



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:57 AM UTC

PDB ID : 9VVR / pdb_00009vvr
EMDB ID : EMD-65388
Title : Structure of the bacteriophage E1004 tail
Authors : Sun, B.N.; Liu, H.R.
Deposited on : 2025-07-16
Resolution : 3.11 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

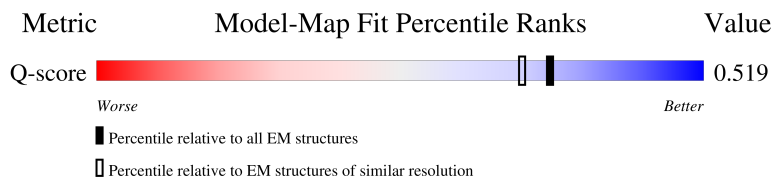
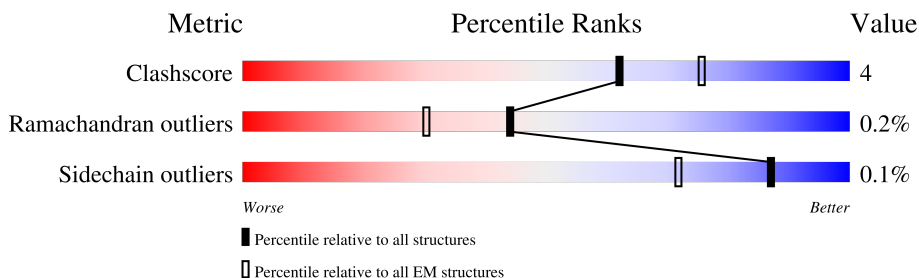
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.11 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.



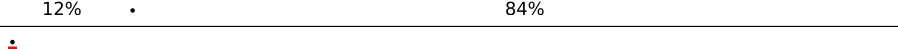
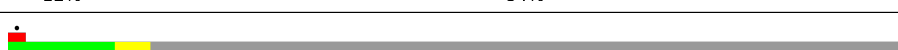
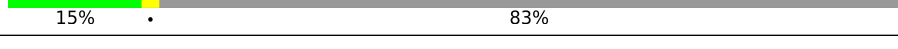
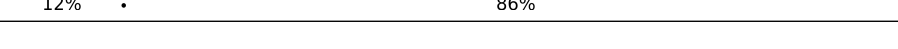
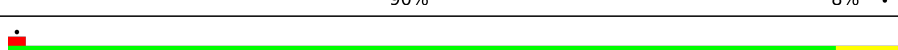
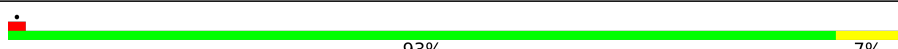
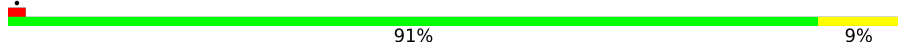
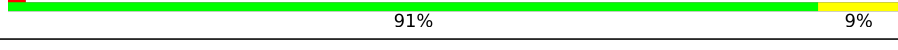
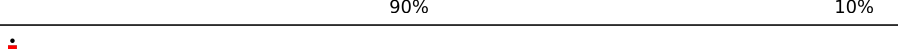
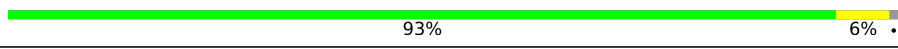
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14465 (2.61 - 3.61)

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	843	 12% 15% 12% 84% 84%
1	B	843	 12% 15% 12% 83% 83%
1	C	843	 12% 15% 12% 86% 86%
1	D	843	 12% 15% 12% 84% 84%

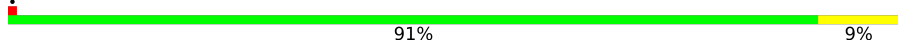
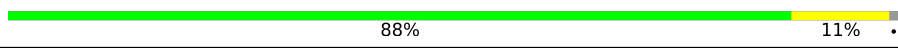
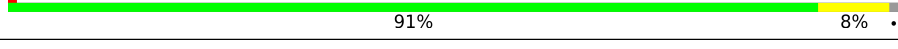
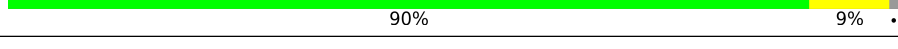
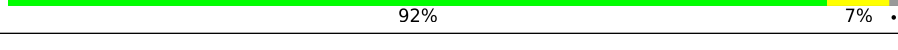
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Mol	Chain	Length	Quality of chain
1	E	843	
1	F	843	
1	G	843	
1	H	843	
1	I	843	
1	J	843	
1	K	843	
1	L	843	
1	M	843	
1	N	843	
1	O	843	
1	P	843	
1	Q	843	
1	R	843	
2	S	785	
2	V	785	
2	X	785	
2	Z	785	
2	b	785	
2	d	785	
3	T	188	
3	U	188	
3	W	188	
3	Y	188	
3	a	188	

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Mol	Chain	Length	Quality of chain
3	c	188	 91%9%
3	e	188	 91%9%
3	f	188	 88%11%.
3	g	188	 89%11%
3	h	188	 91%8%.
3	i	188	 90%9%.
3	j	188	 92%7%.

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 72911 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 Tail spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	131	Total	C	N	O	S	0	0
			1017	629	178	208	2		
1	B	140	Total	C	N	O	S	0	0
			1092	672	193	225	2		
1	C	121	Total	C	N	O	S	0	0
			956	596	166	192	2		
1	D	131	Total	C	N	O	S	0	0
			1017	629	178	208	2		
1	E	140	Total	C	N	O	S	0	0
			1092	672	193	225	2		
1	F	121	Total	C	N	O	S	0	0
			956	596	166	192	2		
1	G	131	Total	C	N	O	S	0	0
			1017	629	178	208	2		
1	H	131	Total	C	N	O	S	0	0
			1017	629	178	208	2		
1	I	131	Total	C	N	O	S	0	0
			1017	629	178	208	2		
1	J	140	Total	C	N	O	S	0	0
			1092	672	193	225	2		
1	K	140	Total	C	N	O	S	0	0
			1092	672	193	225	2		
1	L	140	Total	C	N	O	S	0	0
			1092	672	193	225	2		
1	M	121	Total	C	N	O	S	0	0
			956	596	166	192	2		
1	N	121	Total	C	N	O	S	0	0
			956	596	166	192	2		
1	O	121	Total	C	N	O	S	0	0
			956	596	166	192	2		
1	P	131	Total	C	N	O	S	0	0
			1017	629	178	208	2		
1	Q	140	Total	C	N	O	S	0	0
			1092	672	193	225	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	121	Total	C	N	O	S	0	0
			956	596	166	192	2		

- Molecule 2 is a protein called Nozzle protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	776	Total	C	N	O	S	0	0
			6048	3831	1027	1177	13		
2	V	784	Total	C	N	O	S	0	0
			6101	3862	1036	1190	13		
2	X	784	Total	C	N	O	S	0	0
			6101	3862	1036	1190	13		
2	Z	784	Total	C	N	O	S	0	0
			6101	3862	1036	1190	13		
2	b	784	Total	C	N	O	S	0	0
			6101	3862	1036	1190	13		
2	d	780	Total	C	N	O	S	0	0
			6069	3842	1031	1183	13		

- Molecule 3 is a protein called Adaptor protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	187	Total	C	N	O	S	0	0
			1496	939	250	298	9		
3	U	188	Total	C	N	O	S	0	0
			1504	944	251	299	10		
3	W	188	Total	C	N	O	S	0	0
			1504	944	251	299	10		
3	Y	187	Total	C	N	O	S	0	0
			1496	939	250	298	9		
3	a	188	Total	C	N	O	S	0	0
			1504	944	251	299	10		
3	c	188	Total	C	N	O	S	0	0
			1504	944	251	299	10		
3	e	188	Total	C	N	O	S	0	0
			1504	944	251	299	10		
3	f	187	Total	C	N	O	S	0	0
			1496	939	250	298	9		
3	g	188	Total	C	N	O	S	0	0
			1504	944	251	299	10		
3	h	187	Total	C	N	O	S	0	0
			1496	939	250	298	9		

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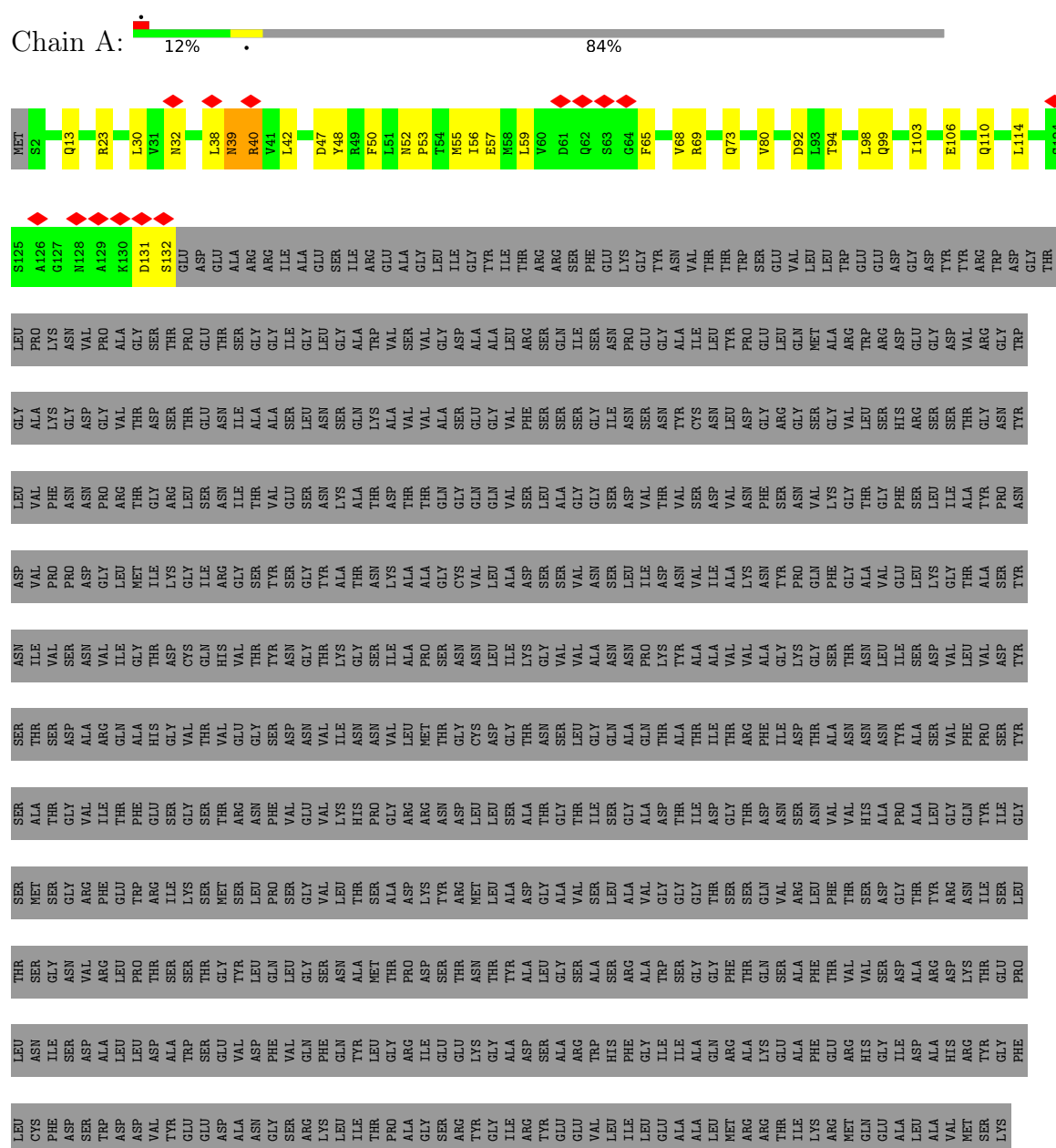
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	i	187	Total	C	N	O	S	0	0
			1496	939	250	298	9		
3	j	187	Total	C	N	O	S	0	0
			1496	939	250	298	9		

