



wwPDB EM Validation Summary Report ⓘ

Jul 14, 2024 – 05:15 pm BST

PDB ID : 8BL4
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:

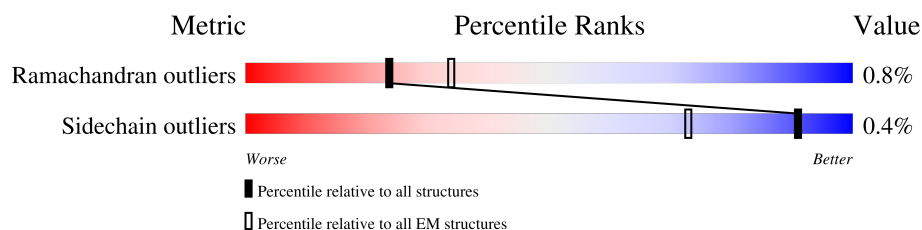
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 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.






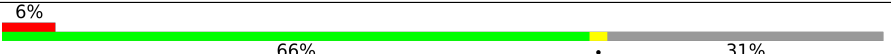
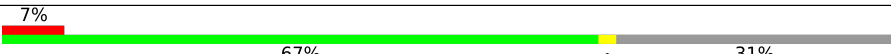
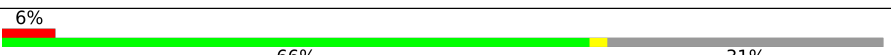
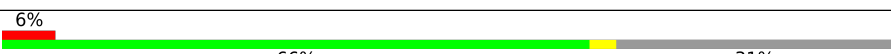
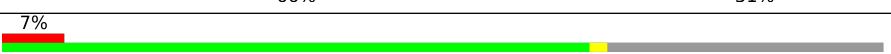

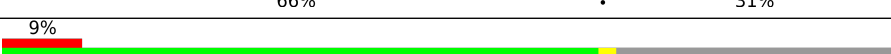
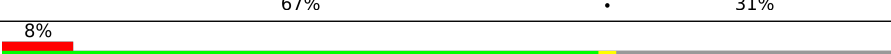
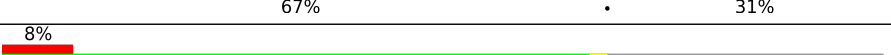
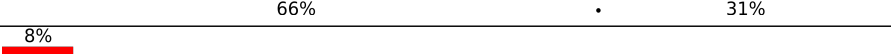
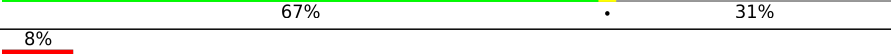


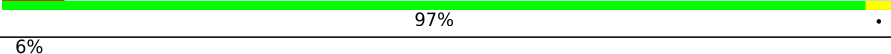
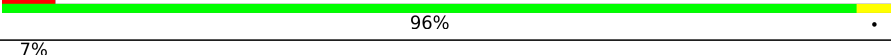
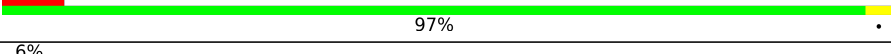
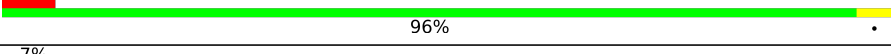
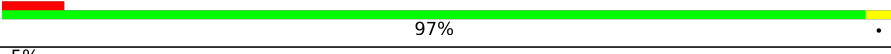
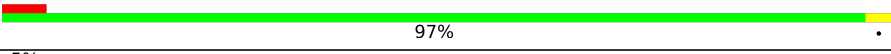
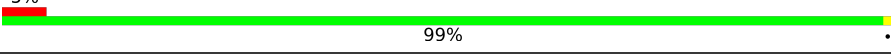
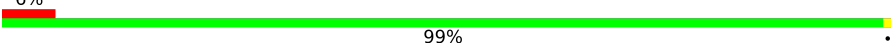
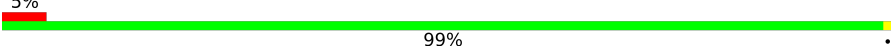
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	<div> <div>5%</div> <div>67%</div> <div>31%</div> </div>
1	B	539	<div> <div>5%</div> <div>66%</div> <div>31%</div> </div>
1	C	539	<div> <div>5%</div> <div>67%</div> <div>31%</div> </div>
1	D	539	<div> <div>5%</div> <div>67%</div> <div>31%</div> </div>
1	E	539	<div> <div>5%</div> <div>67%</div> <div>31%</div> </div>
1	F	539	<div> <div>5%</div> <div>67%</div> <div>31%</div> </div>
1	G	539	<div> <div>5%</div> <div>66%</div> <div>31%</div> </div>
1	H	539	<div> <div>6%</div> <div>66%</div> <div>31%</div> </div>
1	I	539	<div> <div>5%</div> <div>66%</div> <div>31%</div> </div>

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Mol	Chain	Length	Quality of chain
1	J	539	
1	K	539	
1	L	539	
1	M	539	
1	N	539	
1	O	539	
1	P	539	
1	Q	539	
1	R	539	
1	S	539	
1	T	539	
1	U	539	
1	V	539	
1	W	539	
1	X	539	
2	a	149	
2	b	149	
2	c	149	
2	d	149	
2	e	149	
2	f	149	
2	g	149	
2	h	149	
2	i	149	
2	j	149	

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Mol	Chain	Length	Quality of chain
2	k	149	 5% 99%
2	l	149	 5% 99%
2	m	149	 7% 97%
2	n	149	 7% 96%
2	o	149	 8% 96%
2	p	149	 8% 96%
2	q	149	 7% 95% 5%
2	r	149	 7% 95% 5%
2	s	149	 9% 99%
2	t	149	 7% 99%
2	u	149	 9% 99%
2	v	149	 9% 99%
2	w	149	 7% 99%
2	x	149	 9% 99%

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

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

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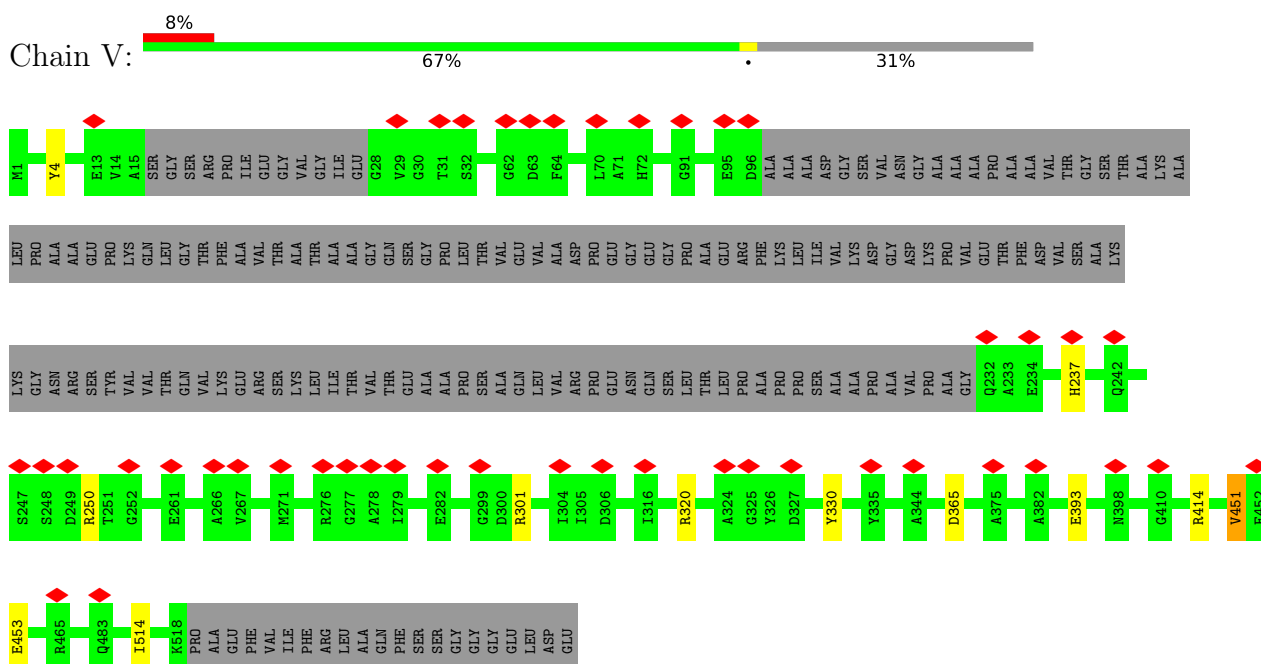
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	g	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	a	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	t	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	n	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
2	h	149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

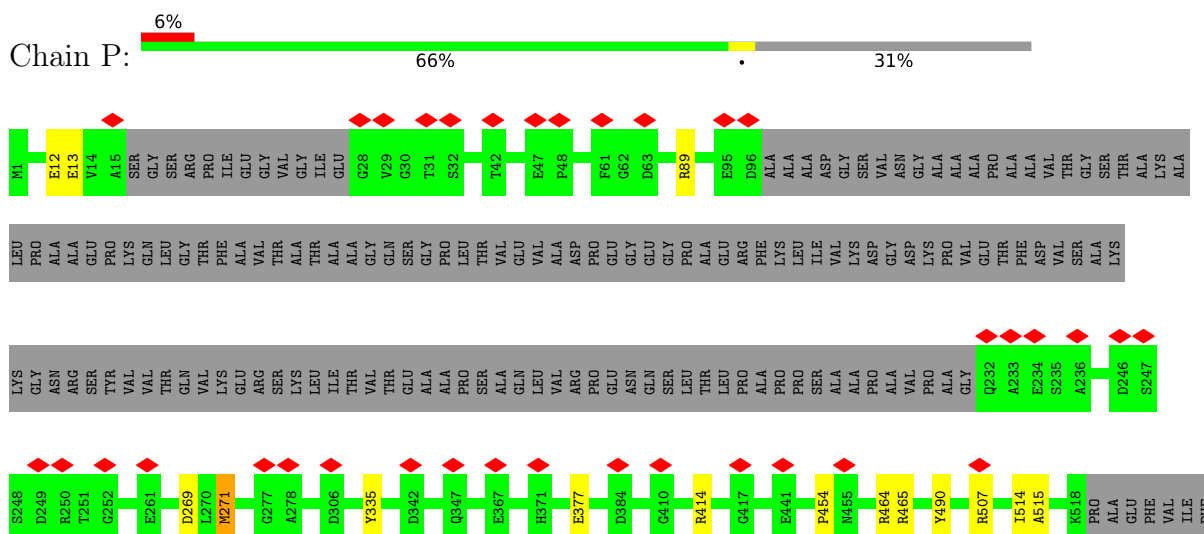
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Phage tail sheath family protein



• Molecule 1: Phage tail sheath family protein



ARG
LEU
ALA
GLN
PHE
SER
SER
GLY
GLY
GLY
LEU
LEU
ASP
GLU

• Molecule 1: Phage tail sheath family protein

Chain J: 

W1 V14 A15 SER GLY THR ARG PRO ILE VAL GLY VAL ILE GLU G28 V29 S32 G43 E47 Y68 R89 V90 G91 A94 E95 D96 ALA ALA ASP ILE VAL GLY SER VAL ASN GLY LYS ALA PRO VAL ALA THR PHE ASP VAL THR LYS LYS ASN

