



## wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:53 PM UTC

PDB ID : 9LU7 / pdb\_00009lu7  
EMDB ID : EMD-63390  
Title : Structure of bacteriophage T4 protal-neck mismatch complex gp20-gp14-gp13  
assembled in vitro in C6 symmetry  
Authors : Han, L.; Mao, Q.; Sun, L.  
Deposited on : 2025-02-07  
Resolution : 3.45 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

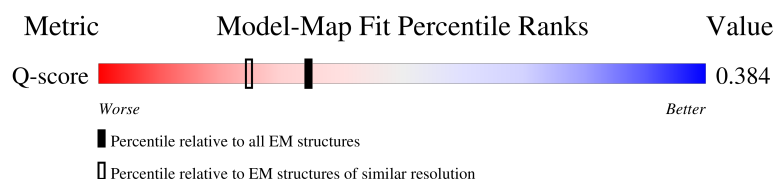
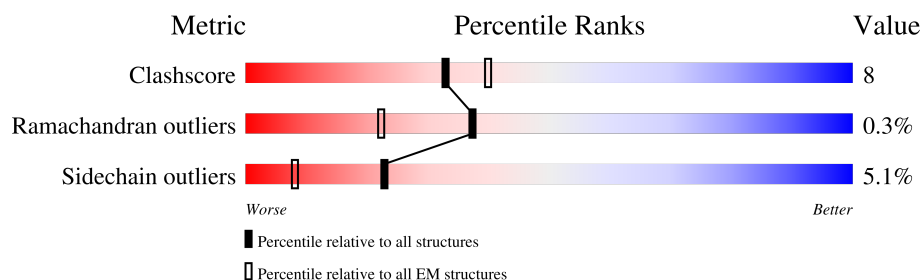
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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




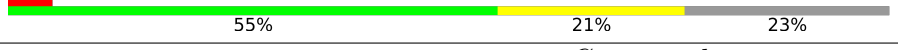
The reported resolution of this entry is 3.45 Å.

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.





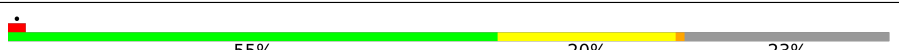
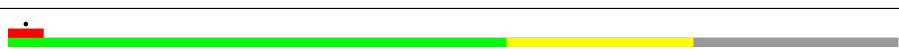

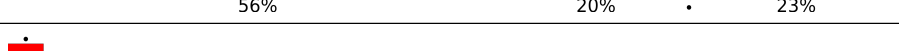
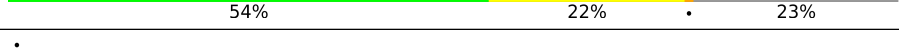


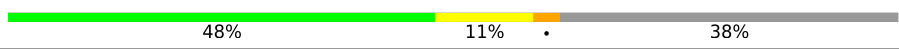
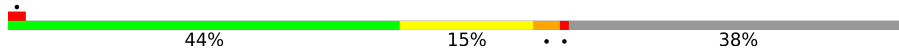
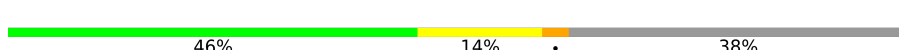
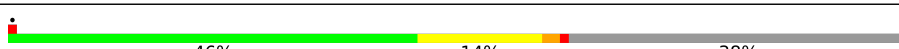
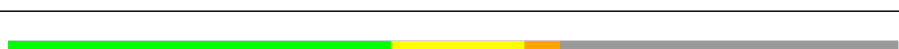
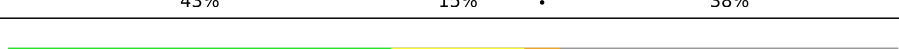
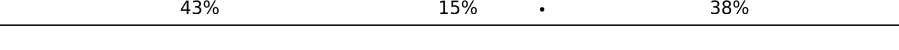








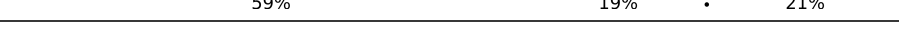
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13836 ( 2.95 - 3.95 )

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

Mol	Chain	Length	Quality of chain
1	A	315	 5% 59% 17% 23%
1	B	315	 5% 56% 21% 23%
1	C	315	 5% 55% 20% 23%
1	D	315	 5% 55% 21% 23%

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Mol	Chain	Length	Quality of chain
1	E	315	
1	F	315	
1	G	315	
1	H	315	
1	I	315	
1	J	315	
1	K	315	
1	L	315	
2	M	265	
2	N	265	
2	O	265	
2	P	265	
2	Q	265	
2	R	265	
3	a	533	
3	b	533	
3	c	533	
3	d	533	
3	e	533	
3	f	533	
3	g	533	
3	h	533	
3	i	533	
3	j	533	
3	k	533	

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Mol	Chain	Length	Quality of chain
3	1	533	<div><div></div><div>61%</div><div>17%</div><div>21%</div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 72372 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 Neck protein gp13.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	241	Total 1937	C 1243	N 326	O 357	S 11	0	0
1	L	241	Total 1937	C 1243	N 326	O 357	S 11	0	0
1	C	241	Total 1937	C 1243	N 326	O 357	S 11	0	0
1	B	241	Total 1937	C 1243	N 326	O 357	S 11	0	0
1	E	241	Total 1937	C 1243	N 326	O 357	S 11	0	0
1	D	241	Total 1937	C 1243	N 326	O 357	S 11	0	0
1	G	241	Total 1937	C 1243	N 326	O 357	S 11	0	0
1	F	241	Total 1937	C 1243	N 326	O 357	S 11	0	0
1	I	241	Total 1937	C 1243	N 326	O 357	S 11	0	0
1	H	241	Total 1937	C 1243	N 326	O 357	S 11	0	0
1	K	241	Total 1937	C 1243	N 326	O 357	S 11	0	0
1	J	241	Total 1937	C 1243	N 326	O 357	S 11	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	HIS	-	expression tag	UNP P11110
A	311	HIS	-	expression tag	UNP P11110
A	312	HIS	-	expression tag	UNP P11110
A	313	HIS	-	expression tag	UNP P11110
A	314	HIS	-	expression tag	UNP P11110
A	315	HIS	-	expression tag	UNP P11110

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Chain	Residue	Modelled	Actual	Comment	Reference
L	310	HIS	-	expression tag	UNP P11110
L	311	HIS	-	expression tag	UNP P11110
L	312	HIS	-	expression tag	UNP P11110
L	313	HIS	-	expression tag	UNP P11110
L	314	HIS	-	expression tag	UNP P11110
L	315	HIS	-	expression tag	UNP P11110
C	310	HIS	-	expression tag	UNP P11110
C	311	HIS	-	expression tag	UNP P11110
C	312	HIS	-	expression tag	UNP P11110
C	313	HIS	-	expression tag	UNP P11110
C	314	HIS	-	expression tag	UNP P11110
C	315	HIS	-	expression tag	UNP P11110
B	310	HIS	-	expression tag	UNP P11110
B	311	HIS	-	expression tag	UNP P11110
B	312	HIS	-	expression tag	UNP P11110
B	313	HIS	-	expression tag	UNP P11110
B	314	HIS	-	expression tag	UNP P11110
B	315	HIS	-	expression tag	UNP P11110
E	310	HIS	-	expression tag	UNP P11110
E	311	HIS	-	expression tag	UNP P11110
E	312	HIS	-	expression tag	UNP P11110
E	313	HIS	-	expression tag	UNP P11110
E	314	HIS	-	expression tag	UNP P11110
E	315	HIS	-	expression tag	UNP P11110
D	310	HIS	-	expression tag	UNP P11110
D	311	HIS	-	expression tag	UNP P11110
D	312	HIS	-	expression tag	UNP P11110
D	313	HIS	-	expression tag	UNP P11110
D	314	HIS	-	expression tag	UNP P11110
D	315	HIS	-	expression tag	UNP P11110
G	310	HIS	-	expression tag	UNP P11110
G	311	HIS	-	expression tag	UNP P11110
G	312	HIS	-	expression tag	UNP P11110
G	313	HIS	-	expression tag	UNP P11110
G	314	HIS	-	expression tag	UNP P11110
G	315	HIS	-	expression tag	UNP P11110
F	310	HIS	-	expression tag	UNP P11110
F	311	HIS	-	expression tag	UNP P11110
F	312	HIS	-	expression tag	UNP P11110
F	313	HIS	-	expression tag	UNP P11110
F	314	HIS	-	expression tag	UNP P11110
F	315	HIS	-	expression tag	UNP P11110

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Chain	Residue	Modelled	Actual	Comment	Reference
I	310	HIS	-	expression tag	UNP P11110
I	311	HIS	-	expression tag	UNP P11110
I	312	HIS	-	expression tag	UNP P11110
I	313	HIS	-	expression tag	UNP P11110
I	314	HIS	-	expression tag	UNP P11110
I	315	HIS	-	expression tag	UNP P11110
H	310	HIS	-	expression tag	UNP P11110
H	311	HIS	-	expression tag	UNP P11110
H	312	HIS	-	expression tag	UNP P11110
H	313	HIS	-	expression tag	UNP P11110
H	314	HIS	-	expression tag	UNP P11110
H	315	HIS	-	expression tag	UNP P11110
K	310	HIS	-	expression tag	UNP P11110
K	311	HIS	-	expression tag	UNP P11110
K	312	HIS	-	expression tag	UNP P11110
K	313	HIS	-	expression tag	UNP P11110
K	314	HIS	-	expression tag	UNP P11110
K	315	HIS	-	expression tag	UNP P11110
J	310	HIS	-	expression tag	UNP P11110
J	311	HIS	-	expression tag	UNP P11110
J	312	HIS	-	expression tag	UNP P11110
J	313	HIS	-	expression tag	UNP P11110
J	314	HIS	-	expression tag	UNP P11110
J	315	HIS	-	expression tag	UNP P11110

- Molecule 2 is a protein called Neck protein gp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	165	Total	C	N	O	S	0	0
			1334	860	219	252	3		
2	N	165	Total	C	N	O	S	0	0
			1334	860	219	252	3		
2	O	165	Total	C	N	O	S	0	0
			1334	860	219	252	3		
2	P	165	Total	C	N	O	S	0	0
			1334	860	219	252	3		
2	Q	165	Total	C	N	O	S	0	0
			1334	860	219	252	3		
2	R	165	Total	C	N	O	S	0	0
			1334	860	219	252	3		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-8	HIS	-	expression tag	UNP P11111
M	-7	HIS	-	expression tag	UNP P11111
M	-6	HIS	-	expression tag	UNP P11111
M	-5	HIS	-	expression tag	UNP P11111
M	-4	HIS	-	expression tag	UNP P11111
M	-3	HIS	-	expression tag	UNP P11111
M	-2	SER	-	expression tag	UNP P11111
M	-1	SER	-	expression tag	UNP P11111
M	0	GLY	-	expression tag	UNP P11111
N	-8	HIS	-	expression tag	UNP P11111
N	-7	HIS	-	expression tag	UNP P11111
N	-6	HIS	-	expression tag	UNP P11111
N	-5	HIS	-	expression tag	UNP P11111
N	-4	HIS	-	expression tag	UNP P11111
N	-3	HIS	-	expression tag	UNP P11111
N	-2	SER	-	expression tag	UNP P11111
N	-1	SER	-	expression tag	UNP P11111
N	0	GLY	-	expression tag	UNP P11111
O	-8	HIS	-	expression tag	UNP P11111
O	-7	HIS	-	expression tag	UNP P11111
O	-6	HIS	-	expression tag	UNP P11111
O	-5	HIS	-	expression tag	UNP P11111
O	-4	HIS	-	expression tag	UNP P11111
O	-3	HIS	-	expression tag	UNP P11111
O	-2	SER	-	expression tag	UNP P11111
O	-1	SER	-	expression tag	UNP P11111
O	0	GLY	-	expression tag	UNP P11111
P	-8	HIS	-	expression tag	UNP P11111
P	-7	HIS	-	expression tag	UNP P11111
P	-6	HIS	-	expression tag	UNP P11111
P	-5	HIS	-	expression tag	UNP P11111
P	-4	HIS	-	expression tag	UNP P11111
P	-3	HIS	-	expression tag	UNP P11111
P	-2	SER	-	expression tag	UNP P11111
P	-1	SER	-	expression tag	UNP P11111
P	0	GLY	-	expression tag	UNP P11111
Q	-8	HIS	-	expression tag	UNP P11111
Q	-7	HIS	-	expression tag	UNP P11111
Q	-6	HIS	-	expression tag	UNP P11111
Q	-5	HIS	-	expression tag	UNP P11111
Q	-4	HIS	-	expression tag	UNP P11111
Q	-3	HIS	-	expression tag	UNP P11111
Q	-2	SER	-	expression tag	UNP P11111

