



wwPDB EM Validation Summary Report ⓘ

May 18, 2024 – 09:18 AM EDT

PDB ID : 7KH1
EMDB ID : EMD-22873
Title : Baseplate Complex for Myoviridae Phage XM1
Authors : Wang, Z.; Klose, T.; Jiang, W.; Kuhn, R.J.
Deposited on : 2020-10-19
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

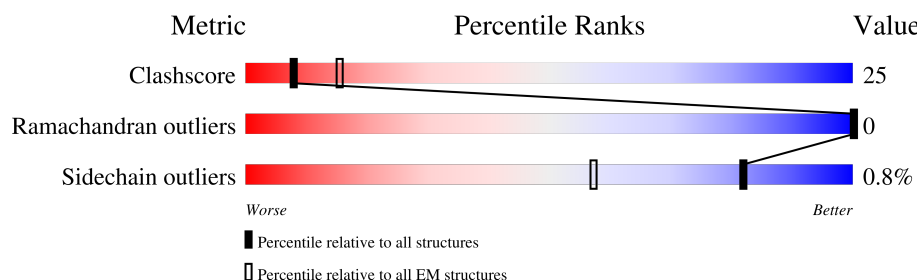
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A1	143	62% 37% ..
1	B1	143	59% 40% ..
1	C1	143	58% 41% ..
1	D1	143	59% 39% ..
1	E1	143	59% 39% ..
1	F1	143	58% 41% ..
2	A2	242	8% 39% 31% 29%
2	B2	242	9% 40% 30% 29%

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Mol	Chain	Length	Quality of chain
2	C2	242	<div> <div>9%</div> <div>39%</div> <div>31%</div> <div>29%</div> </div>
2	D2	242	<div> <div>8%</div> <div>36%</div> <div>34%</div> <div>29%</div> </div>
2	E2	242	<div> <div>10%</div> <div>39%</div> <div>31%</div> <div>29%</div> </div>
2	F2	242	<div> <div>9%</div> <div>39%</div> <div>31%</div> <div>29%</div> </div>
3	A3	250	<div> <div>57%</div> <div>43%</div> </div>
3	B3	250	<div> <div>5%</div> <div>60%</div> <div>40%</div> </div>
3	C3	250	<div> <div>5%</div> <div>57%</div> <div>42%</div> </div>
3	D3	250	<div> <div>5%</div> <div>59%</div> <div>40%</div> </div>
3	E3	250	<div> <div>5%</div> <div>56%</div> <div>44%</div> </div>
3	F3	250	<div> <div>58%</div> <div>41%</div> </div>
4	A4	118	<div> <div>52%</div> <div>48%</div> </div>
4	B4	118	<div> <div>50%</div> <div>50%</div> </div>
4	C4	118	<div> <div>51%</div> <div>49%</div> </div>
4	D4	118	<div> <div>53%</div> <div>47%</div> </div>
4	E4	118	<div> <div>51%</div> <div>49%</div> </div>
4	F4	118	<div> <div>51%</div> <div>49%</div> </div>
5	A5	404	<div> <div>9%</div> <div>51%</div> <div>48%</div> </div>
5	B5	404	<div> <div>13%</div> <div>56%</div> <div>44%</div> </div>
5	C5	404	<div> <div>8%</div> <div>51%</div> <div>48%</div> </div>
5	D5	404	<div> <div>12%</div> <div>53%</div> <div>46%</div> </div>
5	E5	404	<div> <div>8%</div> <div>53%</div> <div>46%</div> </div>
5	F5	404	<div> <div>12%</div> <div>53%</div> <div>46%</div> </div>
5	G5	404	<div> <div>9%</div> <div>52%</div> <div>47%</div> </div>
5	H5	404	<div> <div>13%</div> <div>57%</div> <div>42%</div> </div>
5	I5	404	<div> <div>8%</div> <div>49%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
5	J5	404	
5	K5	404	
5	L5	404	
6	A6	497	
6	B6	497	
6	C6	497	
6	D6	497	
6	E6	497	
6	F6	497	
7	A7	117	
7	B7	117	
7	C7	117	
7	D7	117	
7	E7	117	
7	F7	117	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 97344 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 tube protein, gp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	142	Total	C	N	O	S	0	0
			1091	673	192	224	2		
1	B1	142	Total	C	N	O	S	0	0
			1091	673	192	224	2		
1	C1	142	Total	C	N	O	S	0	0
			1091	673	192	224	2		
1	D1	142	Total	C	N	O	S	0	0
			1091	673	192	224	2		
1	E1	142	Total	C	N	O	S	0	0
			1091	673	192	224	2		
1	F1	142	Total	C	N	O	S	0	0
			1091	673	192	224	2		

- Molecule 2 is a protein called baseplate wedge protein, gp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	173	Total	C	N	O	S	0	0
			1416	917	226	271	2		
2	B2	173	Total	C	N	O	S	0	0
			1416	917	226	271	2		
2	C2	173	Total	C	N	O	S	0	0
			1416	917	226	271	2		
2	D2	173	Total	C	N	O	S	0	0
			1416	917	226	271	2		
2	E2	173	Total	C	N	O	S	0	0
			1416	917	226	271	2		
2	F2	173	Total	C	N	O	S	0	0
			1416	917	226	271	2		

- Molecule 3 is a protein called baseplate organization protein, gp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A3	250	Total	C	N	O	S	0	0
			1944	1204	337	399	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	B3	250	Total	C	N	O	S	0	0
			1944	1204	337	399	4		
3	C3	250	Total	C	N	O	S	0	0
			1944	1204	337	399	4		
3	D3	250	Total	C	N	O	S	0	0
			1944	1204	337	399	4		
3	E3	250	Total	C	N	O	S	0	0
			1944	1204	337	399	4		
3	F3	250	Total	C	N	O	S	0	0
			1944	1204	337	399	4		

- Molecule 4 is a protein called baseplate stabilizing protein, gp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A4	118	Total	C	N	O	S	0	0
			965	616	160	183	6		
4	B4	118	Total	C	N	O	S	0	0
			965	616	160	183	6		
4	C4	118	Total	C	N	O	S	0	0
			965	616	160	183	6		
4	D4	118	Total	C	N	O	S	0	0
			965	616	160	183	6		
4	E4	118	Total	C	N	O	S	0	0
			965	616	160	183	6		
4	F4	118	Total	C	N	O	S	0	0
			965	616	160	183	6		

- Molecule 5 is a protein called baseplate wedge protein, gp16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A5	404	Total	C	N	O	S	0	0
			3101	1929	518	650	4		
5	B5	404	Total	C	N	O	S	0	0
			3103	1931	518	650	4		
5	C5	404	Total	C	N	O	S	0	0
			3101	1929	518	650	4		
5	D5	404	Total	C	N	O	S	0	0
			3103	1931	518	650	4		
5	E5	404	Total	C	N	O	S	0	0
			3101	1929	518	650	4		
5	F5	404	Total	C	N	O	S	0	0
			3103	1931	518	650	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	G5	404	Total	C	N	O	S	0	0
			3101	1929	518	650	4		
5	H5	404	Total	C	N	O	S	0	0
			3103	1931	518	650	4		
5	I5	404	Total	C	N	O	S	0	0
			3101	1929	518	650	4		
5	J5	404	Total	C	N	O	S	0	0
			3103	1931	518	650	4		
5	K5	404	Total	C	N	O	S	0	0
			3101	1929	518	650	4		
5	L5	404	Total	C	N	O	S	0	0
			3103	1931	518	650	4		

- Molecule 6 is a protein called tail sheath protein, gp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A6	497	Total	C	N	O	S	0	0
			3721	2321	616	772	12		
6	B6	497	Total	C	N	O	S	0	0
			3721	2321	616	772	12		
6	C6	497	Total	C	N	O	S	0	0
			3721	2321	616	772	12		
6	D6	497	Total	C	N	O	S	0	0
			3721	2321	616	772	12		
6	E6	497	Total	C	N	O	S	0	0
			3721	2321	616	772	12		
6	F6	497	Total	C	N	O	S	0	0
			3721	2321	616	772	12		

- Molecule 7 is a protein called tail sheath initiator protein, gp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A7	110	Total	C	N	O	S	0	0
			883	549	156	176	2		
7	B7	110	Total	C	N	O	S	0	0
			883	549	156	176	2		
7	C7	110	Total	C	N	O	S	0	0
			883	549	156	176	2		
7	D7	110	Total	C	N	O	S	0	0
			883	549	156	176	2		
7	E7	110	Total	C	N	O	S	0	0
			883	549	156	176	2		