ARG SER TYR VAL THR GLN VAL LYS GLU ARG SER LYS LEU ILE THR VAL THR GLN THR VAL THR GLU ALA PRO SER THR LEU VAL ARG ASN GLN SER LEU LEU PRO ALA PRO ILE SER ALA PRO VAL VAL GLY Q232 A233 E234 P240 A241 Q242 G245 D246

D249 R250 T251 R276 I279 V284 R301 D306 R314 Y330 D342 T345 G346 Q347 R349 R363 D384 R414 Y438 V450 V451 F452 P454 E474 K518 PRO ALA PHE VAL ILE PHE ARG LEU ALA GLN PHE SER SER GLY GLY

GLU
LEU
ASP
GLU

• Molecule 1: Phage tail sheath family protein

Chain D: 

W1 Y4 A15 SER GLY THR SER ARG PRO ILE VAL GLY VAL ILE GLU G28 V29 G30 T31 I39 P44 F61 G81 A94 E95 D96 ALA ALA ASP ILE VAL GLY SER VAL ASN GLY ALA ALA PRO VAL THR PHE LEU LYS LEU LEU PRO ALA PRO ILE SER ALA PRO VAL ASP GLY ASP LYS VAL THR PHE ASP VAL THR GLY SER LYS LYS ASN ARG

SER TYR VAL VAL THR GLN VAL LYS GLU ARG SER LYS ILE THR VAL THR GLU ALA ALA PRO SER GLN VAL VAL ARG PRO GLU ASN GLN SER LEU THR LEU PRO ALA PRO SER ALA VAL VAL GLY Q232 A233 E234 H237 Q242 Y243 L244 G245 D246 S247

S248 G252 A273 A278 I279 D280 R314 R317 A324 Y330 A344 T345 R363 R368 R391 R414 D426 V451 N455 R464 E511 K518 PRO ALA PHE ILE VAL PHE ARG LEU ALA ALA ALA ASP GLY SER VAL VAL GLY THR GLY THR GLY GLY GLY ASP

GLU

• Molecule 1: Phage tail sheath family protein

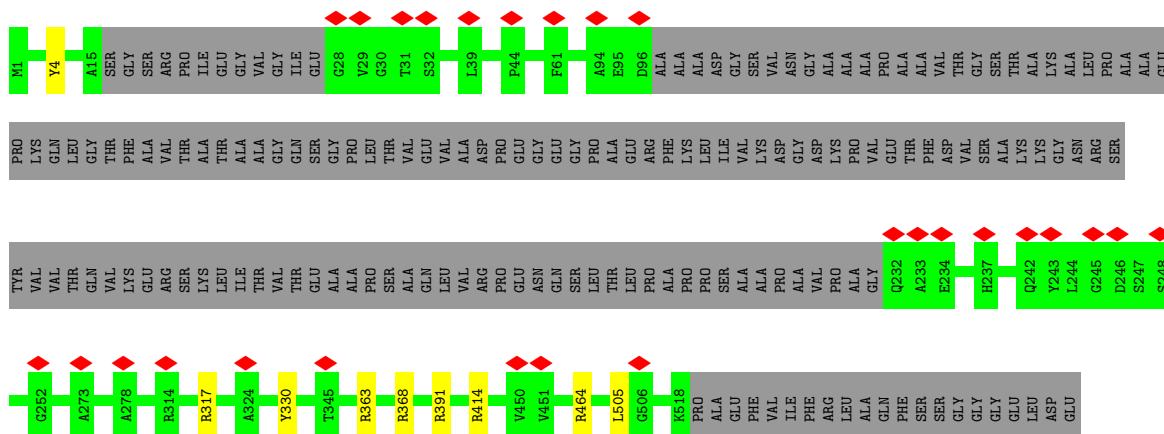
Chain W: 

W1 Y4 F13 V14 A15 SER GLY SER ARG PRO ILE VAL GLY VAL ILE GLU G28 V29 G30 T31 S32 G62 D63 F64 L70 A71 H72 G91 E95 D96 ALA ALA ALA ASP GLY SER VAL VAL ASN GLY ALA ALA ALA PRO VAL VAL THR GLY SER THR LYS ALA

GLY
GLU
LEU
ASP
GLU

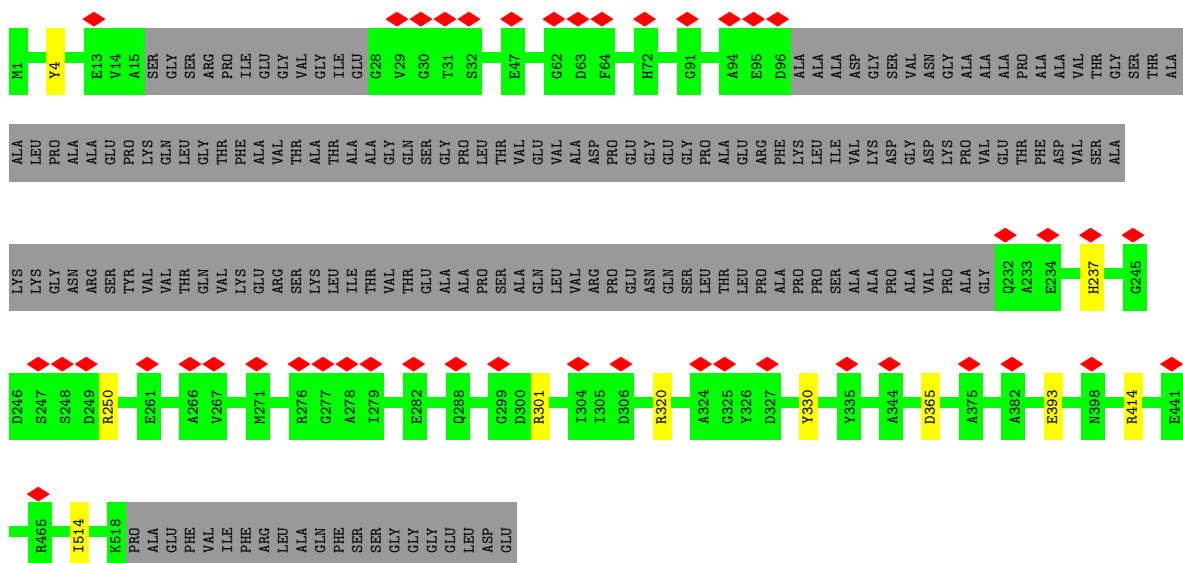
• Molecule 1: Phage tail sheath family protein

Chain E:  5% 67% 31%



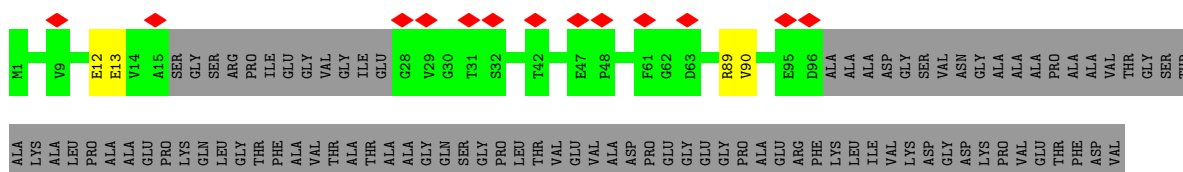
• Molecule 1: Phage tail sheath family protein

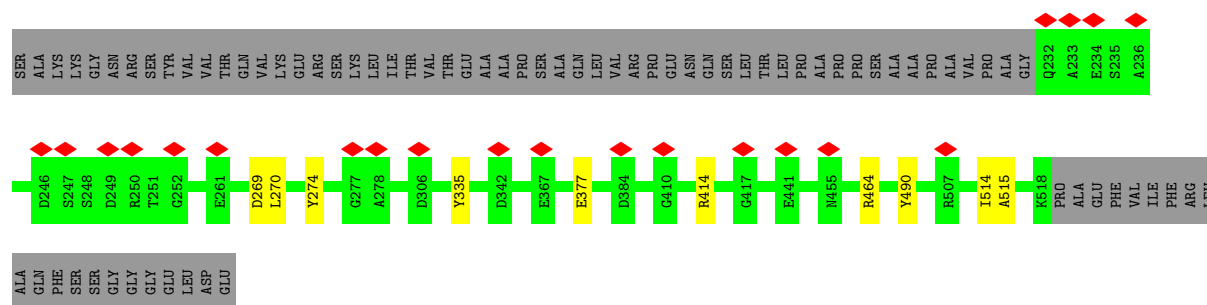
Chain X:  8% 67% 31%



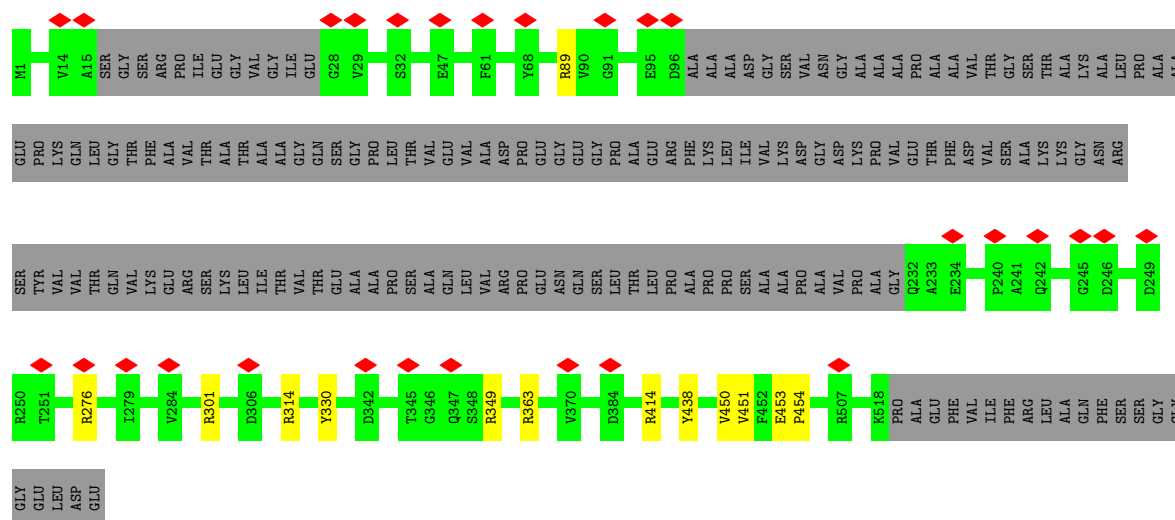
• Molecule 1: Phage tail sheath family protein