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: Tail spike protein



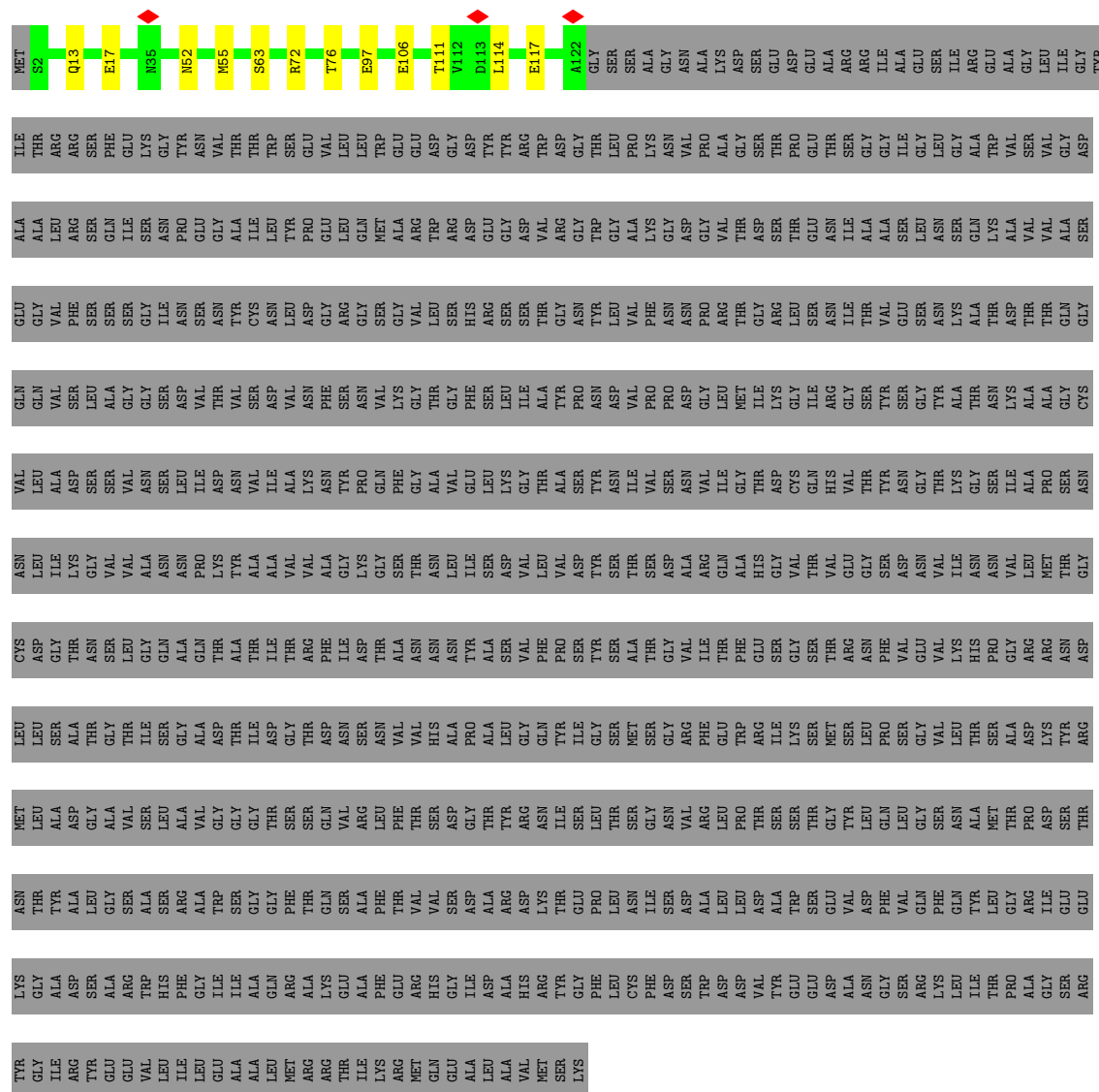
[illegible]

- Molecule 1: Tail spike protein

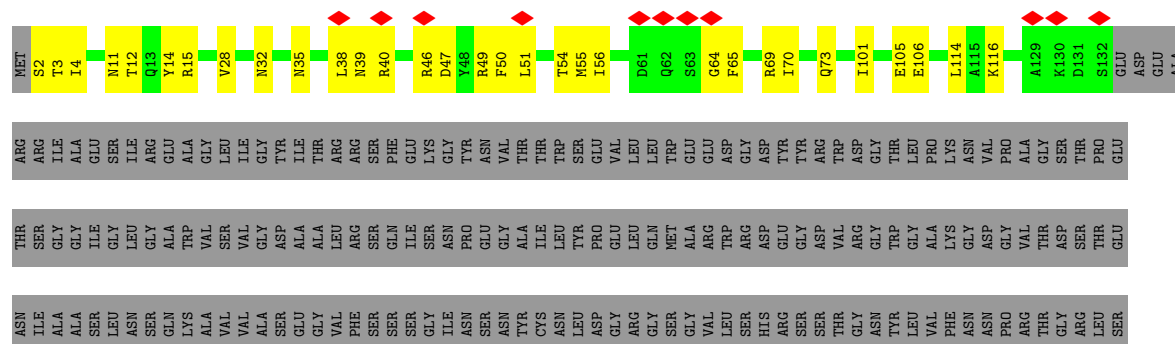


ARG	TYR	GLY	GLY	GLY	ASP	GLY	ASN	ASN	CYS	GLY	SER	ASP	TYR	MET
TYR	GLY	GLY	GLY	LEU	LEU	CYS	ASN	ASN	VAL	GLN	GLY	ALA	ILE	S2
ILE	ALA	ALA	TYR	SER	ALA	GLY	ILE	ILE	ALA	VAL	PHE	LEU	ARG	E17
ARG	ASP	ASP	ALA	THR	GLY	ASN	GLY	VAL	ASP	SER	SER	ARG	ARG	L30
TYR	SER	SER	GLY	THR	GLY	SER	VAL	VAL	SER	ALA	SER	GLN	PHE	V31
GLU	ARG	ARG	GLY	THR	THR	ALA	THR	TYR	ASN	GLY	SER	ILE	GLU	
GLU	ARG	ARG	SER	ILE	ILE	GLY	ALA	ASN	ASN	GLY	GLY	SER	LYS	Ea3
VAL	TRP	TRP	SER	SER	SER	GLN	ASN	ASN	ASN	ASN	ASN	PRO	TYR	R46
LEU	ILE	PHE	ALA	GLY	GLY	ALA	ASN	ASN	ILE	VAL	SER	GLU	ASN	
GLU	GLY	GLY	ALA	ALA	ASP	THR	LYS	LYS	ASP	THR	ASN	GLY	VAL	L51
ALA	ALA	ALA	GLY	THR	THR	ALA	TYR	ALA	ASN	VAL	TYR	ALA	THR	
LEU	GLN	GLN	PHE	GLY	ASP	ILE	THR	VAL	SER	SER	CYS	ILE	THR	E57
MET	ARG	ARG	SER	THR	GLY	ILE	VAL	ALA	ASN	ASP	ASN	LEU	TRP	M58
ARG	ALA	LYS	GLN	ASP	PHE	ASN	VAL	ALA	LYS	PHE	ASP	PRO	GLU	Q62
THR	GLU	GLU	SER	ASN	ASN	ILE	GLY	GLY	TYR	SER	ARG	LEU	VAL	F65
ILE	ALA	ALA	ALA	SER	ASN	ASP	LYS	LYS	PRO	ASN	GLY	GLN	LEU	D66
ILE	PHE	PHE	THR	ASN	THR	THR	GLY	GLN	GLN	VAL	GLY	NET	TRP	I67
ARG	GLU	GLU	VAL	VAL	VAL	ASN	SER	PHE	PHE	LYS	GLY	ALA	GLU	
MET	ARG	ARG	THR	THR	VAL	ASN	THR	GLY	GLY	GLY	VAL	ARG	GLU	R72
GLN	HIS	HIS	VAL	HIS	ASN	ASN	ASN	ALA	ALA	THR	LEU	TRP	ASP	
GLY	GLY	GLY	ASP	ALA	ASN	ASN	LEU	VAL	VAL	GLY	SER	ARG	GLY	V80
ALA	ILE	ILE	ASP	GLY	TYR	ILE	ILE	GLU	GLU	PHE	HIS	ASP	ASP	
LEU	ALA	ALA	THR	GLY	ALA	SER	SER	LEU	LEU	SER	ARG	GLU	TYR	D92
ALA	ALA	THR	THR	LEU	LEU	ASP	ASN	ASN	LYS	LEU	SER	GLY	TYR	
VAL	HIS	ASP	ARG	GLY	GLY	VAL	VAL	ILE	GLY	ILE	SER	ASP	TYR	E106
MET	MET	HIS	ASN	ASN	GLN	ASN	VAL	THR	THR	ALA	THR	VAL	ARG	
SER	SER	TYR	ILE	ILE	TYR	VAL	VAL	ALA	ALA	TYR	ASN	ARG	ASP	
LYS	LYS	GLY	SER	ILE	ILE	SER	TYR	ASN	SER	PRO	GLY	GLY	GLY	D113
	PHE	PHE	GLU	THR	GLY	SER	TYR	ASN	TYR	ASN	TYR	TRP	THR	I114
LEU	LEU	ASN	LEU	SER	GLY	SER	SER	ASN	ASN	LEU	LEU	GLY	LEU	A115
CYS	ASN	SER	ASN	MET	GLY	ALA	THR	THR	ILE	VAL	VAL	ALA	PRO	K116
PHE	PHE	ILE	GLY	SER	THR	THR	THR	THR	VAL	PRO	PHE	LYS	ASN	E117
ASP	ASP	ASP	ASP	GLY	GLY	GLY	ASP	ASP	SER	PRO	GLY	ASN	ASN	Y118
SER	TRP	TRP	VAL	ARG	ILE	ILE	ALA	ALA	VAL	ASN	ASN	ASP	VAL	
ASP	ASP	THR	ALA	PHE	PHE	THR	GLN	GLN	ILE	GLY	PRO	GLY	PRO	K130
ASP	ASP	LEU	LEU	GLU	THR	THR	ASN	THR	ILE	LEU	ARG	VAL	ALA	D131
VAL	VAL	THR	THR	ARG	TRP	PHE	ALA	HIS	GLY	MET	THR	THR	GLY	S132
TYR	TYR	ALA	SER	ILE	ILE	SER	GLY	GLY	ASP	LYS	ARG	SER	THR	E133
GLU	GLU	TRP	SER	LYS	GLY	GLY	VAL	VAL	CYS	GLY	LEU	THR	PRO	D134
ASP	GLU	SER	THR	SER	THR	THR	THR	VAL	HIS	ILE	SER	GLU	THR	E135
ALA	ALA	VAL	TYR	SER	ARG		GLU	VAL	VAL	GLY	ILE	ILE	SER	A136
ASN	ASN	ASP	LEU	SER	THR	ASN	GLY	THR	THR	SER	THR	ALA	GLY	R137
ASN	GLY	PHE	LEU	PRO	PHE	ASN	SER	THR	TYR	TYR	THR	ALA	GLY	R138
GLY	GLY	GLY	GLY	GLY	GLY	ASN	ASN	GLY	ASN	SER	GLU	SER	ILE	I139
ARG	ARG	LEU	LEU	VAL	VAL	VAL	ASN	THR	THR	TYR	ASN	ASN	LEU	A140
LYS	LYS	PHE	GLN	ASN	LYS	LYS	ILE	LYS	GLY	THR	ASN	SER	GLY	E141
ILE	ILE	THR	TYR	ALA	HIS	ASN	ASN	GLY	GLY	THR	ALA	GLN	ALA	SER
THR	THR	GLY	LEU	THR	SER	PRO	ASN	ILE	THR	ASN	THR	LYS	TRP	ILE
PRO	PRO	GLY	GLY	ALA	ALA	GLY	VAL	ILE	THR	ASP	THR	ALA	VAL	ARG
ALA	ALA	ARG	ARG	ASP	ASP	GLY	MET	THR	PRO	LEU	THR	VAL	SER	GLU
ALA	ALA	ILE	ILE	LYS	LYS	ARG	ARG	ARG	PRO	VAL	THR	VAL	VAL	ALA
GLY	GLY	ILE	ILE	THR	THR	ASN	THR	THR	THR	ALA	GLN	GLY	GLY	TYR
SER	SER	THR	THR	THR	THR	ASN	THR	THR	THR	ALA	GLN	GLY	GLY	GLY