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-1	SER	-	expression tag	UNP P11111
Q	0	GLY	-	expression tag	UNP P11111
R	-8	HIS	-	expression tag	UNP P11111
R	-7	HIS	-	expression tag	UNP P11111
R	-6	HIS	-	expression tag	UNP P11111
R	-5	HIS	-	expression tag	UNP P11111
R	-4	HIS	-	expression tag	UNP P11111
R	-3	HIS	-	expression tag	UNP P11111
R	-2	SER	-	expression tag	UNP P11111
R	-1	SER	-	expression tag	UNP P11111
R	0	GLY	-	expression tag	UNP P11111

- Molecule 3 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	420	Total	C	N	O	S	0	0
			3427	2165	602	641	19		
3	l	420	Total	C	N	O	S	0	0
			3427	2165	602	641	19		
3	k	420	Total	C	N	O	S	0	0
			3427	2165	602	641	19		
3	j	420	Total	C	N	O	S	0	0
			3427	2165	602	641	19		
3	i	420	Total	C	N	O	S	0	0
			3427	2165	602	641	19		
3	h	420	Total	C	N	O	S	0	0
			3427	2165	602	641	19		
3	g	420	Total	C	N	O	S	0	0
			3427	2165	602	641	19		
3	f	420	Total	C	N	O	S	0	0
			3427	2165	602	641	19		
3	e	420	Total	C	N	O	S	0	0
			3427	2165	602	641	19		
3	d	420	Total	C	N	O	S	0	0
			3427	2165	602	641	19		
3	c	420	Total	C	N	O	S	0	0
			3427	2165	602	641	19		
3	b	420	Total	C	N	O	S	0	0
			3427	2165	602	641	19		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	525	SER	-	expression tag	UNP A0A7S9SW10
a	526	SER	-	expression tag	UNP A0A7S9SW10
a	527	GLY	-	expression tag	UNP A0A7S9SW10
a	528	HIS	-	expression tag	UNP A0A7S9SW10
a	529	HIS	-	expression tag	UNP A0A7S9SW10
a	530	HIS	-	expression tag	UNP A0A7S9SW10
a	531	HIS	-	expression tag	UNP A0A7S9SW10
a	532	HIS	-	expression tag	UNP A0A7S9SW10
a	533	HIS	-	expression tag	UNP A0A7S9SW10
l	525	SER	-	expression tag	UNP A0A7S9SW10
l	526	SER	-	expression tag	UNP A0A7S9SW10
l	527	GLY	-	expression tag	UNP A0A7S9SW10
l	528	HIS	-	expression tag	UNP A0A7S9SW10
l	529	HIS	-	expression tag	UNP A0A7S9SW10
l	530	HIS	-	expression tag	UNP A0A7S9SW10
l	531	HIS	-	expression tag	UNP A0A7S9SW10
l	532	HIS	-	expression tag	UNP A0A7S9SW10
l	533	HIS	-	expression tag	UNP A0A7S9SW10
k	525	SER	-	expression tag	UNP A0A7S9SW10
k	526	SER	-	expression tag	UNP A0A7S9SW10
k	527	GLY	-	expression tag	UNP A0A7S9SW10
k	528	HIS	-	expression tag	UNP A0A7S9SW10
k	529	HIS	-	expression tag	UNP A0A7S9SW10
k	530	HIS	-	expression tag	UNP A0A7S9SW10
k	531	HIS	-	expression tag	UNP A0A7S9SW10
k	532	HIS	-	expression tag	UNP A0A7S9SW10
k	533	HIS	-	expression tag	UNP A0A7S9SW10
j	525	SER	-	expression tag	UNP A0A7S9SW10
j	526	SER	-	expression tag	UNP A0A7S9SW10
j	527	GLY	-	expression tag	UNP A0A7S9SW10
j	528	HIS	-	expression tag	UNP A0A7S9SW10
j	529	HIS	-	expression tag	UNP A0A7S9SW10
j	530	HIS	-	expression tag	UNP A0A7S9SW10
j	531	HIS	-	expression tag	UNP A0A7S9SW10
j	532	HIS	-	expression tag	UNP A0A7S9SW10
j	533	HIS	-	expression tag	UNP A0A7S9SW10
i	525	SER	-	expression tag	UNP A0A7S9SW10
i	526	SER	-	expression tag	UNP A0A7S9SW10
i	527	GLY	-	expression tag	UNP A0A7S9SW10
i	528	HIS	-	expression tag	UNP A0A7S9SW10
i	529	HIS	-	expression tag	UNP A0A7S9SW10
i	530	HIS	-	expression tag	UNP A0A7S9SW10
i	531	HIS	-	expression tag	UNP A0A7S9SW10

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Chain	Residue	Modelled	Actual	Comment	Reference
i	532	HIS	-	expression tag	UNP A0A7S9SW10
i	533	HIS	-	expression tag	UNP A0A7S9SW10
h	525	SER	-	expression tag	UNP A0A7S9SW10
h	526	SER	-	expression tag	UNP A0A7S9SW10
h	527	GLY	-	expression tag	UNP A0A7S9SW10
h	528	HIS	-	expression tag	UNP A0A7S9SW10
h	529	HIS	-	expression tag	UNP A0A7S9SW10
h	530	HIS	-	expression tag	UNP A0A7S9SW10
h	531	HIS	-	expression tag	UNP A0A7S9SW10
h	532	HIS	-	expression tag	UNP A0A7S9SW10
h	533	HIS	-	expression tag	UNP A0A7S9SW10
g	525	SER	-	expression tag	UNP A0A7S9SW10
g	526	SER	-	expression tag	UNP A0A7S9SW10
g	527	GLY	-	expression tag	UNP A0A7S9SW10
g	528	HIS	-	expression tag	UNP A0A7S9SW10
g	529	HIS	-	expression tag	UNP A0A7S9SW10
g	530	HIS	-	expression tag	UNP A0A7S9SW10
g	531	HIS	-	expression tag	UNP A0A7S9SW10
g	532	HIS	-	expression tag	UNP A0A7S9SW10
g	533	HIS	-	expression tag	UNP A0A7S9SW10
f	525	SER	-	expression tag	UNP A0A7S9SW10
f	526	SER	-	expression tag	UNP A0A7S9SW10
f	527	GLY	-	expression tag	UNP A0A7S9SW10
f	528	HIS	-	expression tag	UNP A0A7S9SW10
f	529	HIS	-	expression tag	UNP A0A7S9SW10
f	530	HIS	-	expression tag	UNP A0A7S9SW10
f	531	HIS	-	expression tag	UNP A0A7S9SW10
f	532	HIS	-	expression tag	UNP A0A7S9SW10
f	533	HIS	-	expression tag	UNP A0A7S9SW10
e	525	SER	-	expression tag	UNP A0A7S9SW10
e	526	SER	-	expression tag	UNP A0A7S9SW10
e	527	GLY	-	expression tag	UNP A0A7S9SW10
e	528	HIS	-	expression tag	UNP A0A7S9SW10
e	529	HIS	-	expression tag	UNP A0A7S9SW10
e	530	HIS	-	expression tag	UNP A0A7S9SW10
e	531	HIS	-	expression tag	UNP A0A7S9SW10
e	532	HIS	-	expression tag	UNP A0A7S9SW10
e	533	HIS	-	expression tag	UNP A0A7S9SW10
d	525	SER	-	expression tag	UNP A0A7S9SW10
d	526	SER	-	expression tag	UNP A0A7S9SW10
d	527	GLY	-	expression tag	UNP A0A7S9SW10
d	528	HIS	-	expression tag	UNP A0A7S9SW10

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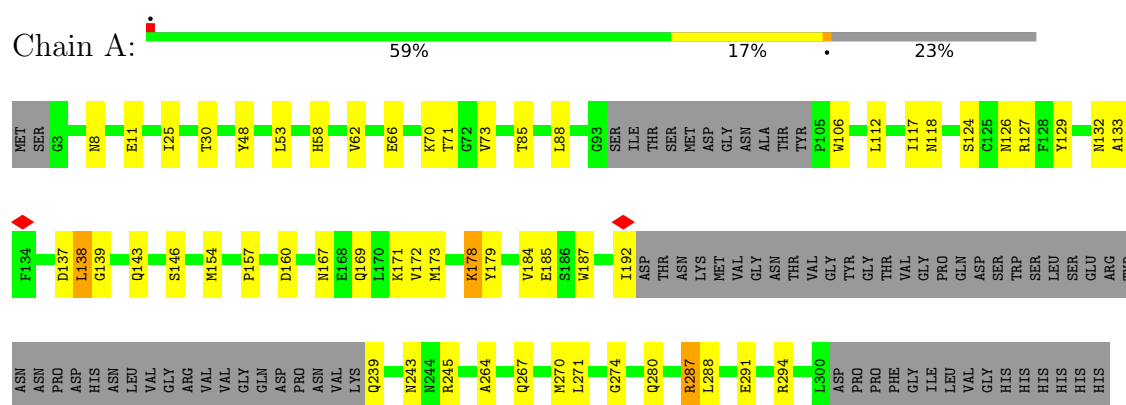
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
d	529	HIS	-	expression tag	UNP A0A7S9SW10
d	530	HIS	-	expression tag	UNP A0A7S9SW10
d	531	HIS	-	expression tag	UNP A0A7S9SW10
d	532	HIS	-	expression tag	UNP A0A7S9SW10
d	533	HIS	-	expression tag	UNP A0A7S9SW10
c	525	SER	-	expression tag	UNP A0A7S9SW10
c	526	SER	-	expression tag	UNP A0A7S9SW10
c	527	GLY	-	expression tag	UNP A0A7S9SW10
c	528	HIS	-	expression tag	UNP A0A7S9SW10
c	529	HIS	-	expression tag	UNP A0A7S9SW10
c	530	HIS	-	expression tag	UNP A0A7S9SW10
c	531	HIS	-	expression tag	UNP A0A7S9SW10
c	532	HIS	-	expression tag	UNP A0A7S9SW10
c	533	HIS	-	expression tag	UNP A0A7S9SW10
b	525	SER	-	expression tag	UNP A0A7S9SW10
b	526	SER	-	expression tag	UNP A0A7S9SW10
b	527	GLY	-	expression tag	UNP A0A7S9SW10
b	528	HIS	-	expression tag	UNP A0A7S9SW10
b	529	HIS	-	expression tag	UNP A0A7S9SW10
b	530	HIS	-	expression tag	UNP A0A7S9SW10
b	531	HIS	-	expression tag	UNP A0A7S9SW10
b	532	HIS	-	expression tag	UNP A0A7S9SW10
b	533	HIS	-	expression tag	UNP A0A7S9SW10