Chain R:  6% 66% 31%

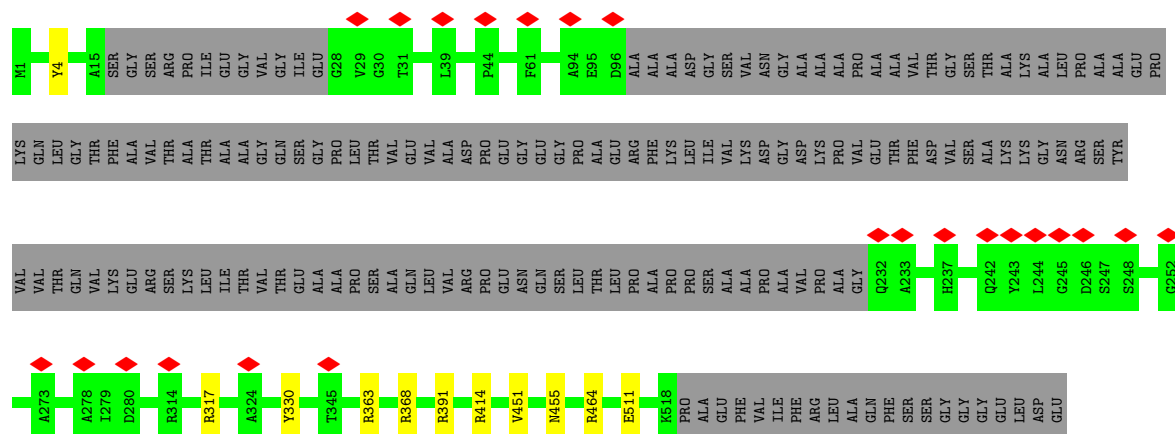




- Molecule 1: Phage tail sheath family protein



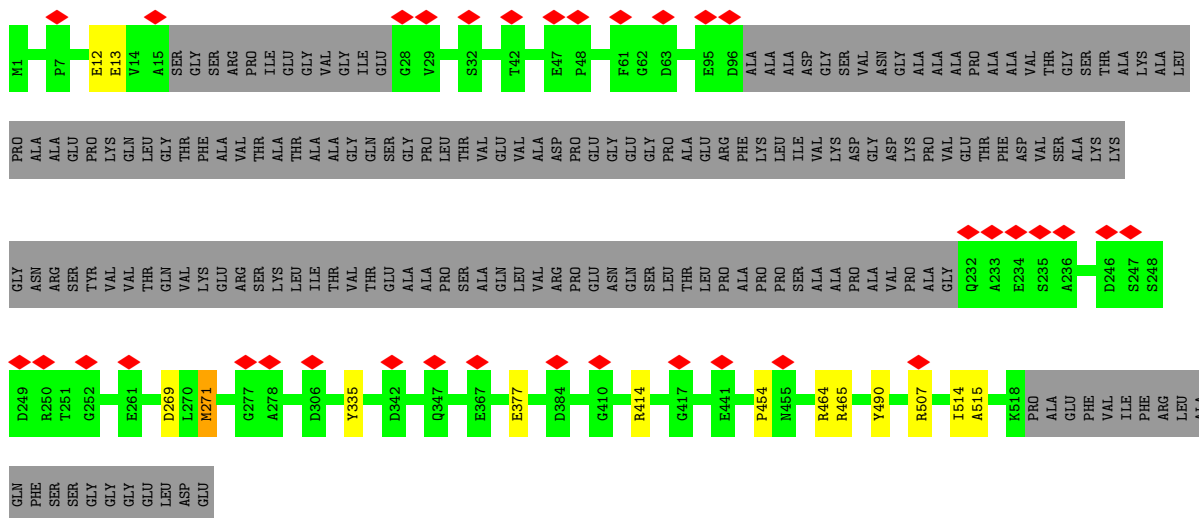
- Molecule 1: Phage tail sheath family protein



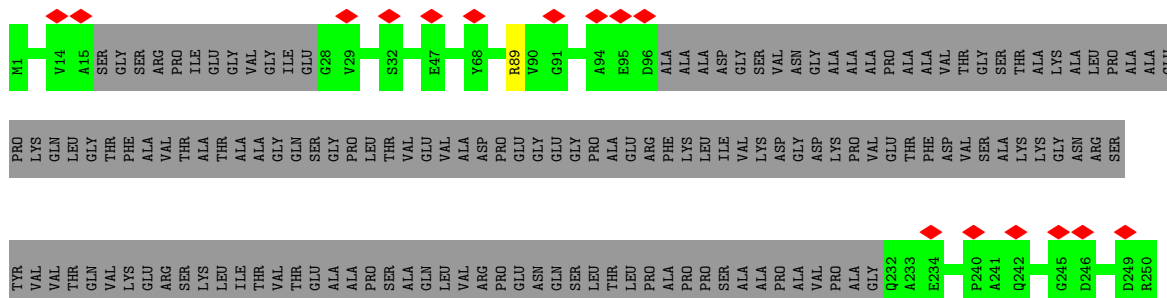
- Molecule 1: Phage tail sheath family protein



- Molecule 1: Phage tail sheath family protein

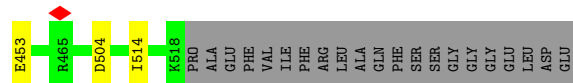
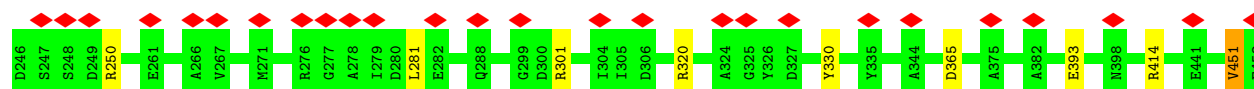
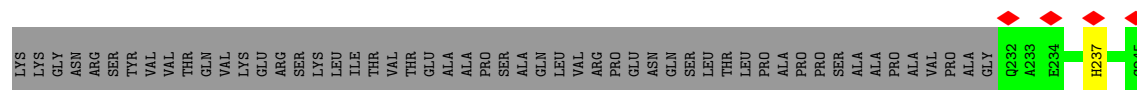
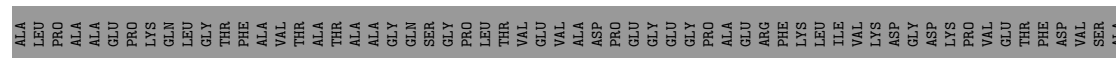
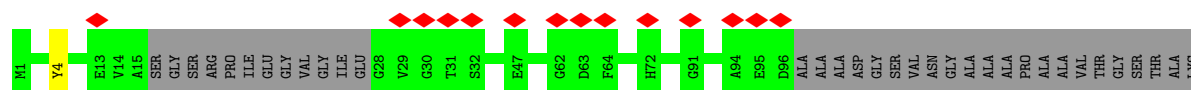


- Molecule 1: Phage tail sheath family protein

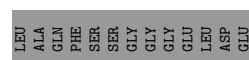
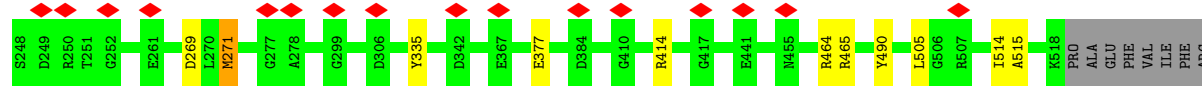
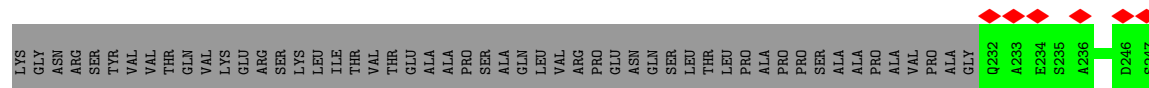
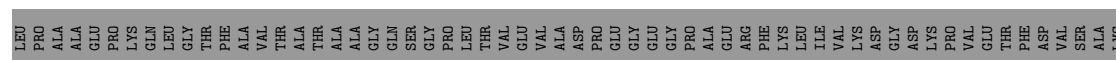
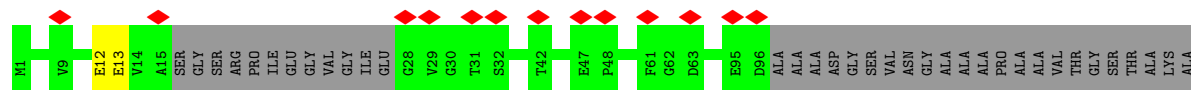




• Molecule 1: Phage tail sheath family protein

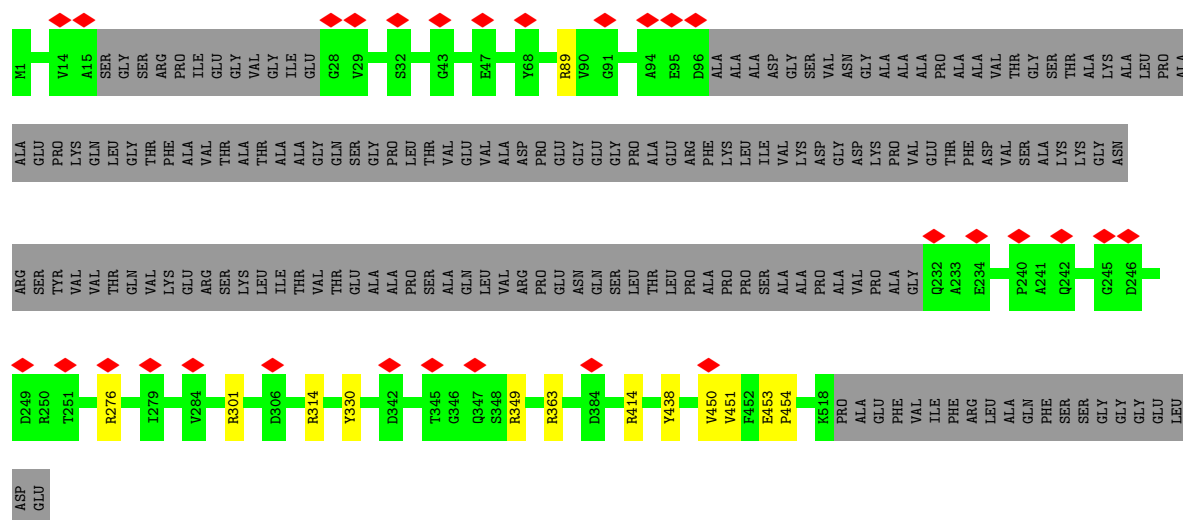


• Molecule 1: Phage tail sheath family protein

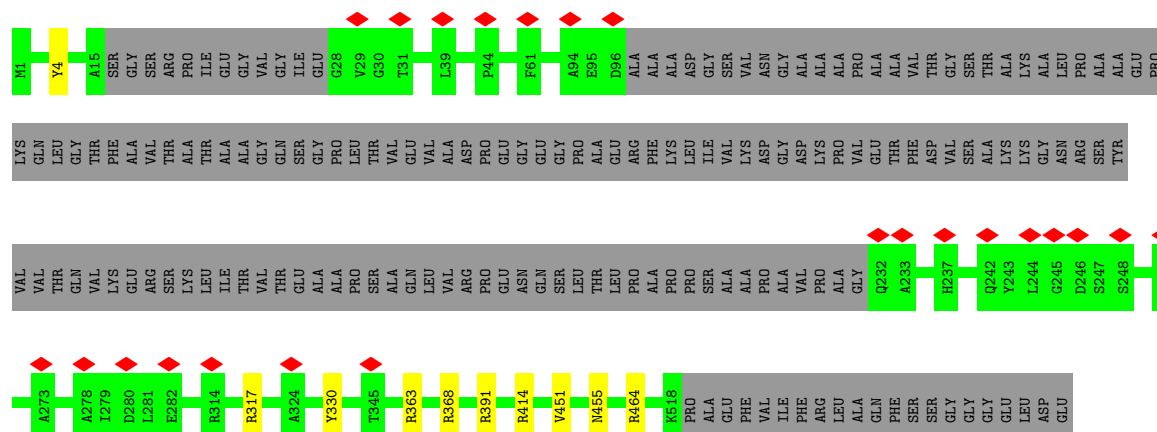


• Molecule 1: Phage tail sheath family protein

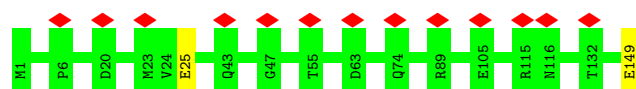




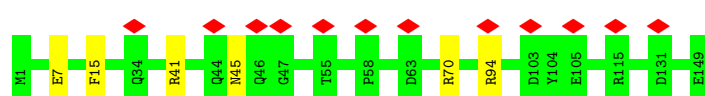
- Molecule 1: Phage tail sheath family protein



