



wwPDB EM Validation Summary Report ⓘ

Mar 13, 2026 – 12:20 AM UTC

PDB ID : 9B45 / pdb_00009b45
EMDB ID : EMD-44168
Title : Pseudomonas phage Pa193 baseplate complex and tail fiber
Authors : Iglesias, S.M.; Cingolani, G.
Deposited on : 2024-03-20
Resolution : 3.30 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:

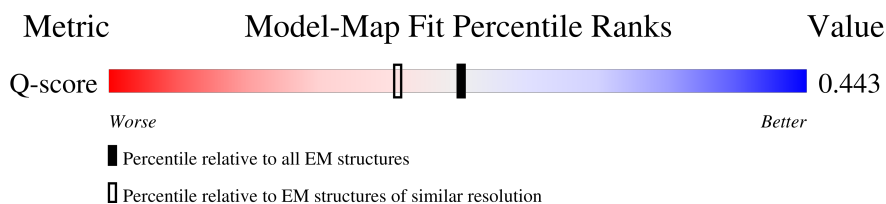
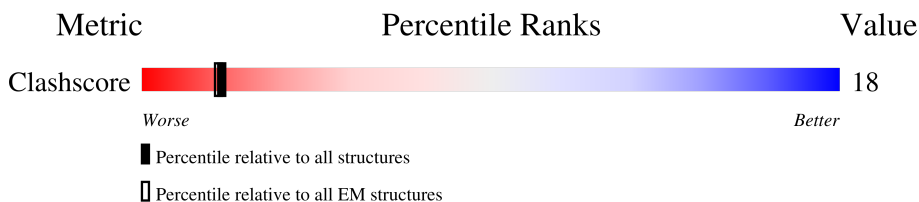
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.30 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	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	j	417	76%	24%
1	k	417	75%	24%
1	l	417	70%	30%
1	m	417	72%	28%
1	n	417	74%	25%
1	o	417	79%	21%

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Mol	Chain	Length	Quality of chain
1	p	417	65% 35%
1	q	417	69% 30% 6%
1	r	417	68% 32% 6%
1	s	417	60% 40%
1	t	417	65% 34% 5%
1	u	417	64% 36% 5%
2	2	962	19% 17% 65% 5%
2	3	962	18% 18% 65% 6%
2	4	962	19% 17% 65% 6%
3	A	107	78% 21%
3	B	107	74% 24%
3	C	107	79% 21%
3	D	107	71% 28%
3	E	107	72% 27%
3	F	107	77% 22%
4	S	180	60% 34% 6%
4	T	180	63% 32% 6%
4	U	180	59% 35% 6%
5	a	858	98%
5	b	858	98%
5	c	858	98%
6	d	287	62% 37%
6	e	287	60% 40%
6	f	287	61% 39%
7	V	197	60% 35% 5%

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Mol	Chain	Length	Quality of chain		
7	W	197	64%	31%	5%
7	X	197	70%	25%	5%
8	l	504	66%	33%	•
8	v	504	63%	36%	•
8	w	504	64%	36%	•
8	x	504	62%	38%	•
8	y	504	60%	39%	•
8	z	504	63%	36%	•
9	M	167	74%	16%	• 10%
9	N	167	67%	23%	10%
9	O	167	74%	17%	10%
9	P	167	74%	16%	10%
9	Q	167	72%	18%	10%
9	R	167	74%	17%	10%
10	G	116	71%	22%	7%
10	H	116	64%	29%	7%
10	I	116	69%	24%	7%
10	J	116	66%	28%	7%
10	K	116	63%	30%	7%
10	L	116	72%	22%	7%
11	g	221	54%	43%	•
11	h	221	56%	41%	•
11	i	221	54%	43%	•

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 104304 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 gp45-a Baseplate wedge 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	j	416	Total 3028	C 1897	N 525	O 596	S 10	0	0
1	k	416	Total 3028	C 1897	N 525	O 596	S 10	0	0
1	l	416	Total 3028	C 1897	N 525	O 596	S 10	0	0
1	m	416	Total 3028	C 1897	N 525	O 596	S 10	0	0
1	n	416	Total 3028	C 1897	N 525	O 596	S 10	0	0
1	o	416	Total 3028	C 1897	N 525	O 596	S 10	0	0
1	q	416	Total 3027	C 1897	N 525	O 595	S 10	0	0
1	p	416	Total 3027	C 1897	N 525	O 595	S 10	0	0
1	r	416	Total 3027	C 1897	N 525	O 595	S 10	0	0
1	s	416	Total 3027	C 1897	N 525	O 595	S 10	0	0
1	t	416	Total 3027	C 1897	N 525	O 595	S 10	0	0
1	u	416	Total 3027	C 1897	N 525	O 595	S 10	0	0

- Molecule 2 is a protein called gp47 Tail fiber.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	340	Total 2547	C 1601	N 450	O 483	S 13	0	0
2	3	340	Total 2547	C 1601	N 450	O 483	S 13	0	0
2	4	340	Total 2547	C 1601	N 450	O 483	S 13	0	0

- Molecule 3 is a protein called gp34 helical bundle.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	106	Total	C	N	O	S	0	0
			854	548	146	154	6		
3	B	106	Total	C	N	O	S	0	0
			854	548	146	154	6		
3	C	106	Total	C	N	O	S	0	0
			854	548	146	154	6		
3	D	106	Total	C	N	O	S	0	0
			854	548	146	154	6		
3	E	106	Total	C	N	O	S	0	0
			854	548	146	154	6		
3	F	106	Total	C	N	O	S	0	0
			854	548	146	154	6		

- Molecule 4 is a protein called gp38 Ripcord-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	170	Total	C	N	O	S	0	0
			1320	823	230	255	12		
4	T	170	Total	C	N	O	S	0	0
			1320	823	230	255	12		
4	U	170	Total	C	N	O	S	0	0
			1320	823	230	255	12		

- Molecule 5 is a protein called gp41 Tape measure protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	a	19	Total	C	N	O	0	0
			146	90	24	32		
5	b	19	Total	C	N	O	0	0
			146	90	24	32		
5	c	19	Total	C	N	O	0	0
			146	90	24	32		

- Molecule 6 is a protein called gp42 Tail hub.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	285	Total	C	N	O	S	0	0
			2261	1430	395	423	13		
6	e	285	Total	C	N	O	S	0	0
			2261	1430	395	423	13		
6	f	285	Total	C	N	O	S	0	0
			2261	1430	395	423	13		

- Molecule 7 is a protein called gp39 Ripcord-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	188	Total	C	N	O	S	0	0
			1436	906	230	293	7		
7	W	188	Total	C	N	O	S	0	0
			1436	906	230	293	7		
7	X	188	Total	C	N	O	S	0	0
			1436	906	230	293	7		

- Molecule 8 is a protein called gp46 Baseplate wedge 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	v	503	Total	C	N	O	S	0	0
			3844	2448	644	738	14		
8	w	503	Total	C	N	O	S	0	0
			3844	2448	644	738	14		
8	x	503	Total	C	N	O	S	0	0
			3844	2448	644	738	14		
8	y	503	Total	C	N	O	S	0	0
			3844	2448	644	738	14		
8	z	503	Total	C	N	O	S	0	0
			3844	2448	644	738	14		
8	1	503	Total	C	N	O	S	0	0
			3844	2448	644	738	14		

- Molecule 9 is a protein called gp37 Baseplate tube.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	151	Total	C	N	O	S	0	0
			1128	723	181	220	4		
9	N	151	Total	C	N	O	S	0	0
			1128	723	181	220	4		
9	O	151	Total	C	N	O	S	0	0
			1128	723	181	220	4		
9	P	151	Total	C	N	O	S	0	0
			1128	723	181	220	4		
9	Q	151	Total	C	N	O	S	0	0
			1128	723	181	220	4		
9	R	151	Total	C	N	O	S	0	0
			1128	723	181	220	4		

- Molecule 10 is a protein called gp35 Sheath initiator.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	108	Total	C	N	O	S	0	0
			823	510	137	172	4		
10	H	108	Total	C	N	O	S	0	0
			823	510	137	172	4		
10	I	108	Total	C	N	O	S	0	0
			823	510	137	172	4		
10	J	108	Total	C	N	O	S	0	0
			823	510	137	172	4		
10	K	108	Total	C	N	O	S	0	0
			823	510	137	172	4		
10	L	108	Total	C	N	O	S	0	0
			823	510	137	172	4		

- Molecule 11 is a protein called gp44 Tail tip.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	g	214	Total	C	N	O	S	0	0
			1650	1026	302	317	5		
11	h	214	Total	C	N	O	S	0	0
			1650	1026	302	317	5		
11	i	214	Total	C	N	O	S	0	0
			1650	1026	302	317	5		

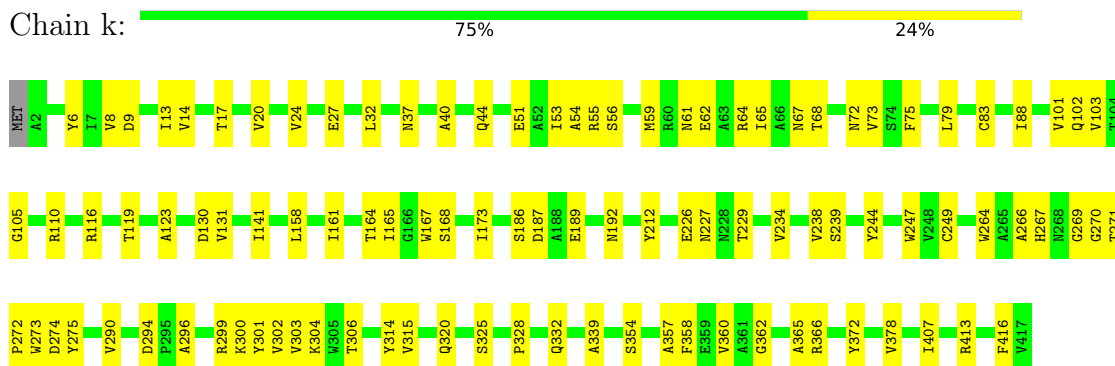
3 Residue-property plots

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.

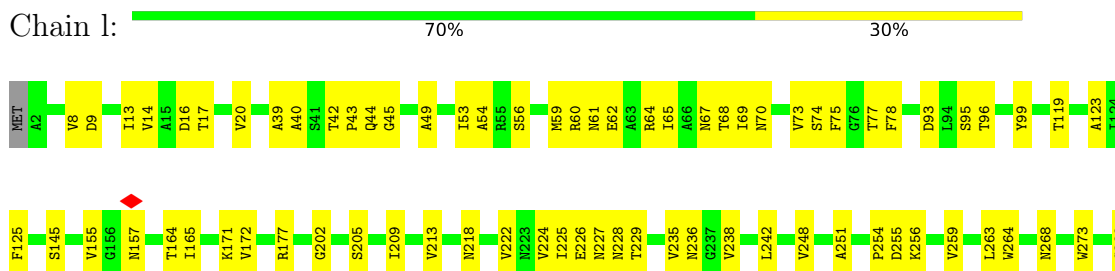
- Molecule 1: gp45-a Baseplate wedge 1

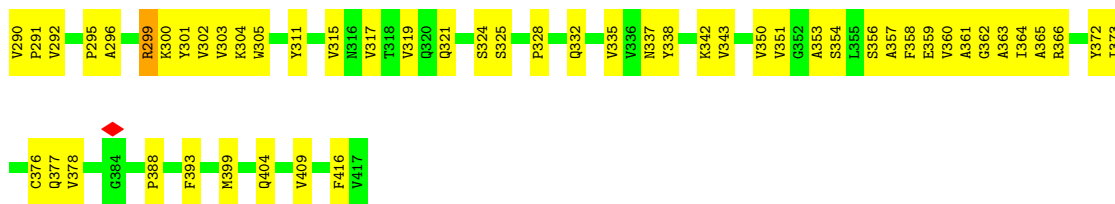


- Molecule 1: gp45-a Baseplate wedge 1



- Molecule 1: gp45-a Baseplate wedge 1

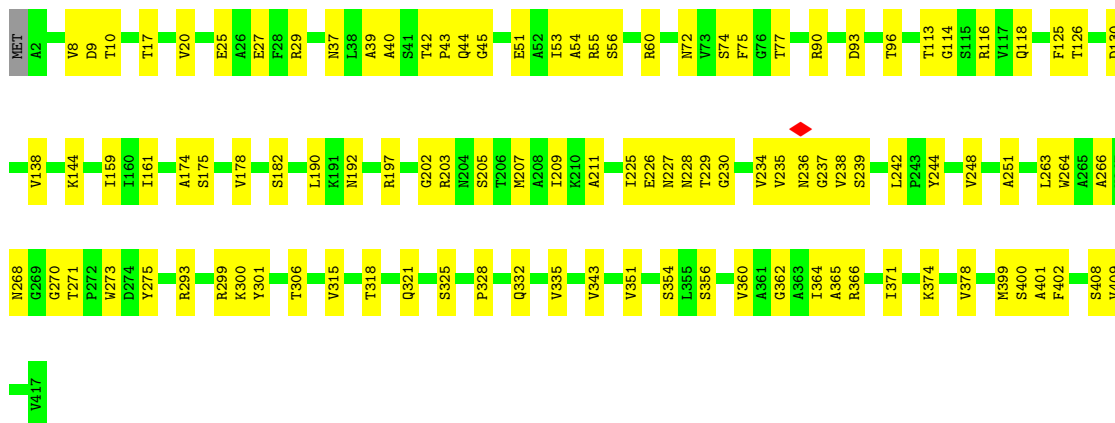




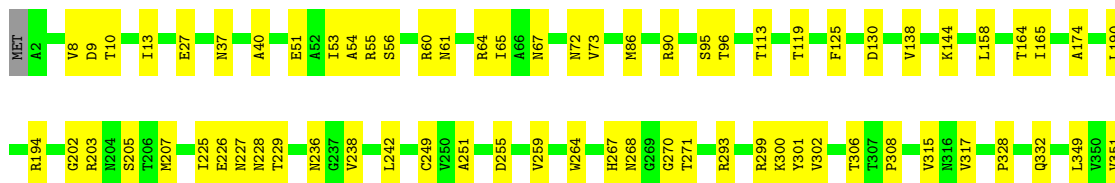
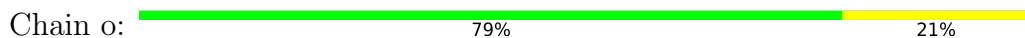
• Molecule 1: gp45-a Baseplate wedge 1