- Molecule 1: Tail spike protein



- Molecule 1: Tail spike protein



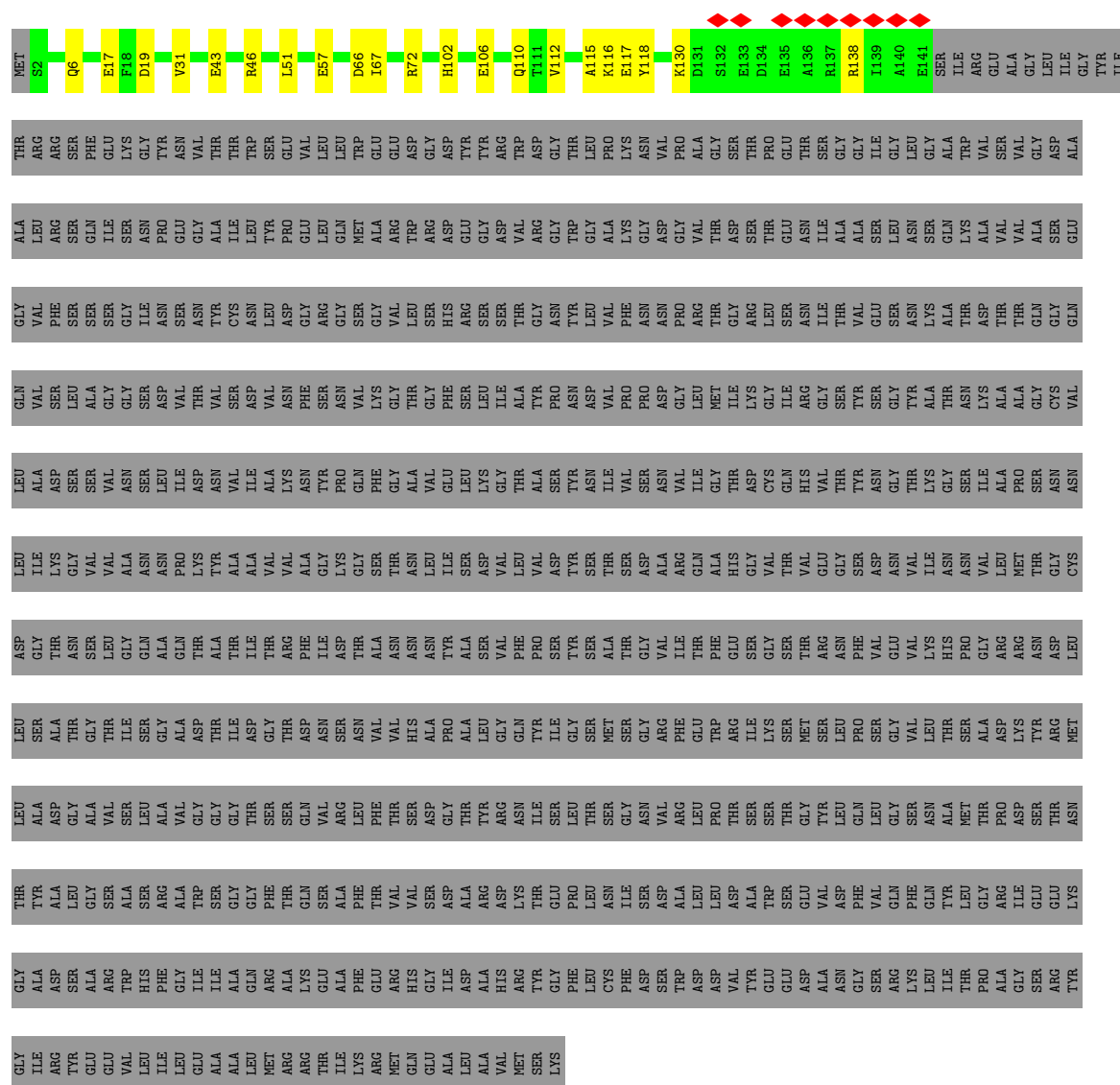
[illegible]

- Molecule 1: Tail spike protein

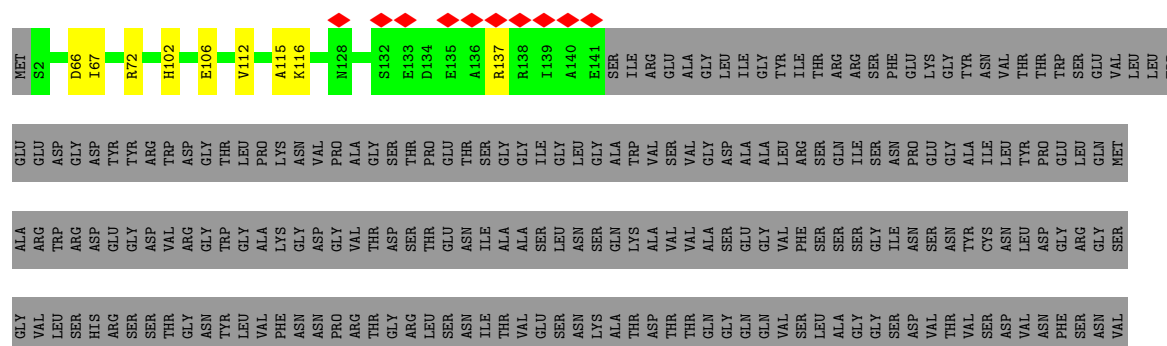
Chain H: 12% 84%

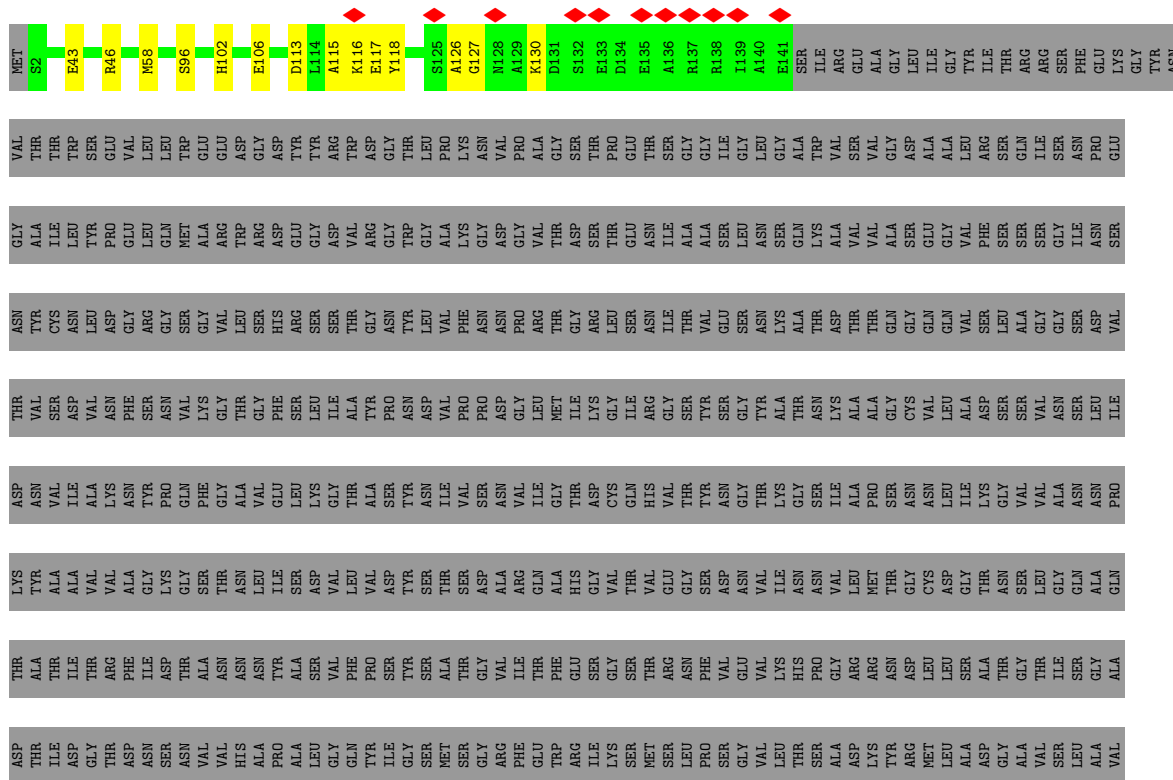
[illegible]

- Molecule 1: Tail spike protein



Chain K: 16% 83%





[illegible]

- Molecule 1: Tail spike protein



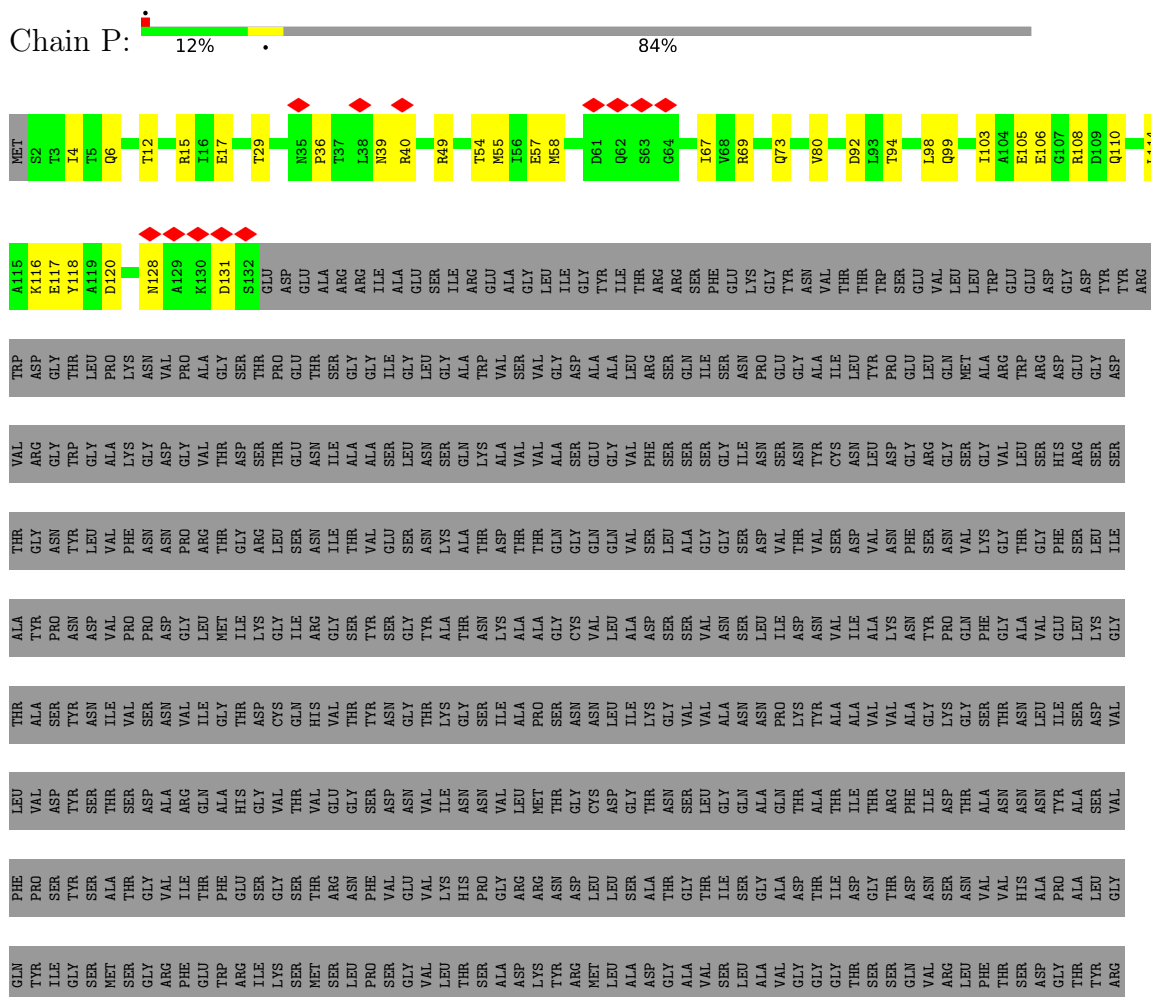
ALA	GLY	SER	ARG	GLU	GLY	TYR	ALA	ASP	ARG	LEU	ALA	ALA	PRO	ALA	ALA	ALA	THR	VAL	SER	LEU	MET
GLY	SER	ARG	GLU	GLY	TYR	ALA	ASP	TYR	ARG	THR	GLY	GLY	SER	ASN	ASN	VAL	GLN	GLU	ALA	GLY	ILE
ARG	GLY	TYR	GLY	GLY	TYR	ALA	ASP	GLY	ASP	LEU	GLY	GLY	ASN	ASN	ILE	ALA	VAL	GLY	LEU	ARG	ARG
ILE	ALA	TYR	ALA	GLY	TYR	ALA	ASP	GLY	SER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