- Molecule 2: Phage tail protein

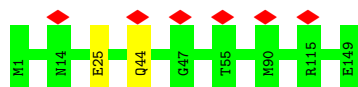


- Molecule 2: Phage tail protein



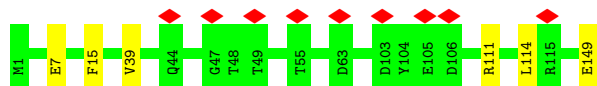
- Molecule 2: Phage tail protein

Chain j:  99%



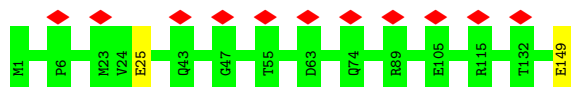
- Molecule 2: Phage tail protein

Chain d:  96%



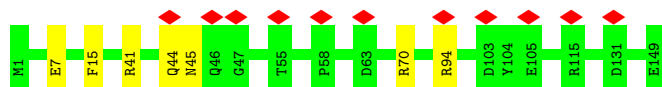
- Molecule 2: Phage tail protein

Chain w:  99%



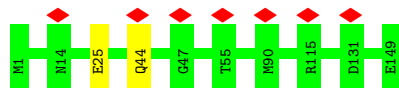
- Molecule 2: Phage tail protein

Chain q:  95% 5%



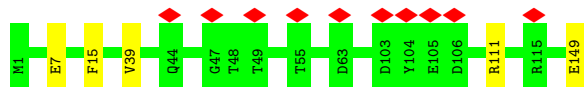
- Molecule 2: Phage tail protein

Chain k:  99%



- Molecule 2: Phage tail protein

Chain e:  97%

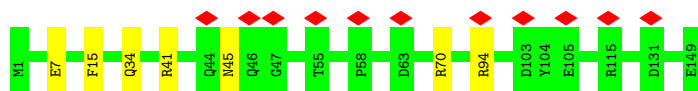
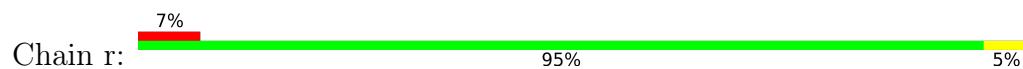


- Molecule 2: Phage tail protein

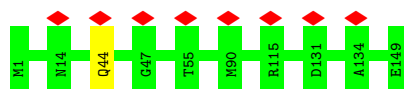
Chain x:  99%



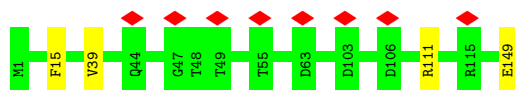
- Molecule 2: Phage tail protein



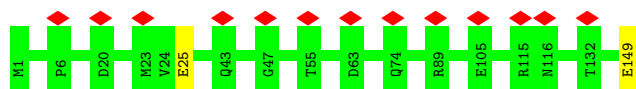
- Molecule 2: Phage tail protein



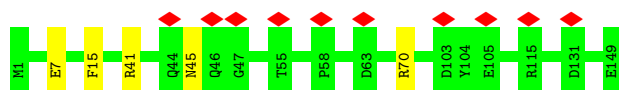
- Molecule 2: Phage tail protein



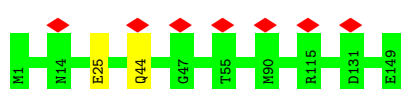
- Molecule 2: Phage tail protein



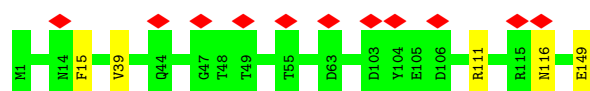
- Molecule 2: Phage tail protein



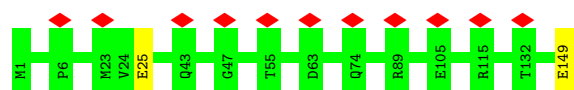
- Molecule 2: Phage tail protein



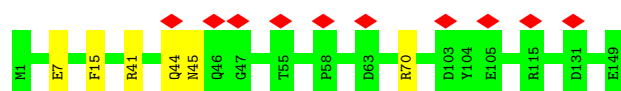
- Molecule 2: Phage tail protein



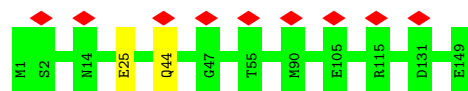
- Molecule 2: Phage tail protein



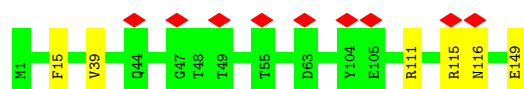
- Molecule 2: Phage tail protein



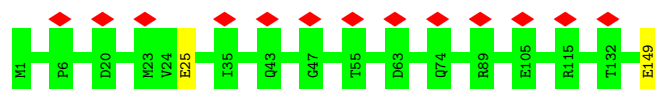
- Molecule 2: Phage tail protein



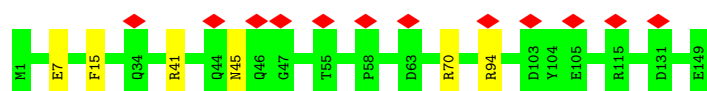
- Molecule 2: Phage tail protein



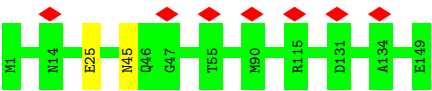
- Molecule 2: Phage tail protein



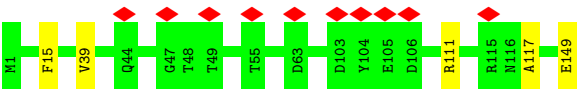
- Molecule 2: Phage tail protein



● 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%)	0.94	11/4014 (0.3%)
1	B	1.01	1/2942 (0.0%)	0.94	11/4014 (0.3%)
1	C	1.01	0/2942	0.95	11/4014 (0.3%)
1	D	1.01	1/2942 (0.0%)	0.94	11/4014 (0.3%)
1	E	1.00	0/2942	0.94	11/4014 (0.3%)
1	F	1.01	1/2942 (0.0%)	0.95	11/4014 (0.3%)
1	G	0.95	1/2942 (0.0%)	0.95	9/4014 (0.2%)
1	H	0.95	1/2942 (0.0%)	0.95	9/4014 (0.2%)
1	I	0.96	1/2942 (0.0%)	0.96	9/4014 (0.2%)
1	J	0.96	1/2942 (0.0%)	0.96	9/4014 (0.2%)
1	K	0.95	1/2942 (0.0%)	0.95	9/4014 (0.2%)
1	L	0.95	1/2942 (0.0%)	0.95	9/4014 (0.2%)
1	M	1.01	4/2942 (0.1%)	0.88	5/4014 (0.1%)
1	N	1.01	4/2942 (0.1%)	0.89	5/4014 (0.1%)
1	O	1.02	5/2942 (0.2%)	0.89	5/4014 (0.1%)
1	P	1.01	5/2942 (0.2%)	0.89	5/4014 (0.1%)
1	Q	1.01	4/2942 (0.1%)	0.88	4/4014 (0.1%)
1	R	1.00	5/2942 (0.2%)	0.88	4/4014 (0.1%)
1	S	0.97	4/2942 (0.1%)	0.93	5/4014 (0.1%)
1	T	0.98	3/2942 (0.1%)	0.95	5/4014 (0.1%)
1	U	0.98	3/2942 (0.1%)	0.95	5/4014 (0.1%)
1	V	0.98	3/2942 (0.1%)	0.95	5/4014 (0.1%)
1	W	0.98	3/2942 (0.1%)	0.95	5/4014 (0.1%)
1	X	0.98	3/2942 (0.1%)	0.95	5/4014 (0.1%)
2	a	0.98	3/1168 (0.3%)	0.96	1/1586 (0.1%)
2	b	0.98	3/1168 (0.3%)	0.95	1/1586 (0.1%)
2	c	0.98	3/1168 (0.3%)	0.95	1/1586 (0.1%)
2	d	1.03	4/1168 (0.3%)	0.96	1/1586 (0.1%)
2	e	0.98	4/1168 (0.3%)	0.96	1/1586 (0.1%)
2	f	0.99	3/1168 (0.3%)	0.95	1/1586 (0.1%)
2	g	1.00	1/1168 (0.1%)	0.96	0/1586
2	h	1.00	1/1168 (0.1%)	0.96	0/1586
2	i	1.00	1/1168 (0.1%)	0.96	0/1586
2	j	1.00	1/1168 (0.1%)	0.96	0/1586

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	k	1.00	1/1168 (0.1%)	0.96	0/1586
2	l	1.00	0/1168	0.96	0/1586
2	m	0.95	2/1168 (0.2%)	0.94	2/1586 (0.1%)
2	n	0.95	2/1168 (0.2%)	0.93	2/1586 (0.1%)
2	o	0.95	2/1168 (0.2%)	0.93	2/1586 (0.1%)
2	p	0.95	2/1168 (0.2%)	0.93	2/1586 (0.1%)
2	q	0.95	2/1168 (0.2%)	0.93	2/1586 (0.1%)
2	r	0.95	2/1168 (0.2%)	0.93	2/1586 (0.1%)
2	s	0.94	3/1168 (0.3%)	0.96	0/1586
2	t	0.94	3/1168 (0.3%)	0.96	0/1586
2	u	0.94	3/1168 (0.3%)	0.95	0/1586
2	v	0.94	3/1168 (0.3%)	0.95	0/1586
2	w	0.94	3/1168 (0.3%)	0.95	0/1586
2	x	0.94	3/1168 (0.3%)	0.96	0/1586
All	All	0.98	111/98640 (0.1%)	0.94	196/134400 (0.1%)

The worst 5 of 111 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	u	25	GLU	CD-OE1	-6.41	1.18	1.25
2	v	25	GLU	CD-OE1	-6.38	1.18	1.25
2	x	25	GLU	CD-OE1	-6.36	1.18	1.25
2	t	25	GLU	CD-OE1	-6.36	1.18	1.25
2	s	25	GLU	CD-OE1	-6.33	1.18	1.25

The worst 5 of 196 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	301	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	V	301	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	W	301	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	S	301	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	U	301	ARG	NE-CZ-NH1	9.97	125.28	120.30

