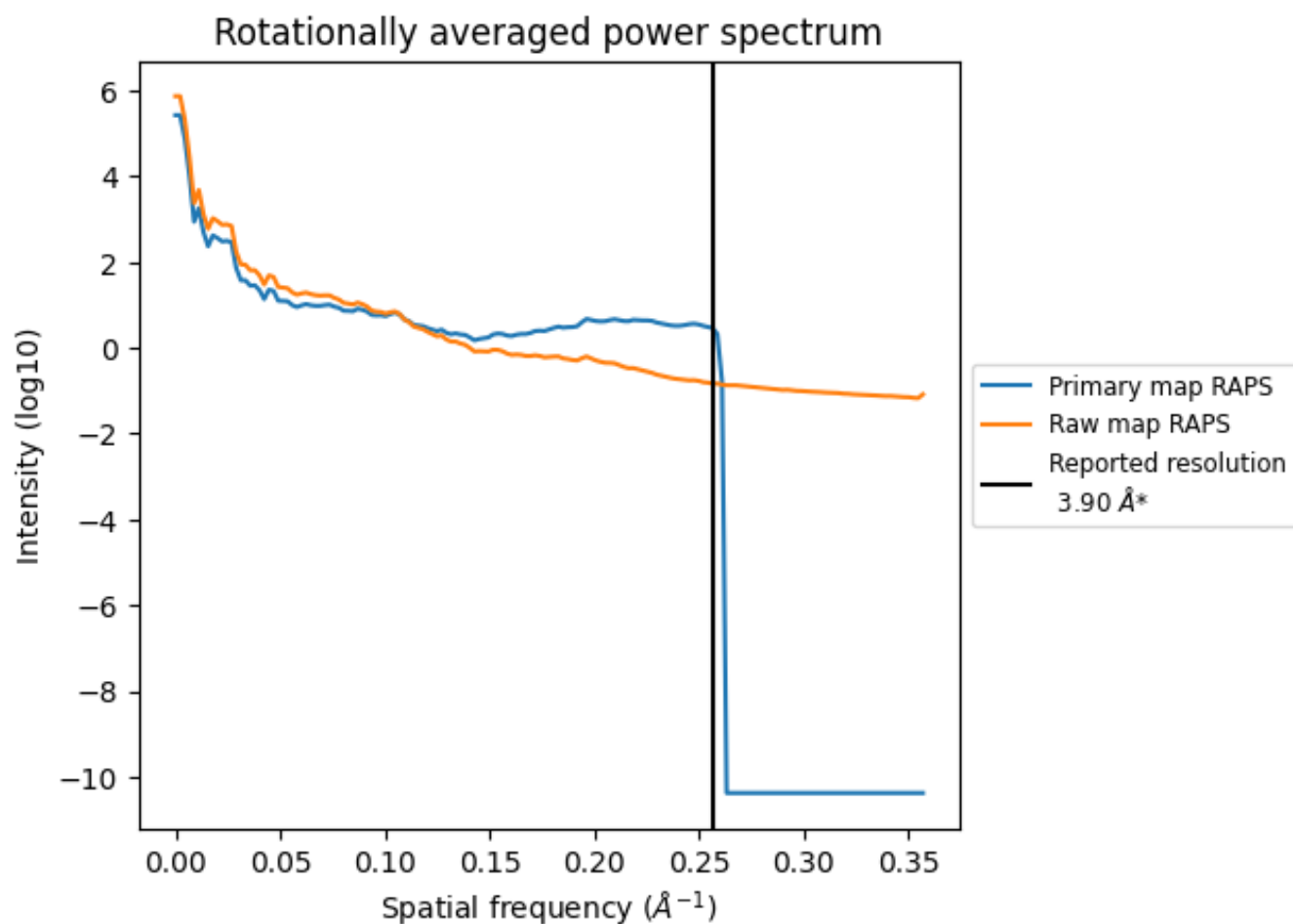
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1828 nm³; this corresponds to an approximate mass of 1651 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](#)