• Molecule 1: gp45-a Baseplate wedge 1

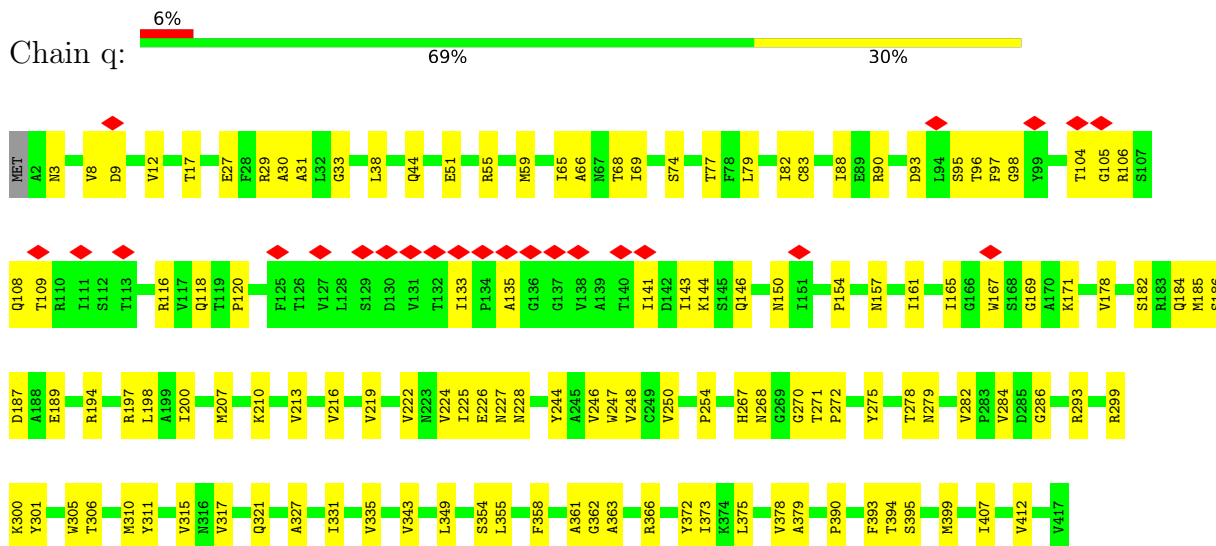


• Molecule 1: gp45-a Baseplate wedge 1

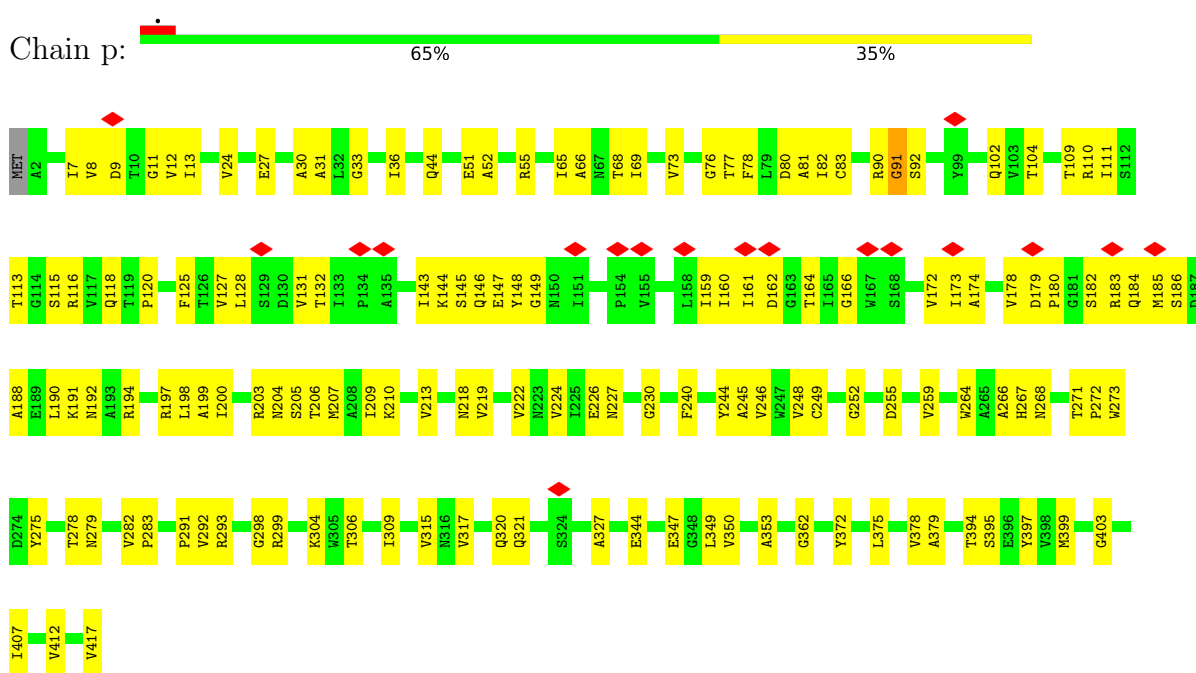




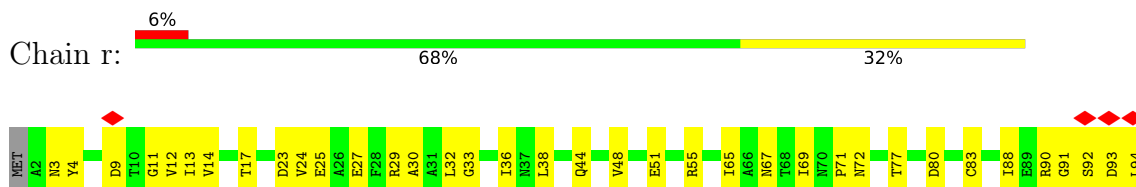
- Molecule 1: gp45-a Baseplate wedge 1

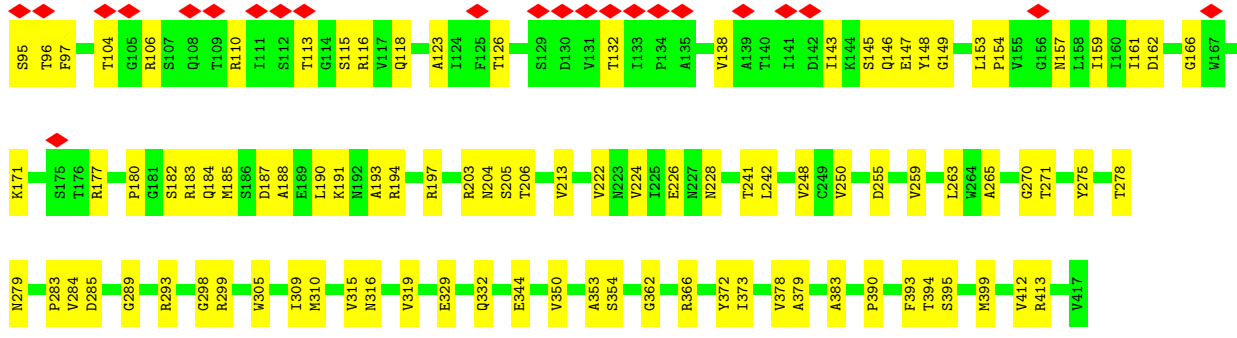


- Molecule 1: gp45-a Baseplate wedge 1

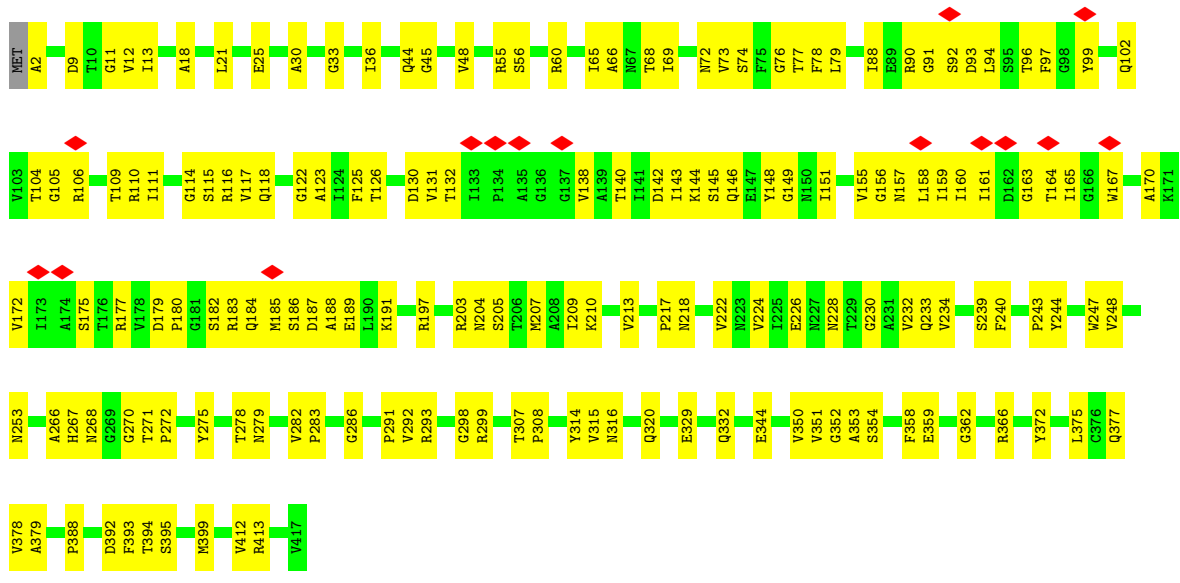


- Molecule 1: gp45-a Baseplate wedge 1

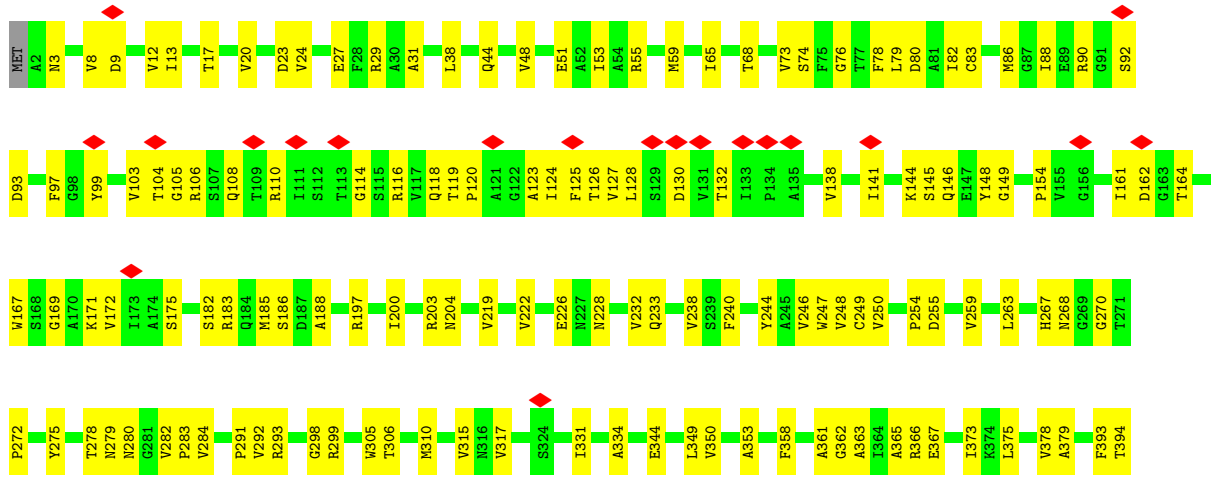




• Molecule 1: gp45-a Baseplate wedge 1

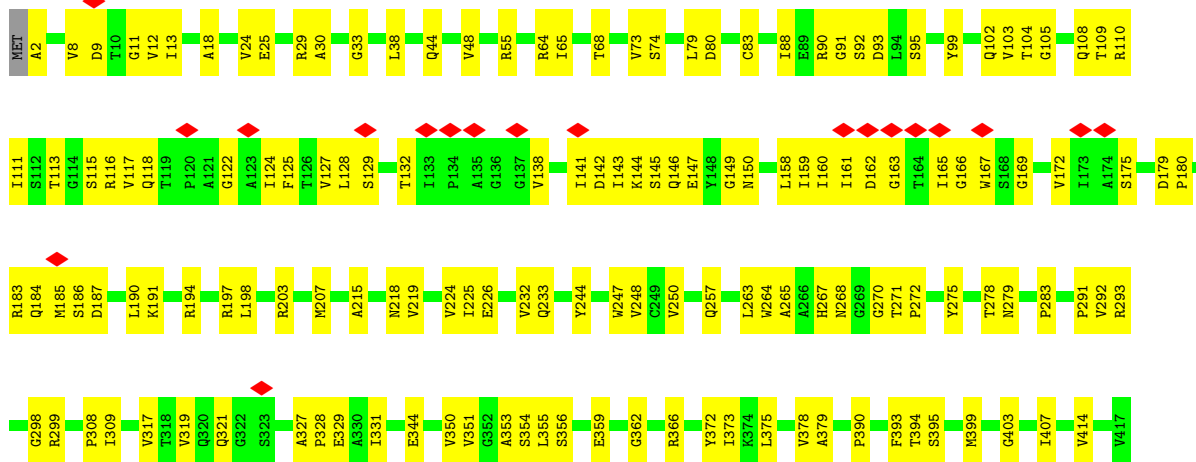


• Molecule 1: gp45-a Baseplate wedge 1

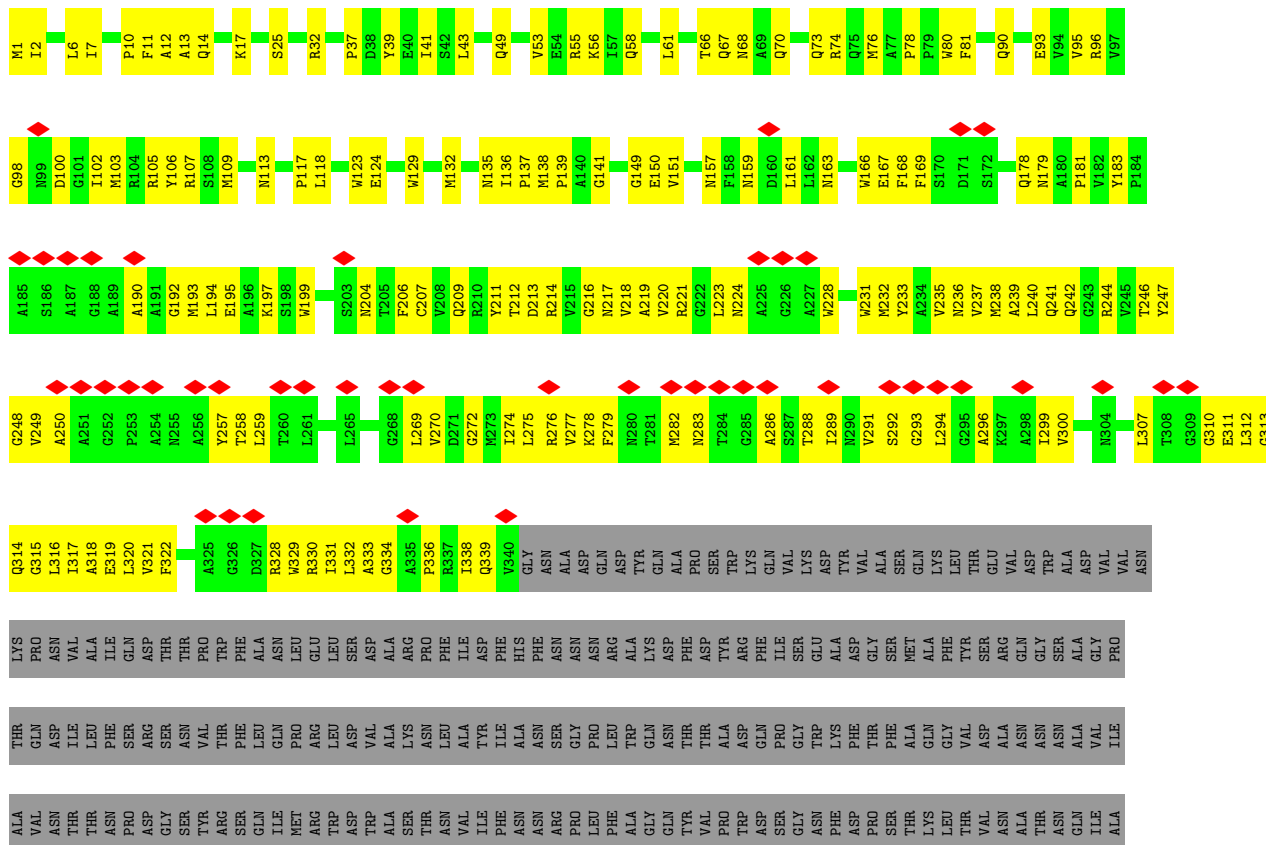




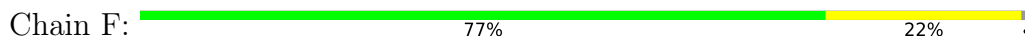
● Molecule 1: gp45-a Baseplate wedge 1



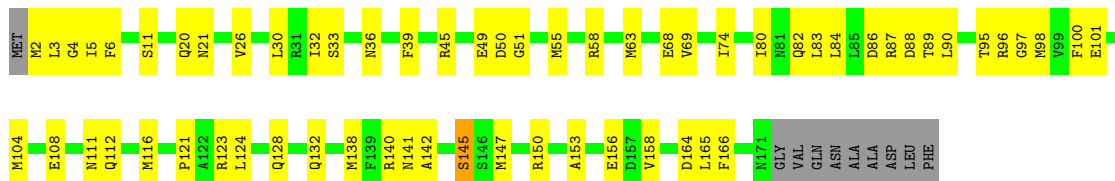
● Molecule 2: gp47 Tail fiber



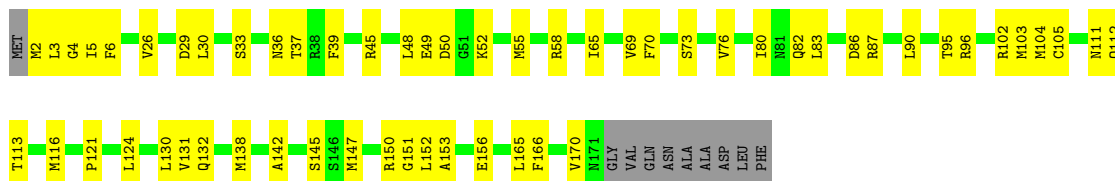
• Molecule 3: gp34 helical bundle



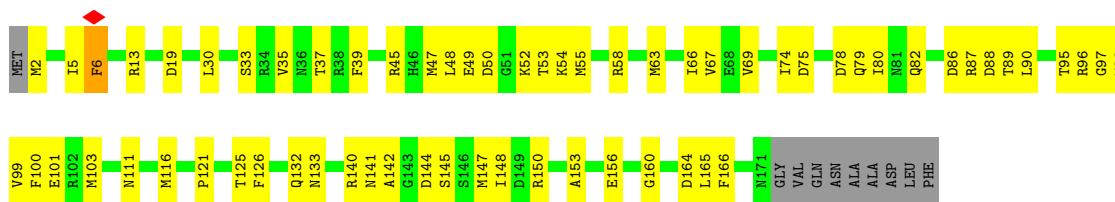
• Molecule 4: gp38 Ripcord-1



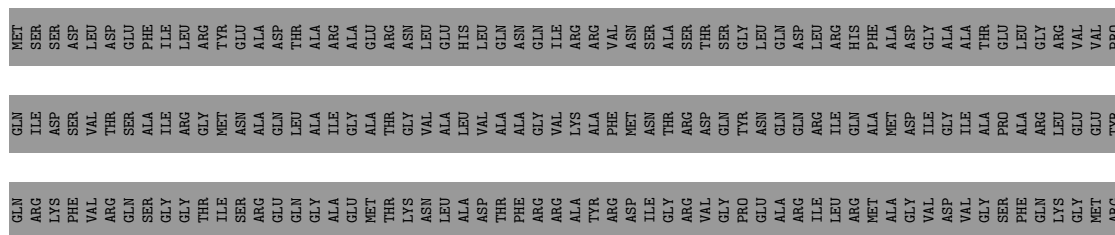
• Molecule 4: gp38 Ripcord-1



• Molecule 4: gp38 Ripcord-1



• Molecule 5: gp41 Tape measure protein



ARG VAL
VAL VAL
GLN R4
VAL R4
PRO I5
GLU L6
ILE R7
ARG M12
ILE M13
PRO M14
ASN M15
GLN M16
ASP M17
ARG M18
MET M19
PRO M20
ARG M21
ASP M22
GLU M23
GLU M24
SER M25
SER M26
ASP M27
GLY M28
SER M29
ILE M30
LEU M31
LEU M32
PHE M33
MET M34
SER M35
TYR M36
ASN M37
ARG M38
GLN M39
GLN M40
LEU M41
LEU M42
ILE M43
ALA M44
LEU M45
GLY M46
ARG M47
ALA M48
LEU M49
SER M50
ASP M51
GLY M52
MET M53
GLY M54
PHE M55
PHE M56
ARG M57
LYS M58
ALA M59
PHE M60
PRO M61
THR M62
GLY M63
THR M64
ASN M65
GLN M66
VAL M67
VAL M68
ASN M69
PRO M70
GLY M71
VAL M72
PHE M73
THR M74
LEU M75
LEU M76
SER M77
PRO M78
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THR M84
GLY M85
ASP M86
ALA M87

ILE
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GLY
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THR