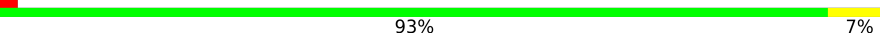
- Molecule 1: Tail spike protein

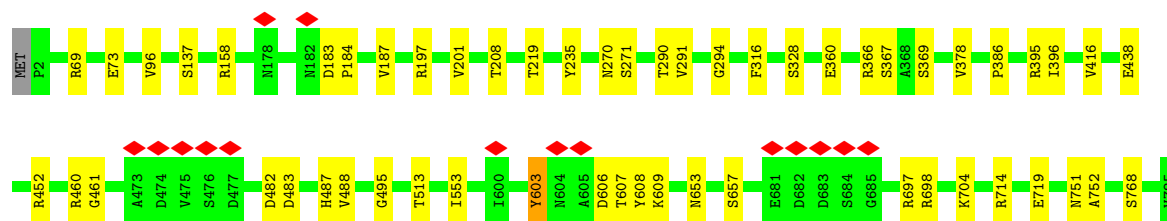




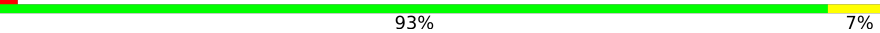
- Molecule 1: Tail spike protein

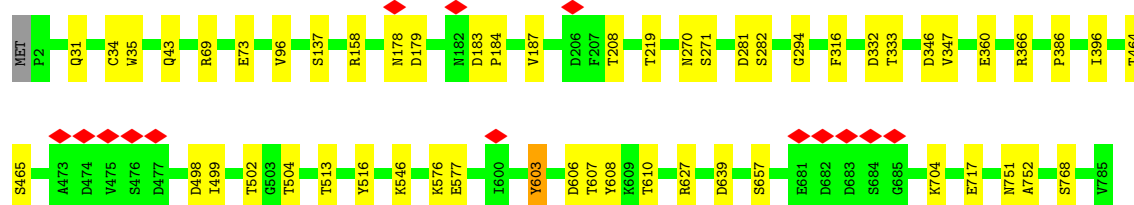


Chain V:  93% 7%



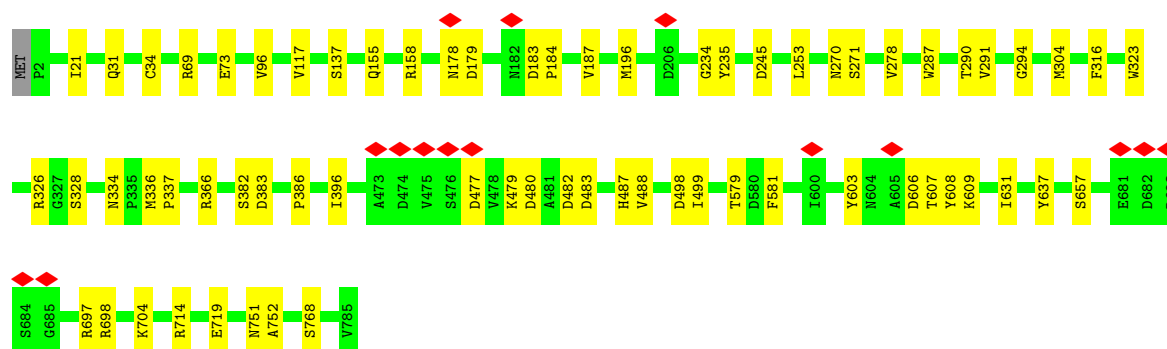
• Molecule 2: Nozzle protein

Chain X:  93% 7%



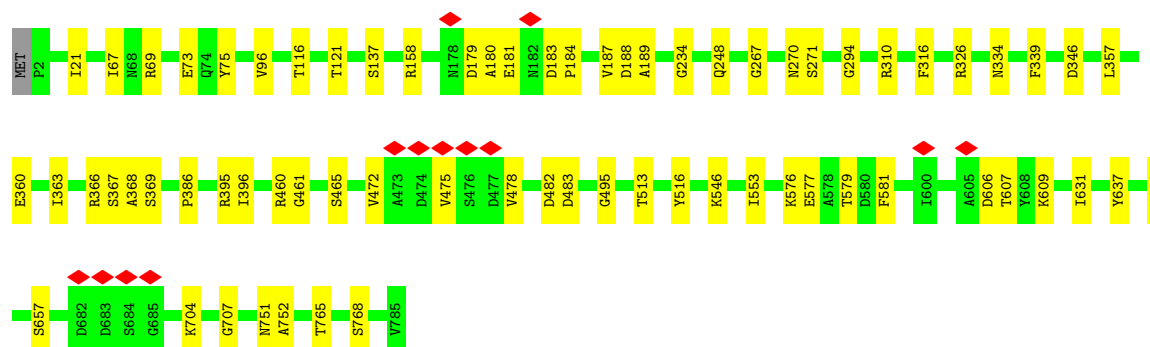
• Molecule 2: Nozzle protein

Chain Z:  91% 9%

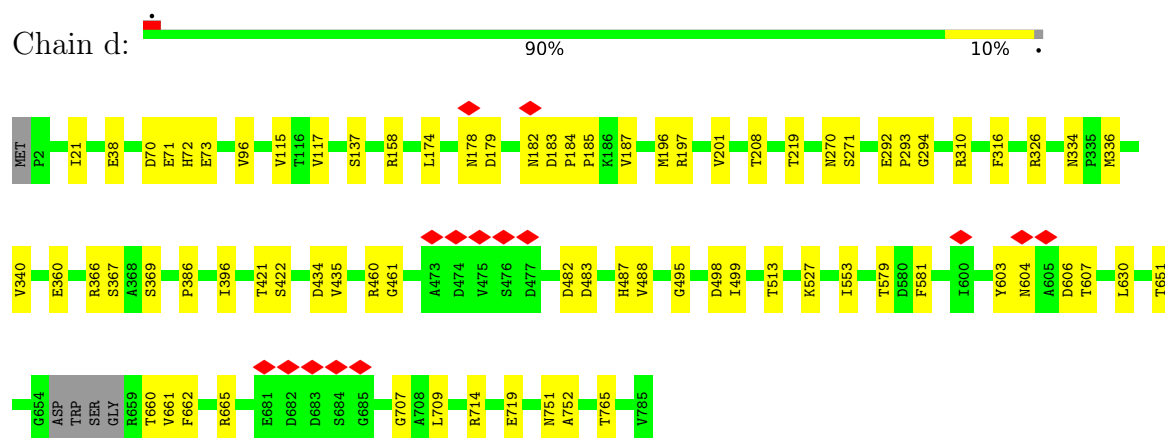


• Molecule 2: Nozzle protein

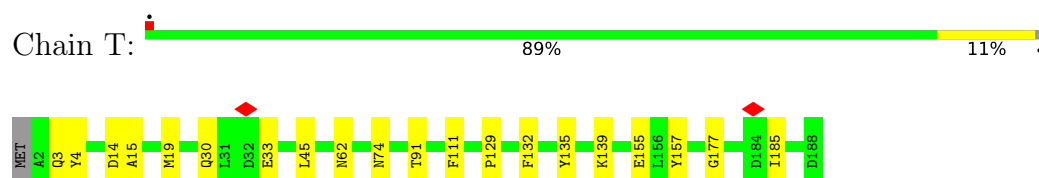
Chain b:  91% 9%



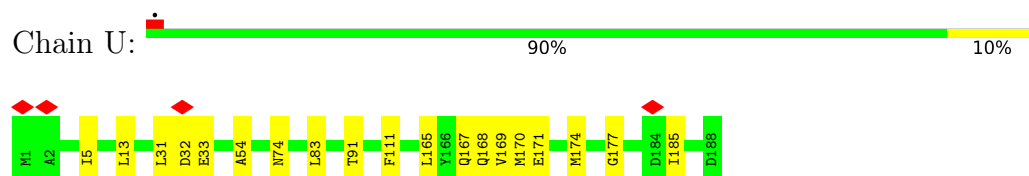
- Molecule 2: Nozzle protein



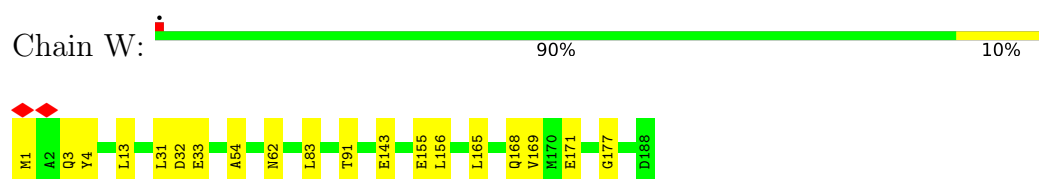
- Molecule 3: Adaptor protein



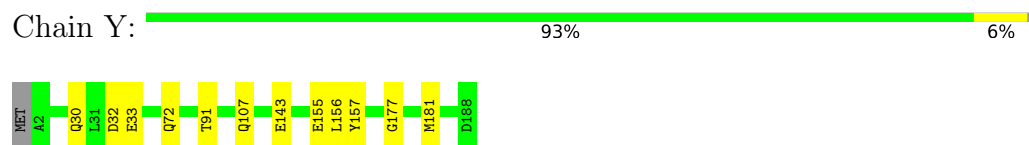
- Molecule 3: Adaptor protein



- Molecule 3: Adaptor protein

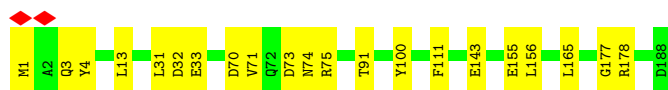


- Molecule 3: Adaptor protein

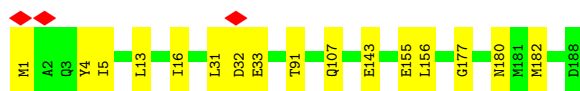
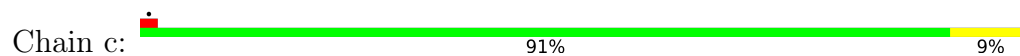


- Molecule 3: Adaptor protein





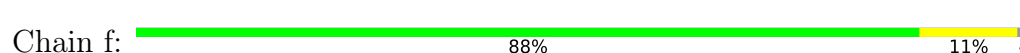
- Molecule 3: Adaptor protein



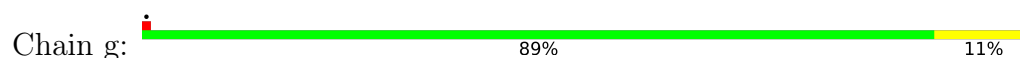
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- Molecule 3: Adaptor protein



- Molecule 3: Adaptor protein



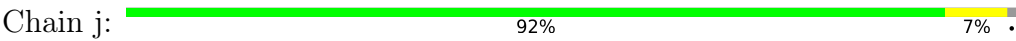
- Molecule 3: Adaptor protein



- Molecule 3: Adaptor protein



- Molecule 3: Adaptor protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50105	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 ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.439	Depositor
Minimum map value	-0.778	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	484.0, 484.0, 484.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.34	0/1031	0.56	0/1400
1	B	0.18	0/1106	0.40	0/1500
1	C	0.14	0/970	0.31	0/1319
1	D	0.28	0/1031	0.51	0/1400
1	E	0.30	0/1106	0.53	0/1500
1	F	0.15	0/970	0.34	0/1319
1	G	0.19	0/1031	0.46	0/1400
1	H	0.35	0/1031	0.60	0/1400
1	I	0.19	0/1031	0.48	0/1400
1	J	0.17	0/1106	0.37	0/1500
1	K	0.16	0/1106	0.36	0/1500
1	L	0.16	0/1106	0.39	0/1500
1	M	0.15	0/970	0.36	0/1319
1	N	0.16	0/970	0.38	0/1319
1	O	0.17	0/970	0.42	0/1319
1	P	0.19	0/1031	0.46	0/1400
1	Q	0.17	0/1106	0.39	0/1500
1	R	0.15	0/970	0.35	0/1319
2	S	0.16	0/6184	0.37	0/8396
2	V	0.15	0/6239	0.36	0/8474
2	X	0.15	0/6239	0.36	0/8474
2	Z	0.19	0/6239	0.41	0/8474
2	b	0.15	0/6239	0.36	0/8474
2	d	0.18	0/6204	0.41	0/8424
3	T	0.14	0/1525	0.36	0/2069
3	U	0.15	0/1533	0.41	0/2079
3	W	0.15	0/1533	0.39	0/2079
3	Y	0.15	0/1525	0.35	0/2069
3	a	0.16	0/1533	0.39	0/2079
3	c	0.15	0/1533	0.40	0/2079
3	e	0.15	0/1533	0.38	0/2079
3	f	0.15	0/1525	0.36	0/2069
3	g	0.15	0/1533	0.38	0/2079
3	h	0.15	0/1525	0.37	0/2069

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	i	0.16	0/1525	0.37	0/2069
3	j	0.15	0/1525	0.37	0/2069
All	All	0.17	0/74334	0.39	0/100918

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1017	0	986	23	0
1	B	1092	0	1055	11	0
1	C	956	0	932	11	0
1	D	1017	0	986	18	0
1	E	1092	0	1055	17	0
1	F	956	0	932	10	0
1	G	1017	0	986	20	0
1	H	1017	0	986	24	0
1	I	1017	0	986	26	0
1	J	1092	0	1055	14	0
1	K	1092	0	1055	6	0
1	L	1092	0	1055	10	0
1	M	956	0	932	13	0
1	N	956	0	932	11	0
1	O	956	0	932	15	0
1	P	1017	0	986	21	0
1	Q	1092	0	1055	11	0
1	R	956	0	932	10	0
2	S	6048	0	5900	41	0
2	V	6101	0	5949	32	0
2	X	6101	0	5949	31	0
2	Z	6101	0	5949	39	0
2	b	6101	0	5949	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	6069	0	5926	51	0
3	T	1496	0	1430	13	0
3	U	1504	0	1442	12	0
3	W	1504	0	1442	13	0
3	Y	1496	0	1430	15	0
3	a	1504	0	1442	15	0
3	c	1504	0	1442	12	0
3	e	1504	0	1442	12	0
3	f	1496	0	1430	19	0
3	g	1504	0	1442	15	0
3	h	1496	0	1430	12	0
3	i	1496	0	1430	11	0
3	j	1496	0	1430	10	0
All	All	72911	0	70692	613	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 4.