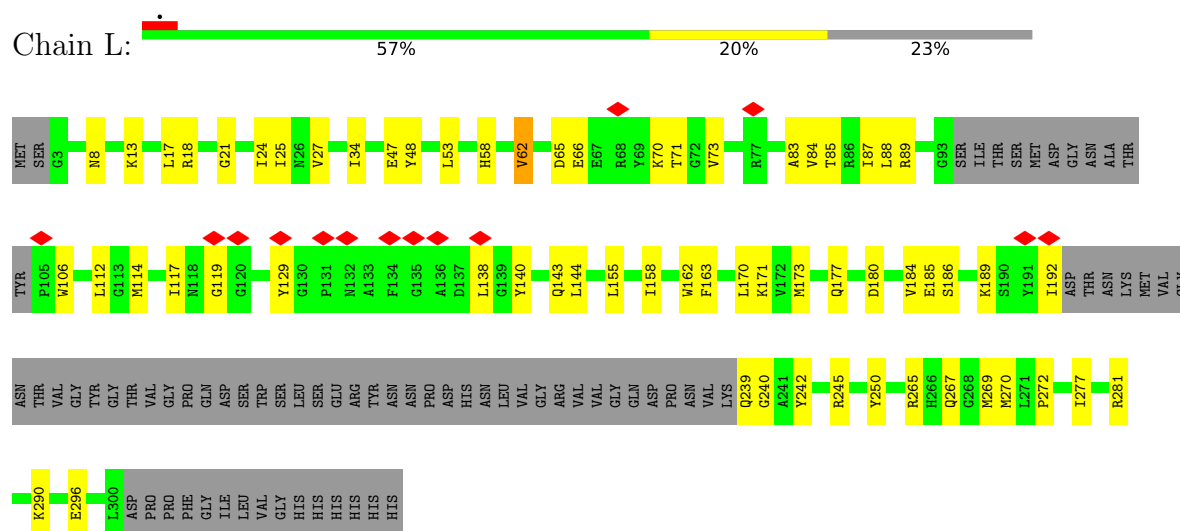
### 3 Residue-property plots

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: Neck protein gp13

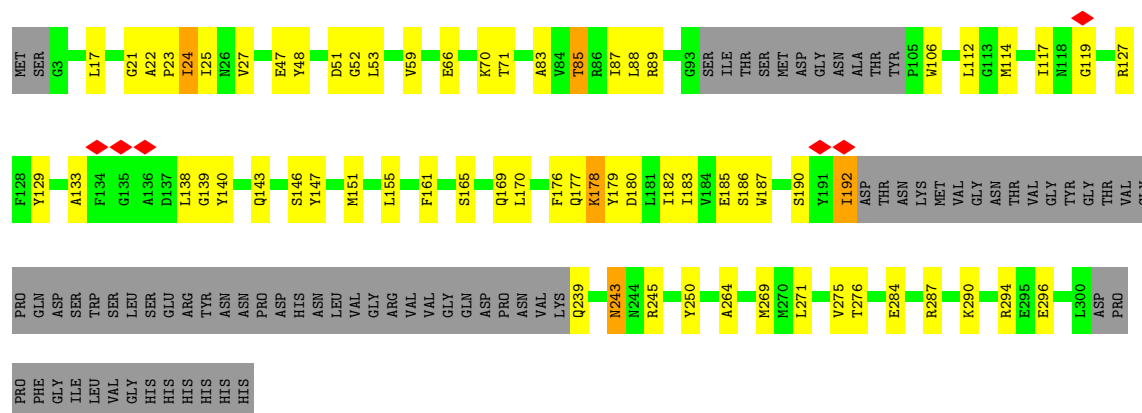


#### • Molecule 1: Neck protein gp13

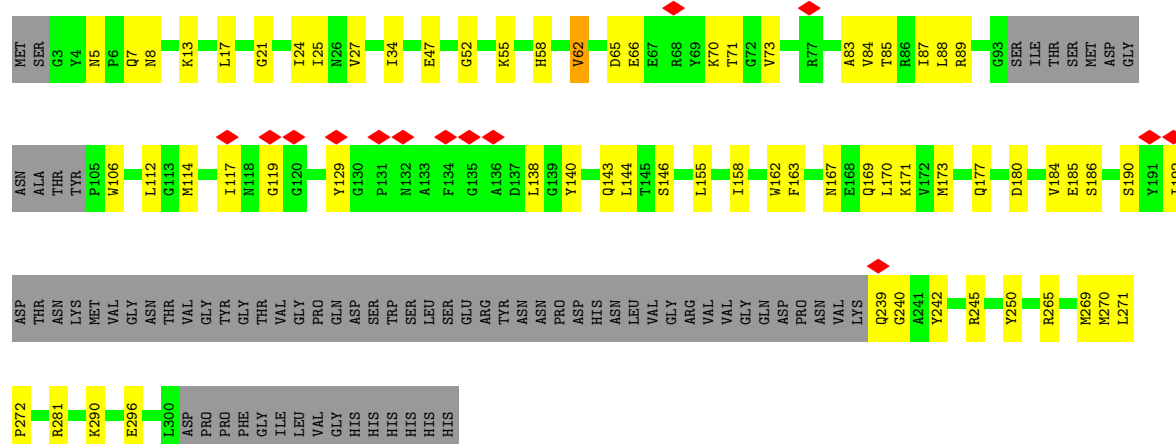


#### • Molecule 1: Neck protein gp13

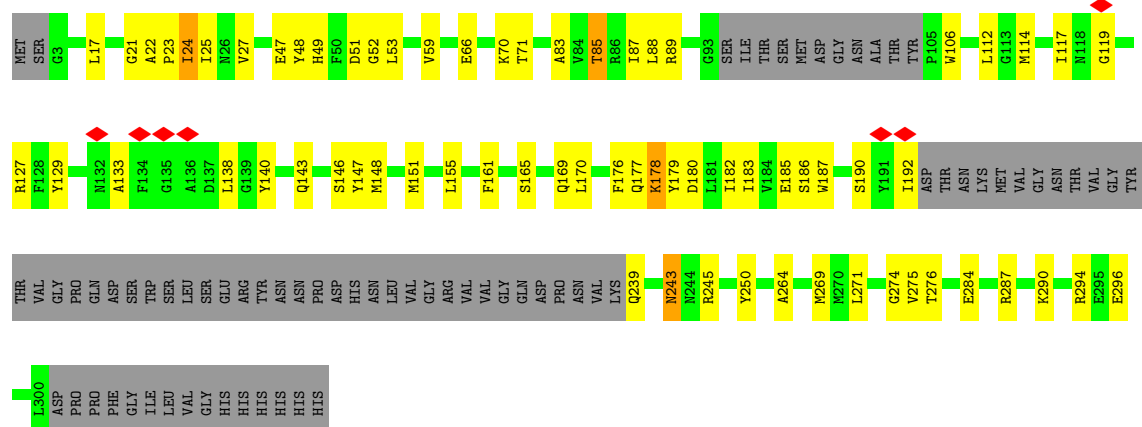




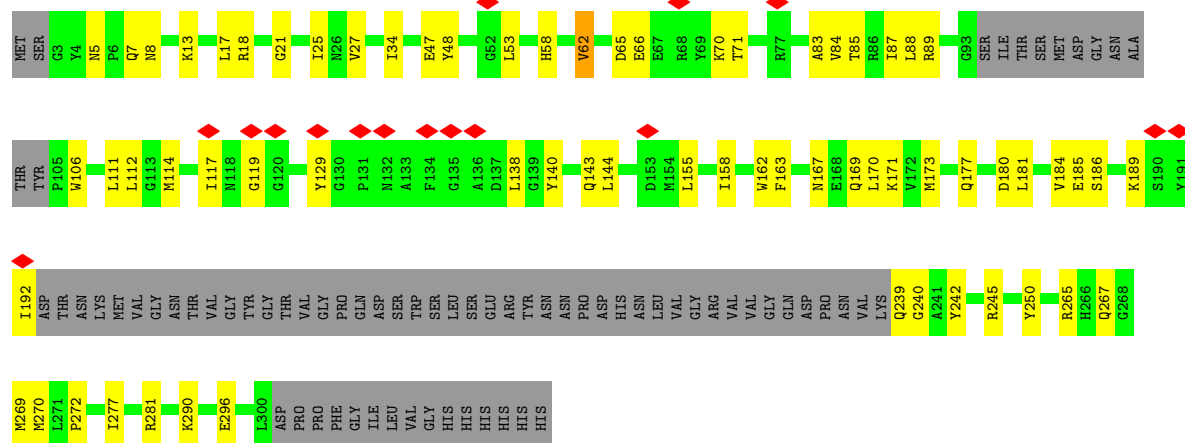
### • Molecule 1: Neck protein gp13



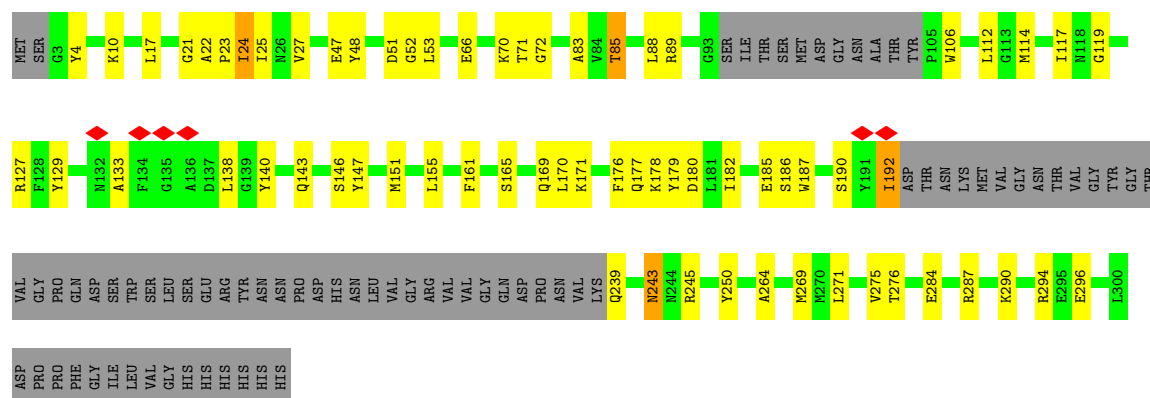
### • Molecule 1: Neck protein gp13



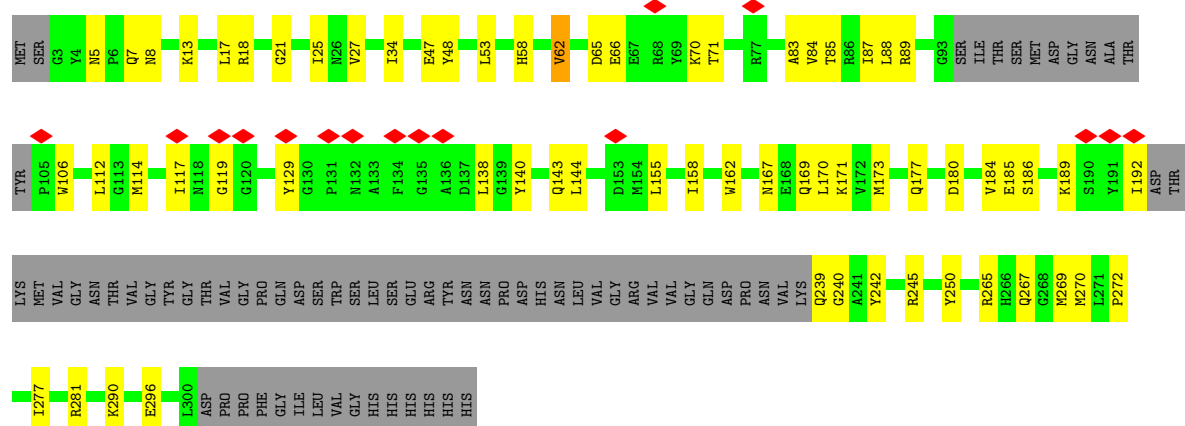
### • Molecule 1: Neck protein gp13



• Molecule 1: Neck protein gp13



• Molecule 1: Neck protein gp13



Chain I:

Chain H:

56% 21% 23%

ALA THR TYR P105 P106 L112 G113 M114 L117 M118 G119 G120 Y129 G130 P131 N132 A133 F134 G135 A136 D137 L138 G139 Y140 Q143 L144 T145 S146 D153 M154 L155 I158 W162 F163 N167 P168 Q169 L170 K171 V172 M173 Q177 D180 V184 E185 S186 K189

M270 L271 P272 I277 R281 K290 E296 L300 ASP PRO PHE ILE LEU VAL GLY HIS HIS HIS HIS HIS HIS

ASP G3 Y4 N5 F6 Q7 N8 K13 L17 R18 G21 T25 N26 V27 I34 Q39 E47 Y48 L53 H58 V62 D65 E66 E67 R68 F69 K70 T71 R77 A83 R84 T85 R86 I87 L88 R89 G93 SER ILE THR SER MET ASP GLY ASN