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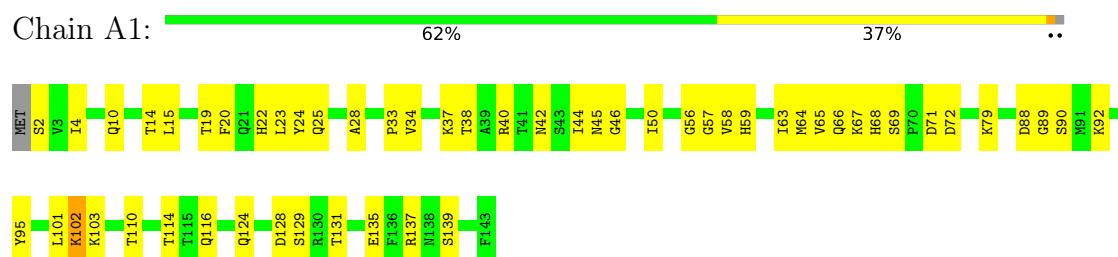
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Mol	Chain	Residues	Atoms					AltConf	Trace
7	F7	110	Total	C	N	O	S	0	0
			883	549	156	176	2		

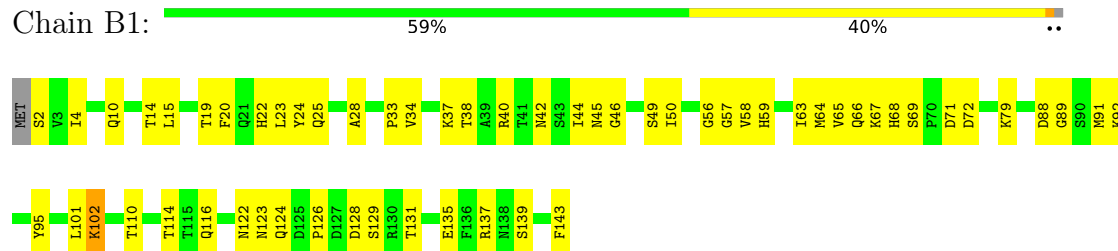
3 Residue-property plots [i](#)

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.

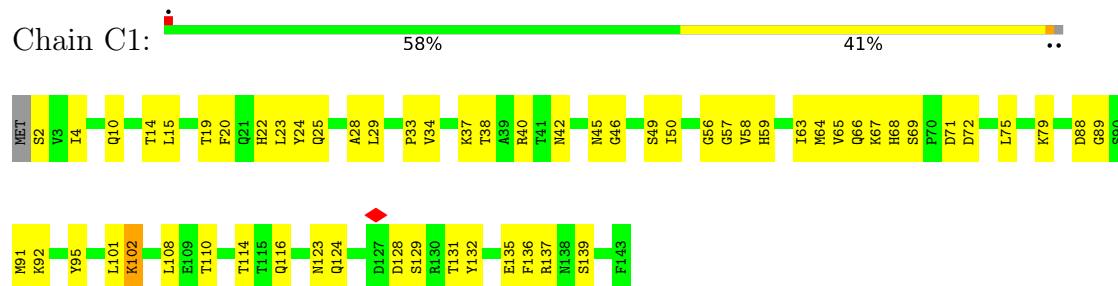
- Molecule 1: tail tube protein, gp7



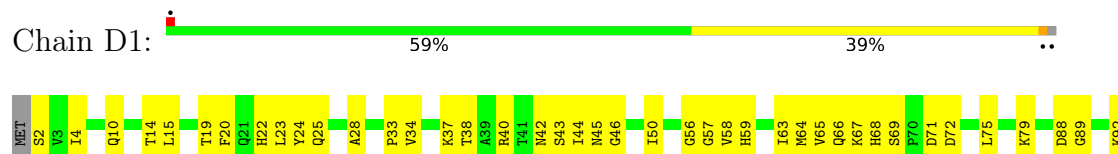
- Molecule 1: tail tube protein, gp7

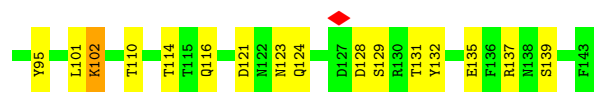


- Molecule 1: tail tube protein, gp7



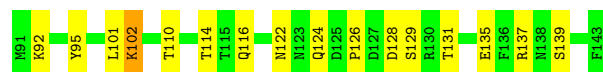
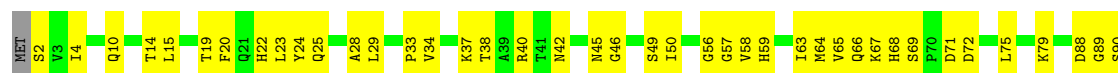
- Molecule 1: tail tube protein, gp7





- Molecule 1: tail tube protein, gp7

Chain E1: 59% 39% ..



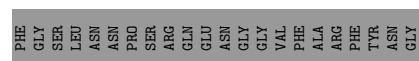
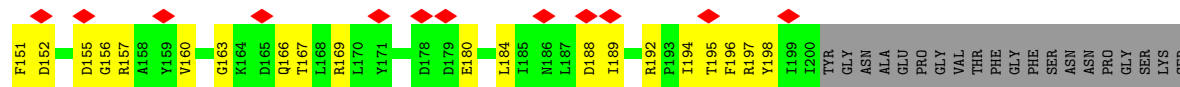
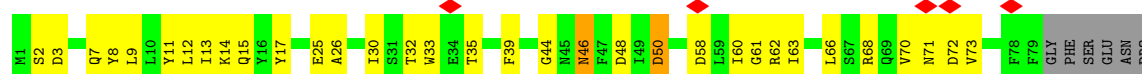
- Molecule 1: tail tube protein, gp7

Chain F1: 58% 41% ..



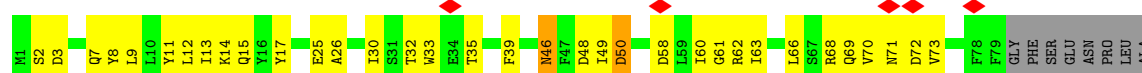
- Molecule 2: baseplate wedge protein, gp17

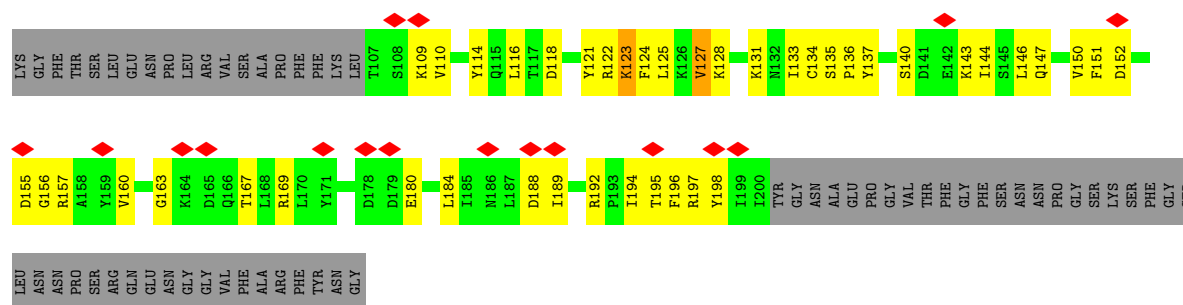
Chain A2: 8% 39% 31% 29%



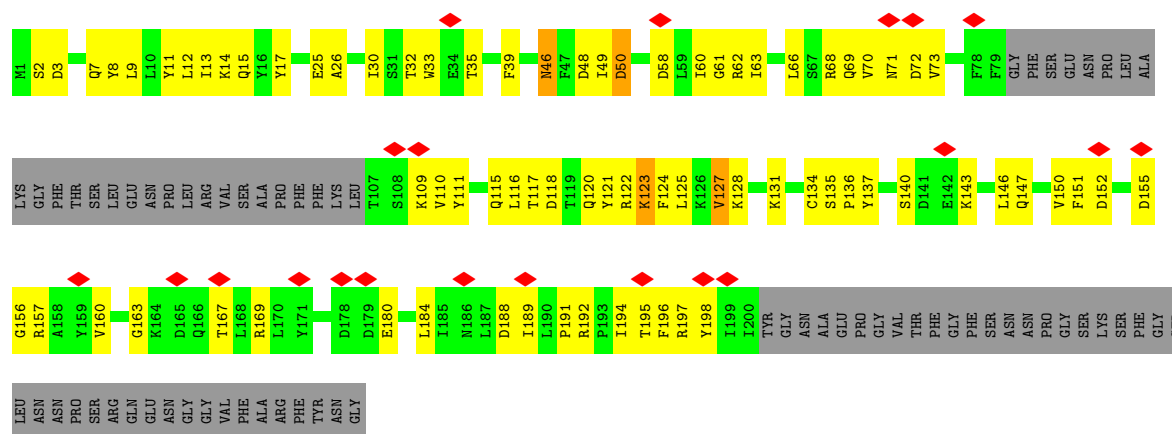
- Molecule 2: baseplate wedge protein, gp17