The worst 5 of 613 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:d:630:LEU:HD11	2:d:661:VAL:HG11	1.16	1.09
2:d:630:LEU:CD1	2:d:661:VAL:HG11	1.85	1.05
2:d:661:VAL:HG12	2:d:662:PHE:N	1.87	0.87
2:d:661:VAL:HG12	2:d:662:PHE:H	1.42	0.83
1:A:32:ASN:HD22	1:A:38:LEU:HD23	1.44	0.81

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	129/843 (15%)	123 (95%)	5 (4%)	1 (1%)	16	45
1	B	138/843 (16%)	135 (98%)	3 (2%)	0	100	100
1	C	119/843 (14%)	118 (99%)	1 (1%)	0	100	100
1	D	129/843 (15%)	120 (93%)	8 (6%)	1 (1%)	16	45
1	E	138/843 (16%)	130 (94%)	8 (6%)	0	100	100
1	F	119/843 (14%)	117 (98%)	1 (1%)	1 (1%)	16	45
1	G	129/843 (15%)	124 (96%)	5 (4%)	0	100	100
1	H	129/843 (15%)	120 (93%)	9 (7%)	0	100	100
1	I	129/843 (15%)	125 (97%)	4 (3%)	0	100	100
1	J	138/843 (16%)	137 (99%)	1 (1%)	0	100	100
1	K	138/843 (16%)	133 (96%)	5 (4%)	0	100	100
1	L	138/843 (16%)	137 (99%)	1 (1%)	0	100	100
1	M	119/843 (14%)	117 (98%)	2 (2%)	0	100	100
1	N	119/843 (14%)	117 (98%)	2 (2%)	0	100	100
1	O	119/843 (14%)	114 (96%)	5 (4%)	0	100	100
1	P	129/843 (15%)	125 (97%)	4 (3%)	0	100	100
1	Q	138/843 (16%)	136 (99%)	2 (1%)	0	100	100
1	R	119/843 (14%)	118 (99%)	1 (1%)	0	100	100
2	S	772/785 (98%)	717 (93%)	51 (7%)	4 (0%)	24	55
2	V	782/785 (100%)	726 (93%)	53 (7%)	3 (0%)	30	60
2	X	782/785 (100%)	728 (93%)	51 (6%)	3 (0%)	30	60
2	Z	782/785 (100%)	726 (93%)	54 (7%)	2 (0%)	36	65
2	b	782/785 (100%)	725 (93%)	54 (7%)	3 (0%)	30	60
2	d	776/785 (99%)	716 (92%)	58 (8%)	2 (0%)	36	65
3	T	185/188 (98%)	175 (95%)	10 (5%)	0	100	100
3	U	186/188 (99%)	171 (92%)	15 (8%)	0	100	100
3	W	186/188 (99%)	176 (95%)	10 (5%)	0	100	100
3	Y	185/188 (98%)	176 (95%)	9 (5%)	0	100	100
3	a	186/188 (99%)	176 (95%)	10 (5%)	0	100	100
3	c	186/188 (99%)	170 (91%)	16 (9%)	0	100	100
3	e	186/188 (99%)	171 (92%)	15 (8%)	0	100	100
3	f	185/188 (98%)	170 (92%)	15 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	g	186/188 (99%)	174 (94%)	12 (6%)	0	100	100
3	h	185/188 (98%)	175 (95%)	10 (5%)	0	100	100
3	i	185/188 (98%)	174 (94%)	11 (6%)	0	100	100
3	j	185/188 (98%)	174 (94%)	11 (6%)	0	100	100
All	All	9218/22140 (42%)	8666 (94%)	532 (6%)	20 (0%)	44	71

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	603	TYR
2	d	603	TYR
1	A	40	ARG
1	D	103	ILE
1	F	63	SER

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	113/685 (16%)	112 (99%)	1 (1%)	70	78
1	B	120/685 (18%)	120 (100%)	0	100	100
1	C	107/685 (16%)	107 (100%)	0	100	100
1	D	113/685 (16%)	113 (100%)	0	100	100
1	E	120/685 (18%)	119 (99%)	1 (1%)	73	80
1	F	107/685 (16%)	107 (100%)	0	100	100
1	G	113/685 (16%)	113 (100%)	0	100	100
1	H	113/685 (16%)	112 (99%)	1 (1%)	70	78
1	I	113/685 (16%)	113 (100%)	0	100	100
1	J	120/685 (18%)	120 (100%)	0	100	100
1	K	120/685 (18%)	120 (100%)	0	100	100
1	L	120/685 (18%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	107/685 (16%)	107 (100%)	0	100	100
1	N	107/685 (16%)	107 (100%)	0	100	100
1	O	107/685 (16%)	107 (100%)	0	100	100
1	P	113/685 (16%)	113 (100%)	0	100	100
1	Q	120/685 (18%)	120 (100%)	0	100	100
1	R	107/685 (16%)	107 (100%)	0	100	100
2	S	663/670 (99%)	663 (100%)	0	100	100
2	V	669/670 (100%)	669 (100%)	0	100	100
2	X	669/670 (100%)	669 (100%)	0	100	100
2	Z	669/670 (100%)	668 (100%)	1 (0%)	88	90
2	b	669/670 (100%)	669 (100%)	0	100	100
2	d	666/670 (99%)	663 (100%)	3 (0%)	81	83
3	T	162/163 (99%)	162 (100%)	0	100	100
3	U	163/163 (100%)	163 (100%)	0	100	100
3	W	163/163 (100%)	163 (100%)	0	100	100
3	Y	162/163 (99%)	162 (100%)	0	100	100
3	a	163/163 (100%)	163 (100%)	0	100	100
3	c	163/163 (100%)	163 (100%)	0	100	100
3	e	163/163 (100%)	163 (100%)	0	100	100
3	f	162/163 (99%)	162 (100%)	0	100	100
3	g	163/163 (100%)	163 (100%)	0	100	100
3	h	162/163 (99%)	162 (100%)	0	100	100
3	i	162/163 (99%)	162 (100%)	0	100	100
3	j	162/163 (99%)	162 (100%)	0	100	100
All	All	7995/18306 (44%)	7988 (100%)	7 (0%)	87	90

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Z	117	VAL
2	d	651	THR
2	d	665	ARG
2	d	660	THR
1	H	11	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
2	d	334	ASN
3	i	60	ASN
2	d	634	GLN
3	a	145	ASN
2	S	311	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

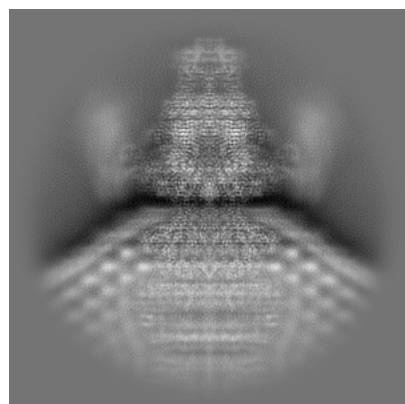
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65388. These allow visual inspection of the internal detail of the map and identification of artifacts.

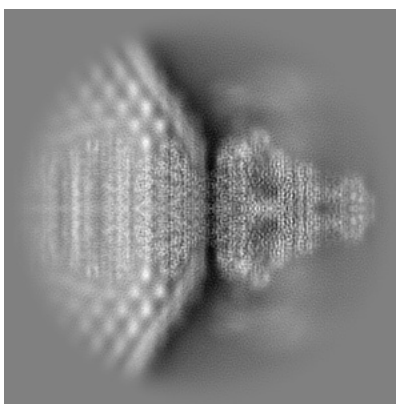
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

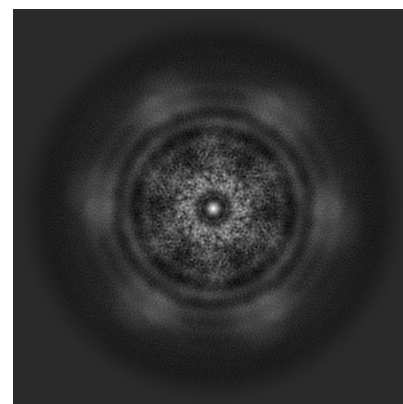
6.1.1 Primary map



X

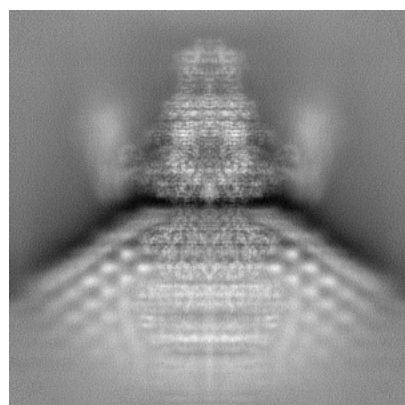


Y

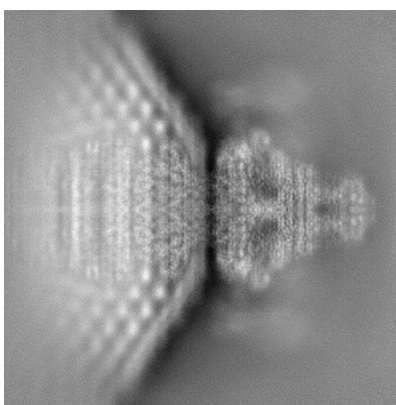


Z

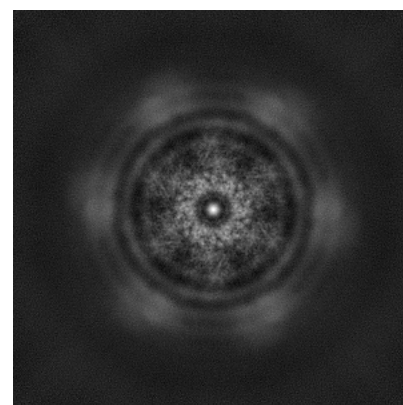
6.1.2 Raw map



X



Y

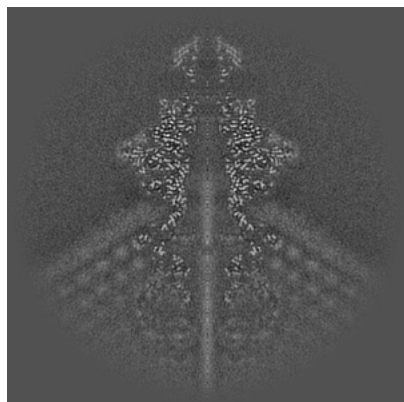


Z

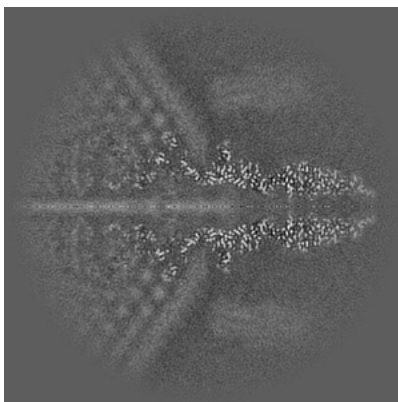
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

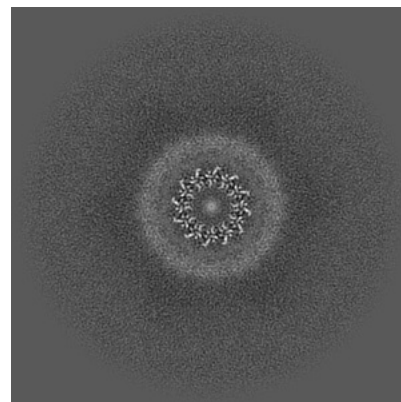
6.2.1 Primary map



X Index: 220

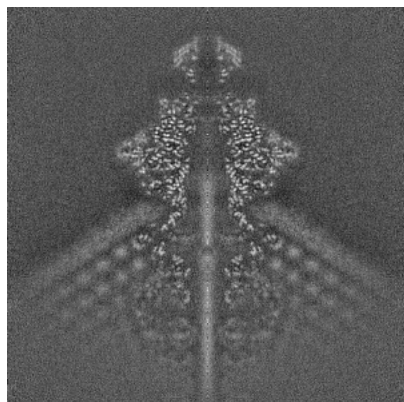


Y Index: 220

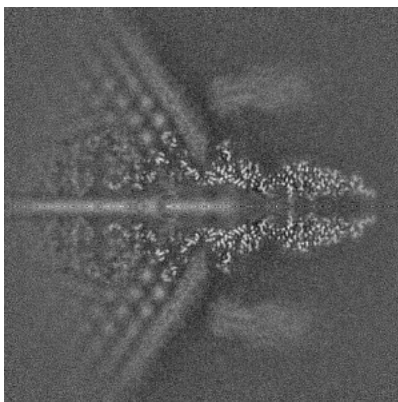


Z Index: 220

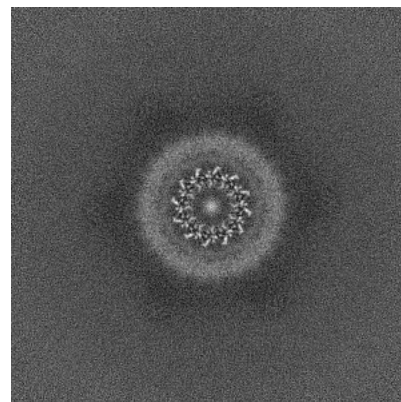
6.2.2 Raw map



X Index: 220



Y Index: 220

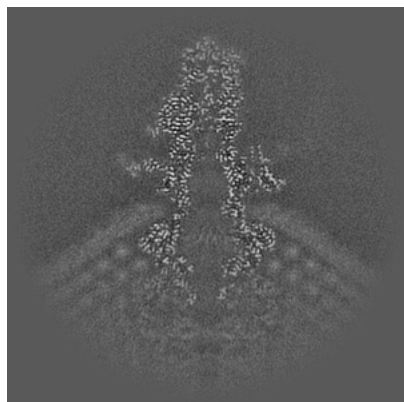


Z Index: 220

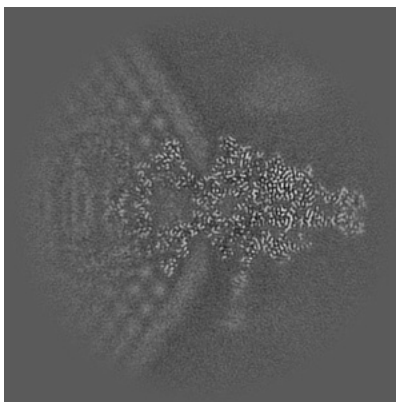
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