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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	365/539 (68%)	343 (94%)	20 (6%)	2 (0%)	29	67
1	B	365/539 (68%)	341 (93%)	21 (6%)	3 (1%)	19	57
1	C	365/539 (68%)	344 (94%)	19 (5%)	2 (0%)	29	67
1	D	365/539 (68%)	343 (94%)	20 (6%)	2 (0%)	29	67
1	E	365/539 (68%)	345 (94%)	20 (6%)	0	100	100
1	F	365/539 (68%)	344 (94%)	19 (5%)	2 (0%)	29	67
1	G	365/539 (68%)	339 (93%)	23 (6%)	3 (1%)	19	57
1	H	365/539 (68%)	335 (92%)	26 (7%)	4 (1%)	14	51
1	I	365/539 (68%)	340 (93%)	22 (6%)	3 (1%)	19	57
1	J	365/539 (68%)	340 (93%)	22 (6%)	3 (1%)	19	57
1	K	365/539 (68%)	341 (93%)	21 (6%)	3 (1%)	19	57
1	L	365/539 (68%)	339 (93%)	23 (6%)	3 (1%)	19	57
1	M	365/539 (68%)	339 (93%)	22 (6%)	4 (1%)	14	51
1	N	365/539 (68%)	342 (94%)	19 (5%)	4 (1%)	14	51
1	O	365/539 (68%)	339 (93%)	22 (6%)	4 (1%)	14	51
1	P	365/539 (68%)	339 (93%)	22 (6%)	4 (1%)	14	51
1	Q	365/539 (68%)	340 (93%)	21 (6%)	4 (1%)	14	51
1	R	365/539 (68%)	342 (94%)	20 (6%)	3 (1%)	19	57
1	S	365/539 (68%)	328 (90%)	35 (10%)	2 (0%)	29	67
1	T	365/539 (68%)	331 (91%)	29 (8%)	5 (1%)	11	46
1	U	365/539 (68%)	331 (91%)	27 (7%)	7 (2%)	8	41
1	V	365/539 (68%)	331 (91%)	29 (8%)	5 (1%)	11	46
1	W	365/539 (68%)	331 (91%)	28 (8%)	6 (2%)	9	44
1	X	365/539 (68%)	331 (91%)	29 (8%)	5 (1%)	11	46
2	a	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	22	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	147/149 (99%)	133 (90%)	13 (9%)	1 (1%)	22	60
2	c	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	22	60
2	d	147/149 (99%)	134 (91%)	12 (8%)	1 (1%)	22	60
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%)	22	60
2	h	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	22	60
2	i	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	22	60
2	j	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	22	60
2	k	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	22	60
2	l	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	22	60
2	m	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	22	60
2	n	147/149 (99%)	138 (94%)	7 (5%)	2 (1%)	11	46
2	o	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	22	60
2	p	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	22	60
2	q	147/149 (99%)	138 (94%)	7 (5%)	2 (1%)	11	46
2	r	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	22	60
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%)	24	57

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 ⓘ

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%)	92	95
1	C	295/417 (71%)	295 (100%)	0	100	100
1	D	295/417 (71%)	295 (100%)	0	100	100
1	E	295/417 (71%)	294 (100%)	1 (0%)	92	95
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%)	295 (100%)	0	100	100
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%)	292 (99%)	3 (1%)	76	86
1	N	295/417 (71%)	293 (99%)	2 (1%)	84	90
1	O	295/417 (71%)	293 (99%)	2 (1%)	84	90
1	P	295/417 (71%)	291 (99%)	4 (1%)	67	81
1	Q	295/417 (71%)	293 (99%)	2 (1%)	84	90
1	R	295/417 (71%)	291 (99%)	4 (1%)	67	81
1	S	295/417 (71%)	292 (99%)	3 (1%)	76	86
1	T	295/417 (71%)	293 (99%)	2 (1%)	84	90
1	U	295/417 (71%)	293 (99%)	2 (1%)	84	90
1	V	295/417 (71%)	293 (99%)	2 (1%)	84	90
1	W	295/417 (71%)	293 (99%)	2 (1%)	84	90
1	X	295/417 (71%)	293 (99%)	2 (1%)	84	90
2	a	129/129 (100%)	129 (100%)	0	100	100
2	b	129/129 (100%)	128 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	129 (100%)	0	100	100
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
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%)	81	89
2	p	129/129 (100%)	128 (99%)	1 (1%)	81	89
2	q	129/129 (100%)	128 (99%)	1 (1%)	81	89
2	r	129/129 (100%)	127 (98%)	2 (2%)	62	79
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%)	10138 (100%)	38 (0%)	91	94

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	451	VAL
1	O	269	ASP
1	N	269	ASP
2	b	115	ARG
2	o	94	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	311	GLN
1	C	311	GLN
2	b	34	GLN
2	u	116	ASN
2	c	116	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

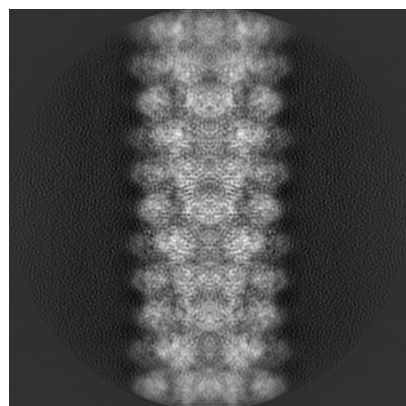
6 Map visualisation [i](#)

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.

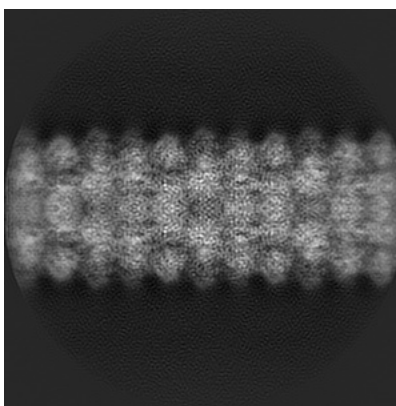
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

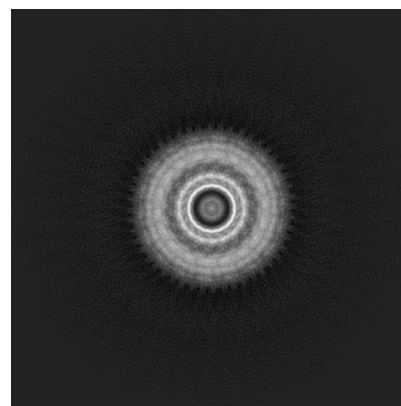
6.1.1 Primary map



X

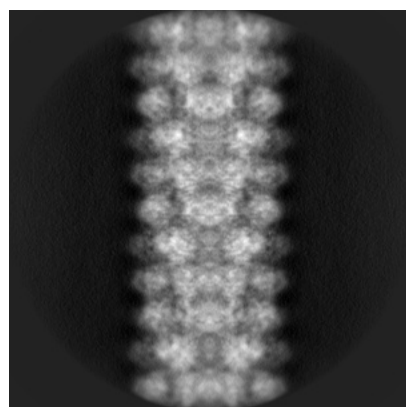


Y

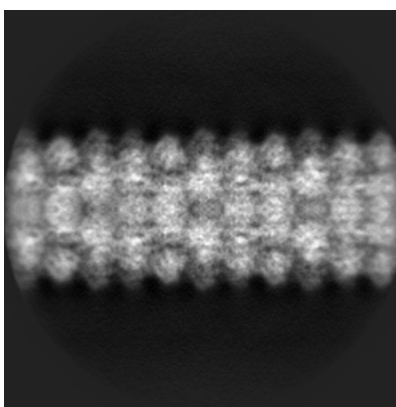


Z

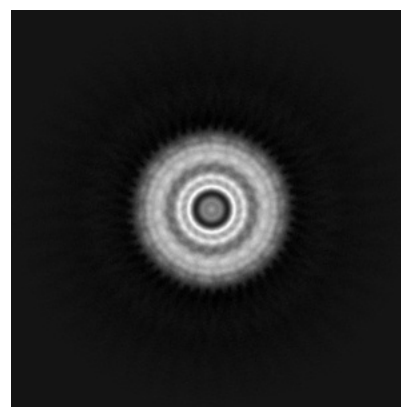
6.1.2 Raw map



X



Y

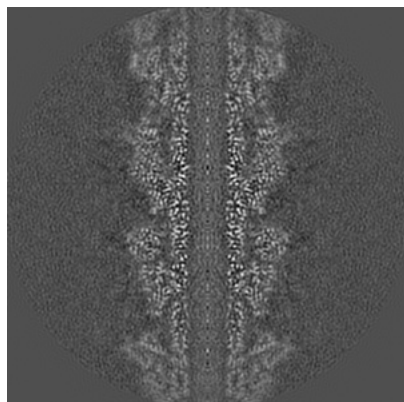


Z

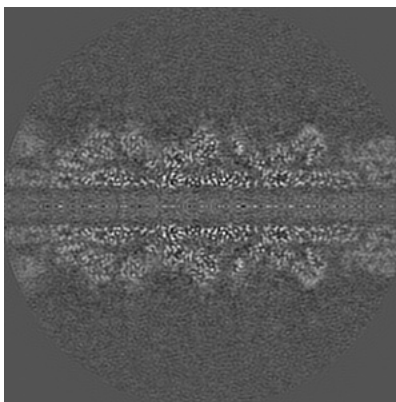
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

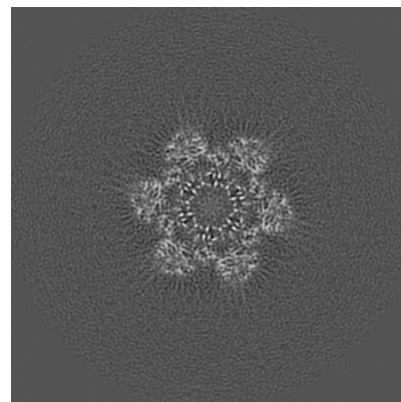
6.2.1 Primary map



X Index: 160

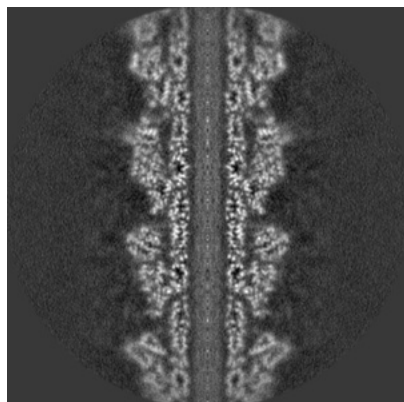


Y Index: 160

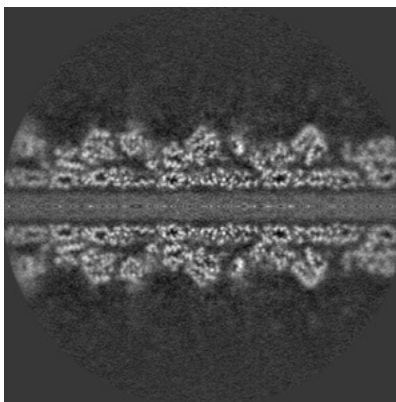


Z Index: 160

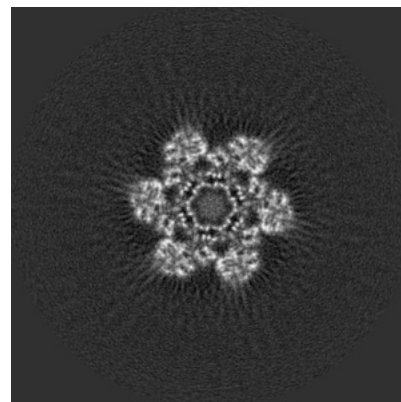
6.2.2 Raw map



X Index: 160



Y Index: 160

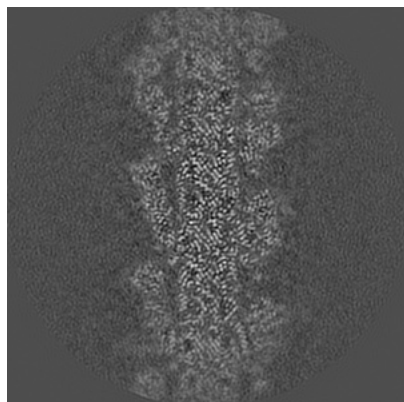


Z Index: 160

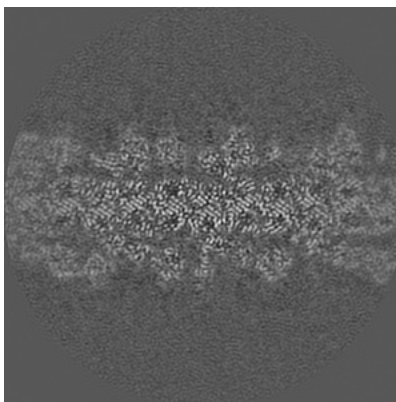
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