Chain B2: 9% 40% 30% 29%

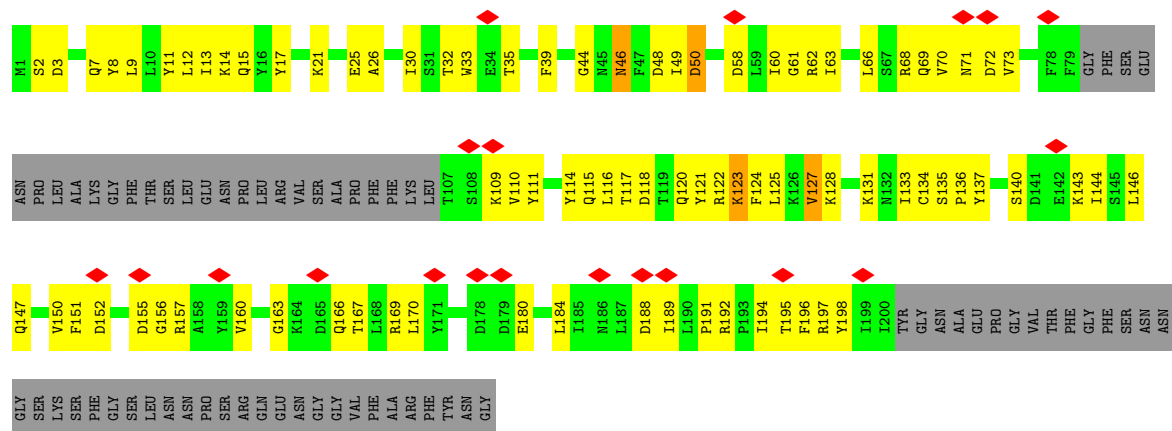




• Molecule 2: baseplate wedge protein, gp17

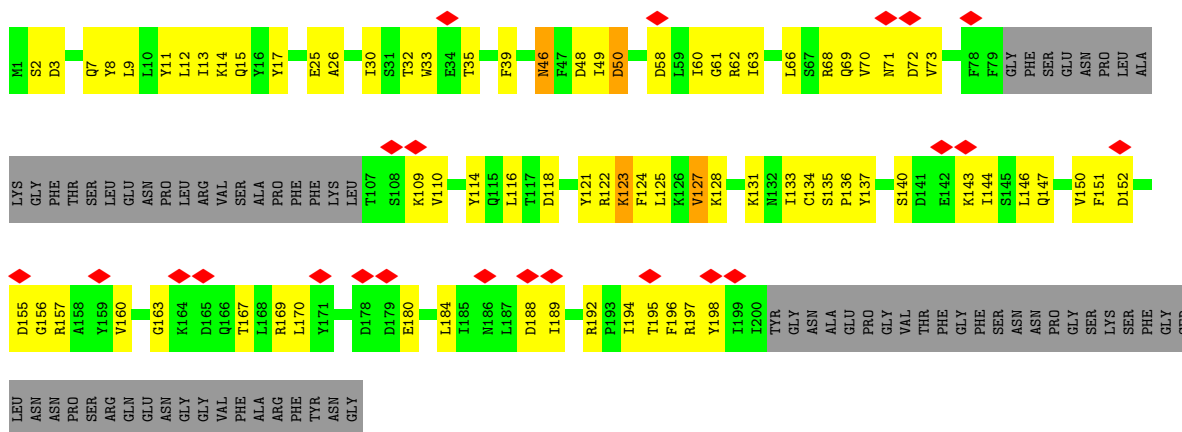


• Molecule 2: baseplate wedge protein, gp17

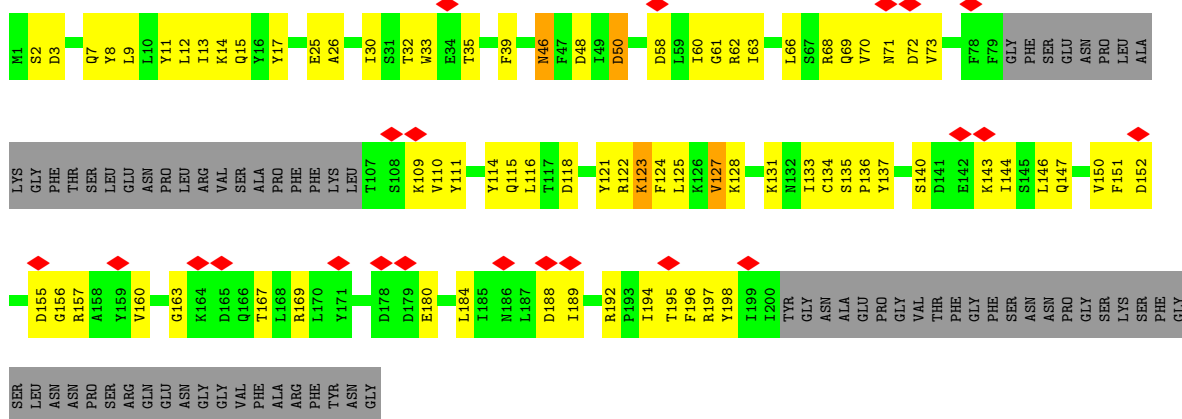


• Molecule 2: baseplate wedge protein, gp17

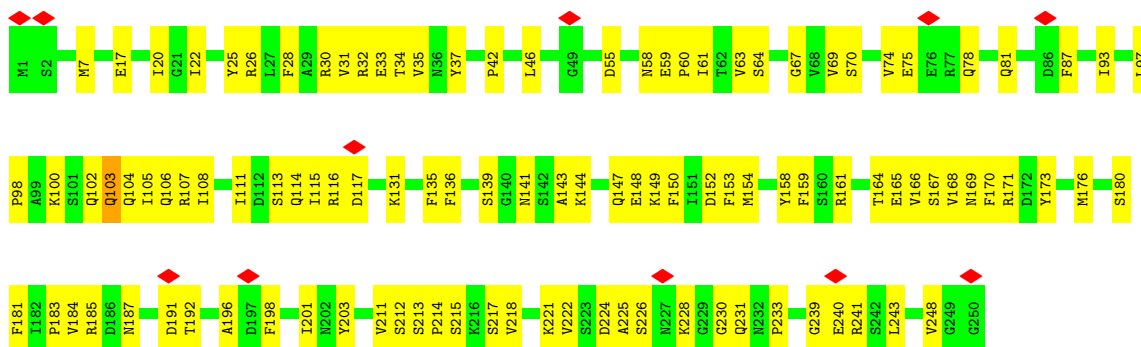




• Molecule 2: baseplate wedge protein, gp17

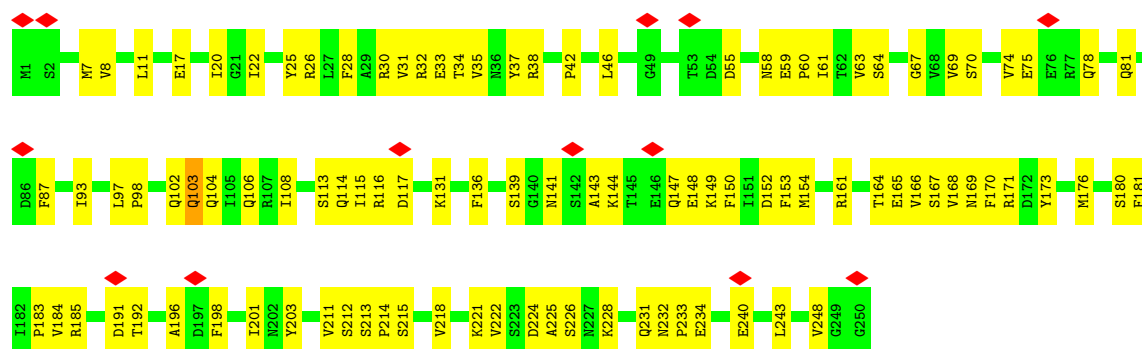


• Molecule 3: baseplate organization protein, gp11

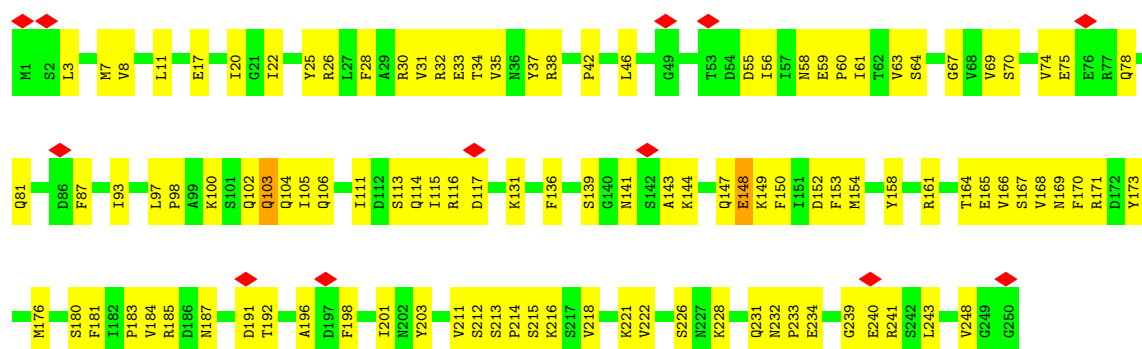