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ARG
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SER
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GLU
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SER
SER
LYS
GLN
LYS
THR
ALA
ASP
ASP
Q840

A848
Q849
T854
K855
L856
Y858

• Molecule 6: gp42 Tail hub



MET
LYS
K3
R4
I5
L6
R7
M12
P13
Y14
D15
I19
R20
E21
D22
L23
D24
V25
R26
V27
R28
L29
M30
L34
N38
R39
A40
T41
M42
E43
I44
F45
T48
L55
L56
W62
R65
Q66
Q68
V69
G70
E74
L75
M76
S80
D87
Q88
G89
R90

S94
F97
V98
G99
E100
V101
A102
P103
V104
D105
I106
P110
R116
T117
Q118
T121
R122
Q123
I124
D125
R126
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R131
P135
A136
V141
K142
E145
T159
M168
P169
S172
I173
T174
S177
Q184
M188
P189
D190
A193
V202
K203

D204
R205
V208
L209
R210
W216
F220
V221
G222
I223
P224
E228
W229
L236
F239
V243
A248
S251
L252
M253
S256
A265
L266
E267
D269
D274
F277
V278
I279
K280
V281
M282
A287

• Molecule 6: gp42 Tail hub



MET
LYS
K3
R4
I5
L6
R7
M12
P13
Y14
E17
V18
I19
D22
L23
D24
V25
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P169
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R171
S172

I173
T174
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D206
K207
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I209
R210
E213
W216
F220
V221
G222
I223
P224
E228
W229
A244
A248
S251
L252
M253
E267
Y268
R273
D274
I279
K280
A287

• Molecule 6: gp42 Tail hub

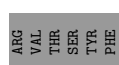


MET
LYS
K3
R4
I5
L6
R7
M12
Y14
E17
V18
I19
R20
E21
D22
L23
D24
V25
R26
I29
M30
K31
A32
A33
L34
R35
I36
Q37
N38
R39
A40
T41
M42
E43
I44
F45
T48
L55
F59
W62
K63
H64
R65
Q66
R67
Q68
V69
G70
M75
L76
I77

S80
D87
Q88
G89
R90
S94
R95
V96
F97
V98
G99
E100
V101
A102
I103
I107
P110
G114
I115
R116
I117
Q118
C119
Y120
T121
R122
Q123
I124
D125
R126
T127
K128
T129
I130
R131
P135
A136
V141
K142
E145
M162
L166
K167
M168
P169
S172
I173
T174