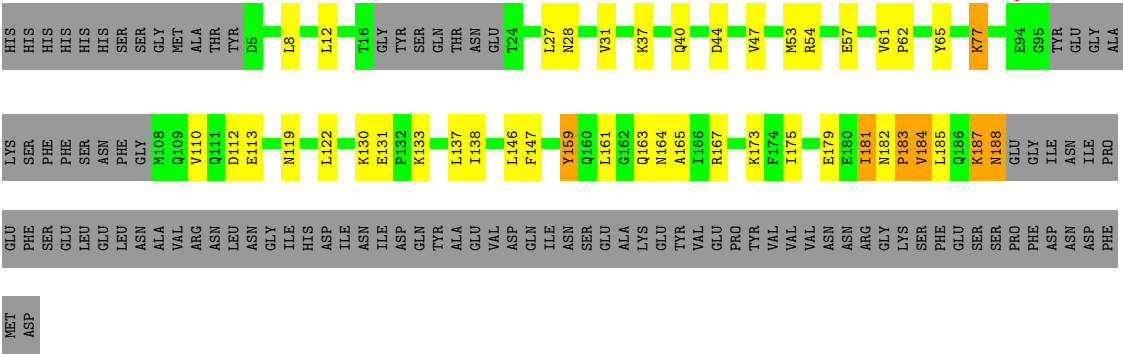
Chain K:

56% 19% 23%

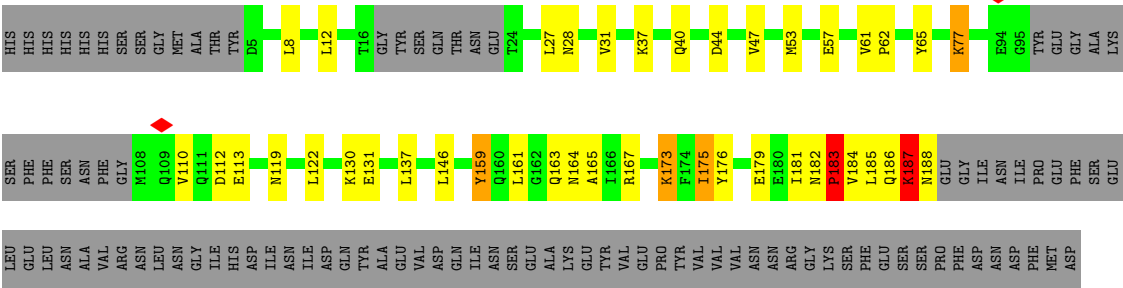
Sequence logo for Chain K, showing amino acid conservation across three regions. The top bar chart indicates overall conservation percentages: 56% (green), 19% (yellow), and 23% (grey). The sequence logo below shows specific amino acid preferences at each position, with color-coded bars indicating conservation levels. Red diamonds highlight specific positions of interest.