• Molecule 3: baseplate organization protein, gp11

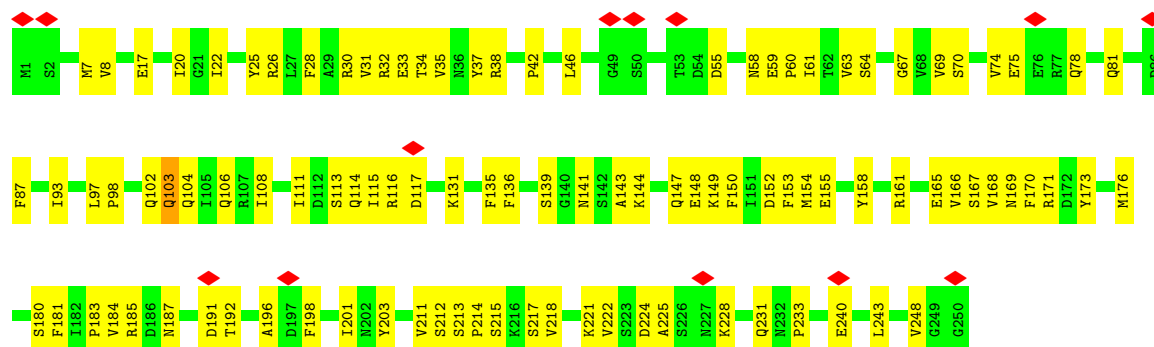




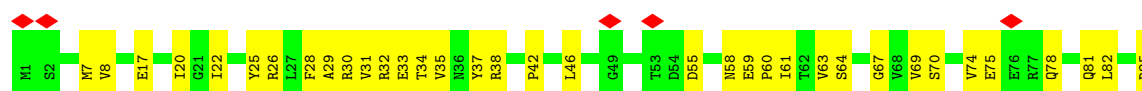
- Molecule 3: baseplate organization protein, gp11

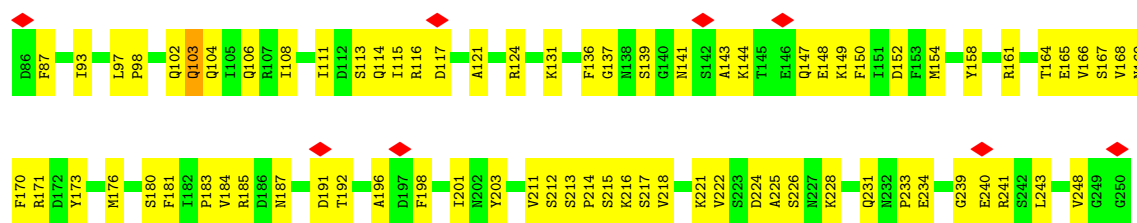


- Molecule 3: baseplate organization protein, gp11

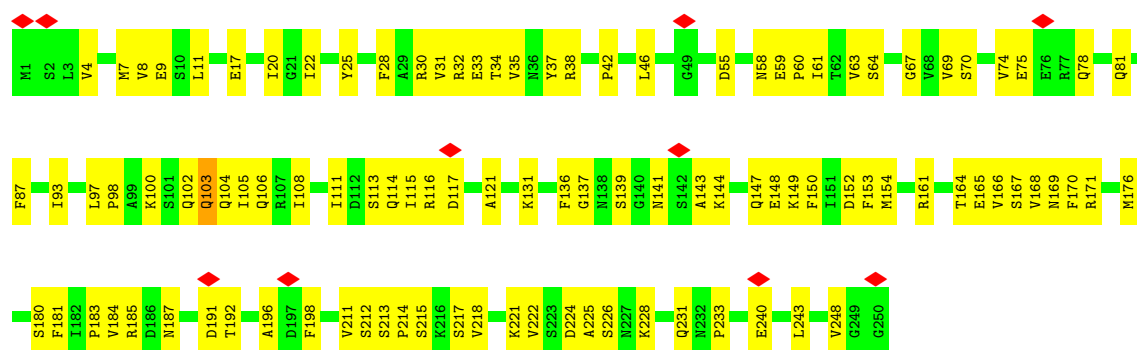


- Molecule 3: baseplate organization protein, gp11

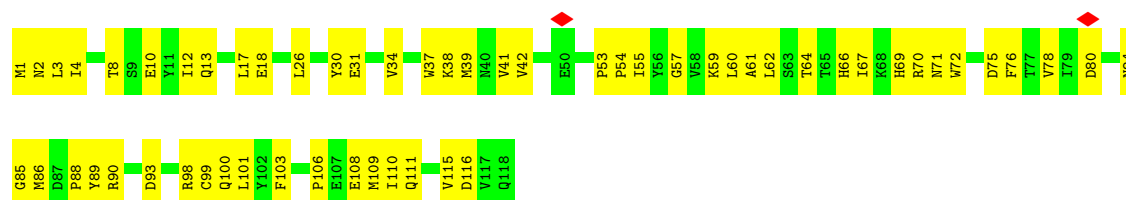




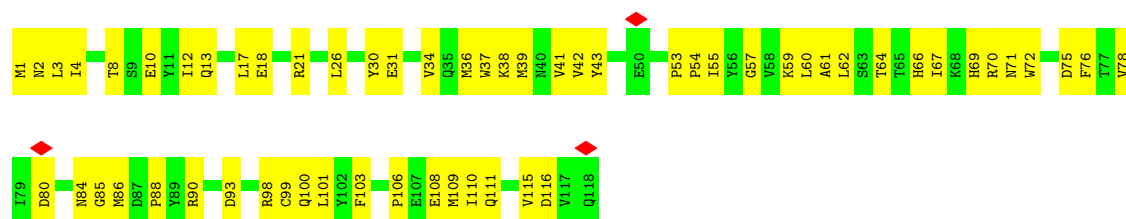
- Molecule 3: baseplate organization protein, gp11