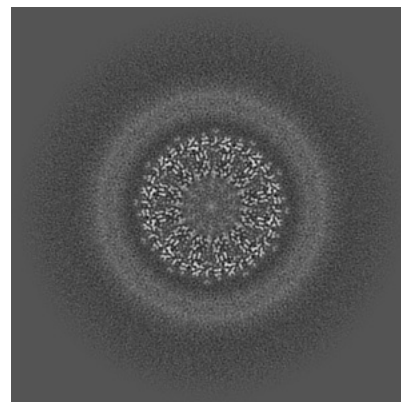
6.3.1 Primary map



X Index: 206

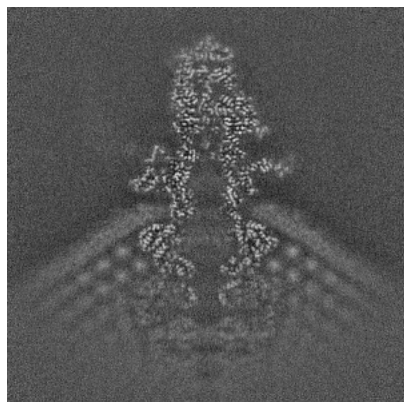


Y Index: 196

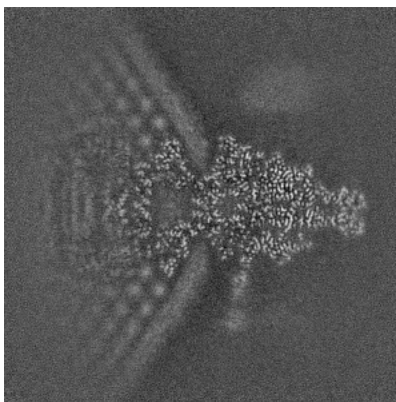


Z Index: 184

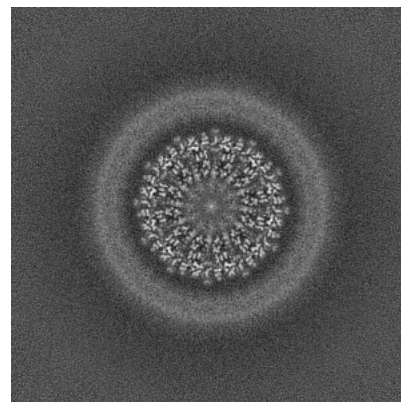
6.3.2 Raw map



X Index: 235



Y Index: 196

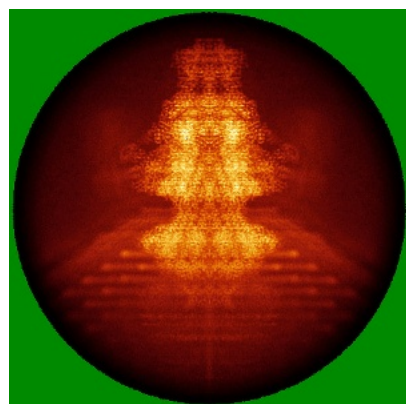


Z Index: 184

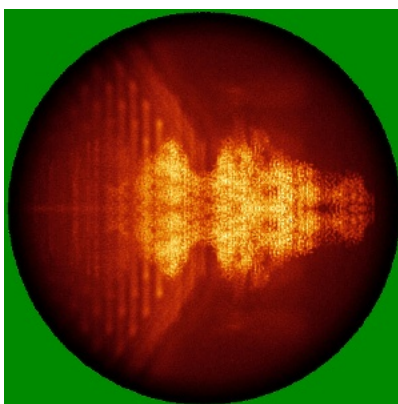
The images above show the largest variance slices of the map in three orthogonal directions.

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

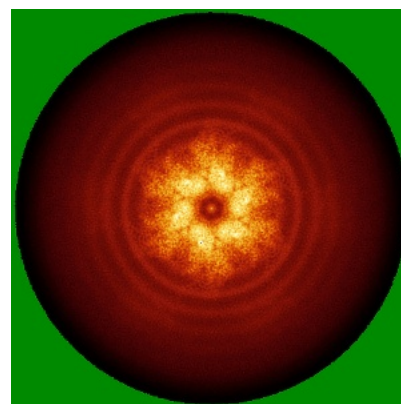
6.4.1 Primary map



X

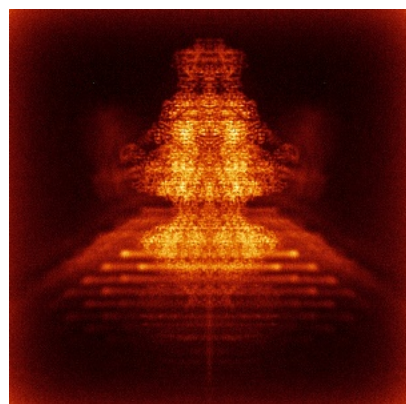


Y

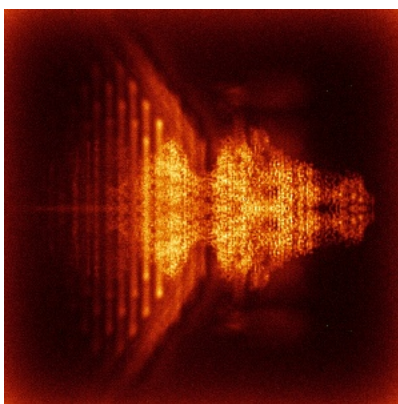


Z

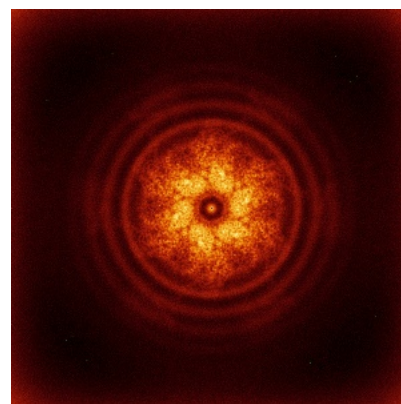
6.4.2 Raw map



X



Y

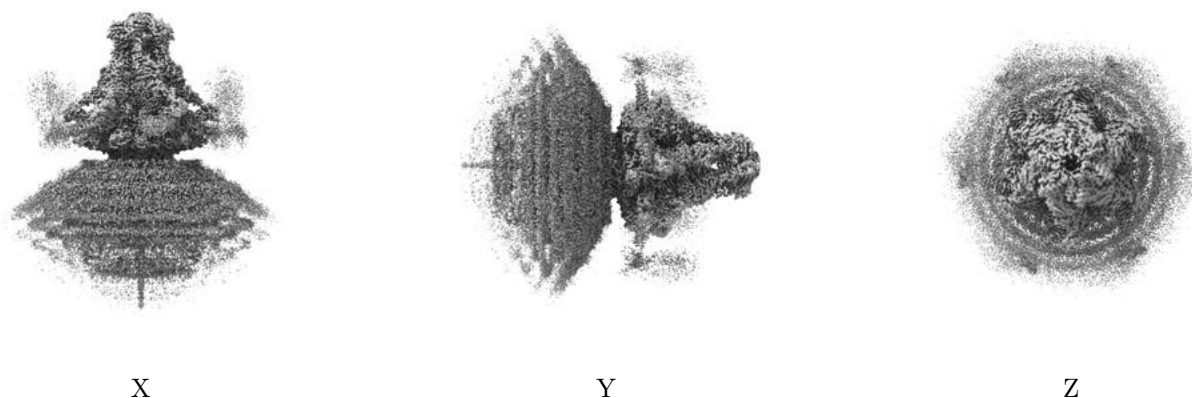


Z

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.

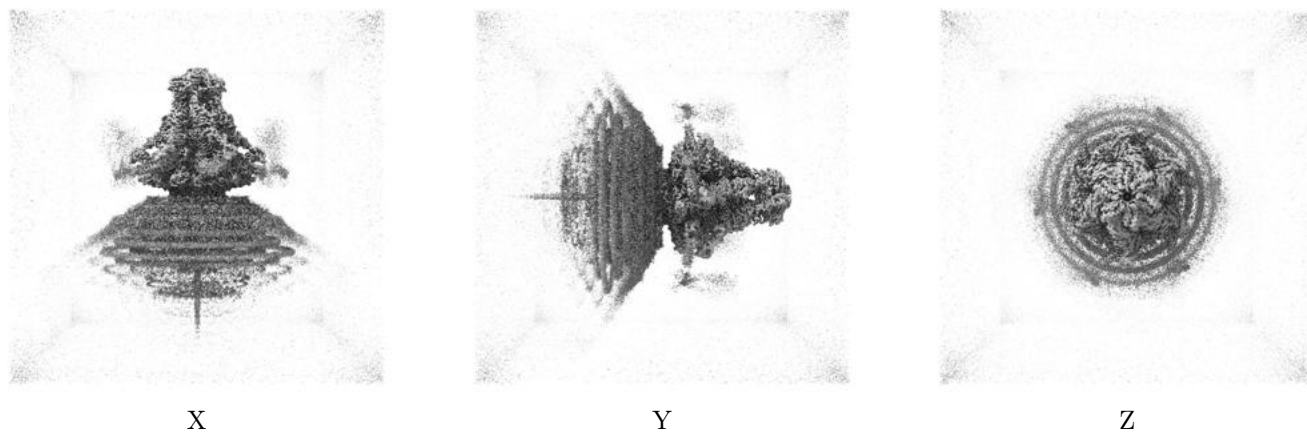
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

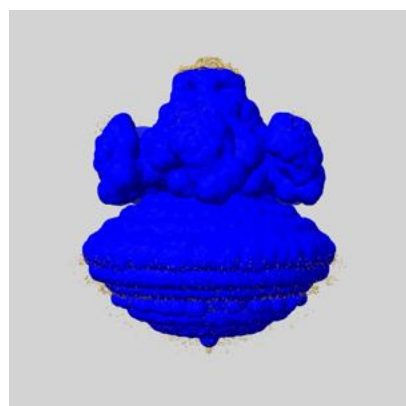
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

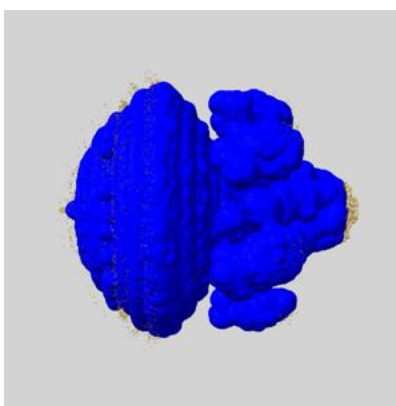
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

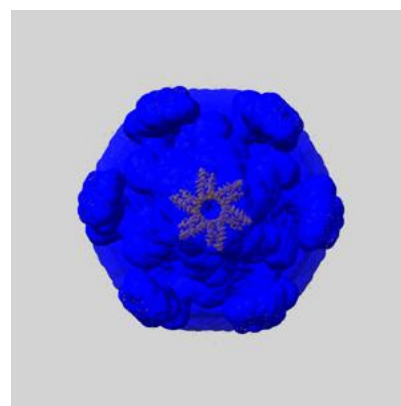
6.6.1 emd_65388_msk_1.map [i](#)