• Molecule 7: gp39 Ripcord-2



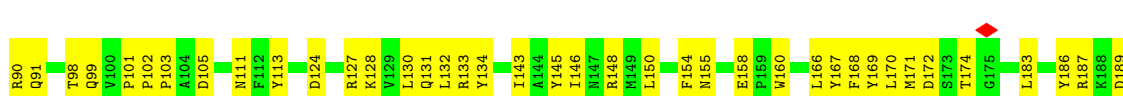
• Molecule 7: gp39 Ripcord-2

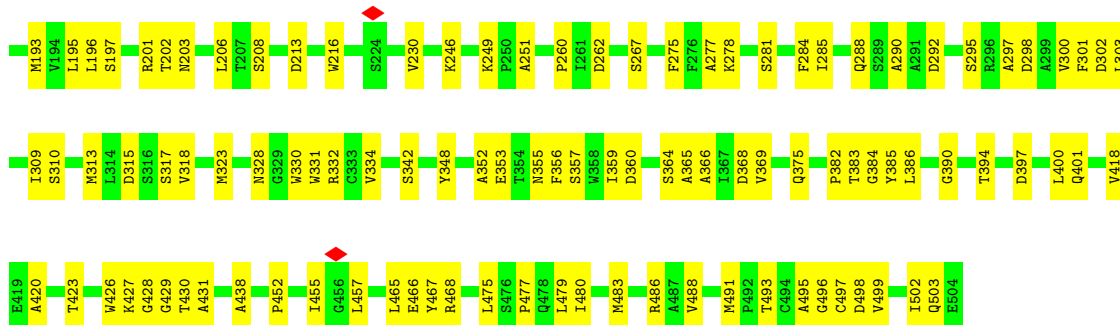


• Molecule 7: gp39 Ripcord-2

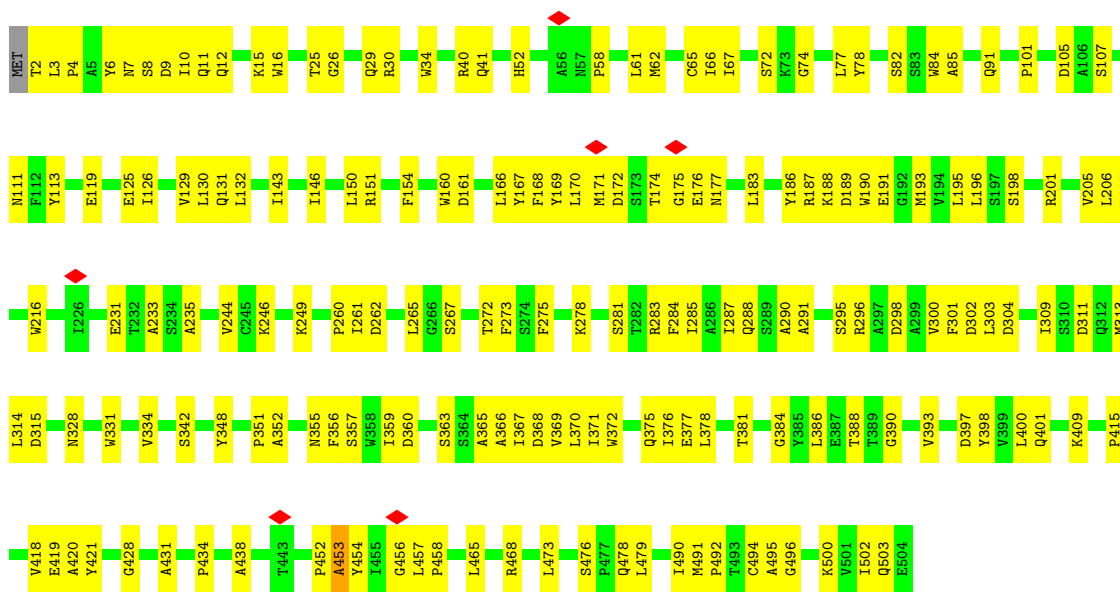


• Molecule 8: gp46 Baseplate wedge 2

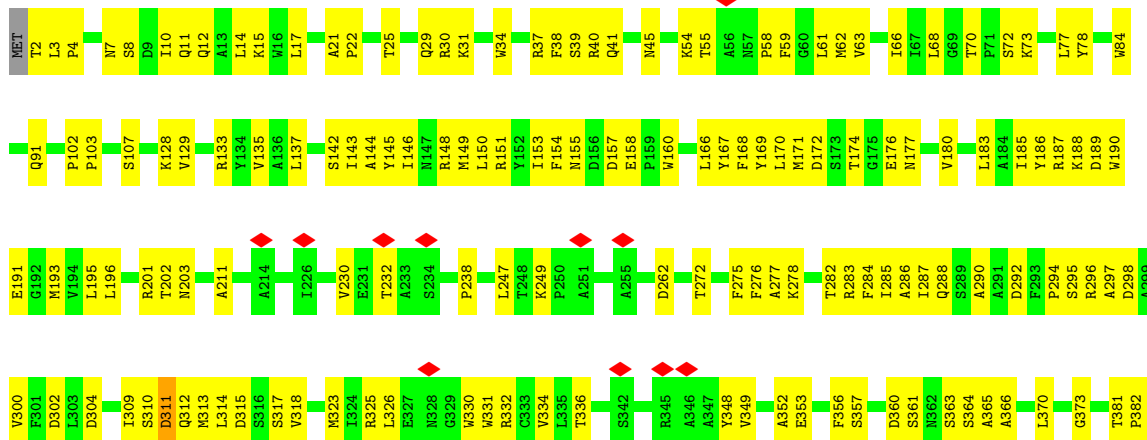


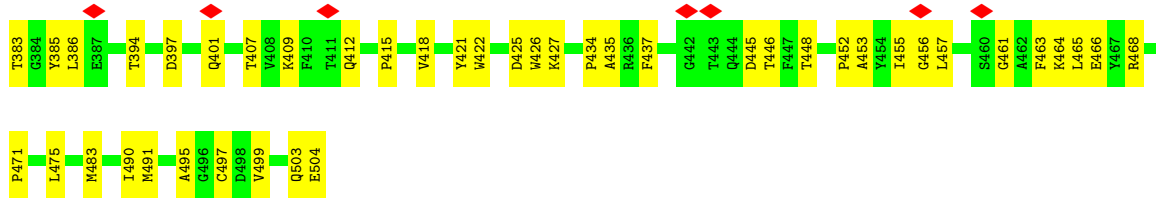


• Molecule 8: gp46 Baseplate wedge 2

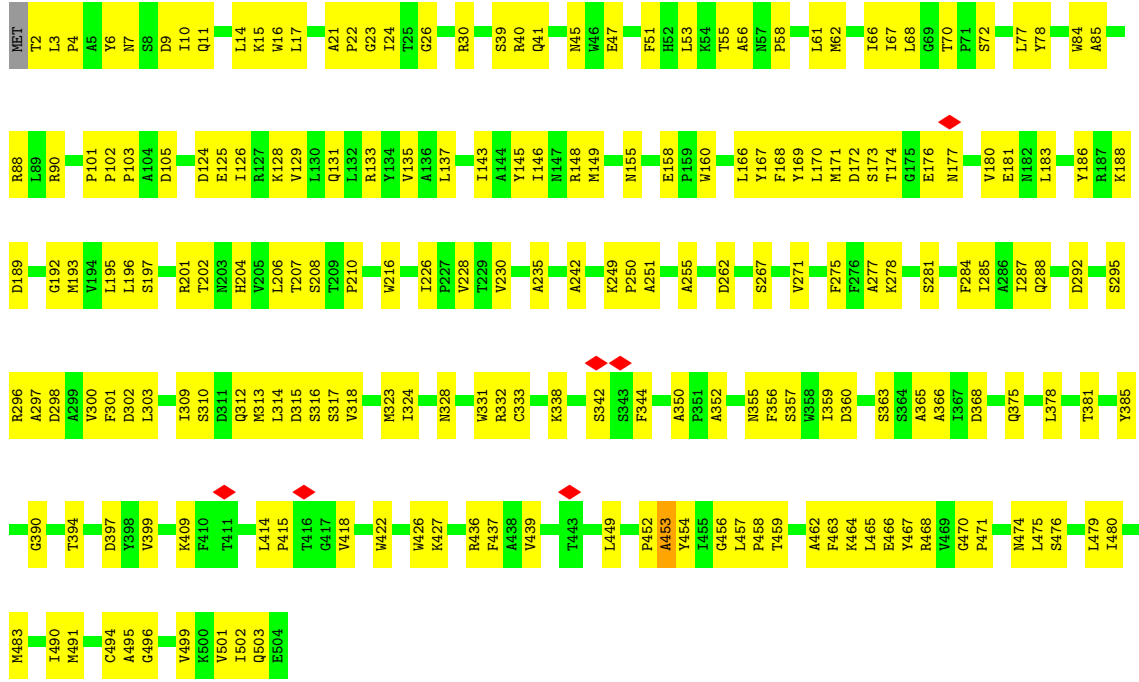


• Molecule 8: gp46 Baseplate wedge 2

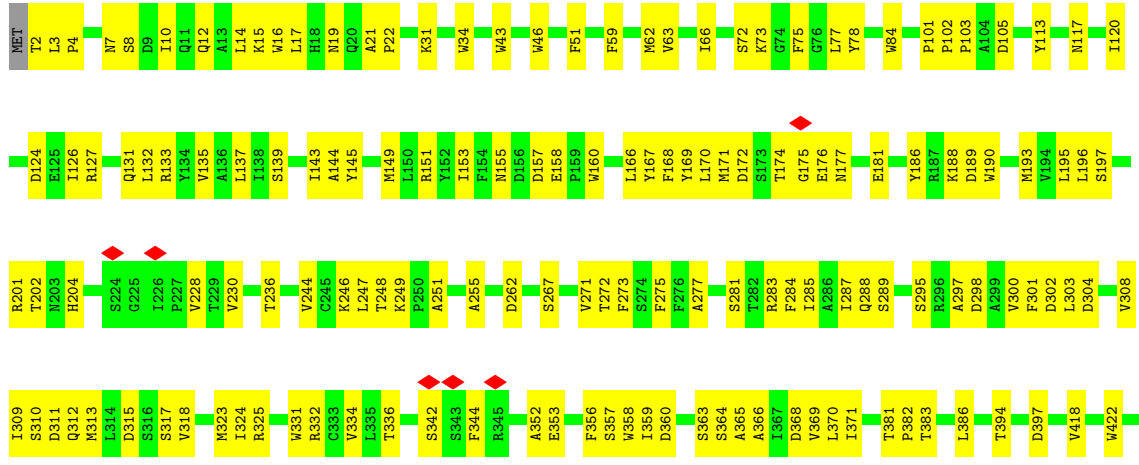




• Molecule 8: gp46 Baseplate wedge 2

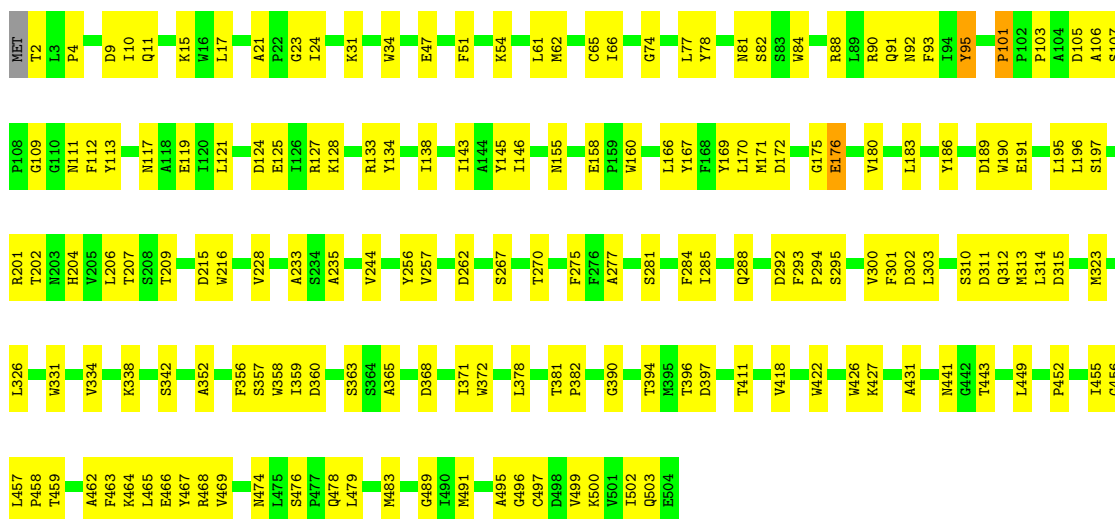


• Molecule 8: gp46 Baseplate wedge 2

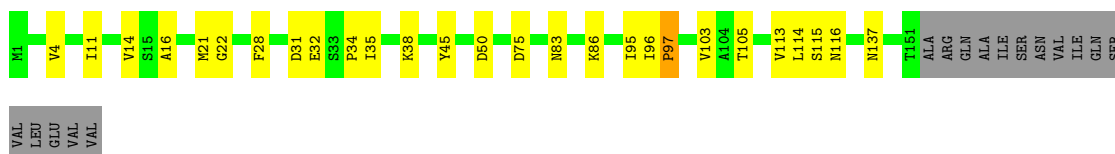




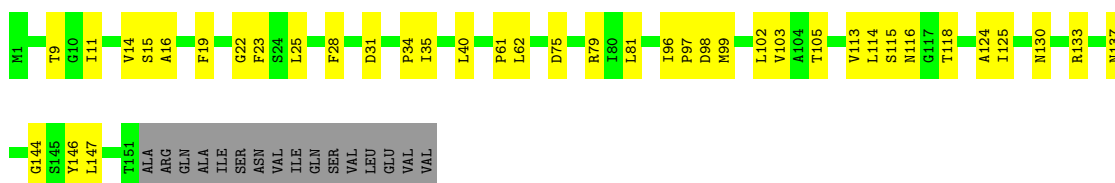
• Molecule 8: gp46 Baseplate wedge 2



• Molecule 9: gp37 Baseplate tube



• Molecule 9: gp37 Baseplate tube



• Molecule 9: gp37 Baseplate tube



VAL
ILE
GLN
SER
GLU
VAL
LEU
GLU
VAL
VAL

- Molecule 9: gp37 Baseplate tube



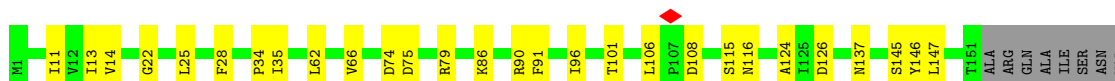
SER
VAL
LEU
GLU
VAL
VAL

- Molecule 9: gp37 Baseplate tube



SER
ASN
VAL
ILE
GLN
SER
VAL
LEU
GLU
VAL

- Molecule 9: gp37 Baseplate tube



ILE
GLN
SER
VAL
LEU
GLU
VAL
VAL

- Molecule 10: gp35 Sheath initiator



- Molecule 10: gp35 Sheath initiator



VAL

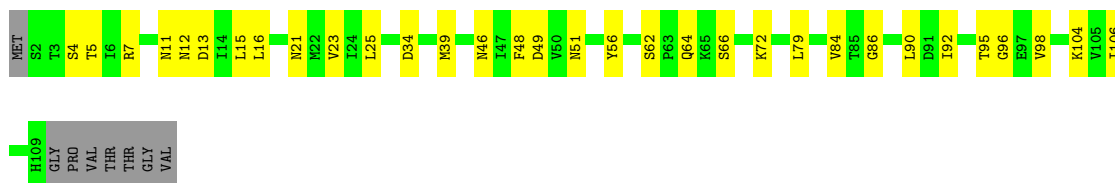
- Molecule 10: gp35 Sheath initiator

Chain I:  69% 24% 7%



- Molecule 10: gp35 Sheath initiator

Chain J:  66% 28% 7%



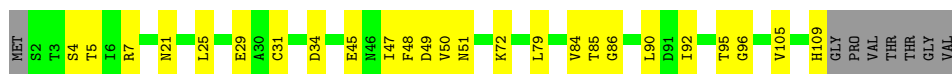
- Molecule 10: gp35 Sheath initiator

Chain K:  63% 30% 7%



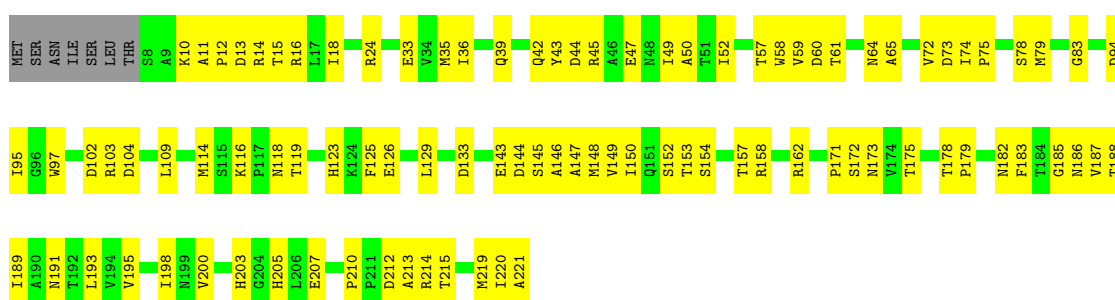
- Molecule 10: gp35 Sheath initiator

Chain L:  72% 22% 7%



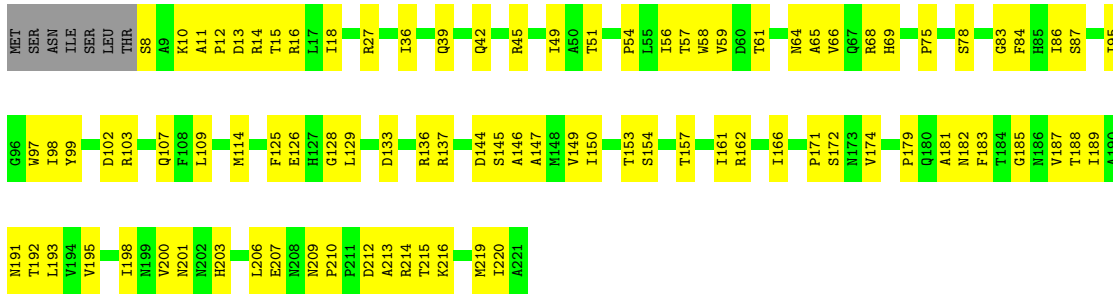
- Molecule 11: gp44 Tail tip

Chain g:  54% 43% 3%

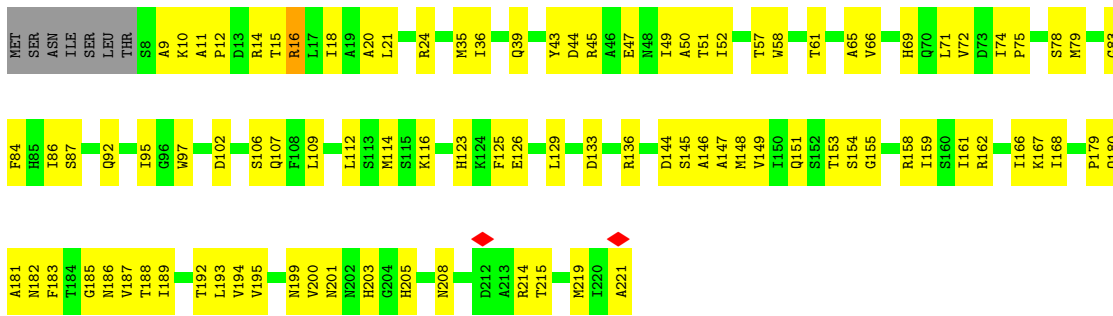


- Molecule 11: gp44 Tail tip

Chain h:  56% 41% 3%



• Molecule 11: gp44 Tail tip



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17175	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 ($e^-/\text{\AA}^2$)	34.4	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	34.243	Depositor
Minimum map value	-13.446	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4	Depositor
Map size (\AA)	643.2, 643.2, 643.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.34, 1.34, 1.34	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	j	0.15	0/3082	0.34	0/4216
1	k	0.22	0/3082	0.39	0/4216
1	l	0.18	0/3082	0.39	0/4216
1	m	0.17	0/3082	0.37	0/4216
1	n	0.16	0/3082	0.33	0/4216
1	o	0.15	0/3082	0.34	0/4216
1	p	0.19	0/3080	0.51	2/4213 (0.0%)
1	q	0.18	0/3080	0.46	0/4213
1	r	0.17	0/3080	0.44	0/4213
1	s	0.20	0/3080	0.48	0/4213
1	t	0.18	0/3081	0.46	0/4216
1	u	0.19	0/3080	0.49	0/4213
2	2	0.18	0/2606	0.44	0/3553
2	3	0.15	0/2606	0.41	0/3553
2	4	0.23	0/2606	0.51	2/3553 (0.1%)
3	A	0.19	0/876	0.42	0/1184
3	B	0.21	0/876	0.54	2/1184 (0.2%)
3	C	0.17	0/876	0.41	0/1184
3	D	0.22	0/876	0.46	0/1184
3	E	0.17	0/876	0.38	0/1184
3	F	0.27	0/876	0.48	0/1184
4	S	0.19	0/1337	0.42	0/1807
4	T	0.20	0/1337	0.43	0/1807
4	U	0.21	0/1337	0.47	0/1807
5	a	0.23	0/146	0.61	0/198
5	b	0.17	0/146	0.62	0/198
5	c	0.34	0/146	0.72	0/198
6	d	0.20	0/2304	0.44	0/3124
6	e	0.18	0/2304	0.44	0/3124
6	f	0.17	0/2304	0.39	0/3124
7	V	0.25	0/1458	0.56	2/1986 (0.1%)
7	W	0.22	0/1458	0.45	0/1986
7	X	0.27	0/1458	0.48	0/1986
8	1	0.26	0/3948	0.53	4/5398 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	v	0.24	0/3948	0.46	0/5398
8	w	0.21	0/3948	0.48	1/5398 (0.0%)
8	x	0.25	0/3948	0.50	3/5398 (0.1%)
8	y	0.23	0/3948	0.48	0/5398
8	z	0.24	0/3948	0.47	0/5398
9	M	0.24	0/1150	0.45	2/1556 (0.1%)