- Molecule 4: baseplate stabilizing protein, gp12

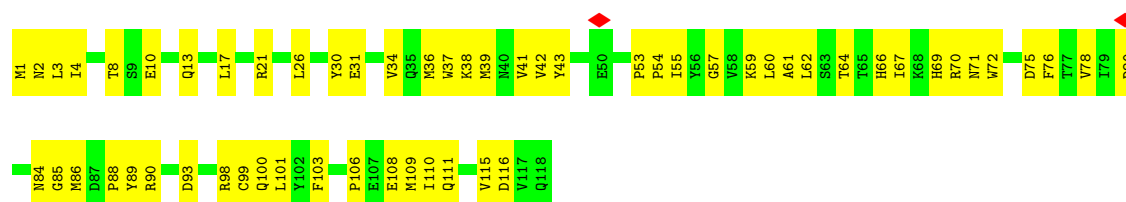


- Molecule 4: baseplate stabilizing protein, gp12

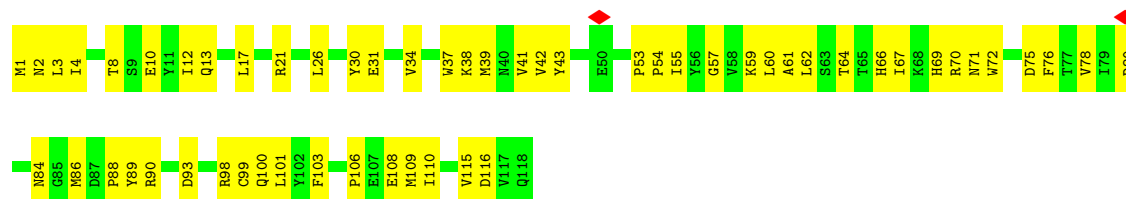


- Molecule 4: baseplate stabilizing protein, gp12

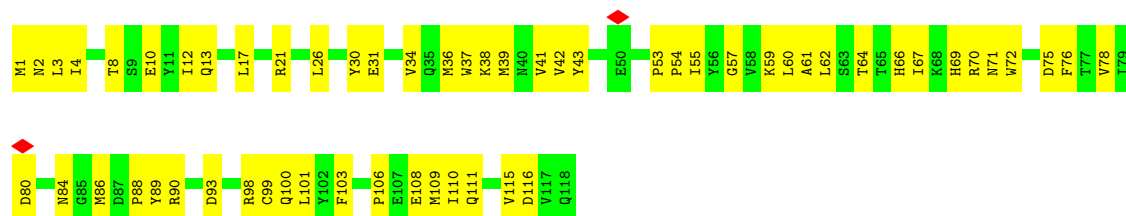




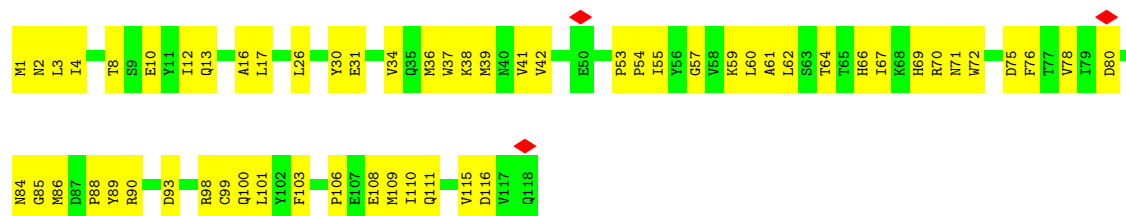
- Molecule 4: baseplate stabilizing protein, gp12



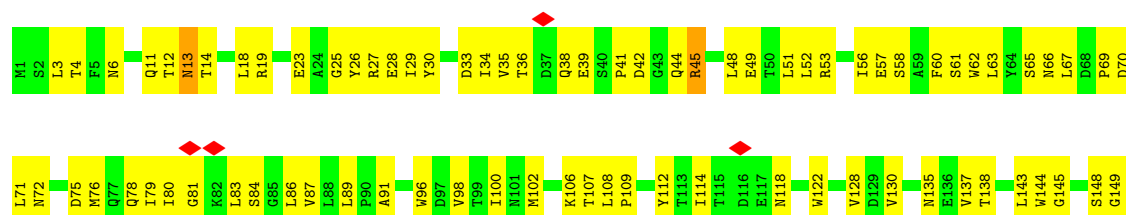
- Molecule 4: baseplate stabilizing protein, gp12