X



Y

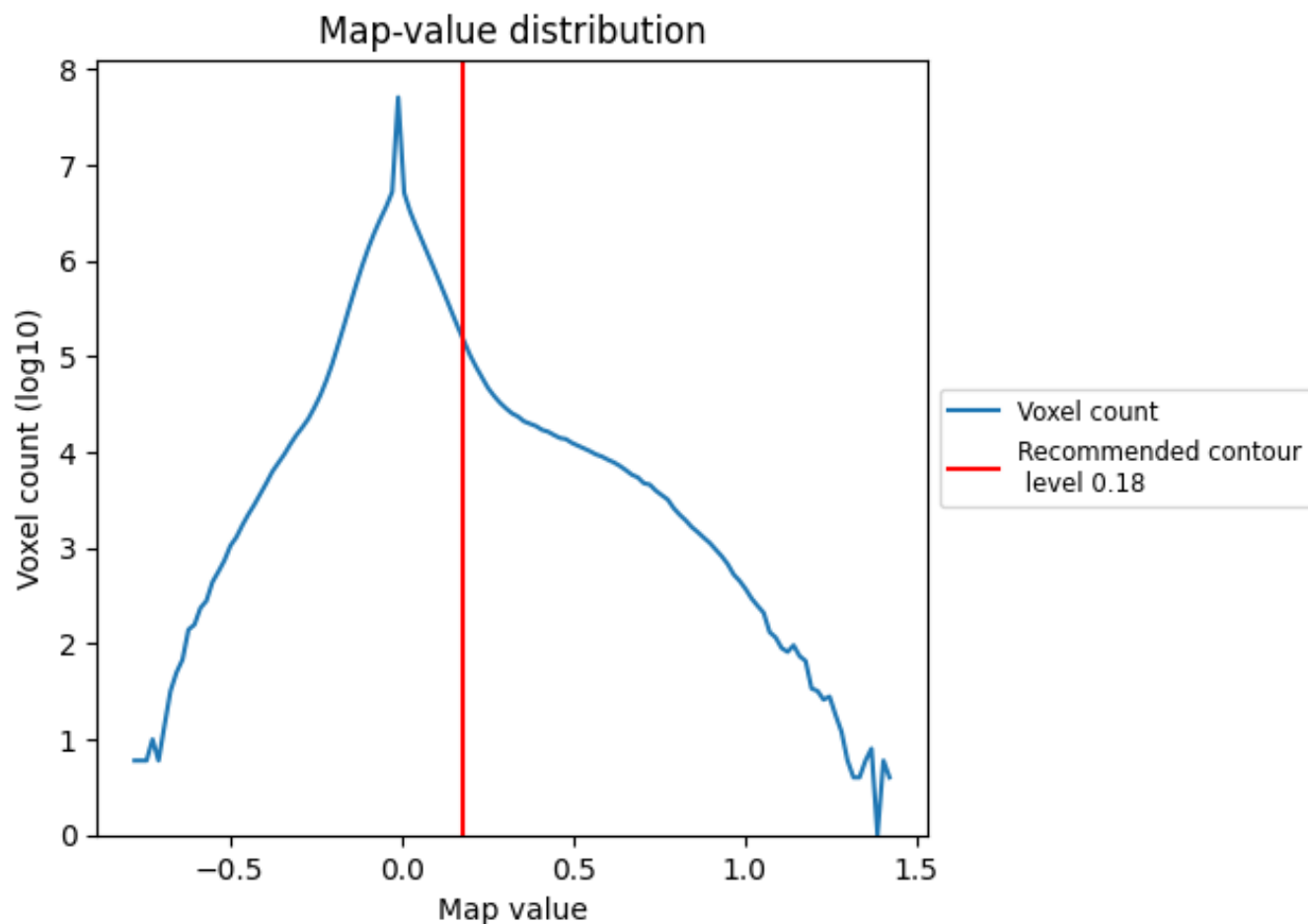


Z

7 Map analysis [i](#)

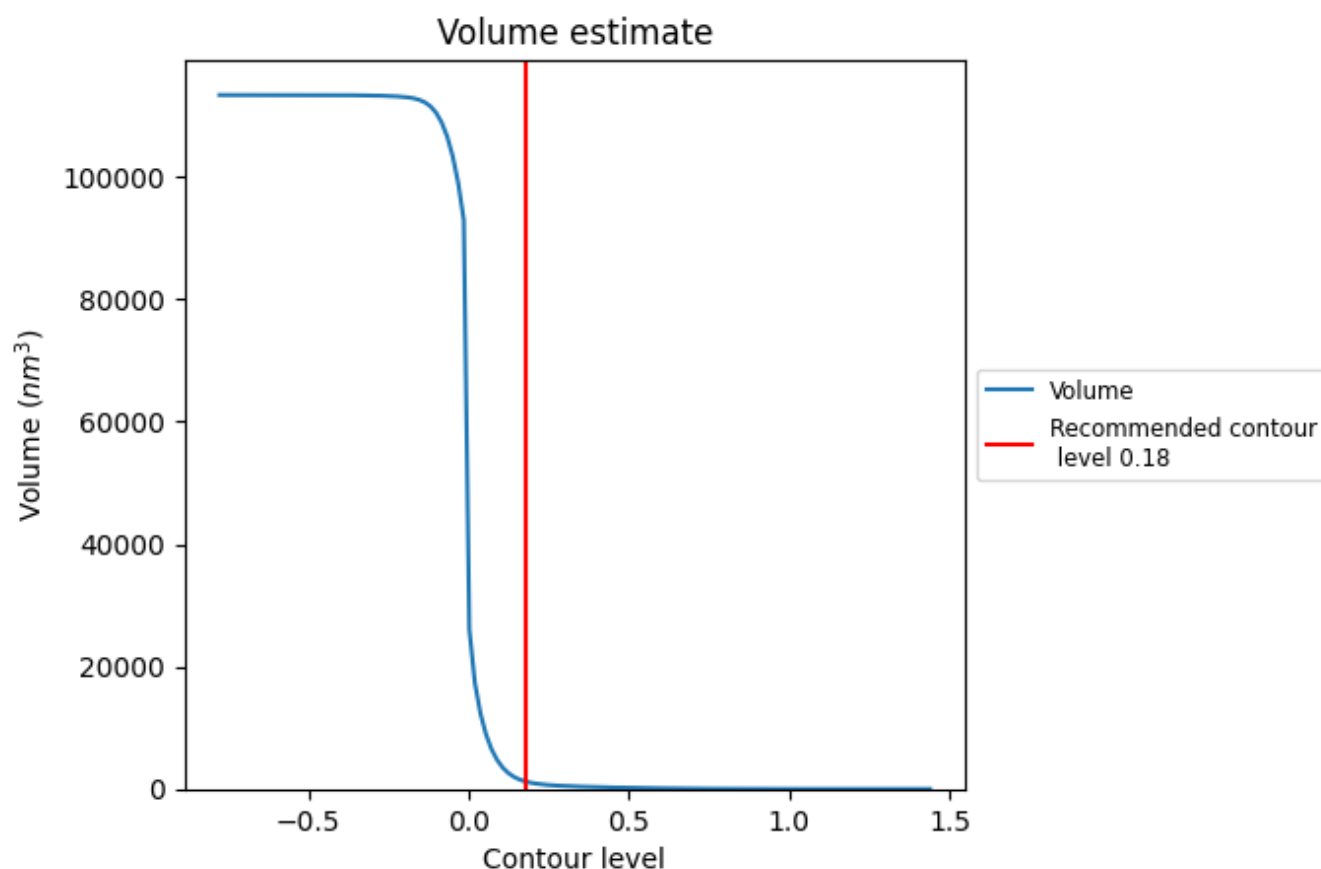
This section contains the results of statistical analysis of the map.

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.

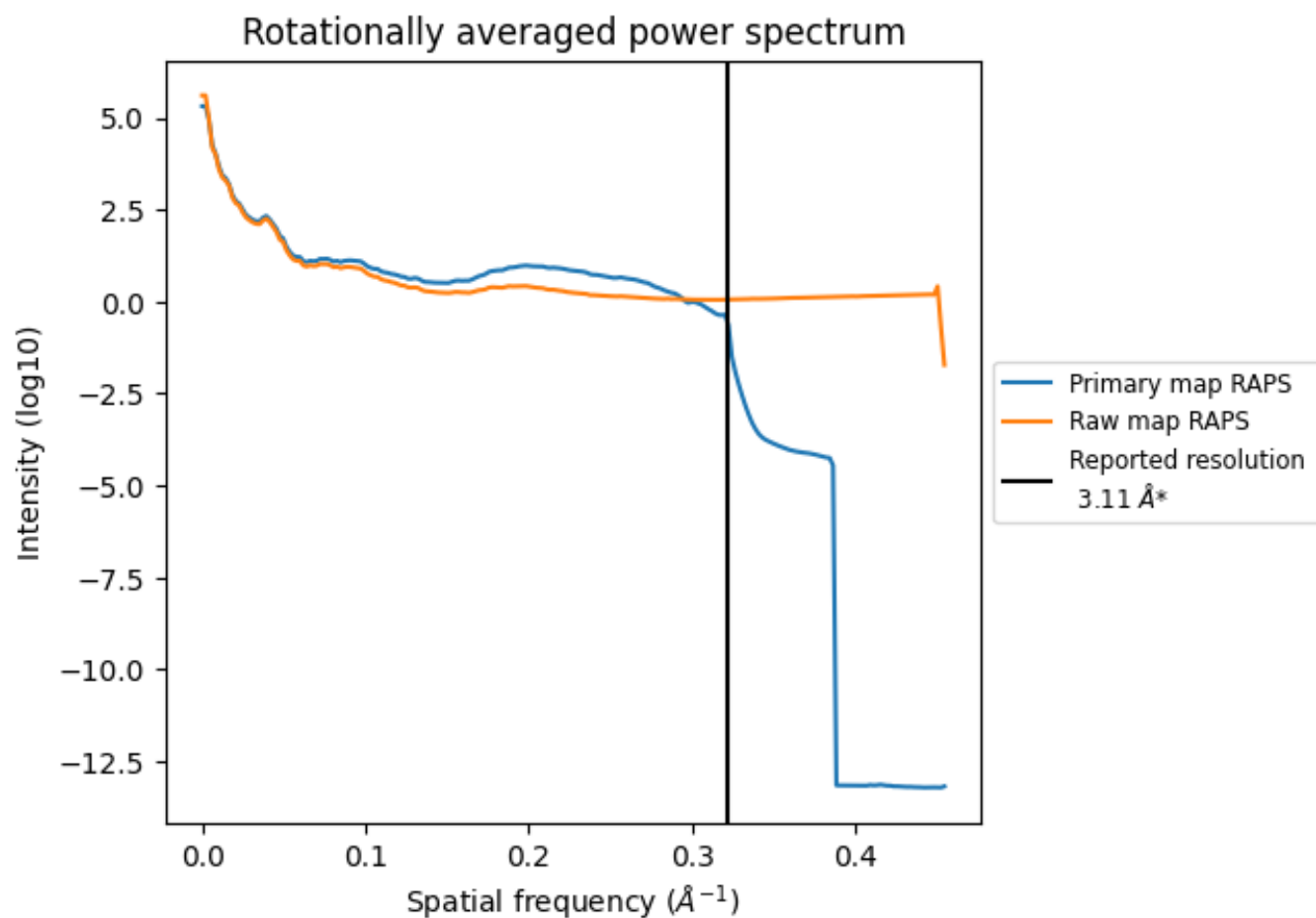
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1184 nm^3 ; this corresponds to an approximate mass of 1069 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 ⓘ