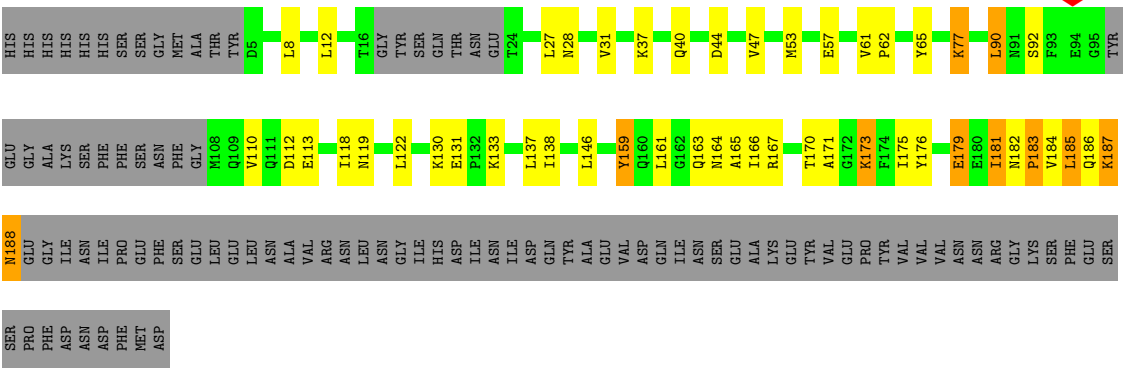




• Molecule 2: Neck protein gp14

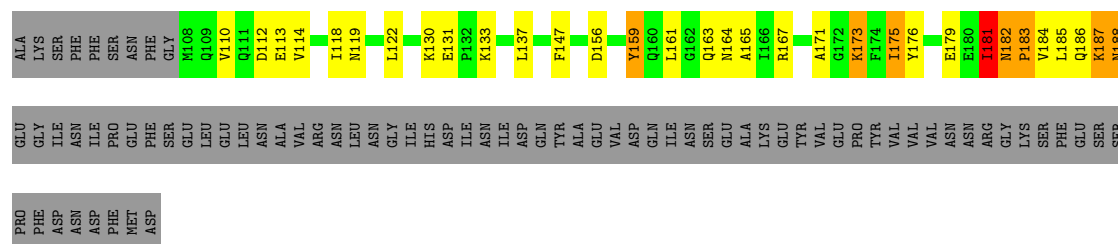


• Molecule 2: Neck protein gp14

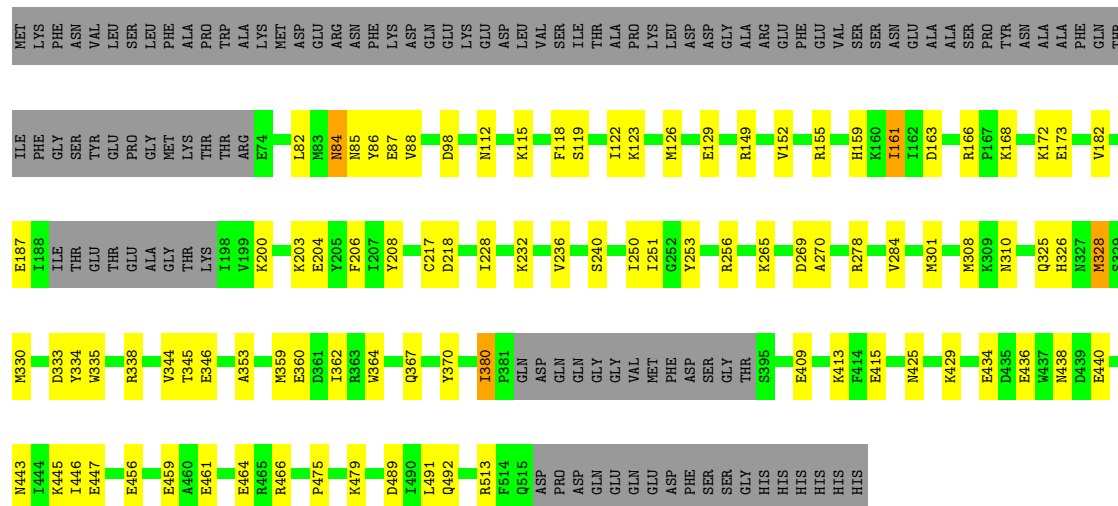


• Molecule 2: Neck protein gp14

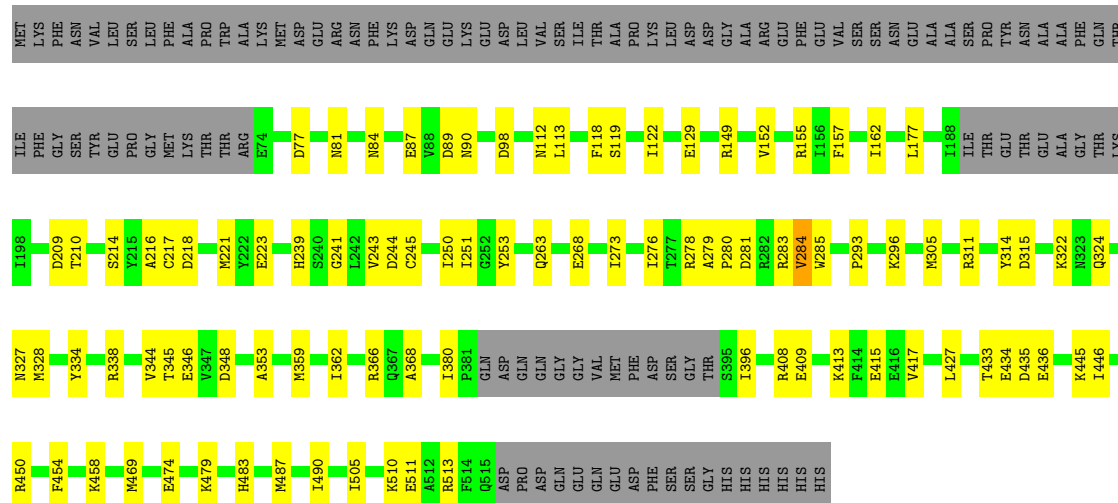




- Molecule 3: Portal protein



- Molecule 3: Portal protein

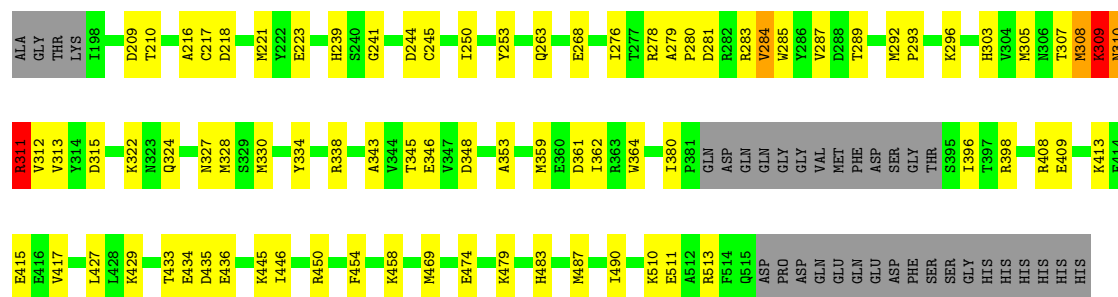


- Molecule 3: Portal protein



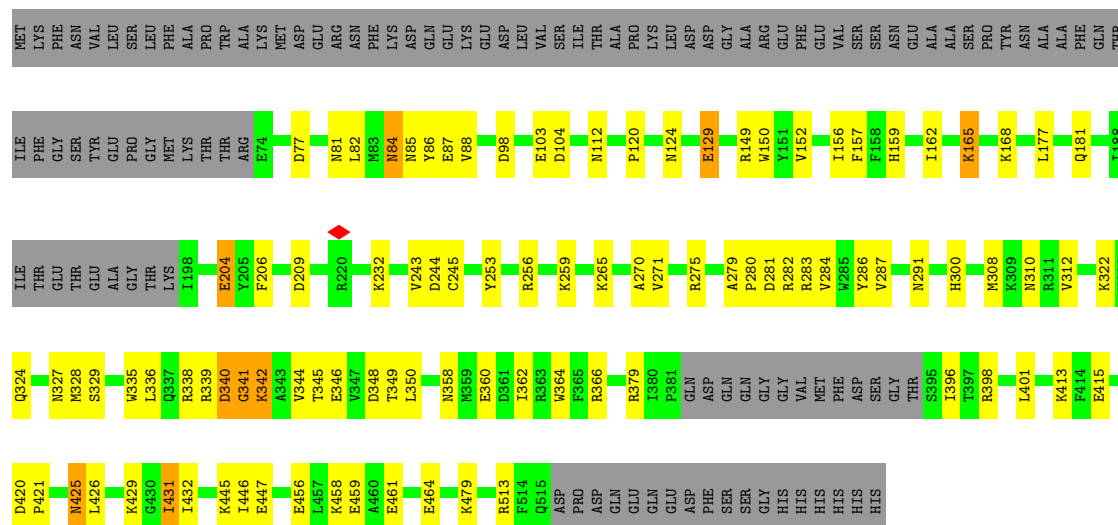






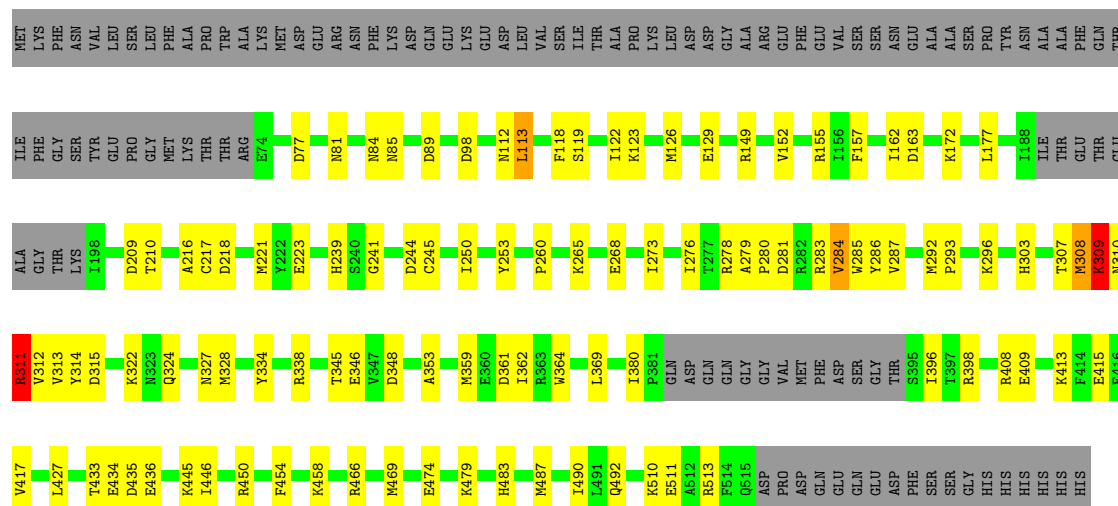
• Molecule 3: Portal protein

Chain e: 60% 17% 21%



• Molecule 3: Portal protein

Chain d: 59% 19% 21%



• Molecule 3: Portal protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13381	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	53	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	17.267	Depositor
Minimum map value	-0.383	Depositor
Average map value	0.101	Depositor
Map value standard deviation	0.843	Depositor
Recommended contour level	0.487	Depositor
Map size (Å)	334.72, 334.72, 334.72	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.046, 1.046, 1.046	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.13	0/1981	0.39	0/2674
1	B	0.09	0/1981	0.23	0/2674
1	C	0.08	0/1981	0.24	0/2674
1	D	0.09	0/1981	0.23	0/2674
1	E	0.08	0/1981	0.23	0/2674
1	F	0.09	0/1981	0.23	0/2674
1	G	0.08	0/1981	0.23	0/2674
1	H	0.09	0/1981	0.23	0/2674
1	I	0.08	0/1981	0.25	0/2674
1	J	0.09	0/1981	0.24	0/2674
1	K	0.08	0/1981	0.25	0/2674
1	L	0.09	0/1981	0.23	0/2674
2	M	0.32	0/1365	0.55	1/1849 (0.1%)
2	N	0.30	0/1365	0.50	1/1849 (0.1%)
2	O	0.28	0/1365	0.56	3/1849 (0.2%)
2	P	0.30	0/1365	0.52	1/1849 (0.1%)
2	Q	0.31	0/1365	0.46	1/1849 (0.1%)
2	R	0.30	0/1365	0.50	1/1849 (0.1%)
3	a	0.17	0/3491	0.41	0/4705
3	b	0.08	0/3491	0.24	0/4705
3	c	0.08	0/3491	0.25	0/4705
3	d	0.14	0/3491	0.30	0/4705
3	e	0.15	0/3491	0.31	0/4705
3	f	0.15	0/3491	0.29	0/4705
3	g	0.16	0/3491	0.32	0/4705
3	h	0.14	0/3491	0.28	0/4705
3	i	0.08	0/3491	0.24	0/4705
3	j	0.14	0/3491	0.28	0/4705
3	k	0.08	0/3491	0.25	0/4705
3	l	0.08	0/3491	0.24	0/4705
All	All	0.15	0/73854	0.31	8/99642 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	d	0	1
3	e	0	1
3	f	0	1
3	g	0	2
3	h	0	1
3	j	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	183	PRO	N-CA-C	6.65	122.10	111.26
2	O	183	PRO	N-CA-C	6.57	121.53	111.15
2	M	183	PRO	N-CA-C	6.41	121.14	111.14
2	N	183	PRO	N-CA-C	6.02	120.65	111.19
2	R	183	PRO	N-CA-C	5.98	120.25	111.03

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	f	311	ARG	Sidechain
3	g	338	ARG	Sidechain
3	g	339	ARG	Sidechain
3	h	311	ARG	Sidechain
3	j	311	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1937	0	1886	38	0
1	B	1937	0	1886	48	0
1	C	1937	0	1886	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1937	0	1886	46	0
1	E	1937	0	1886	49	0
1	F	1937	0	1886	44	0
1	G	1937	0	1886	49	0
1	H	1937	0	1886	44	0
1	I	1937	0	1886	46	0
1	J	1937	0	1886	50	0
1	K	1937	0	1886	46	0
1	L	1937	0	1886	44	0
2	M	1334	0	1282	33	0
2	N	1334	0	1282	34	0
2	O	1334	0	1282	37	0
2	P	1334	0	1282	38	0
2	Q	1334	0	1282	34	0
2	R	1334	0	1282	37	0
3	a	3427	0	3378	57	0
3	b	3427	0	3378	56	0
3	c	3427	0	3378	56	0
3	d	3427	0	3378	59	0
3	e	3427	0	3378	61	0
3	f	3427	0	3378	62	0
3	g	3427	0	3378	72	0
3	h	3427	0	3378	60	0
3	i	3427	0	3378	64	0
3	j	3427	0	3378	60	0
3	k	3427	0	3378	58	0
3	l	3427	0	3378	60	0
All	All	72372	0	70860	1202	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 8.

The worst 5 of 1202 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)
2:P:185:LEU:HD13	3:g:333:ASP:HB3	1.34	1.06
2:O:185:LEU:HD13	3:i:333:ASP:HB3	1.39	1.00
2:O:185:LEU:HD11	3:i:335:TRP:CD1	2.00	0.96
2:O:185:LEU:HD11	3:i:335:TRP:NE1	1.87	0.89
2:P:185:LEU:HD11	3:g:335:TRP:CD1	2.07	0.89

There are no symmetry-related clashes.

## 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	235/315 (75%)	225 (96%)	10 (4%)	0	100	100
1	B	235/315 (75%)	223 (95%)	12 (5%)	0	100	100
1	C	235/315 (75%)	218 (93%)	17 (7%)	0	100	100
1	D	235/315 (75%)	223 (95%)	12 (5%)	0	100	100
1	E	235/315 (75%)	218 (93%)	17 (7%)	0	100	100
1	F	235/315 (75%)	223 (95%)	12 (5%)	0	100	100
1	G	235/315 (75%)	217 (92%)	18 (8%)	0	100	100
1	H	235/315 (75%)	223 (95%)	12 (5%)	0	100	100
1	I	235/315 (75%)	218 (93%)	17 (7%)	0	100	100
1	J	235/315 (75%)	223 (95%)	12 (5%)	0	100	100
1	K	235/315 (75%)	217 (92%)	18 (8%)	0	100	100
1	L	235/315 (75%)	222 (94%)	13 (6%)	0	100	100
2	M	159/265 (60%)	146 (92%)	11 (7%)	2 (1%)	9	39
2	N	159/265 (60%)	146 (92%)	9 (6%)	4 (2%)	4	28
2	O	159/265 (60%)	147 (92%)	10 (6%)	2 (1%)	9	39
2	P	159/265 (60%)	150 (94%)	6 (4%)	3 (2%)	6	33
2	Q	159/265 (60%)	149 (94%)	7 (4%)	3 (2%)	6	33
2	R	159/265 (60%)	148 (93%)	8 (5%)	3 (2%)	6	33
3	a	414/533 (78%)	408 (99%)	6 (1%)	0	100	100
3	b	414/533 (78%)	406 (98%)	8 (2%)	0	100	100
3	c	414/533 (78%)	392 (95%)	22 (5%)	0	100	100
3	d	414/533 (78%)	400 (97%)	13 (3%)	1 (0%)	43	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	e	414/533 (78%)	391 (94%)	22 (5%)	1 (0%)	43	74
3	f	414/533 (78%)	404 (98%)	9 (2%)	1 (0%)	43	74
3	g	414/533 (78%)	389 (94%)	23 (6%)	2 (0%)	24	57
3	h	414/533 (78%)	404 (98%)	9 (2%)	1 (0%)	43	74
3	i	414/533 (78%)	392 (95%)	22 (5%)	0	100	100
3	j	414/533 (78%)	403 (97%)	10 (2%)	1 (0%)	43	74
3	k	414/533 (78%)	392 (95%)	22 (5%)	0	100	100
3	l	414/533 (78%)	403 (97%)	11 (3%)	0	100	100
All	All	8742/11766 (74%)	8320 (95%)	398 (5%)	24 (0%)	37	67

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	176	TYR
2	M	187	LYS
3	g	339	ARG
3	g	341	GLY
2	Q	176	TYR

### 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	202/266 (76%)	190 (94%)	12 (6%)	18	45
1	B	202/266 (76%)	195 (96%)	7 (4%)	32	58
1	C	202/266 (76%)	193 (96%)	9 (4%)	24	52
1	D	202/266 (76%)	195 (96%)	7 (4%)	32	58
1	E	202/266 (76%)	192 (95%)	10 (5%)	22	49
1	F	202/266 (76%)	195 (96%)	7 (4%)	32	58
1	G	202/266 (76%)	192 (95%)	10 (5%)	22	49
1	H	202/266 (76%)	195 (96%)	7 (4%)	32	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	202/266 (76%)	193 (96%)	9 (4%)	24	52
1	J	202/266 (76%)	195 (96%)	7 (4%)	32	58
1	K	202/266 (76%)	193 (96%)	9 (4%)	24	52
1	L	202/266 (76%)	195 (96%)	7 (4%)	32	58
2	M	143/237 (60%)	129 (90%)	14 (10%)	7	30
2	N	143/237 (60%)	125 (87%)	18 (13%)	4	22
2	O	143/237 (60%)	131 (92%)	12 (8%)	10	35
2	P	143/237 (60%)	130 (91%)	13 (9%)	9	32
2	Q	143/237 (60%)	126 (88%)	17 (12%)	5	24
2	R	143/237 (60%)	126 (88%)	17 (12%)	5	24
3	a	368/473 (78%)	352 (96%)	16 (4%)	26	52
3	b	368/473 (78%)	355 (96%)	13 (4%)	32	58
3	c	368/473 (78%)	354 (96%)	14 (4%)	29	57
3	d	368/473 (78%)	350 (95%)	18 (5%)	22	50
3	e	368/473 (78%)	351 (95%)	17 (5%)	24	51
3	f	368/473 (78%)	348 (95%)	20 (5%)	20	47
3	g	368/473 (78%)	348 (95%)	20 (5%)	20	47
3	h	368/473 (78%)	350 (95%)	18 (5%)	22	50
3	i	368/473 (78%)	354 (96%)	14 (4%)	29	57
3	j	368/473 (78%)	350 (95%)	18 (5%)	22	50
3	k	368/473 (78%)	352 (96%)	16 (4%)	26	52
3	l	368/473 (78%)	354 (96%)	14 (4%)	29	57
All	All	7698/10290 (75%)	7308 (95%)	390 (5%)	23	49

5 of 390 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	g	243	VAL
2	Q	170	THR
3	g	339	ARG
3	f	510	LYS
3	e	165	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 243 such sidechains are listed below:

Mol	Chain	Res	Type
3	h	85	ASN
1	J	259	ASN
2	P	164	ASN
1	J	175	ASN
3	c	425	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 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.

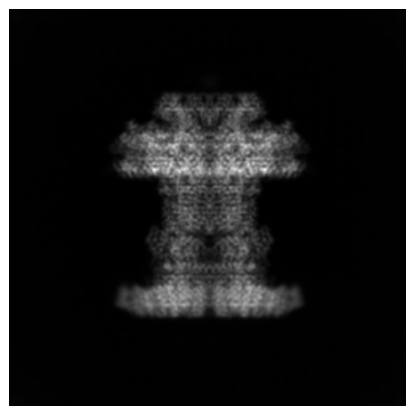
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63390. These allow visual inspection of the internal detail of the map and identification of artifacts.