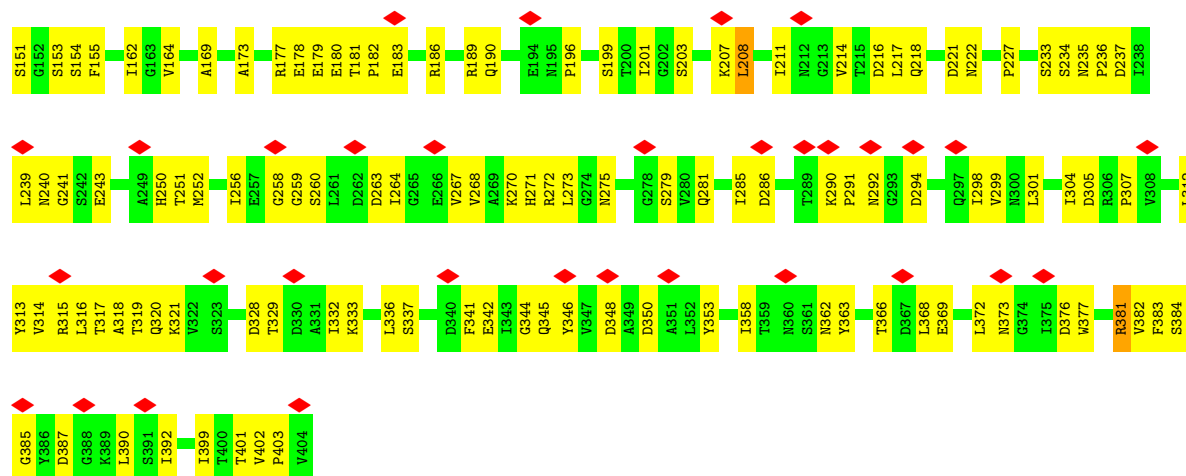


- Molecule 4: baseplate stabilizing protein, gp12

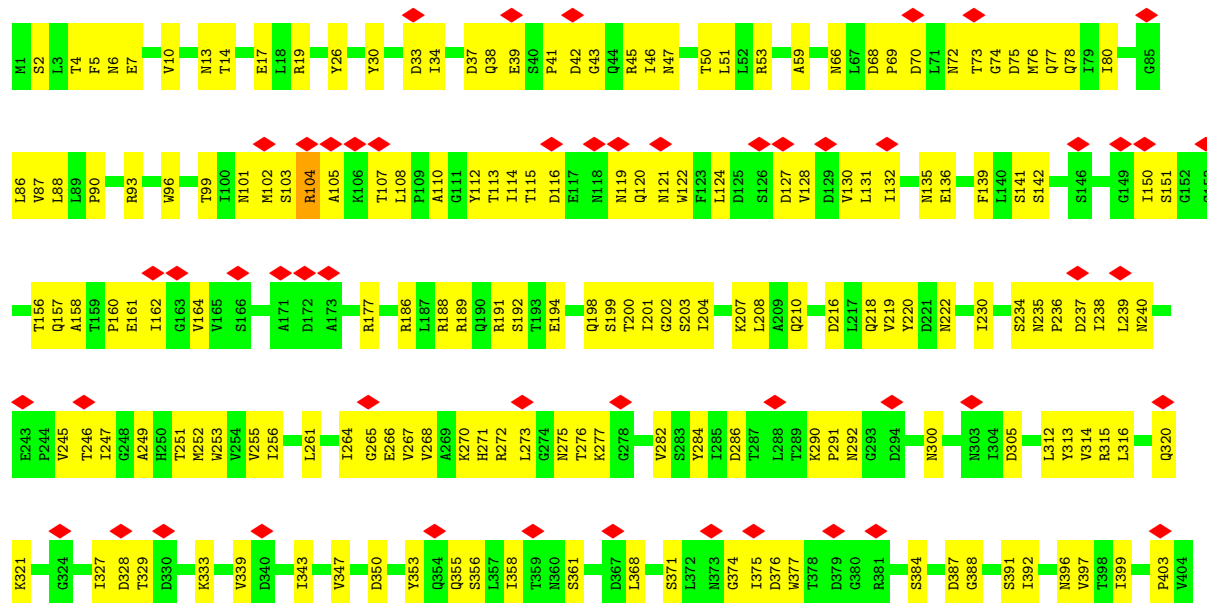


- Molecule 5: baseplate wedge protein, gp16

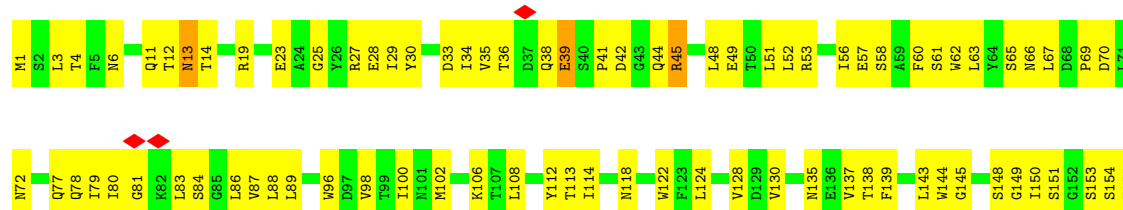


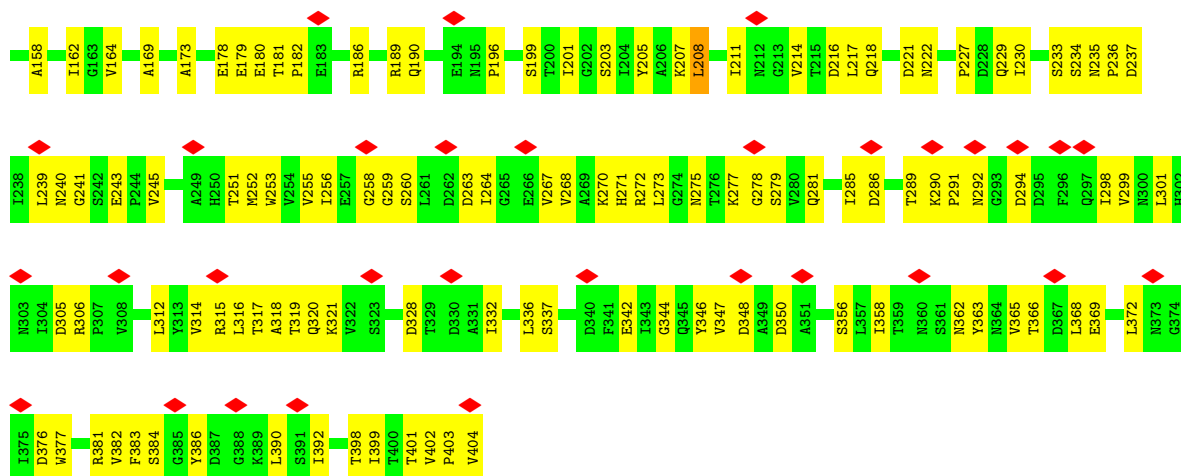


- Molecule 5: baseplate wedge protein, gp16

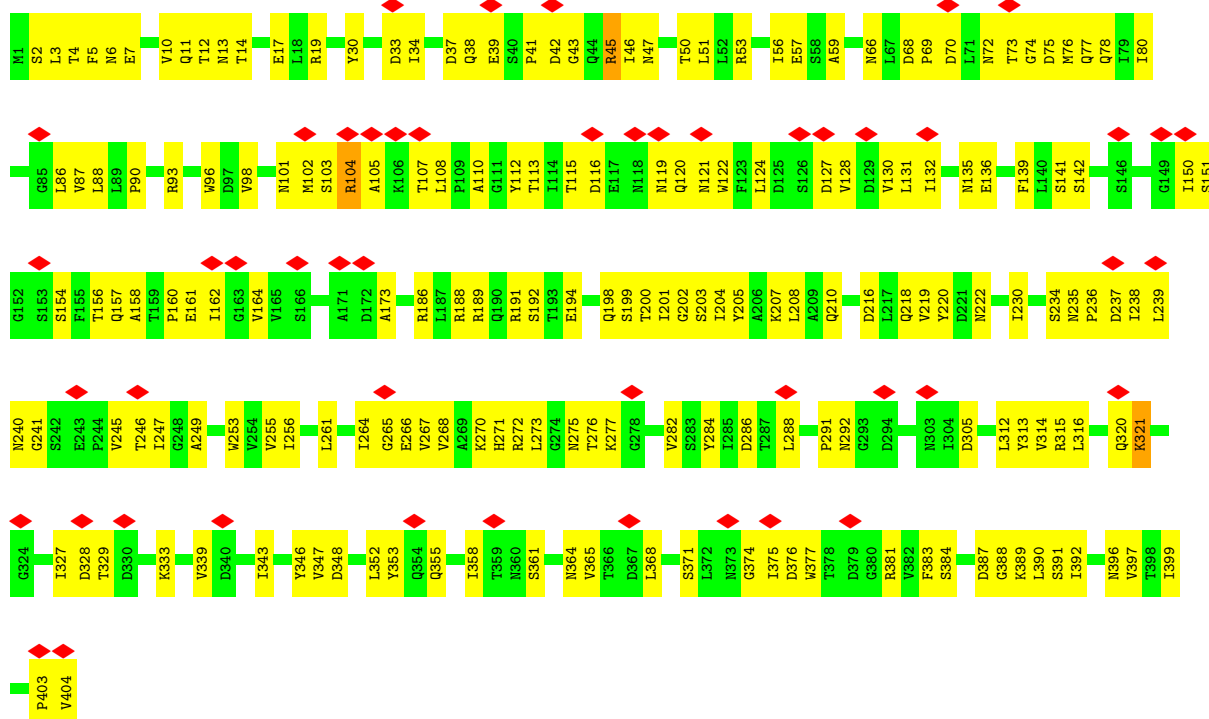


- Molecule 5: baseplate wedge protein, gp16