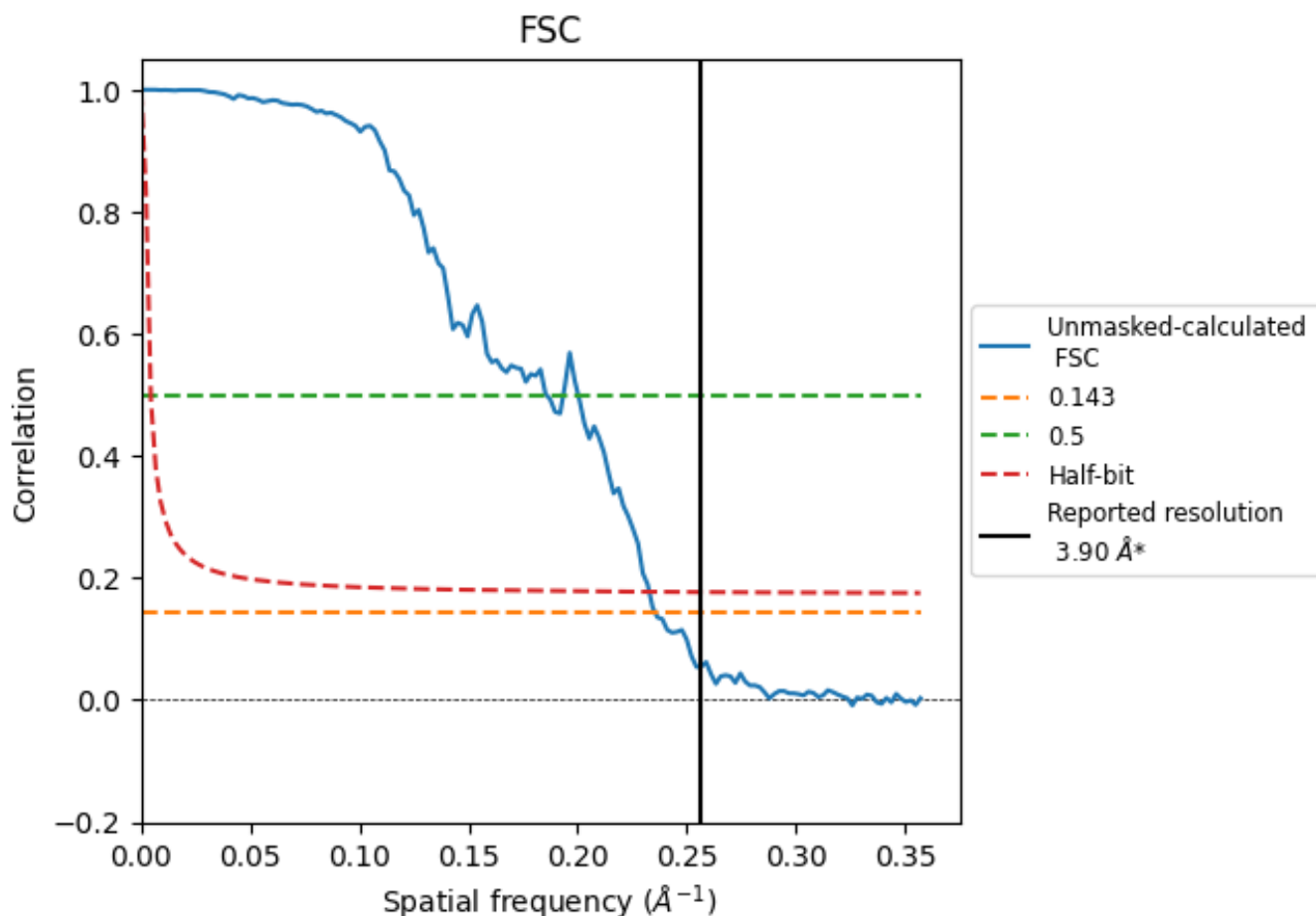


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

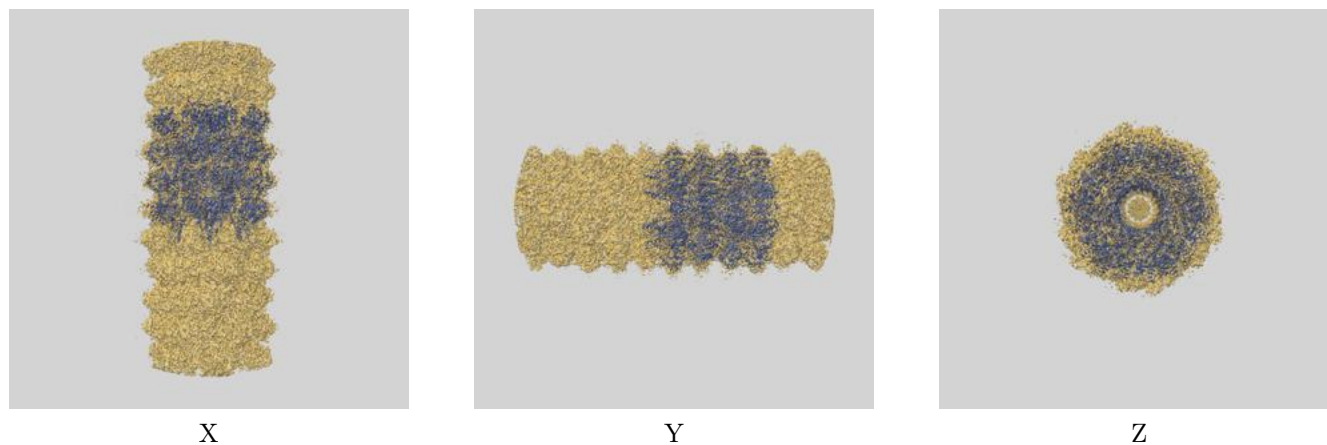
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	5.39	4.29