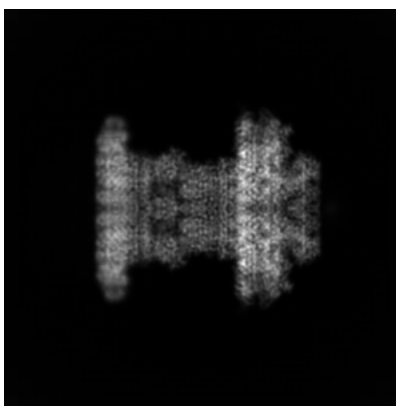
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

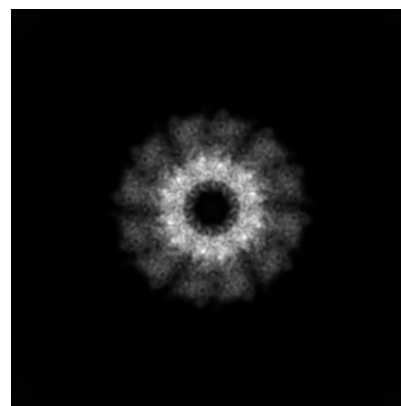
#### 6.1.1 Primary map



X

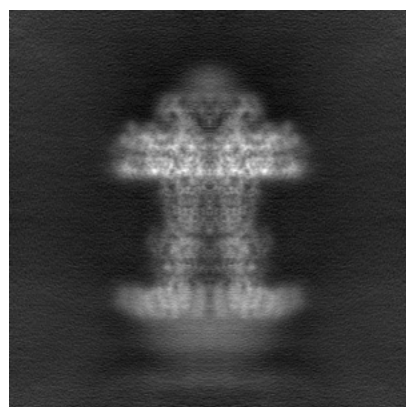


Y

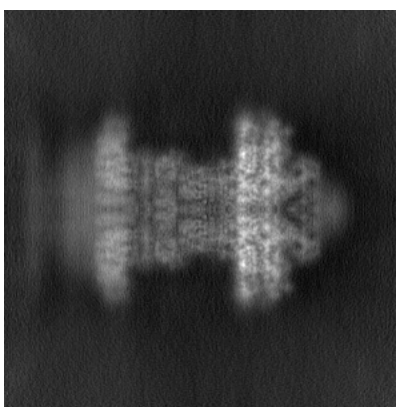


Z

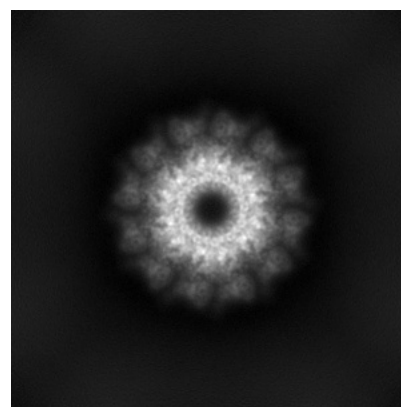
#### 6.1.2 Raw map



X



Y



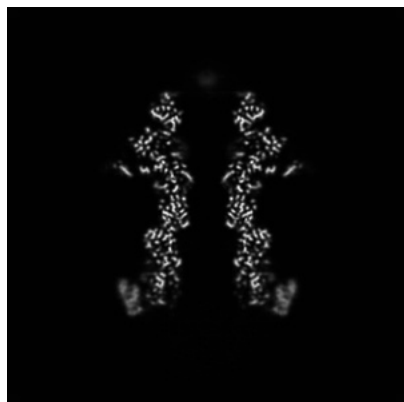
Z

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

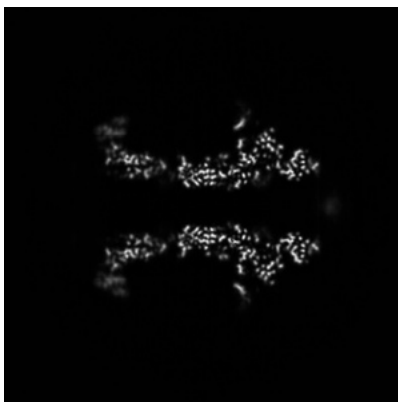


## 6.2 Central slices [i](#)

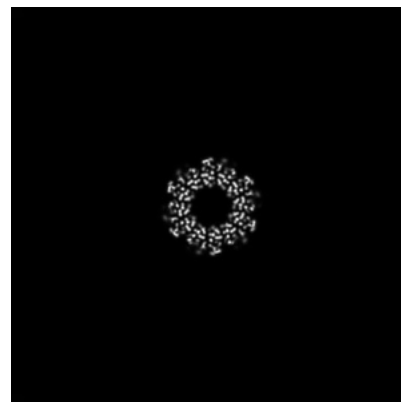
### 6.2.1 Primary map



X Index: 160

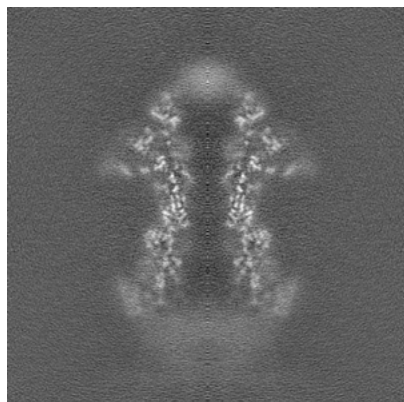


Y Index: 160

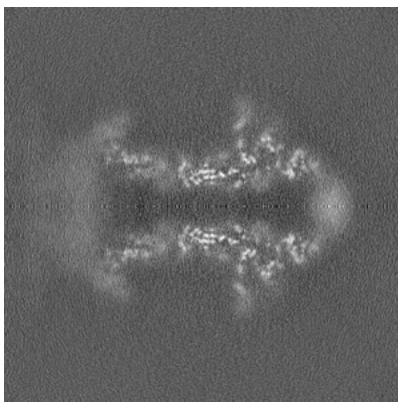


Z Index: 160

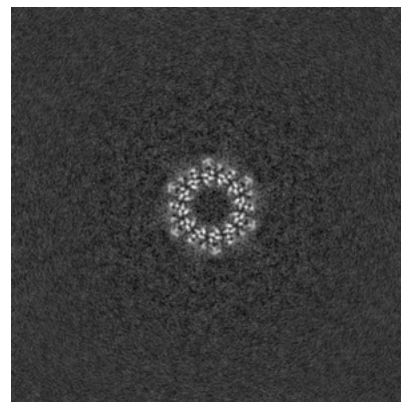
### 6.2.2 Raw map



X Index: 160



Y Index: 160

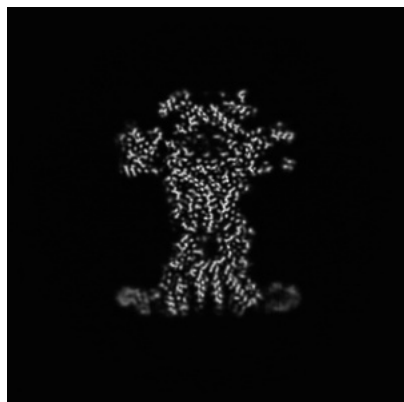


Z Index: 160

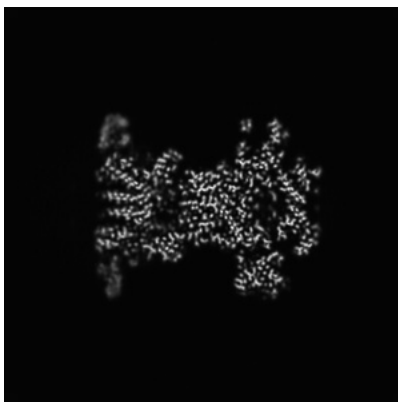
The images above show central slices of the map in three orthogonal directions.

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

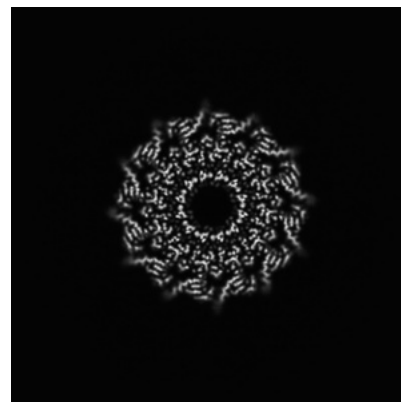
### 6.3.1 Primary map



X Index: 184

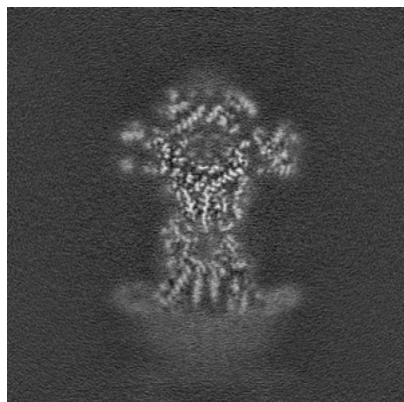


Y Index: 136

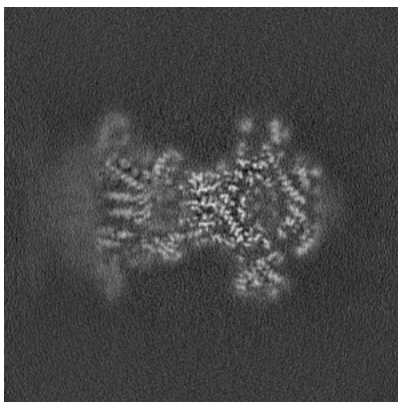


Z Index: 191

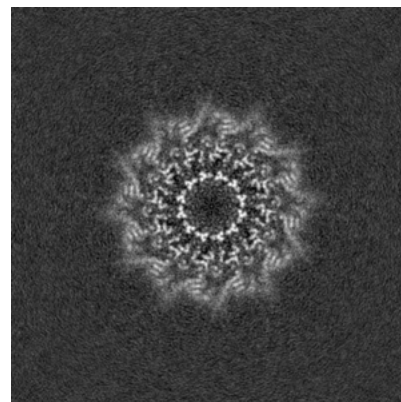
### 6.3.2 Raw map



X Index: 136



Y Index: 136

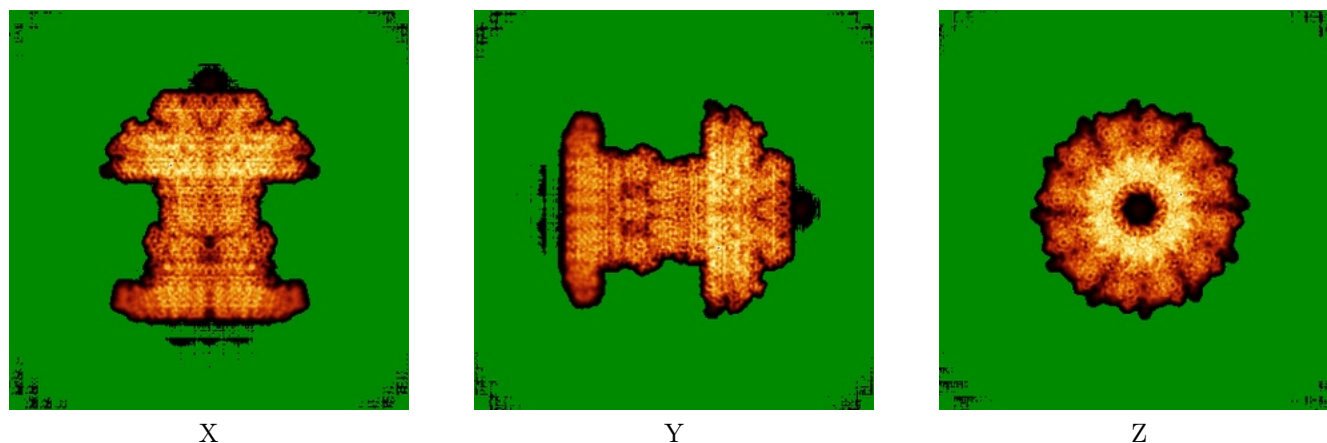


Z Index: 191

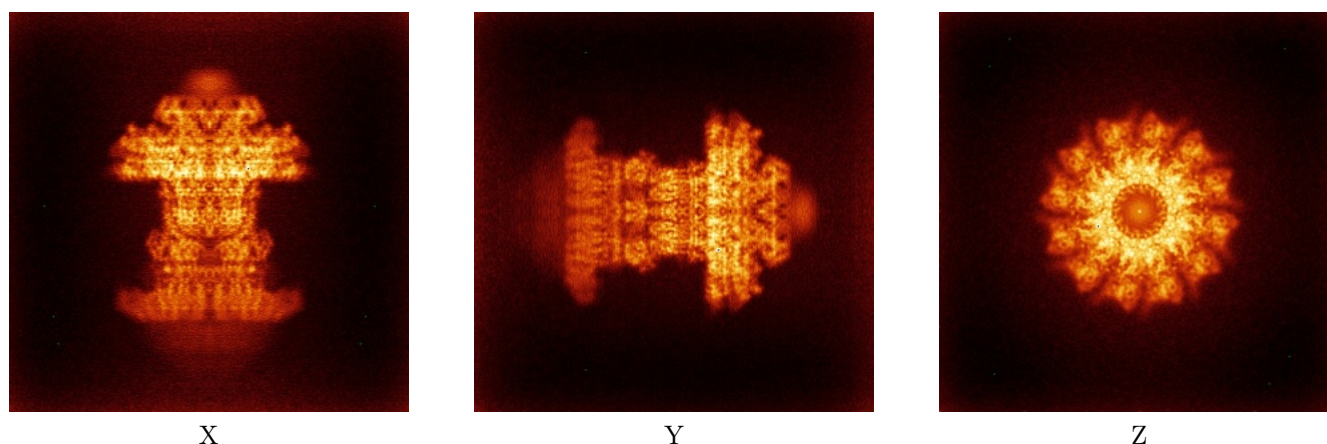
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