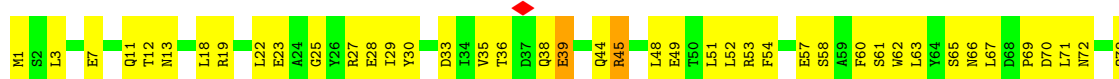


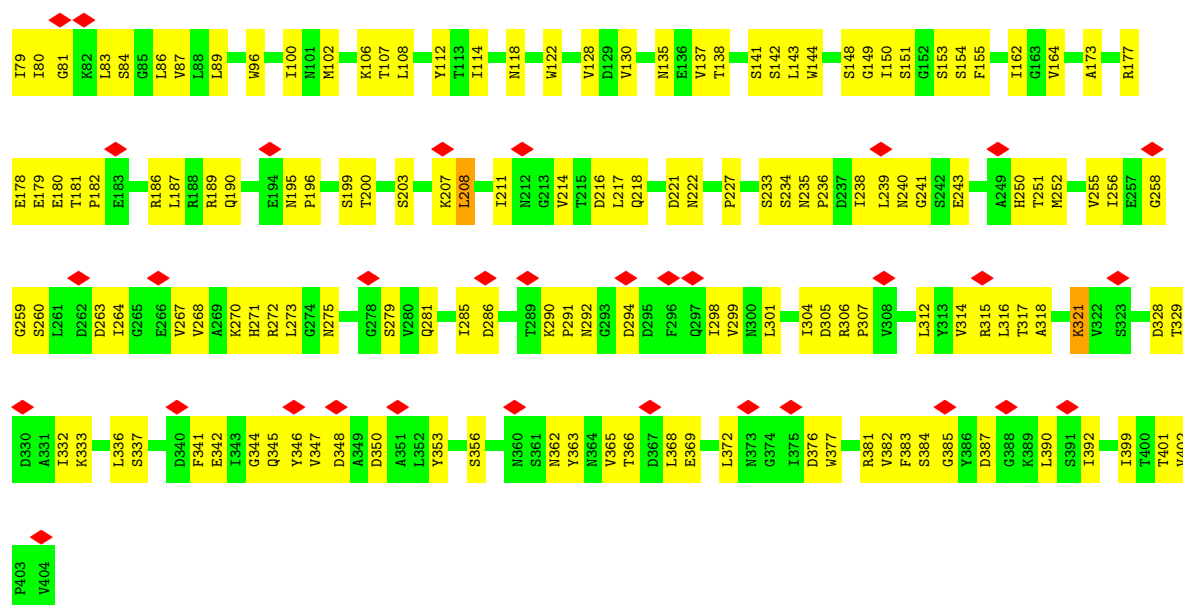


- Molecule 5: baseplate wedge protein, gp16

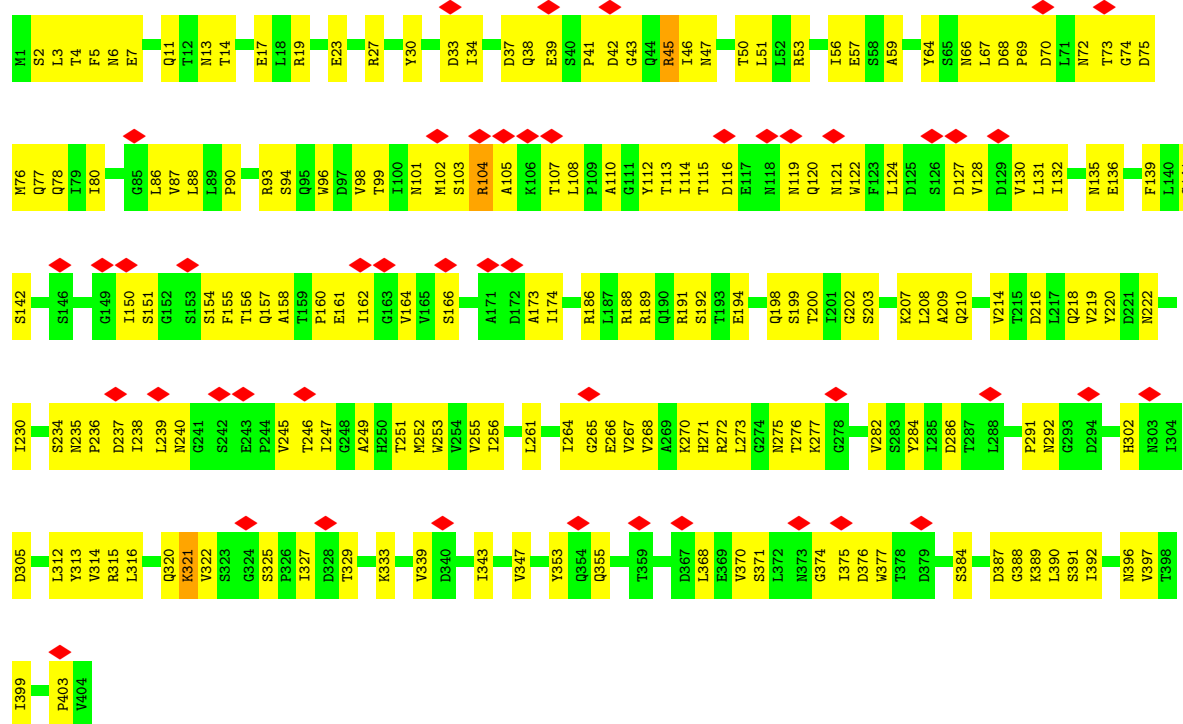


- Molecule 5: baseplate wedge protein, gp16



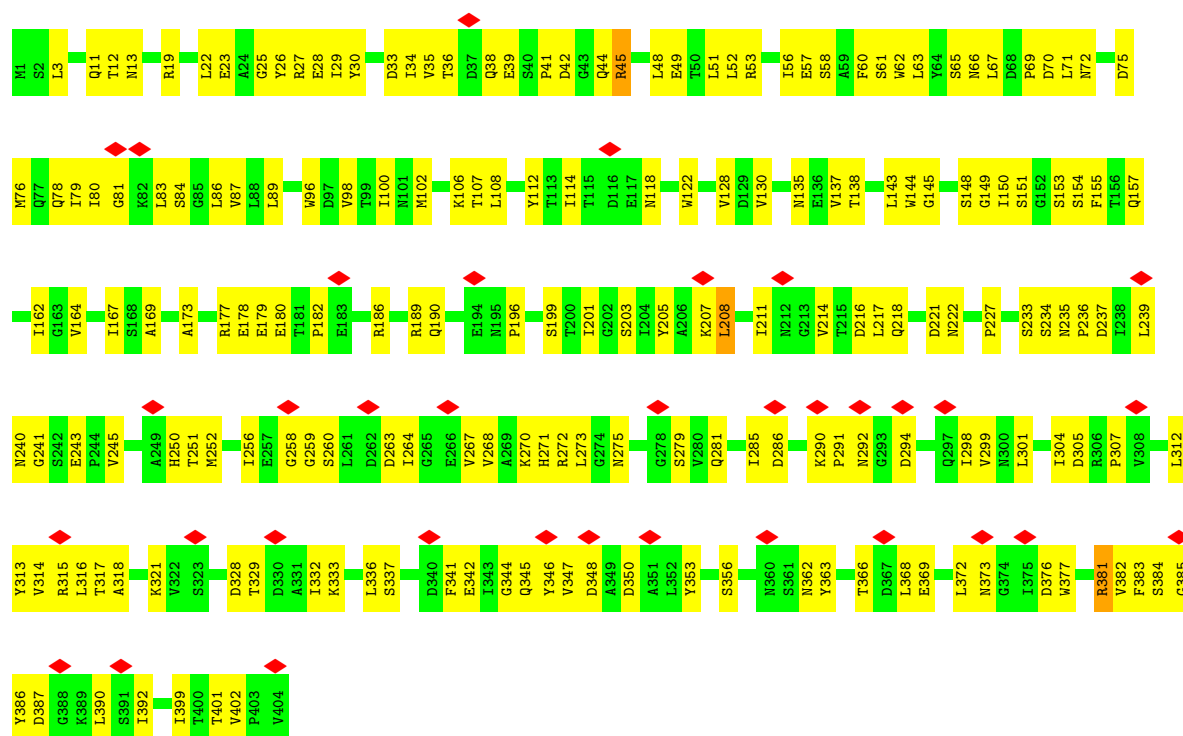


- Molecule 5: baseplate wedge protein, gp16

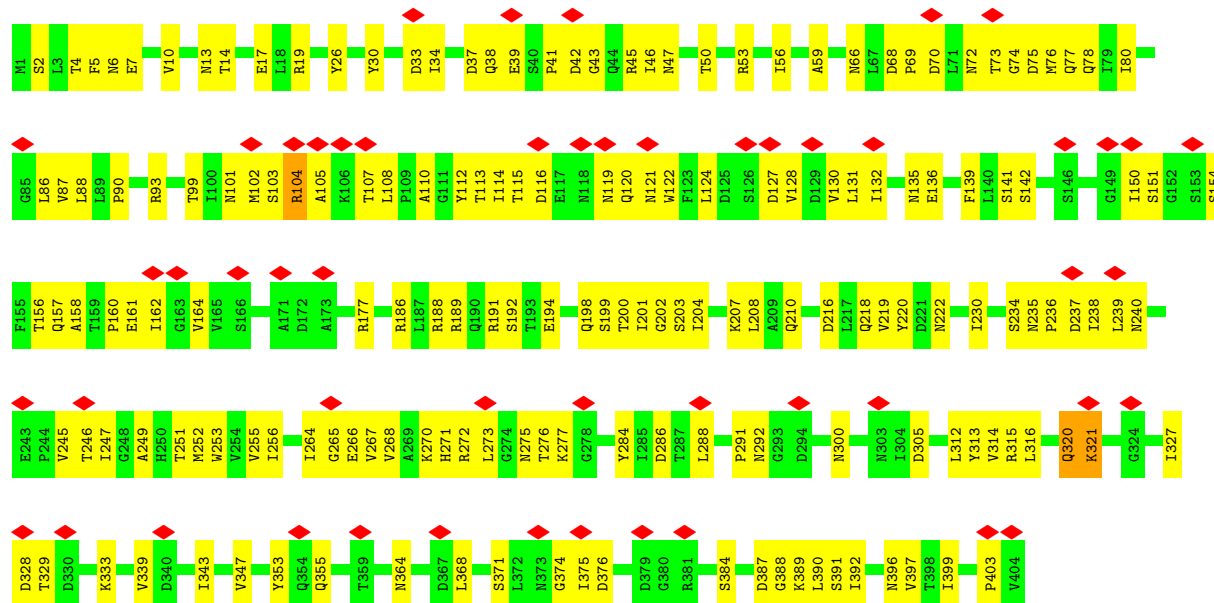