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

9 Map-model fit [i](#)

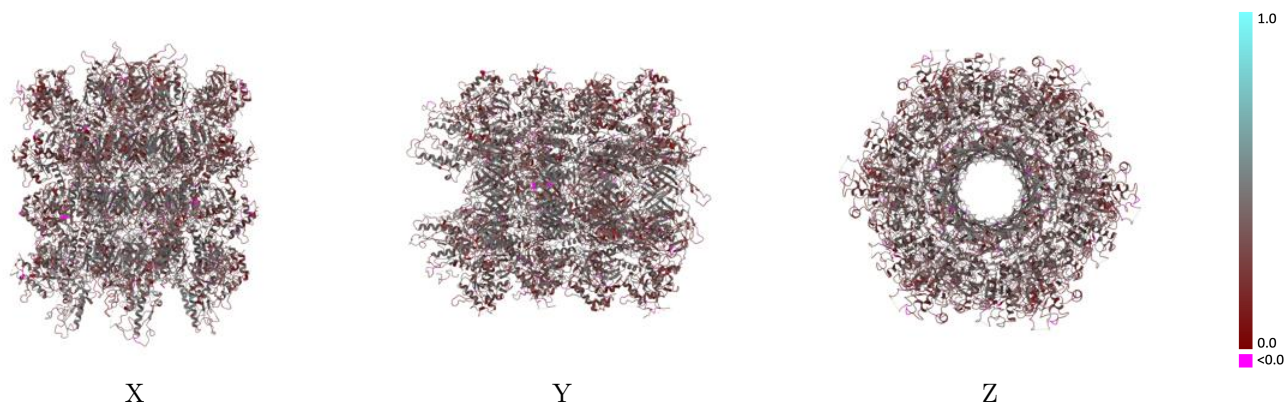
This section contains information regarding the fit between EMDB map EMD-16101 and PDB model 8BL4. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



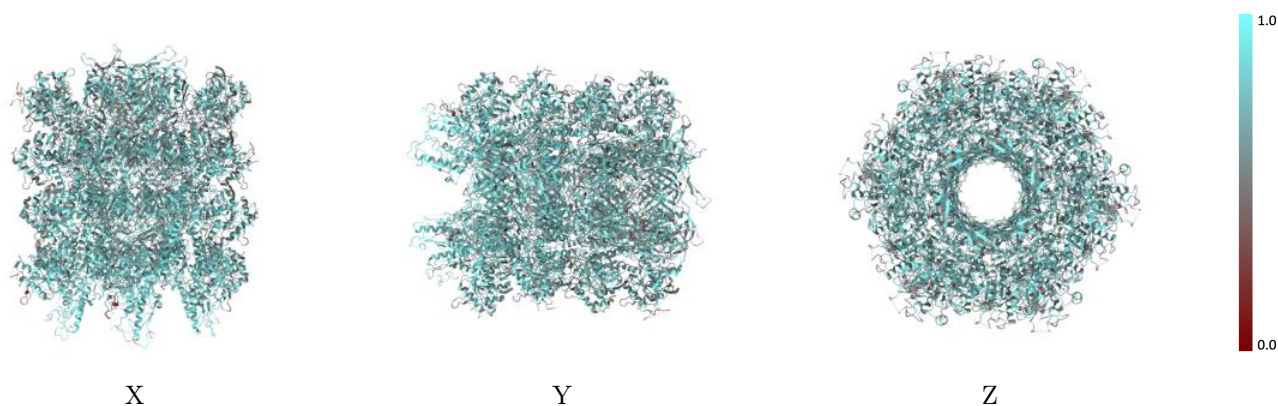
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