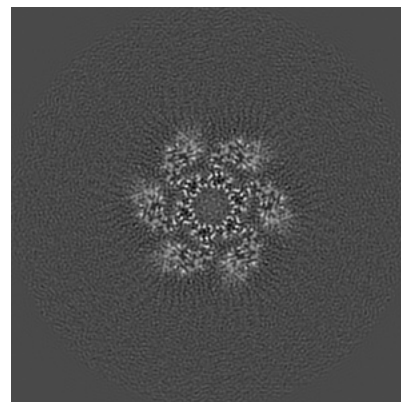
6.3.1 Primary map



X Index: 143

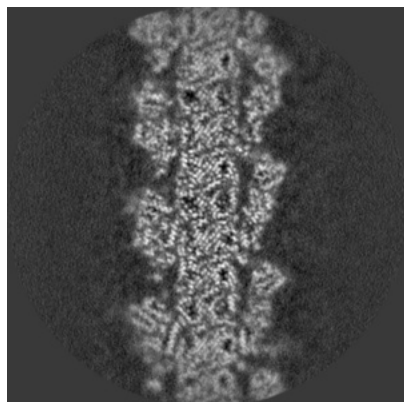


Y Index: 178

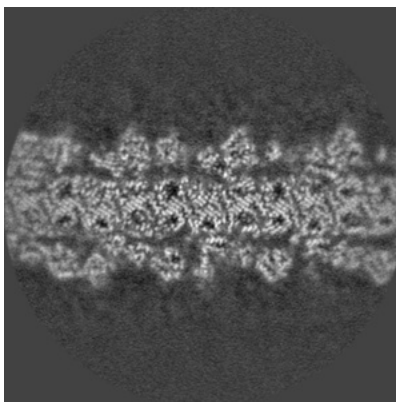


Z Index: 163

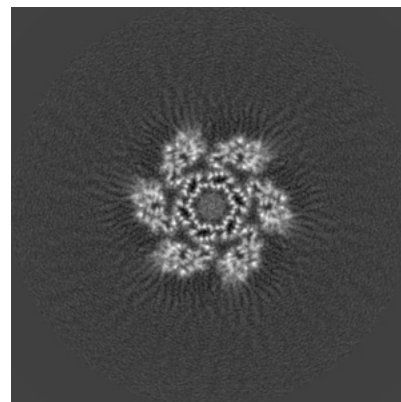
6.3.2 Raw map



X Index: 177



Y Index: 178

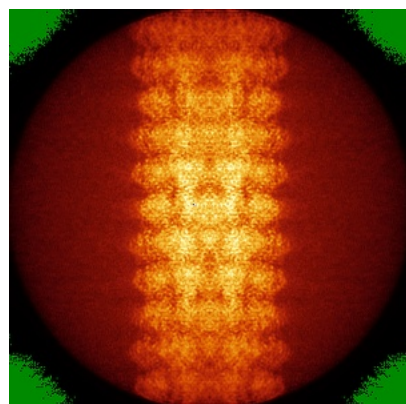


Z Index: 163

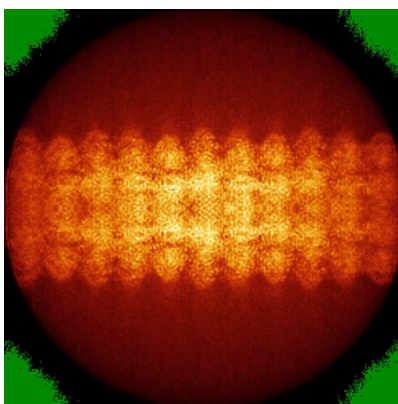
The images above show the largest variance slices of the map in three orthogonal directions.

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

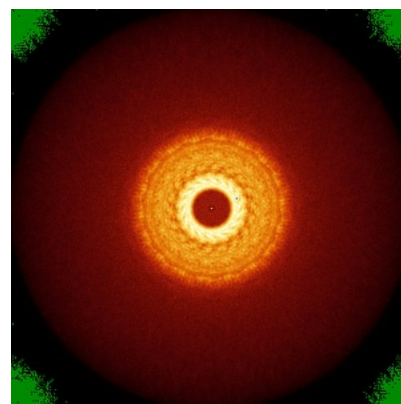
6.4.1 Primary map



X

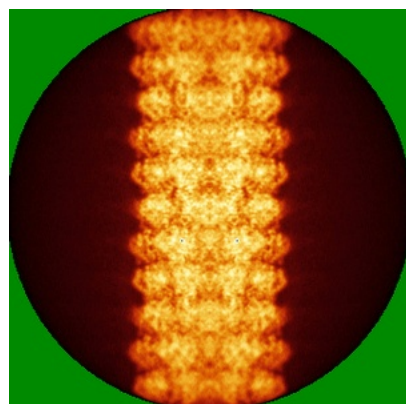


Y

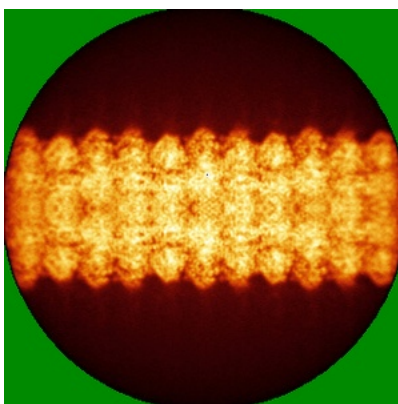


Z

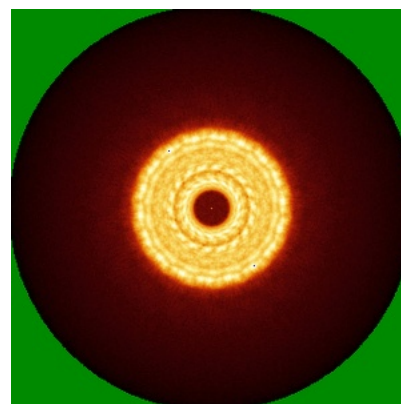
6.4.2 Raw map



X



Y

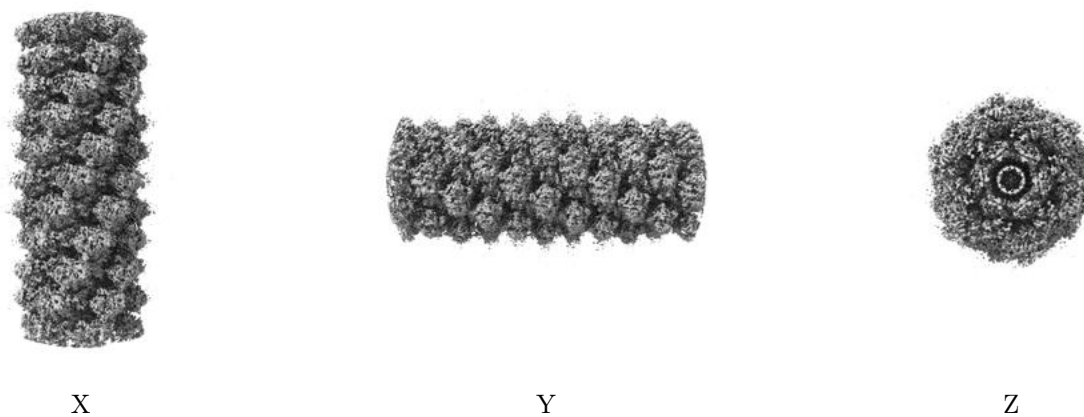


Z

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.

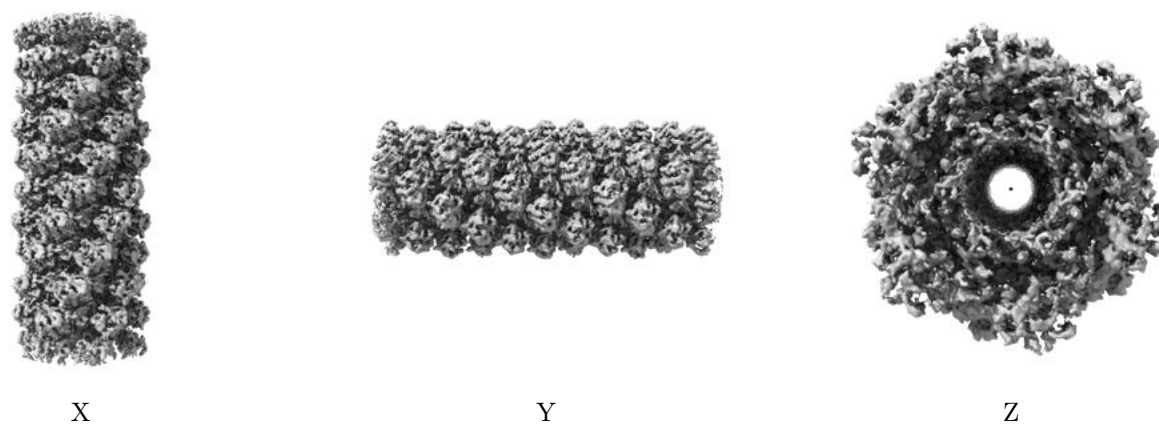
6.5 Orthogonal surface views [i](#)

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.