9	N	0.20	0/1150	0.42	0/1556
9	O	0.17	0/1150	0.33	0/1556
9	P	0.19	0/1150	0.45	0/1556
9	Q	0.17	0/1150	0.38	0/1556
9	R	0.19	0/1150	0.41	0/1556
10	G	0.19	0/832	0.45	0/1128
10	H	0.16	0/832	0.34	0/1128
10	I	0.16	0/832	0.38	0/1128
10	J	0.15	0/832	0.35	0/1128
10	K	0.15	0/832	0.34	0/1128
10	L	0.17	0/832	0.40	0/1128
11	g	0.16	0/1682	0.38	0/2288
11	h	0.16	0/1682	0.40	0/2288
11	i	0.21	0/1682	0.46	0/2288
All	All	0.20	0/106408	0.44	18/145041 (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
1	l	0	1
1	q	0	1
1	t	0	1
2	4	0	1
4	S	0	1
4	U	0	2
5	a	0	1
6	d	0	1
8	w	0	1
8	x	0	1
8	y	0	1
8	z	0	1
11	i	0	1
All	All	0	14

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	w	7	ASN	CB-CA-C	-7.78	106.65	117.23
3	B	64	TYR	CA-C-N	-7.70	108.32	123.56
3	B	64	TYR	C-N-CA	-7.70	108.32	123.56
1	p	91	GLY	CA-C-N	7.69	136.23	121.54
1	p	91	GLY	C-N-CA	7.69	136.23	121.54

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	4	39	TYR	Peptide
4	S	145	SER	Peptide
4	U	45	ARG	Sidechain
4	U	6	PHE	Peptide
1	l	299	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	3028	0	3003	84	0
1	k	3028	0	3003	96	0
1	l	3028	0	3003	119	0
1	m	3028	0	3003	93	0
1	n	3028	0	3003	100	0
1	o	3028	0	3003	83	0
1	p	3027	0	3002	149	0
1	q	3027	0	3002	118	0
1	r	3027	0	3002	109	0
1	s	3027	0	3002	188	0
1	t	3027	0	3003	131	0
1	u	3027	0	3002	153	0
2	2	2547	0	2485	221	0
2	3	2547	0	2485	187	0
2	4	2547	0	2485	204	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	854	0	824	36	0
3	B	854	0	824	47	0
3	C	854	0	824	32	0
3	D	854	0	824	53	0
3	E	854	0	824	33	0
3	F	854	0	824	44	0
4	S	1320	0	1331	70	0
4	T	1320	0	1331	62	0
4	U	1320	0	1331	74	0
5	a	146	0	144	16	0
5	b	146	0	144	15	0
5	c	146	0	144	7	0
6	d	2261	0	2269	102	0
6	e	2261	0	2269	104	0
6	f	2261	0	2269	104	0
7	V	1436	0	1454	69	0
7	W	1436	0	1454	73	0
7	X	1436	0	1454	68	0
8	l	3844	0	3720	176	0
8	v	3844	0	3720	167	0
8	w	3844	0	3720	150	0
8	x	3844	0	3720	184	0
8	y	3844	0	3720	195	0
8	z	3844	0	3720	167	0
9	M	1128	0	1132	27	0
9	N	1128	0	1132	36	0
9	O	1128	0	1132	20	0
9	P	1128	0	1132	22	0
9	Q	1128	0	1132	20	0
9	R	1128	0	1132	24	0
10	G	823	0	800	31	0
10	H	823	0	800	36	0
10	I	823	0	800	25	0
10	J	823	0	800	36	0
10	K	823	0	800	30	0
10	L	823	0	800	32	0
11	g	1650	0	1624	118	0
11	h	1650	0	1624	108	0
11	i	1650	0	1624	117	0
All	All	104304	0	102808	3709	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 18.

The worst 5 of 3709 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)
8:w:494:CYS:SG	1:u:268:ASN:ND2	2.22	1.13
3:F:62:ARG:HD3	1:u:183:ARG:HD2	1.36	1.05
6:d:30:MET:SD	11:i:16:ARG:HG3	1.97	1.04
8:1:62:MET:HG2	1:s:9:ASP:HA	1.40	1.03
1:n:236:ASN:HB2	1:s:299:ARG:HG2	1.43	0.97

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	p	1
1	q	1
1	s	1
1	u	1
1	r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	p	184:GLN	C	185:MET	N	8.90
1	q	184:GLN	C	185:MET	N	7.08
1	s	184:GLN	C	185:MET	N	5.61
1	u	184:GLN	C	185:MET	N	5.37
1	r	184:GLN	C	185:MET	N	5.33

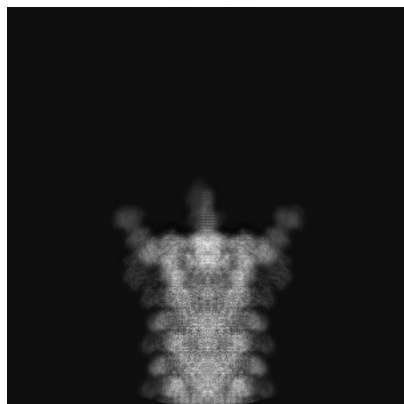
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44168. These allow visual inspection of the internal detail of the map and identification of artifacts.

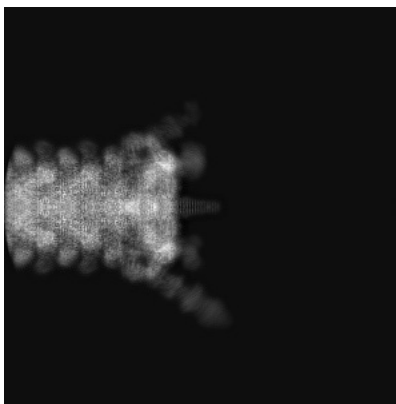
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

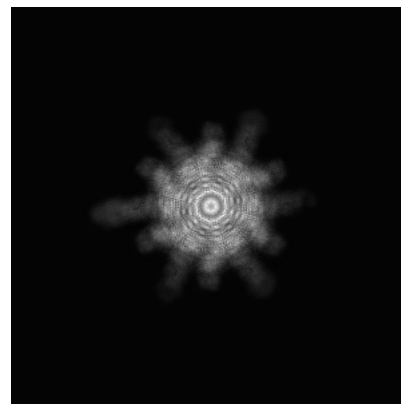
6.1.1 Primary map



X

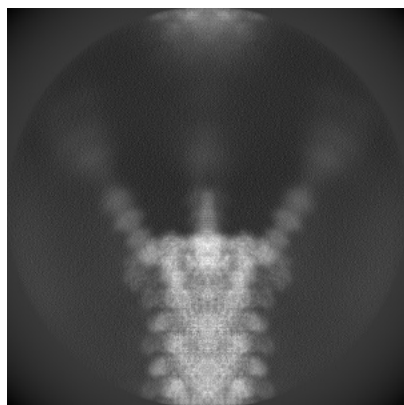


Y

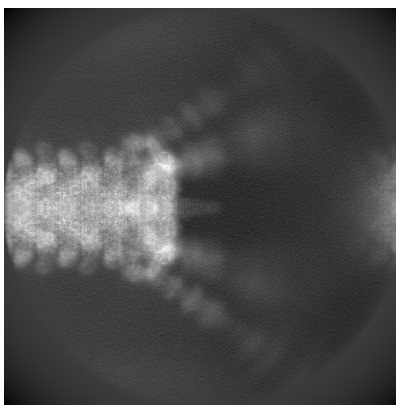


Z

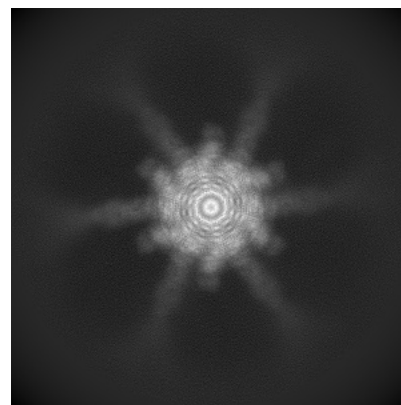
6.1.2 Raw map



X



Y

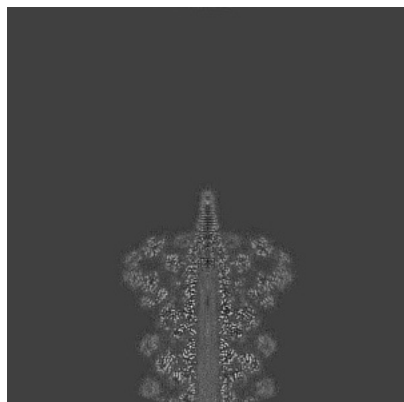


Z

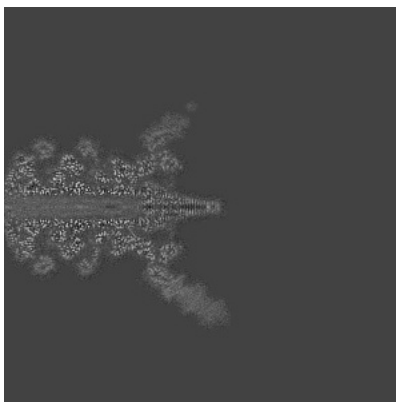
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