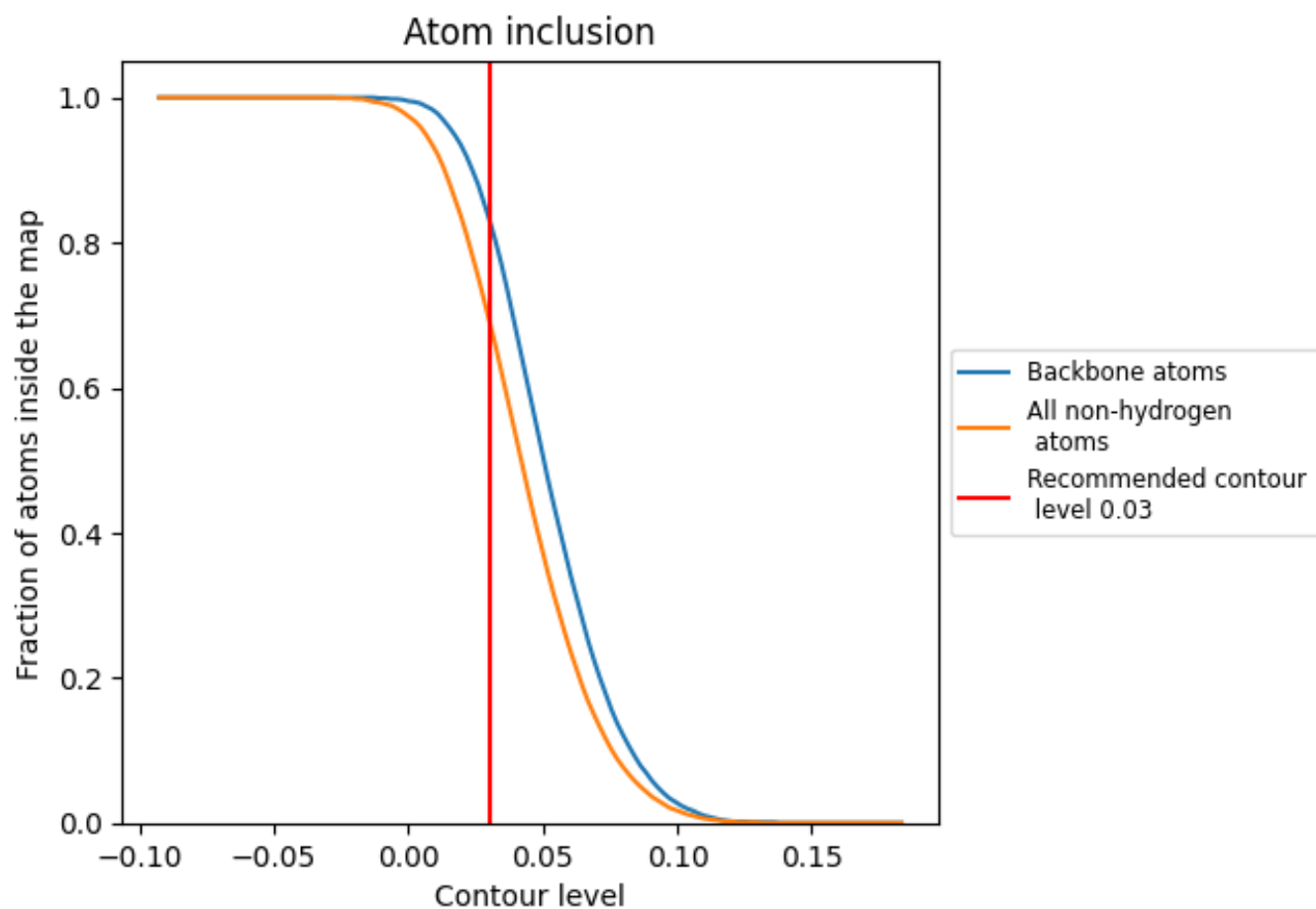
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





























The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6950	 0.3350
A	 0.7310	 0.3450
B	 0.7310	 0.3390
C	 0.7380	 0.3420
D	 0.7310	 0.3440
E	 0.7260	 0.3390
F	 0.7410	 0.3450
G	 0.7140	 0.3290
H	 0.7160	 0.3260
I	 0.7180	 0.3300
J	 0.7150	 0.3300
K	 0.7190	 0.3260
L	 0.7170	 0.3260
M	 0.6920	 0.3200
N	 0.6920	 0.3220
O	 0.6900	 0.3200
P	 0.6900	 0.3210
Q	 0.6910	 0.3230
R	 0.6920	 0.3230
S	 0.6460	 0.3050
T	 0.6550	 0.3090
U	 0.6530	 0.3110
V	 0.6500	 0.3120
W	 0.6490	 0.3120
X	 0.6510	 0.3110
a	 0.7240	 0.3750
b	 0.7130	 0.3710
c	 0.7210	 0.3730
d	 0.7300	 0.3750
e	 0.7270	 0.3740
f	 0.7300	 0.3730
g	 0.7090	 0.3600
h	 0.7100	 0.3630
i	 0.7220	 0.3640
j	 0.7100	 0.3620



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Chain	Atom inclusion	Q-score
k	 0.7150	 0.3640
l	 0.7140	 0.3620
m	 0.6650	 0.3540
n	 0.6690	 0.3550
o	 0.6620	 0.3510
p	 0.6650	 0.3500
q	 0.6700	 0.3560
r	 0.6630	 0.3510
s	 0.6580	 0.3520
t	 0.6510	 0.3490
u	 0.6540	 0.3500
v	 0.6540	 0.3500
w	 0.6490	 0.3510
x	 0.6550	 0.3500