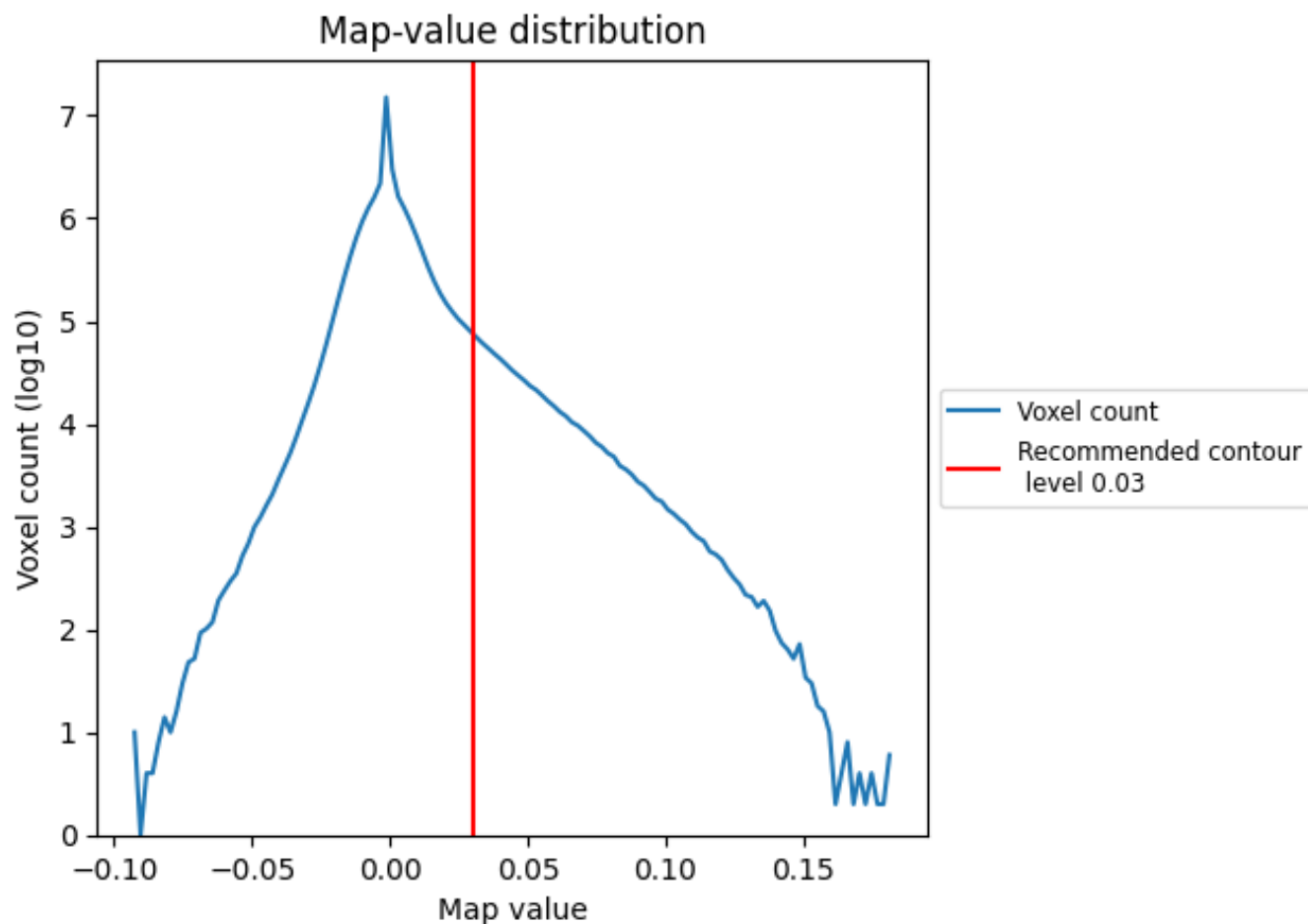
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

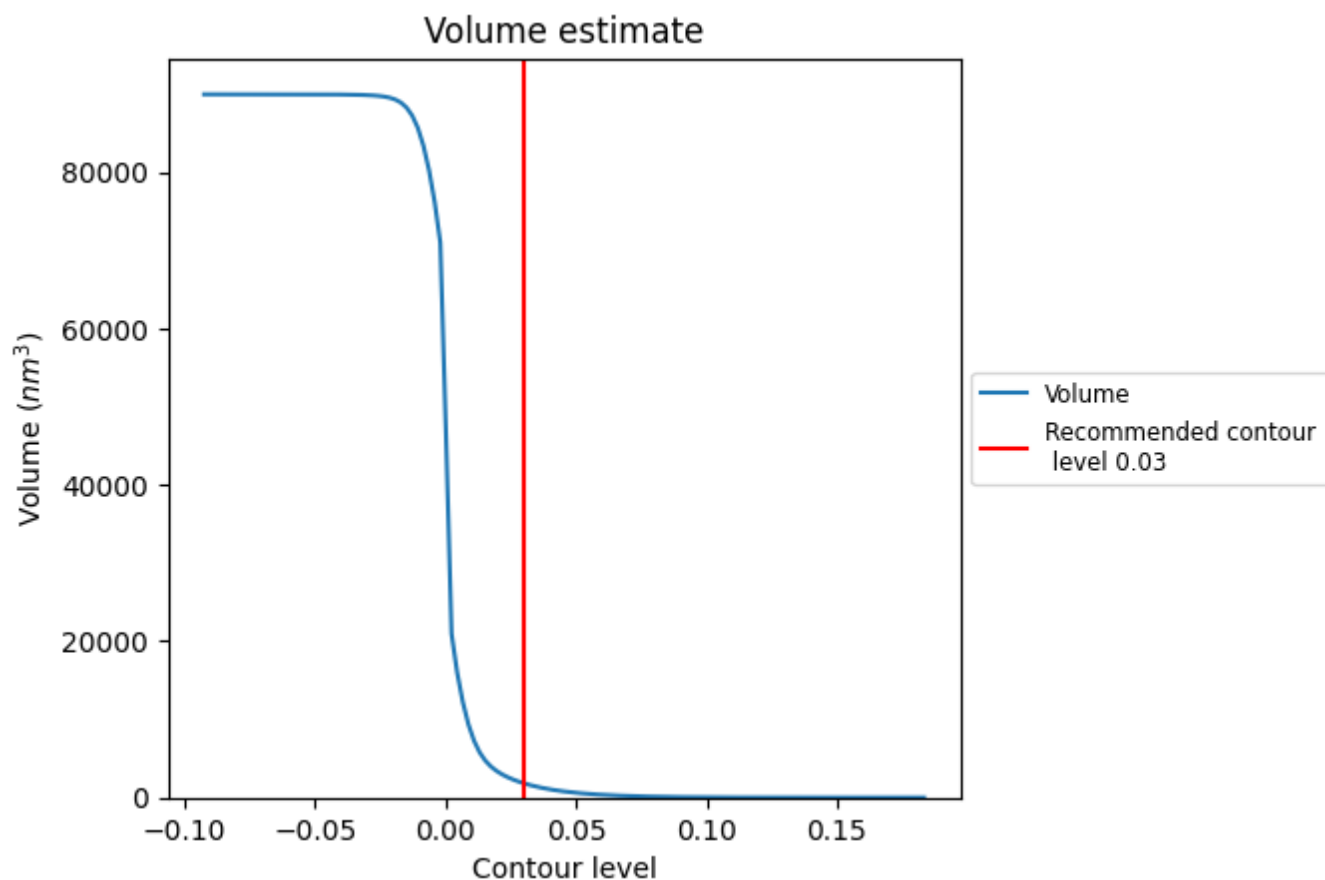
This section contains the results of statistical analysis of the map.

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.

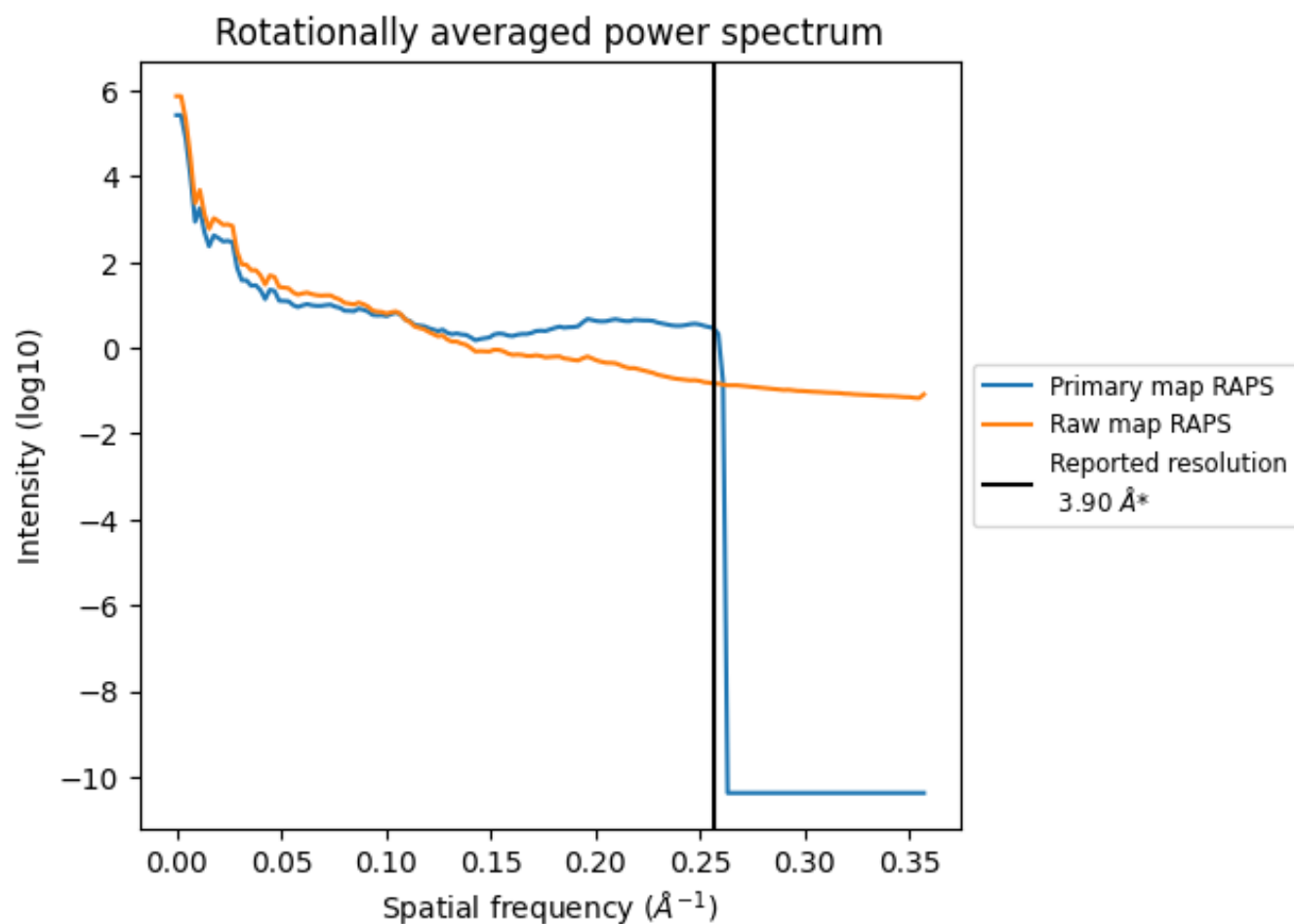
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1828 nm^3 ; 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 ⓘ