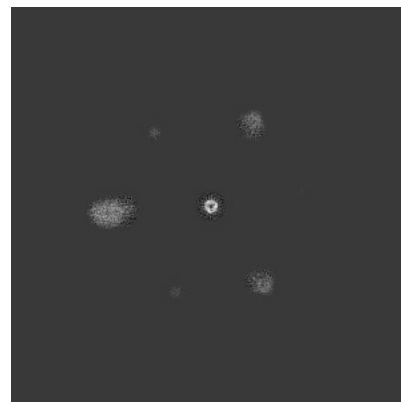
6.2.1 Primary map



X Index: 240

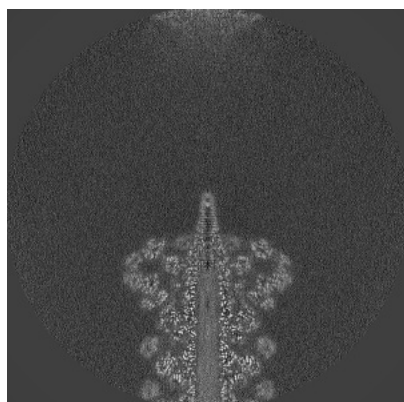


Y Index: 240

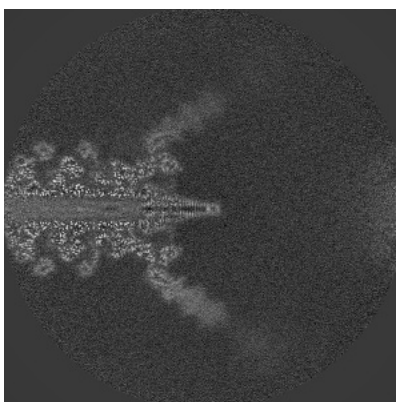


Z Index: 240

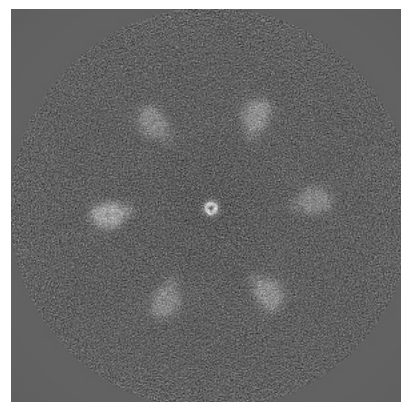
6.2.2 Raw map



X Index: 240



Y Index: 240

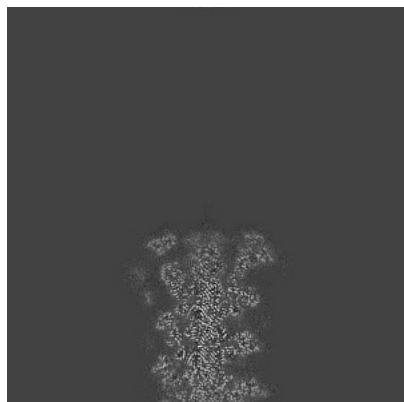


Z Index: 240

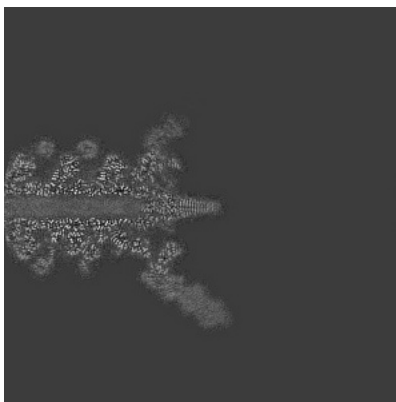
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

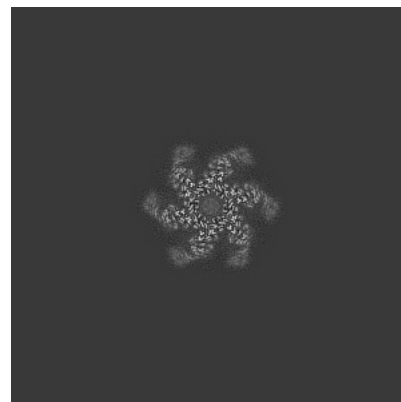
6.3.1 Primary map



X Index: 222

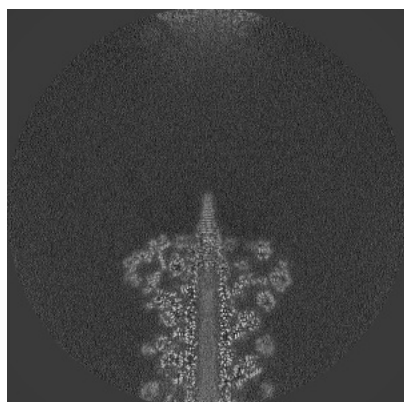


Y Index: 236

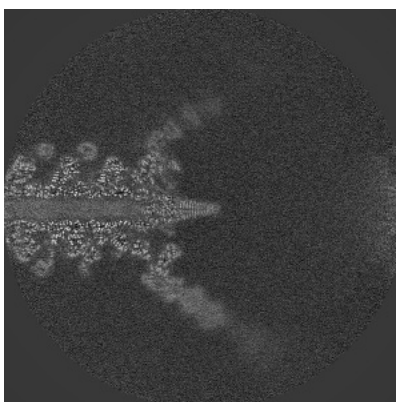


Z Index: 94

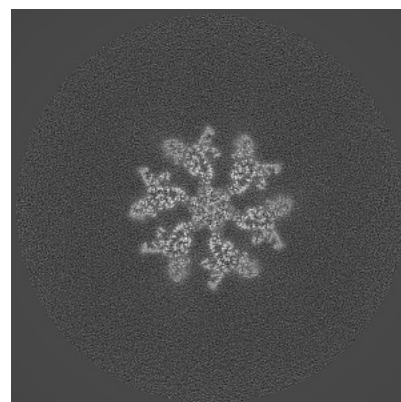
6.3.2 Raw map



X Index: 245



Y Index: 236

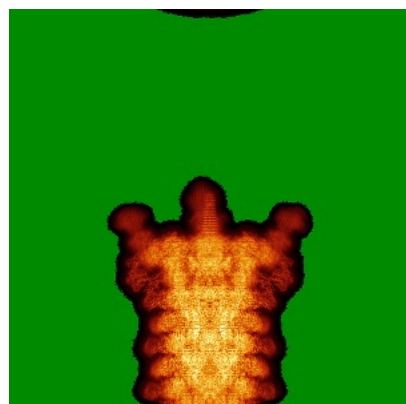


Z Index: 180

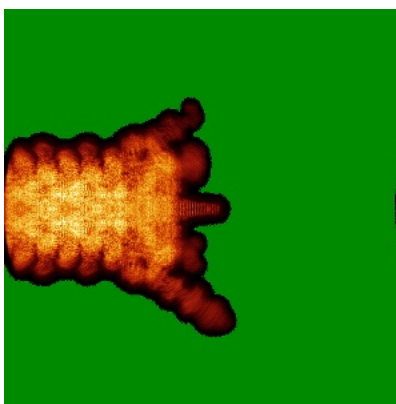
The images above show the largest variance slices of the map in three orthogonal directions.

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

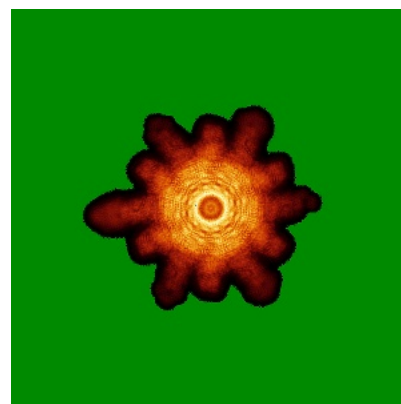
6.4.1 Primary map



X

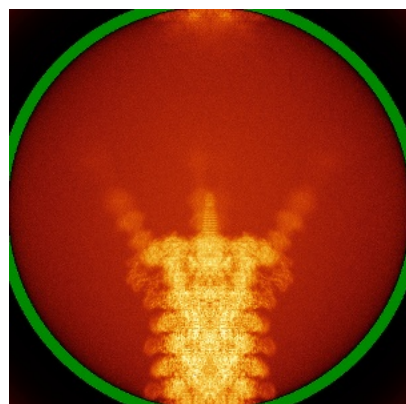


Y

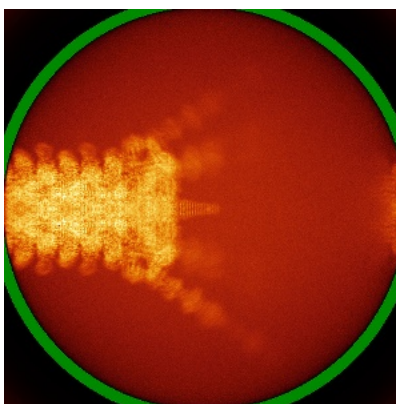


Z

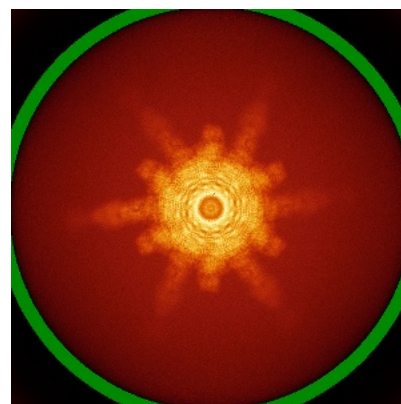
6.4.2 Raw map



X



Y

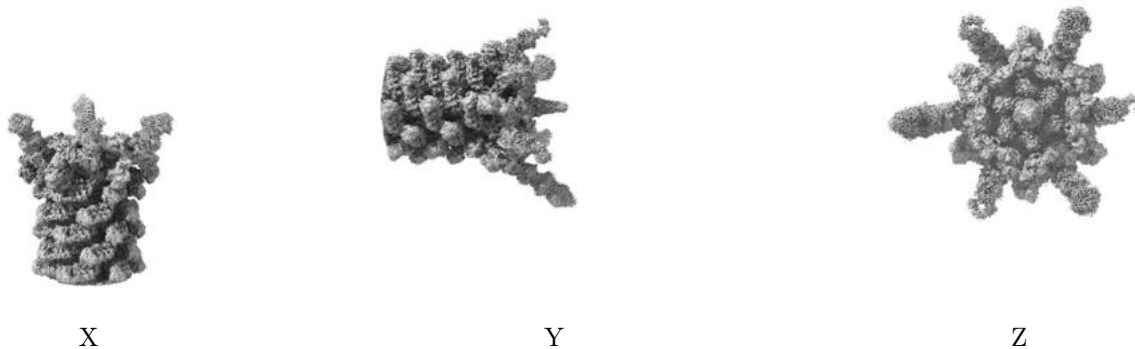


Z

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.

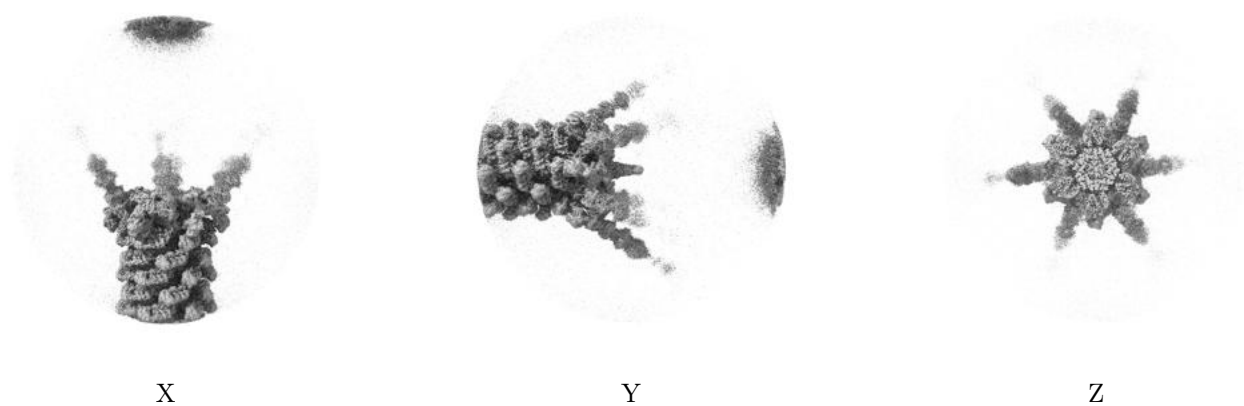
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. 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.