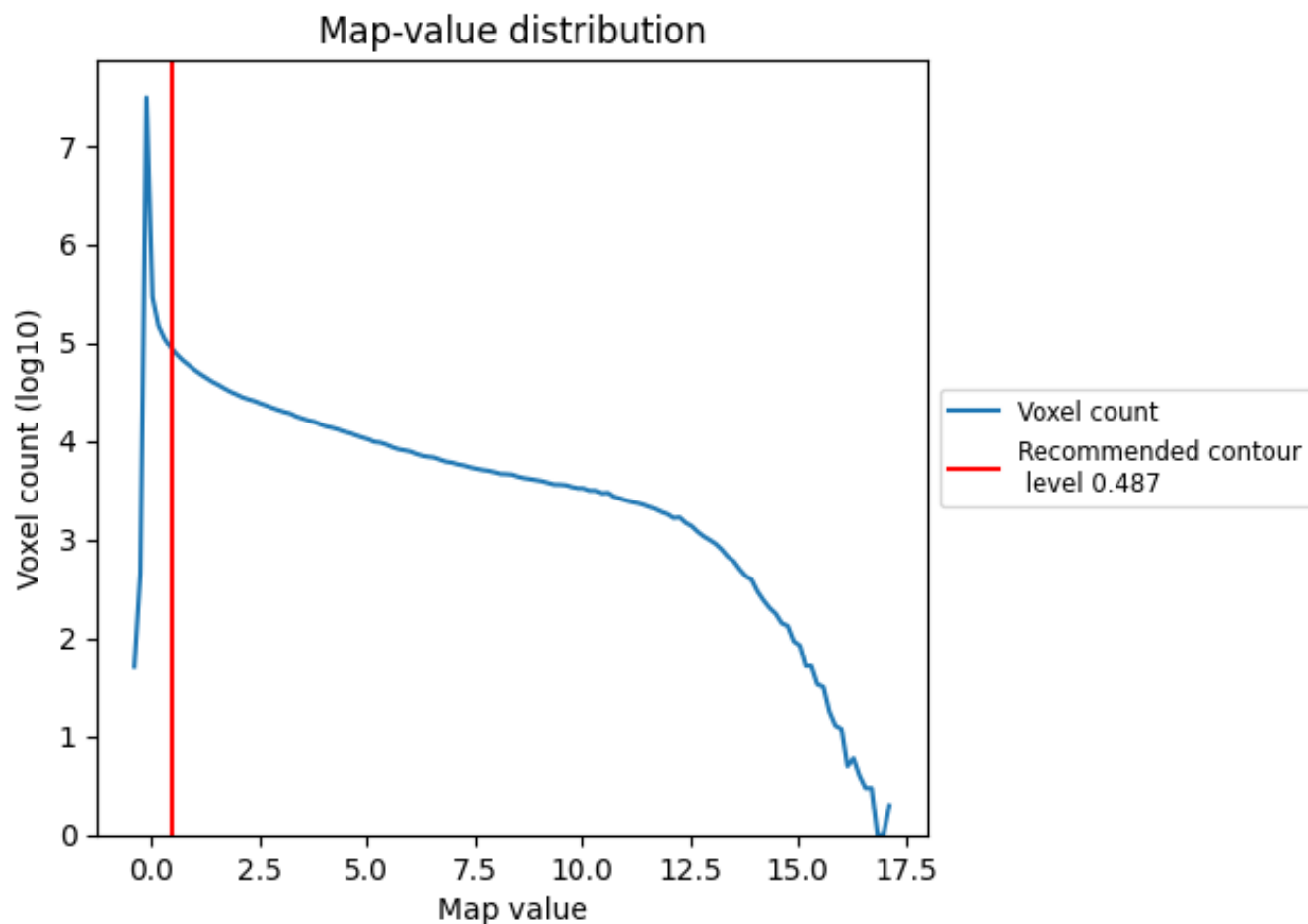
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

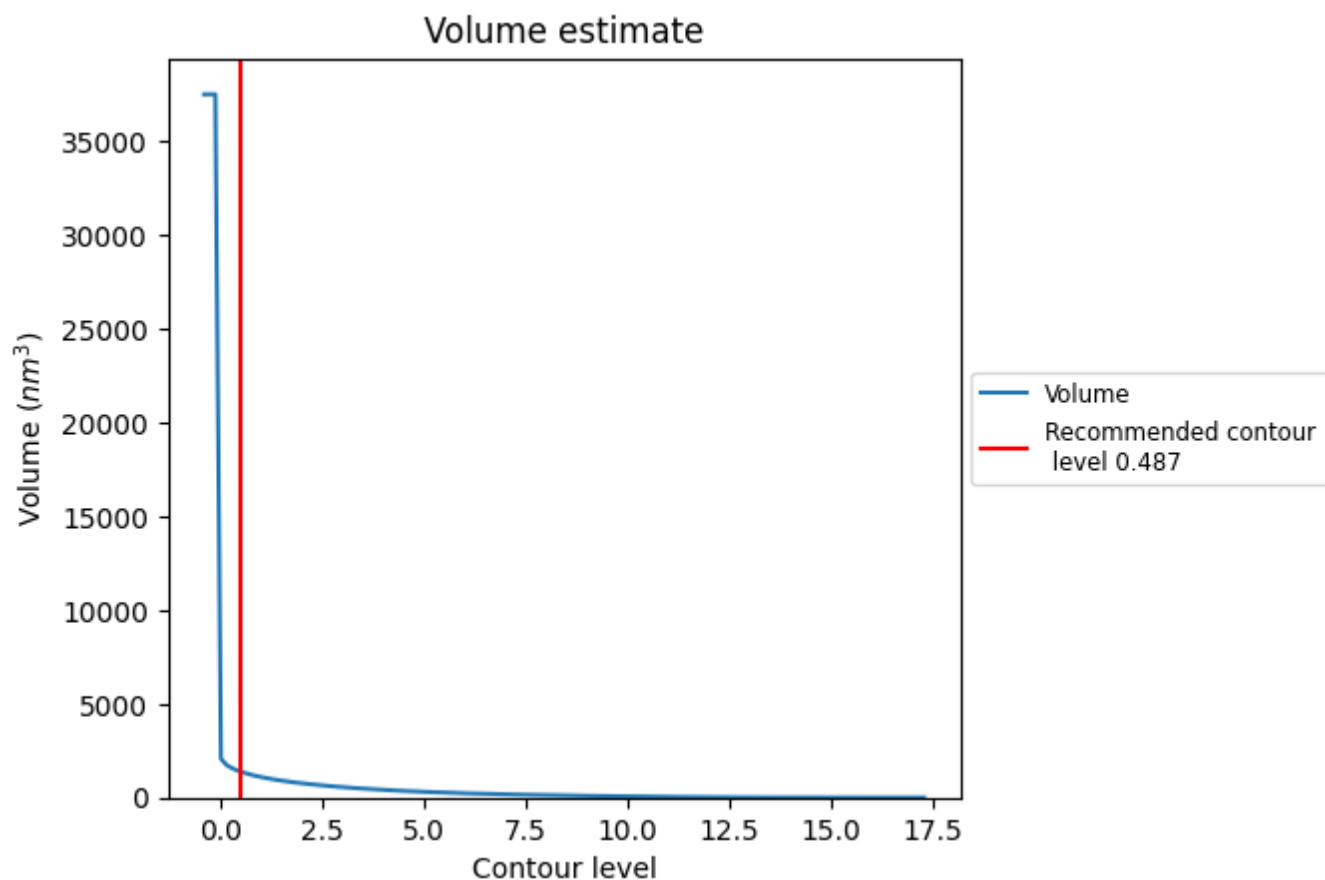
This section contains the results of statistical analysis of the map.

### 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.

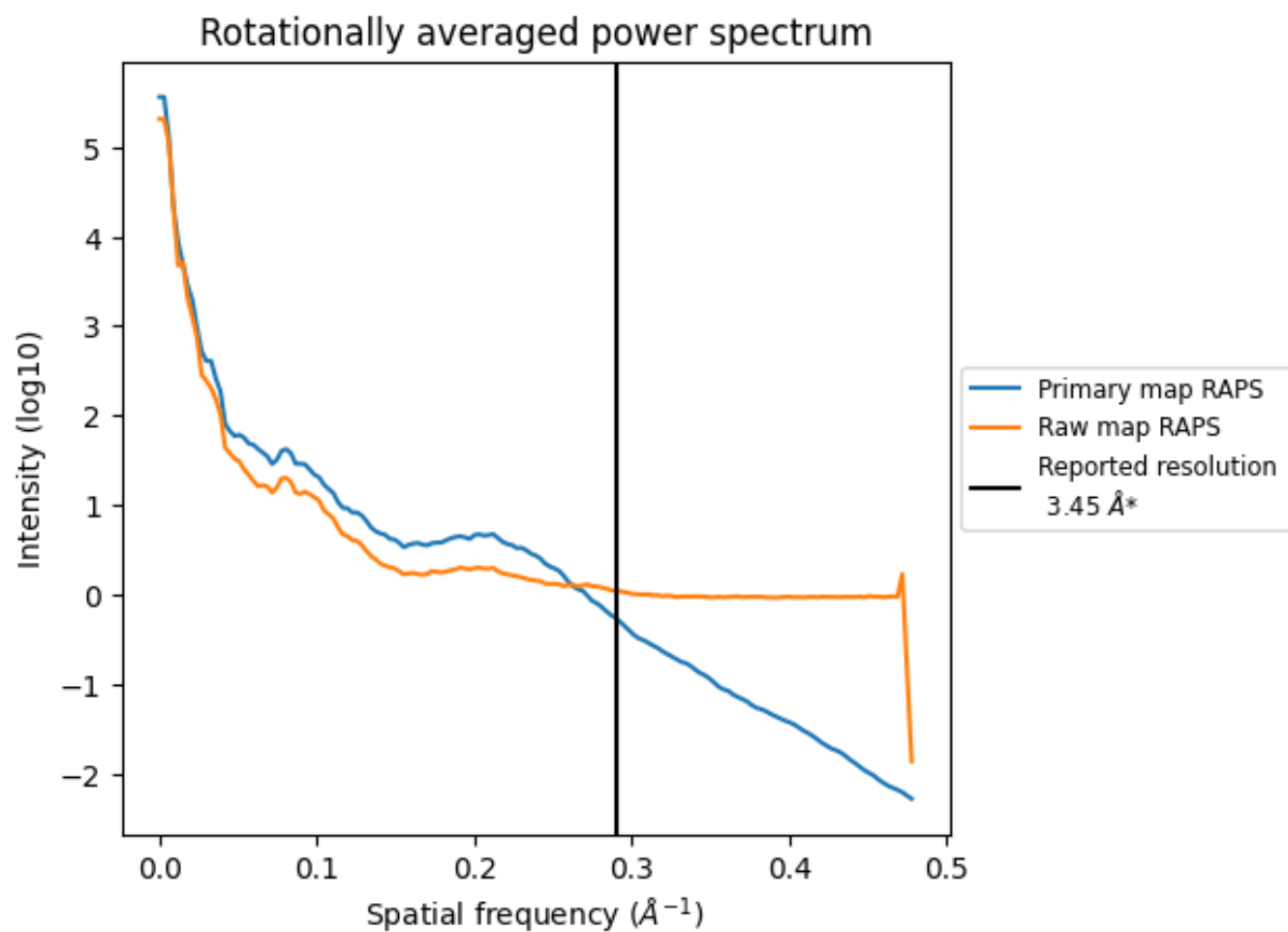
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $1402 \text{ nm}^3$ ; this corresponds to an approximate mass of 1267 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 ⓘ