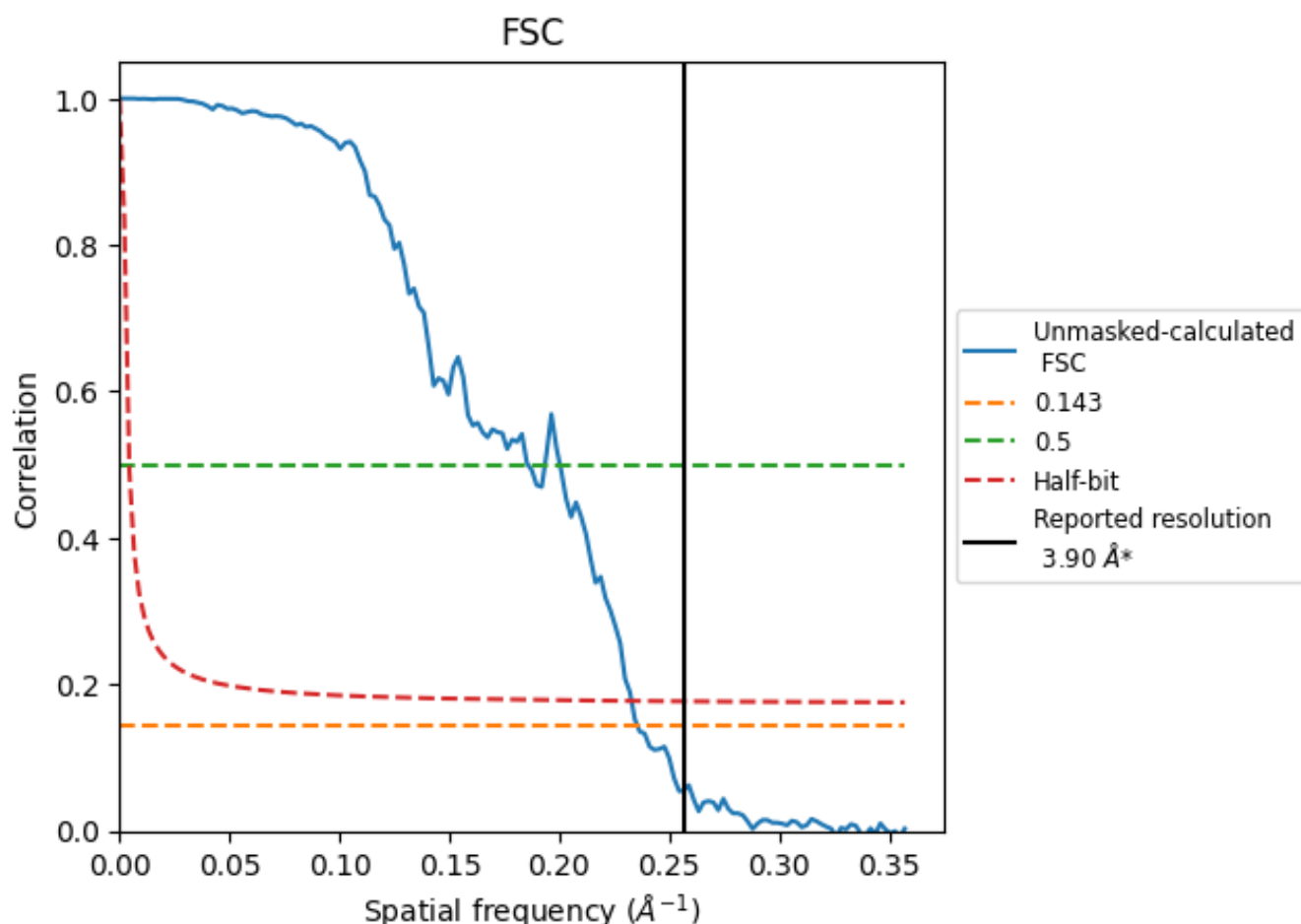


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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](#)

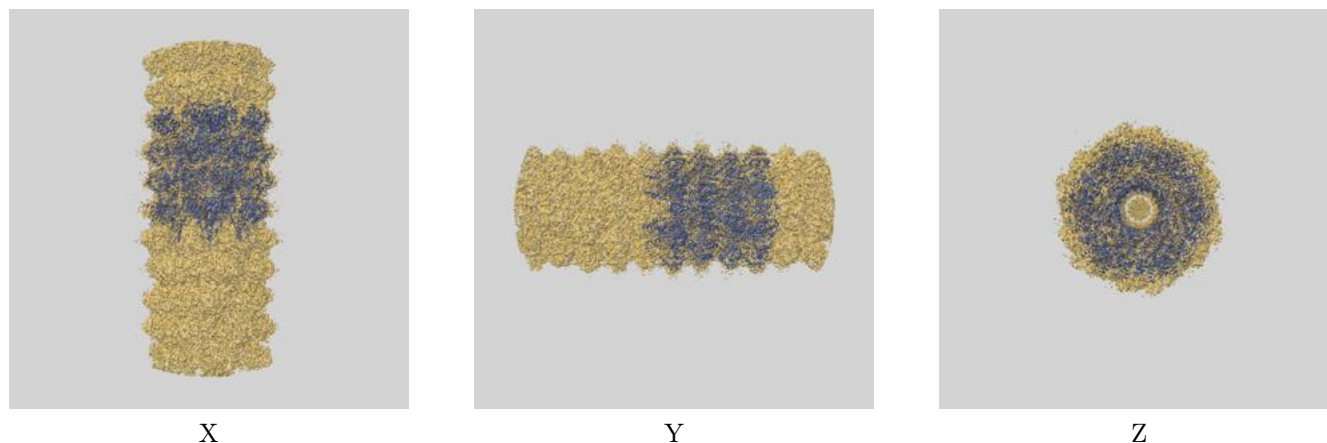
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	5.39	4.29

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

9 Map-model fit [i](#)

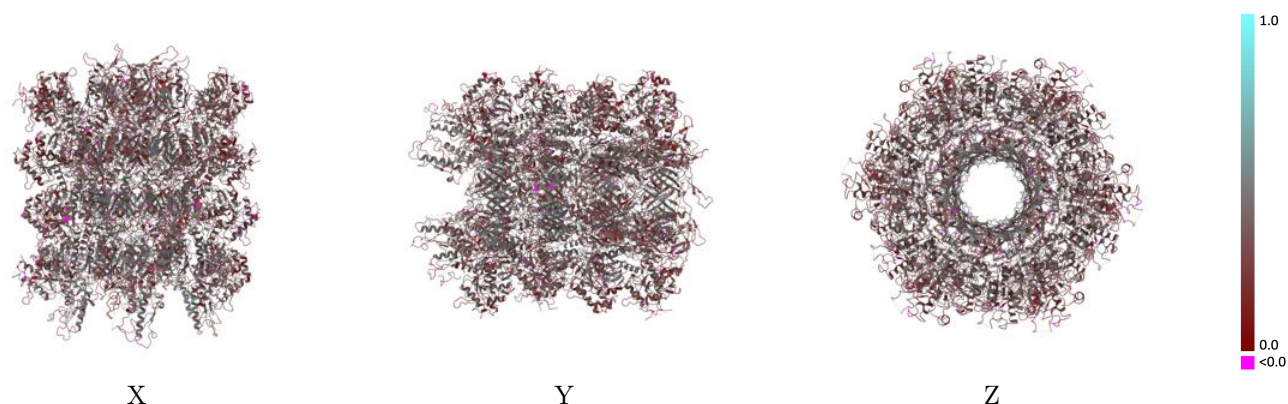
This section contains information regarding the fit between EMDB map EMD-16101 and PDB model 8BL4. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



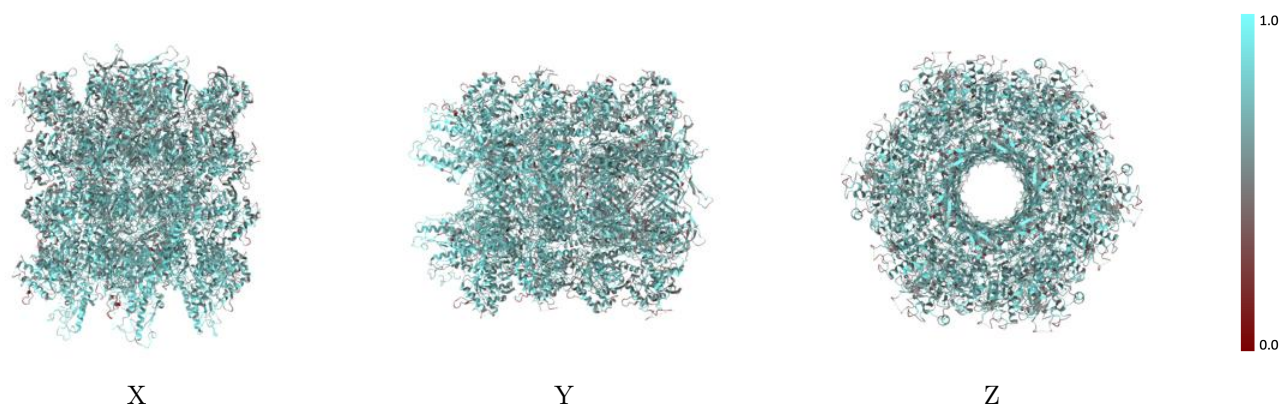
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



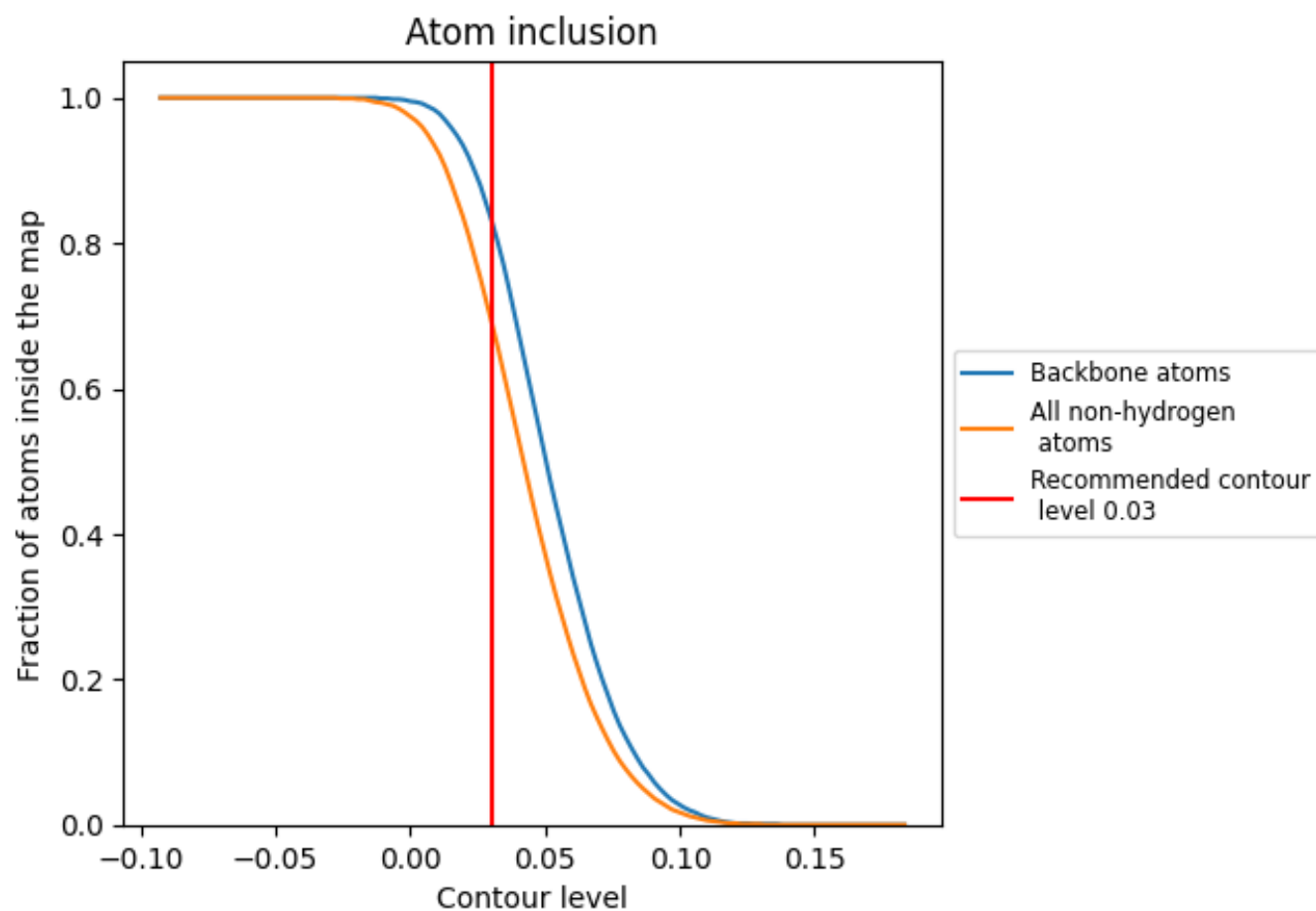
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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