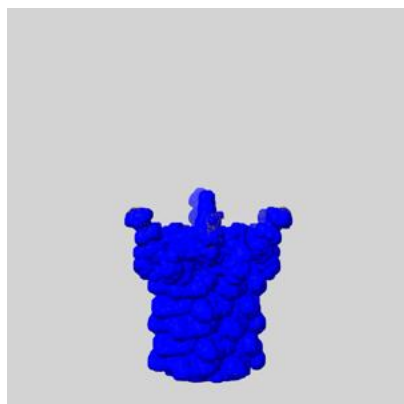
6.6 Mask visualisation [i](#)

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

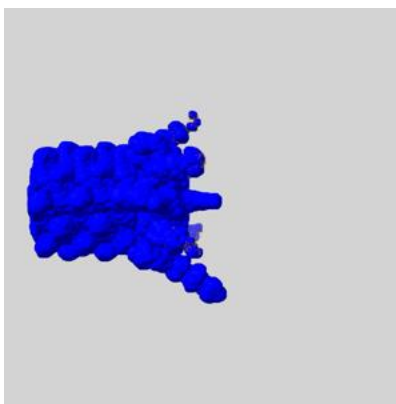
A mask typically either:

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

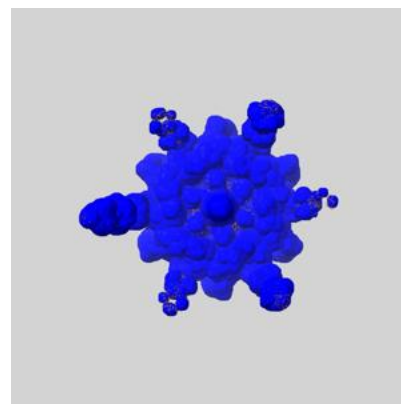
6.6.1 emd_44168_msk_1.map [i](#)



X



Y

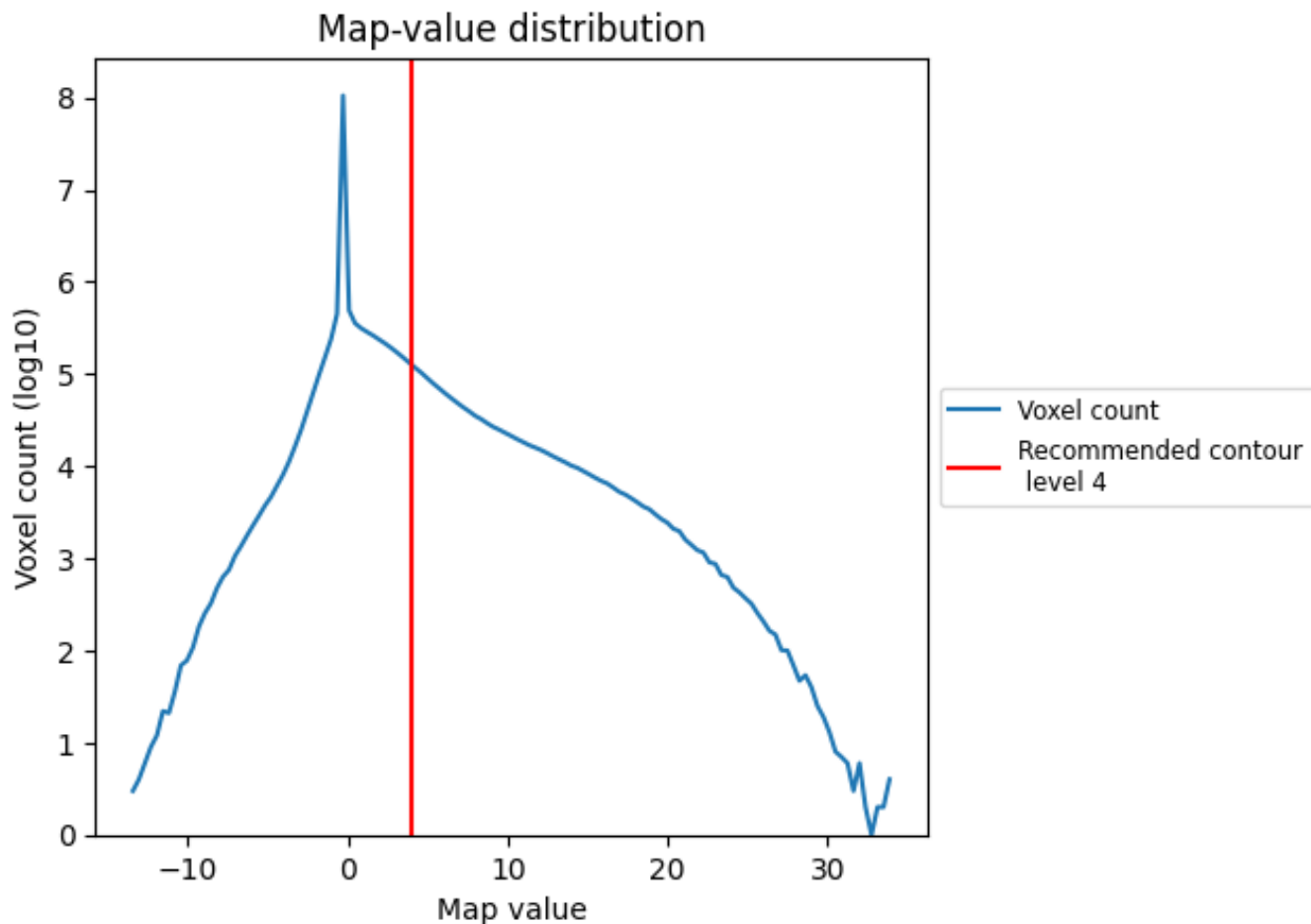


Z

7 Map analysis [i](#)

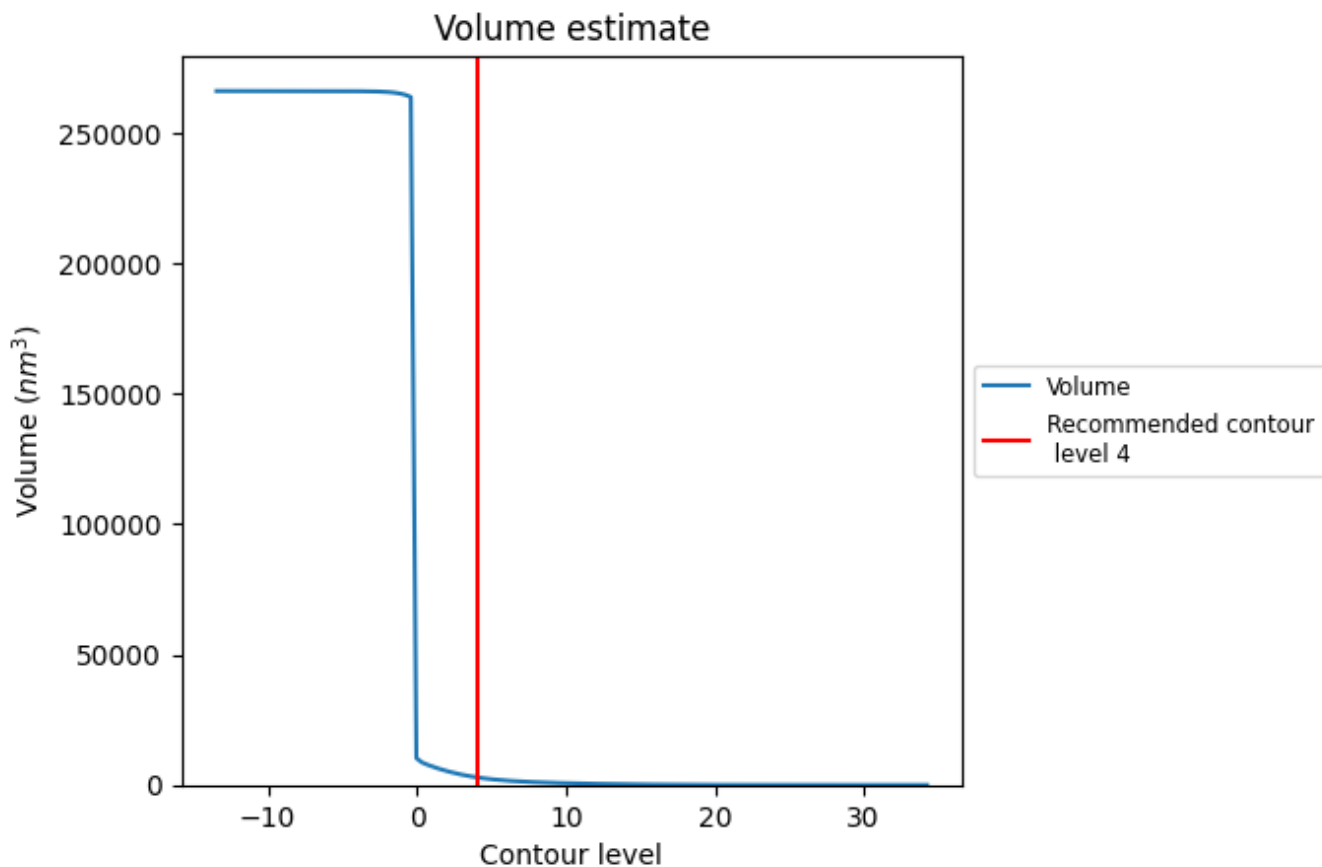
This section contains the results of statistical analysis of the map.

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.

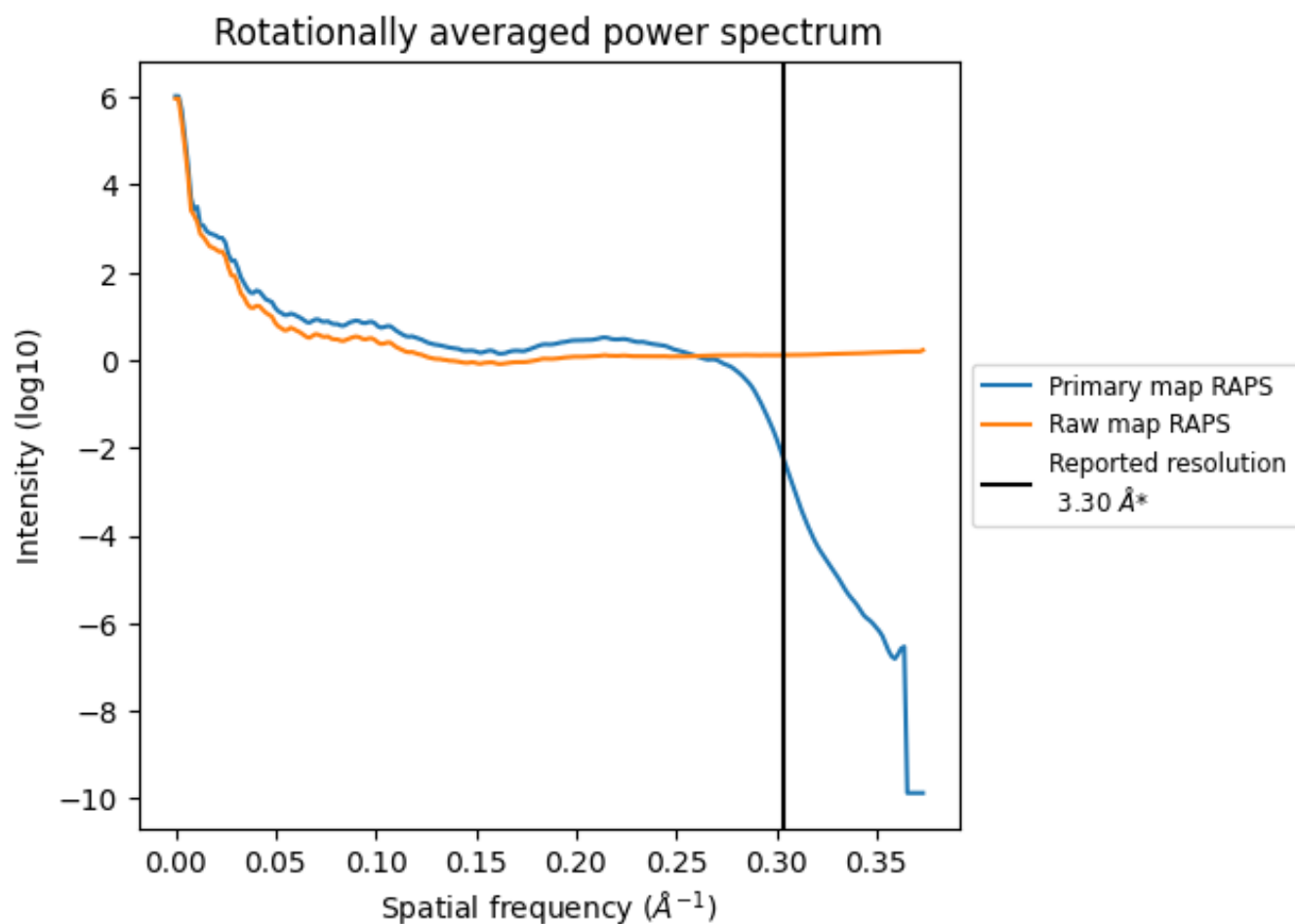
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2941 nm³; this corresponds to an approximate mass of 2657 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