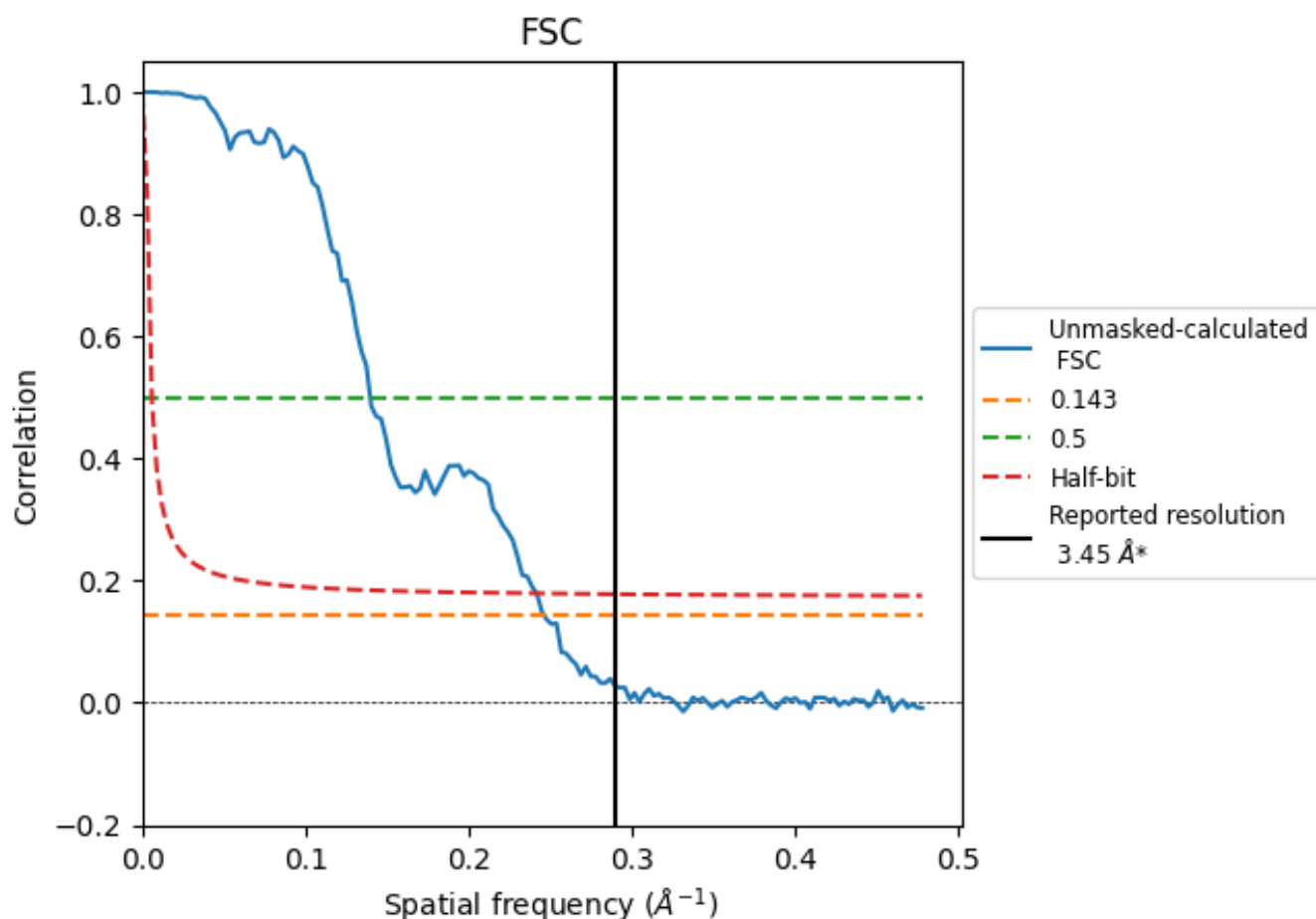


\*Reported resolution corresponds to spatial frequency of 0.290  $\text{\AA}^{-1}$

## 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 0.290 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.06	7.15	4.14

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.06 differs from the reported value 3.45 by more than 10 %



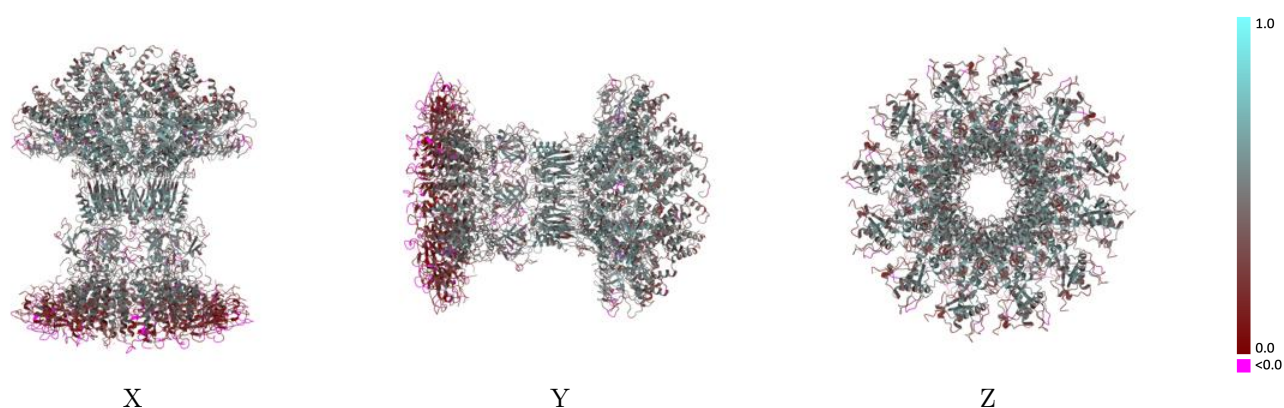
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-63390 and PDB model 9LU7. Per-residue inclusion information can be found in section 3 on page 13.

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

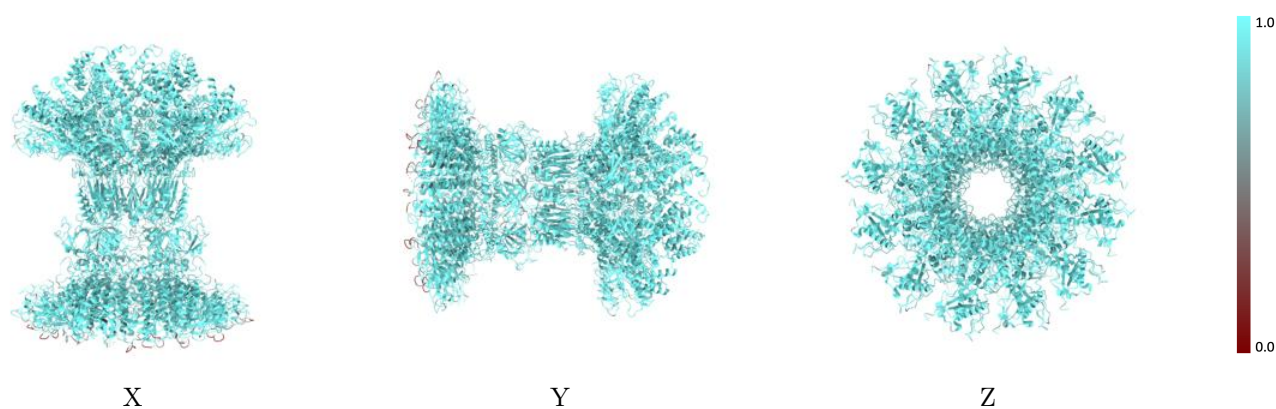
This section was not generated.

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



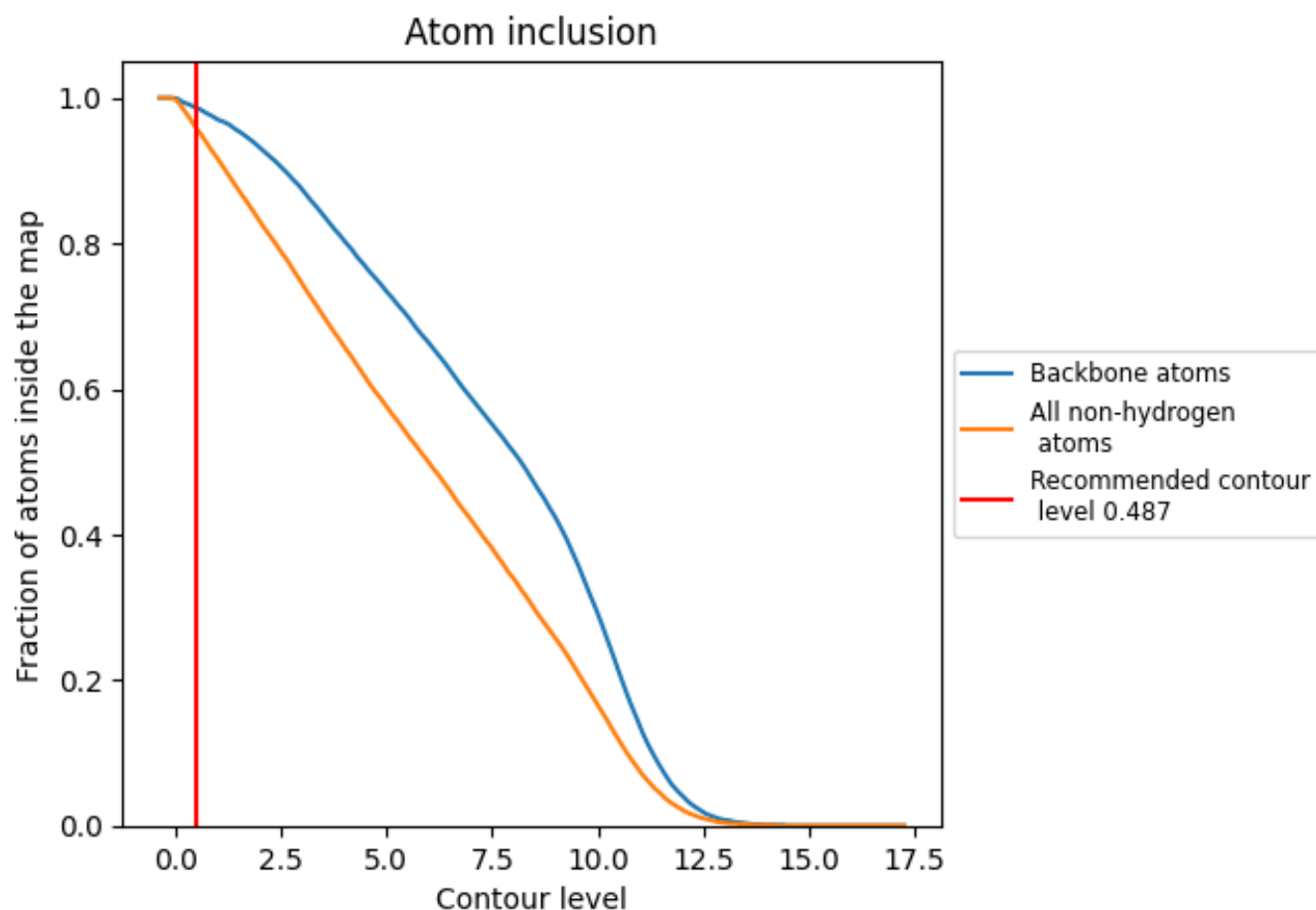
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.487).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.487) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9580	 0.3840
A	 0.9710	 0.3040
B	 0.8940	 0.2330
C	 0.9450	 0.2650
D	 0.8890	 0.2280
E	 0.9420	 0.2680
F	 0.8910	 0.2320
G	 0.9460	 0.2690
H	 0.8970	 0.2360
I	 0.9470	 0.2720
J	 0.8960	 0.2340
K	 0.9430	 0.2680
L	 0.8910	 0.2330
M	 0.9750	 0.4210
N	 0.9570	 0.3880
O	 0.9700	 0.3900
P	 0.9650	 0.3920
Q	 0.9680	 0.3960
R	 0.9730	 0.3960
a	 0.9850	 0.5000
b	 0.9760	 0.4560
c	 0.9750	 0.4410
d	 0.9780	 0.4560
e	 0.9770	 0.4480
f	 0.9760	 0.4570
g	 0.9770	 0.4490
h	 0.9780	 0.4550
i	 0.9760	 0.4430
j	 0.9780	 0.4550
k	 0.9760	 0.4400
l	 0.9760	 0.4560