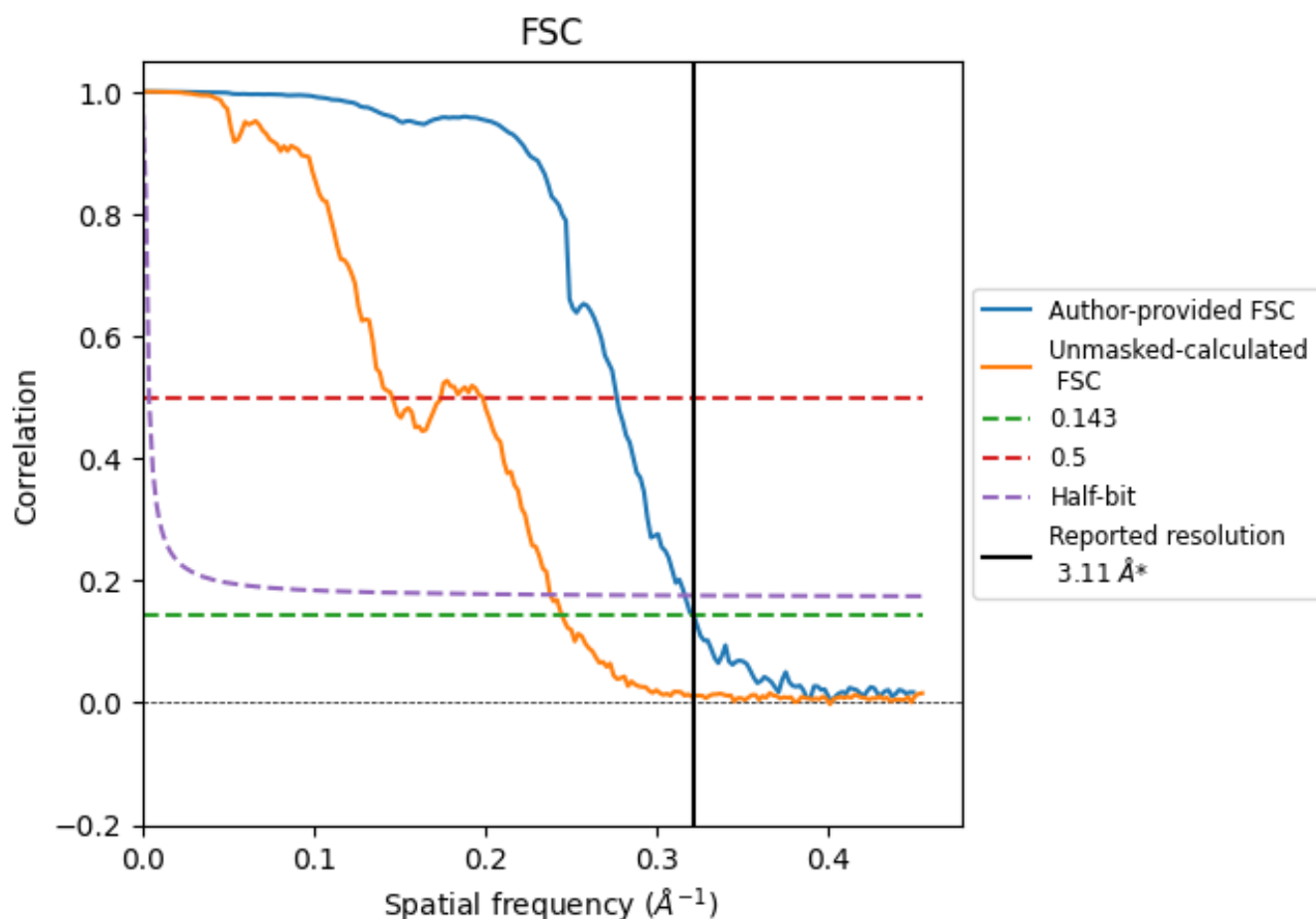


*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

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 0.322 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

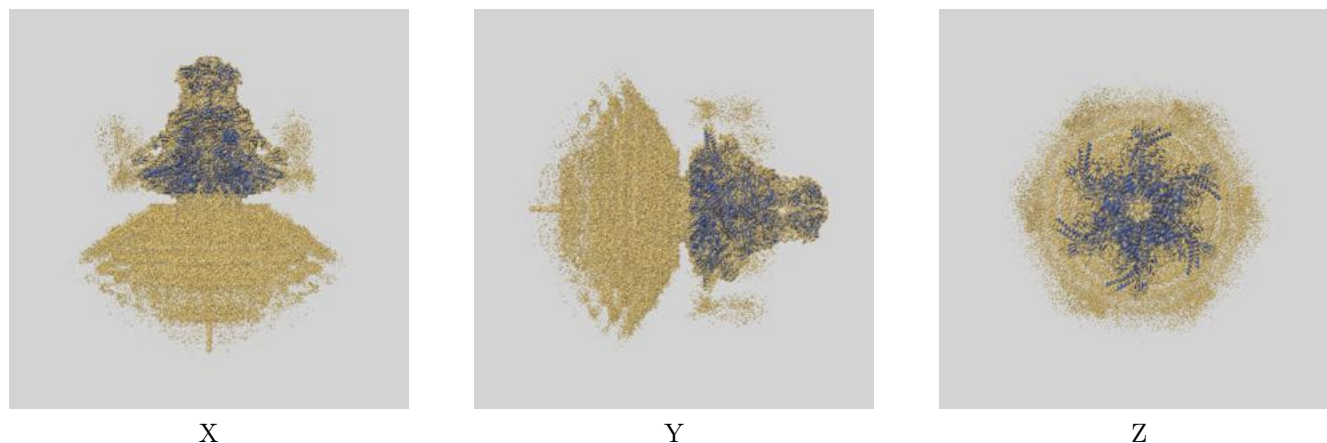
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.11	3.62	3.16
Unmasked-calculated*	4.09	6.87	4.21

*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 4.09 differs from the reported value 3.11 by more than 10 %

9 Map-model fit [i](#)

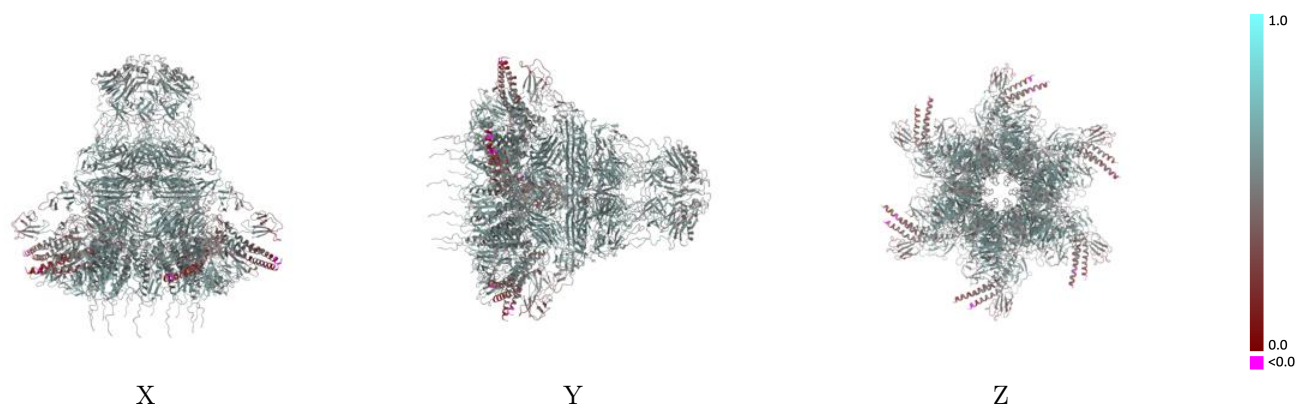
This section contains information regarding the fit between EMDB map EMD-65388 and PDB model 9VVR. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



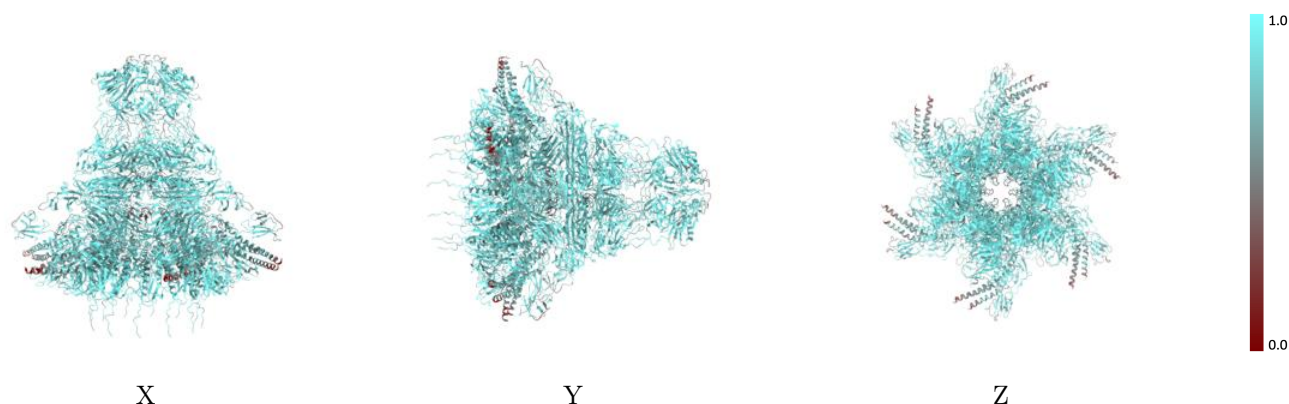
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



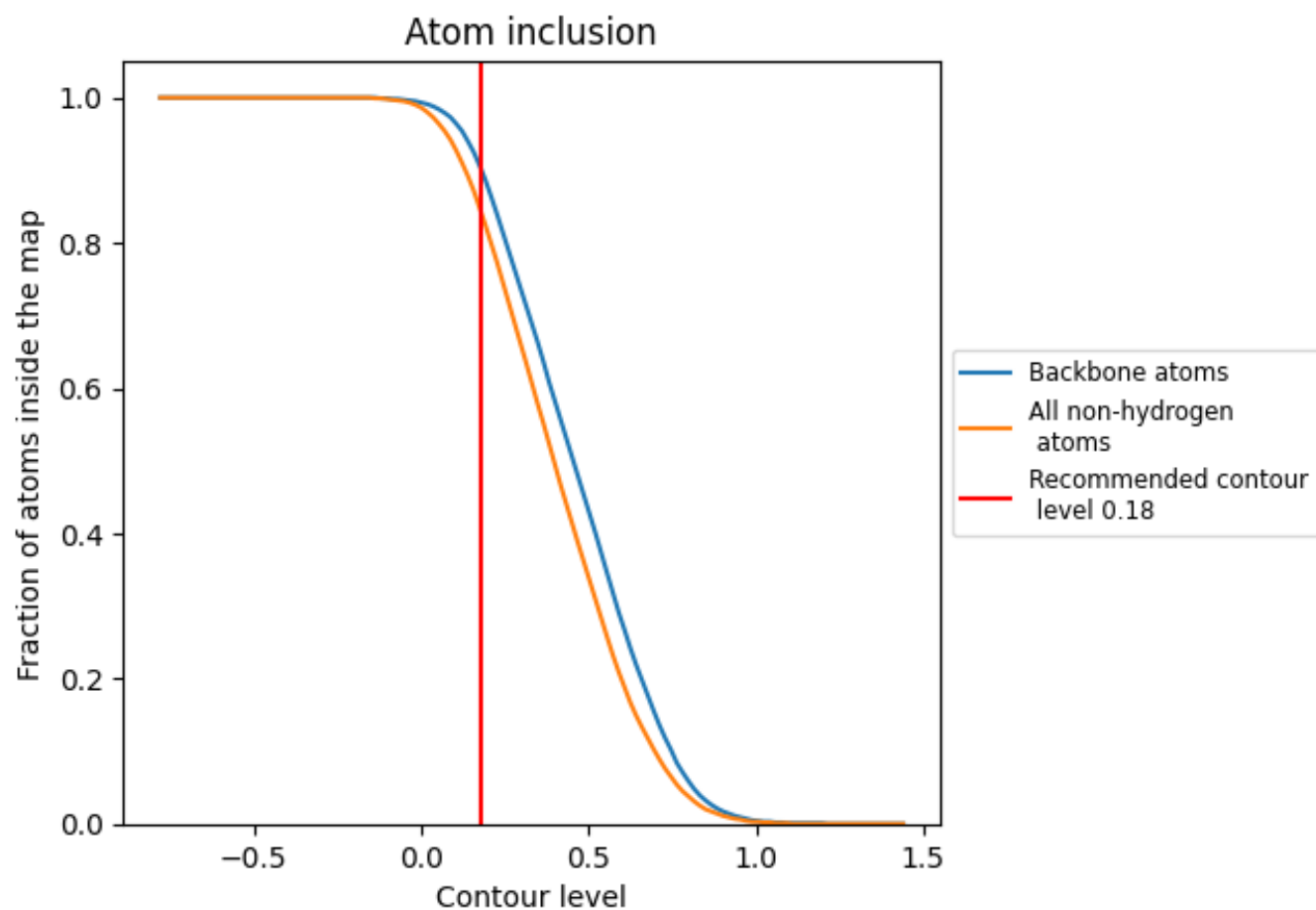
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.5190
A	 0.7240	 0.4060
B	 0.7920	 0.4770
C	 0.8190	 0.4950
D	 0.7340	 0.4020
E	 0.7870	 0.4870
F	 0.8260	 0.4940
G	 0.7290	 0.4070
H	 0.7240	 0.4100
I	 0.7110	 0.3940
J	 0.7940	 0.4820
K	 0.7920	 0.4840
L	 0.7840	 0.4820
M	 0.8230	 0.5020
N	 0.8190	 0.5010
O	 0.8260	 0.4940
P	 0.7270	 0.4100
Q	 0.7890	 0.4780
R	 0.8220	 0.4990
S	 0.8660	 0.5380
T	 0.8630	 0.5410
U	 0.8500	 0.5370
V	 0.8660	 0.5380
W	 0.8540	 0.5380
X	 0.8670	 0.5370
Y	 0.8640	 0.5420
Z	 0.8680	 0.5390
a	 0.8500	 0.5370
b	 0.8670	 0.5360
c	 0.8450	 0.5340
d	 0.8690	 0.5380
e	 0.8520	 0.5330
f	 0.8610	 0.5440
g	 0.8540	 0.5370
h	 0.8620	 0.5420



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Chain	Atom inclusion	Q-score
i	 0.8630	 0.5410
j	 0.8670	 0.5400