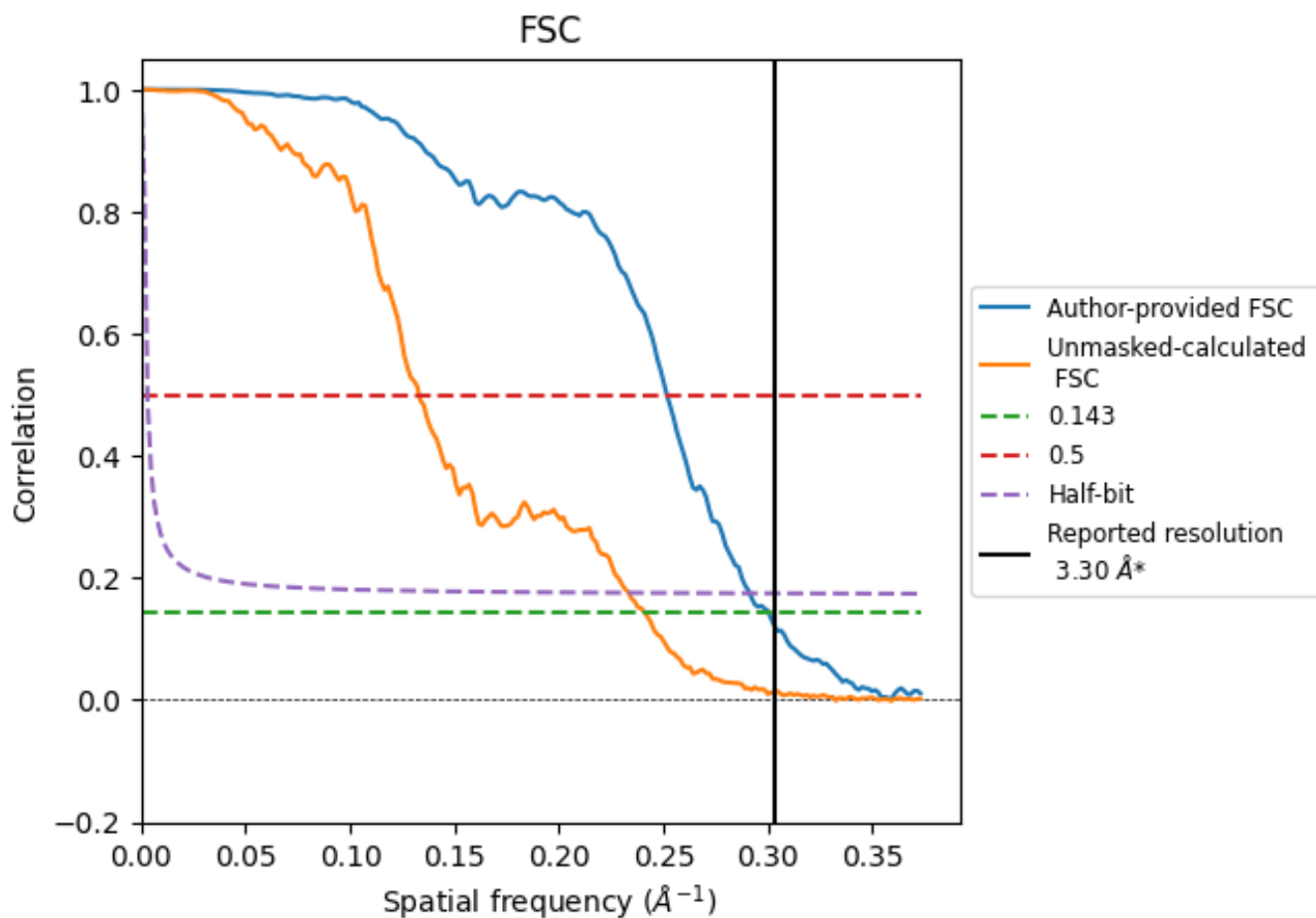


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

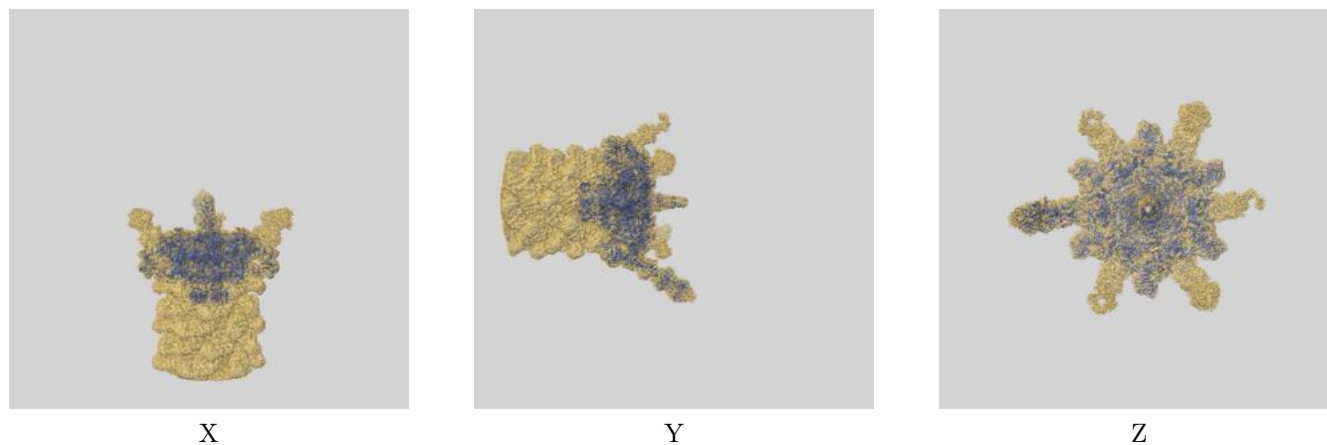
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	3.97	3.43
Unmasked-calculated*	4.15	7.51	4.28

*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 4.15 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

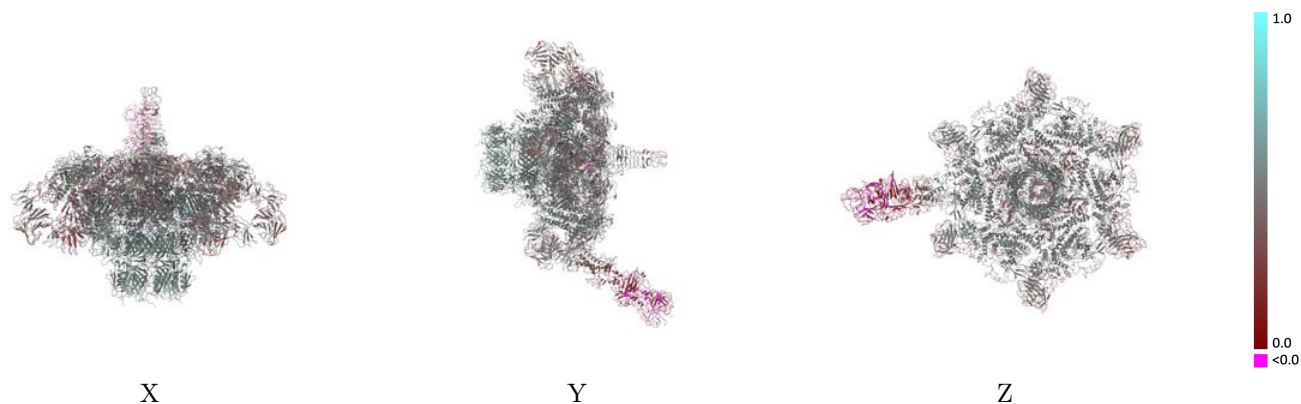
This section contains information regarding the fit between EMDB map EMD-44168 and PDB model 9B45. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



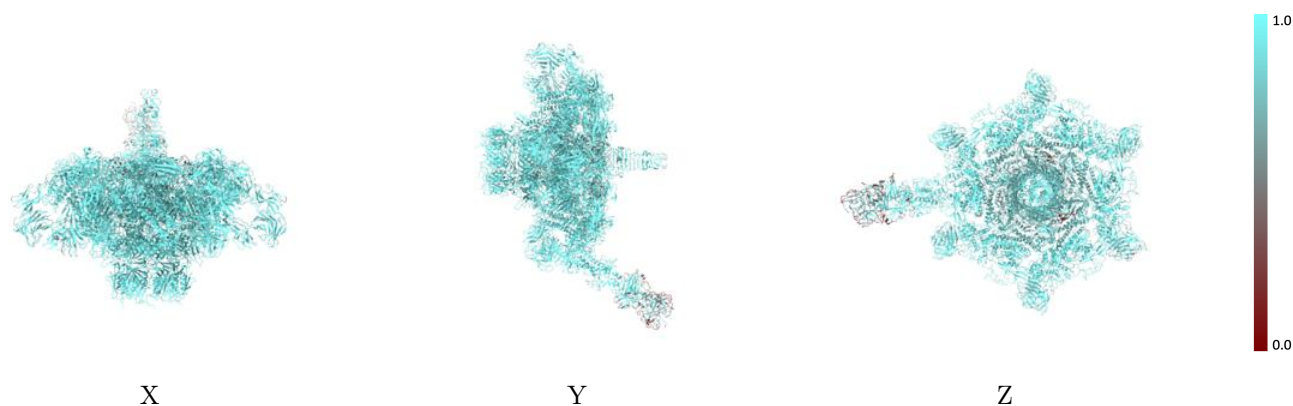
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



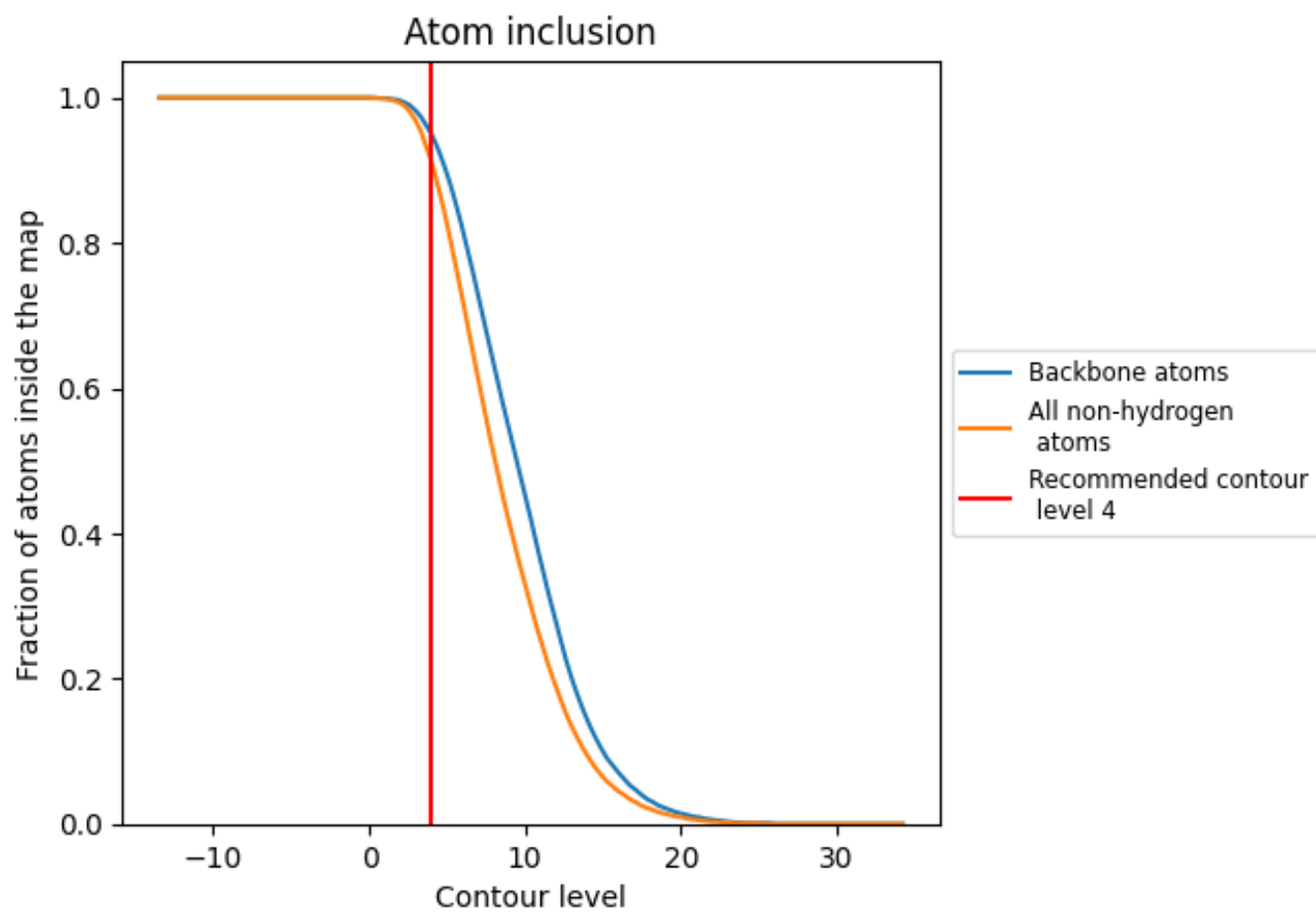
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9120	 0.4430
1	 0.9340	 0.4360
2	 0.7870	 0.2300
3	 0.7800	 0.2400
4	 0.7570	 0.2120
A	 0.9660	 0.5100
B	 0.9700	 0.5080
C	 0.9760	 0.5100
D	 0.9690	 0.5050
E	 0.9700	 0.5080
F	 0.9600	 0.5060
G	 0.9560	 0.5100
H	 0.9480	 0.5120
I	 0.9590	 0.5110
J	 0.9530	 0.5170
K	 0.9620	 0.5150
L	 0.9480	 0.5150
M	 0.9540	 0.5390
N	 0.9520	 0.5300
O	 0.9690	 0.5420
P	 0.9600	 0.5370
Q	 0.9570	 0.5390
R	 0.9570	 0.5360
S	 0.9580	 0.5220
T	 0.9550	 0.5220
U	 0.9490	 0.5190
V	 0.9290	 0.4980
W	 0.9250	 0.4970
X	 0.9310	 0.5000
a	 0.9240	 0.4660
b	 0.9240	 0.4890
c	 0.9380	 0.4920
d	 0.9350	 0.4950
e	 0.9310	 0.4870
f	 0.9340	 0.4920



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Chain	Atom inclusion	Q-score
g	 0.9310	 0.4700
h	 0.9290	 0.4580
i	 0.9230	 0.4630
j	 0.9530	 0.4850
k	 0.9450	 0.4710
l	 0.9340	 0.4560
m	 0.9420	 0.4750
n	 0.9540	 0.4860
o	 0.9640	 0.5050
p	 0.8740	 0.4280
q	 0.8650	 0.4250
r	 0.8570	 0.4180
s	 0.8850	 0.4330
t	 0.8630	 0.4320
u	 0.8900	 0.4410
v	 0.9270	 0.4160
w	 0.9080	 0.3980
x	 0.8650	 0.3450
y	 0.9000	 0.3950
z	 0.9020	 0.3940