- Molecule 5: baseplate wedge protein, gp16



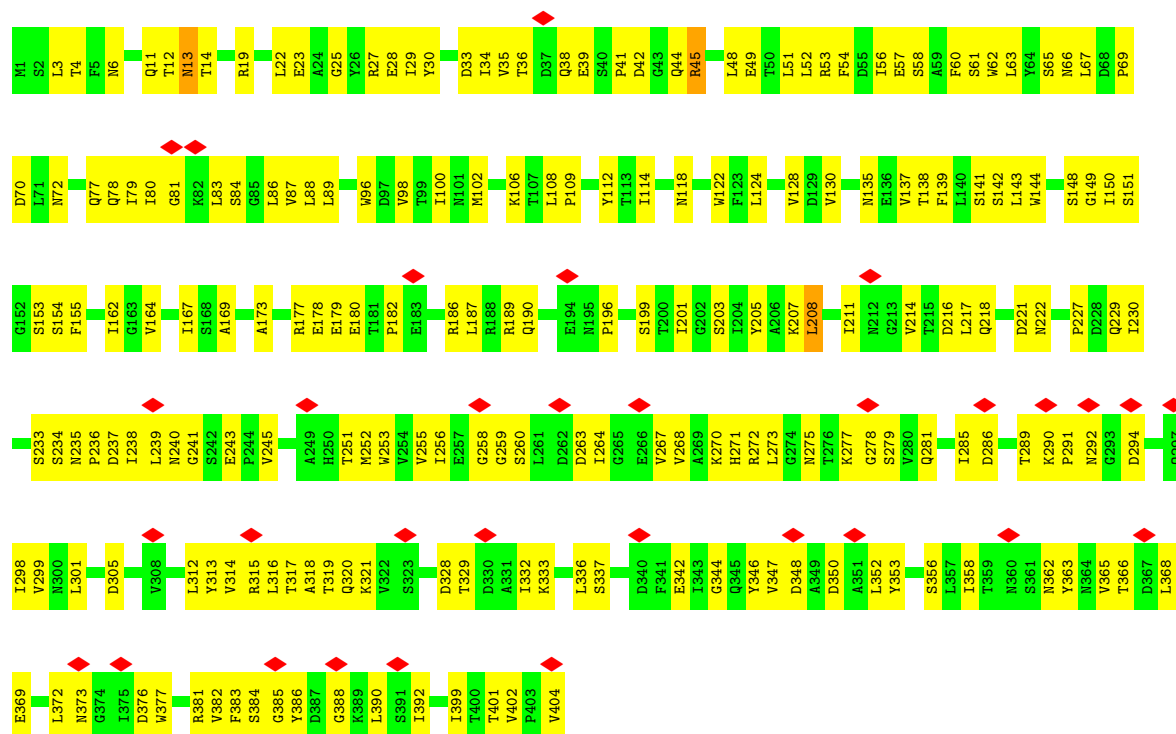


• Molecule 5: baseplate wedge protein, gp16

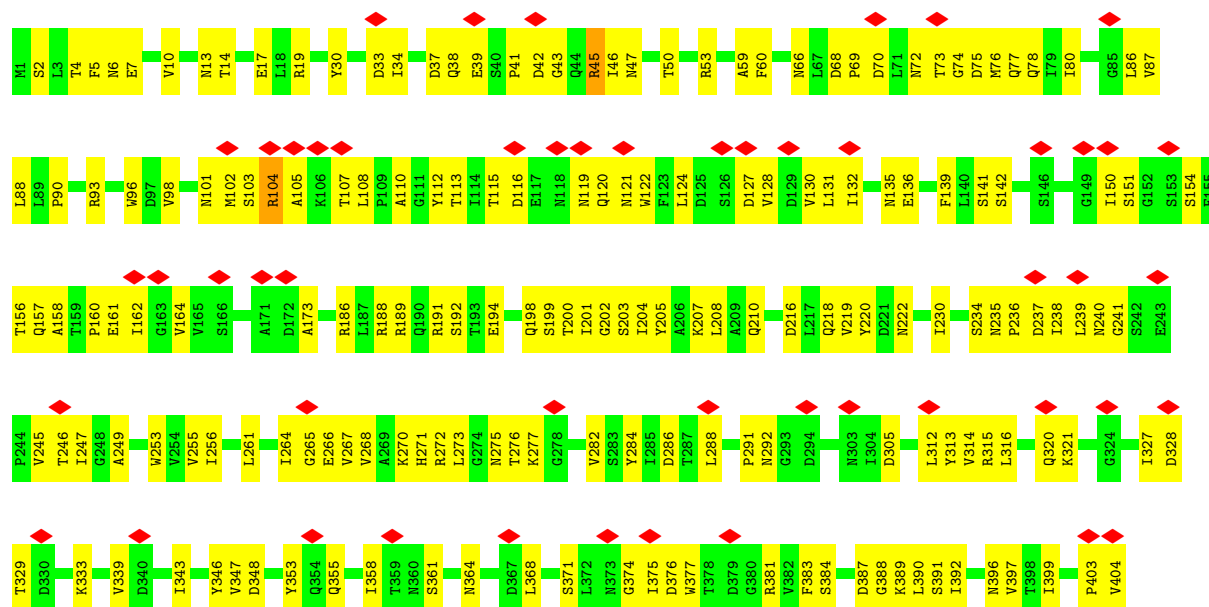


• Molecule 5: baseplate wedge protein, gp16



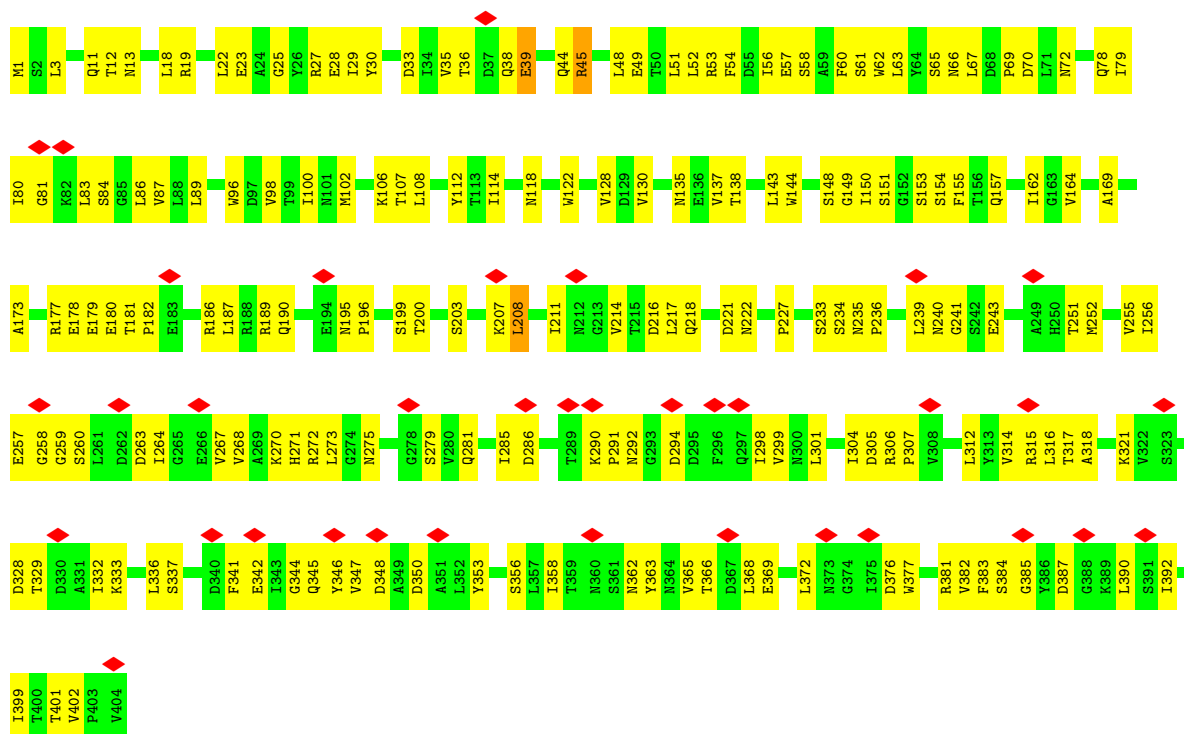


• Molecule 5: baseplate wedge protein, gp16

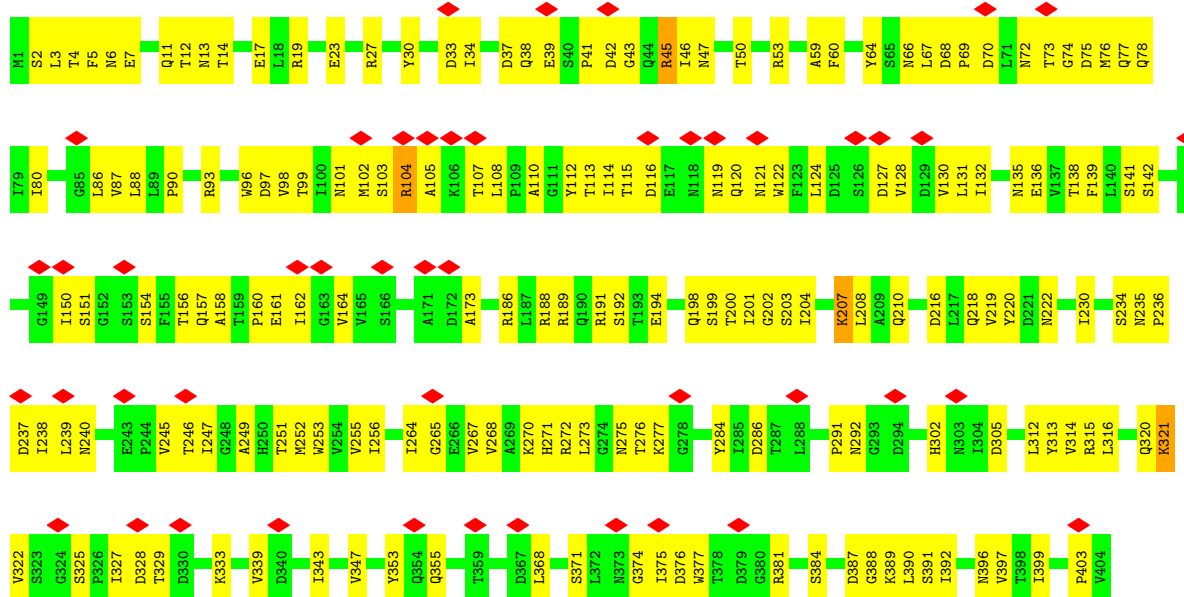


• Molecule 5: baseplate wedge protein, gp16



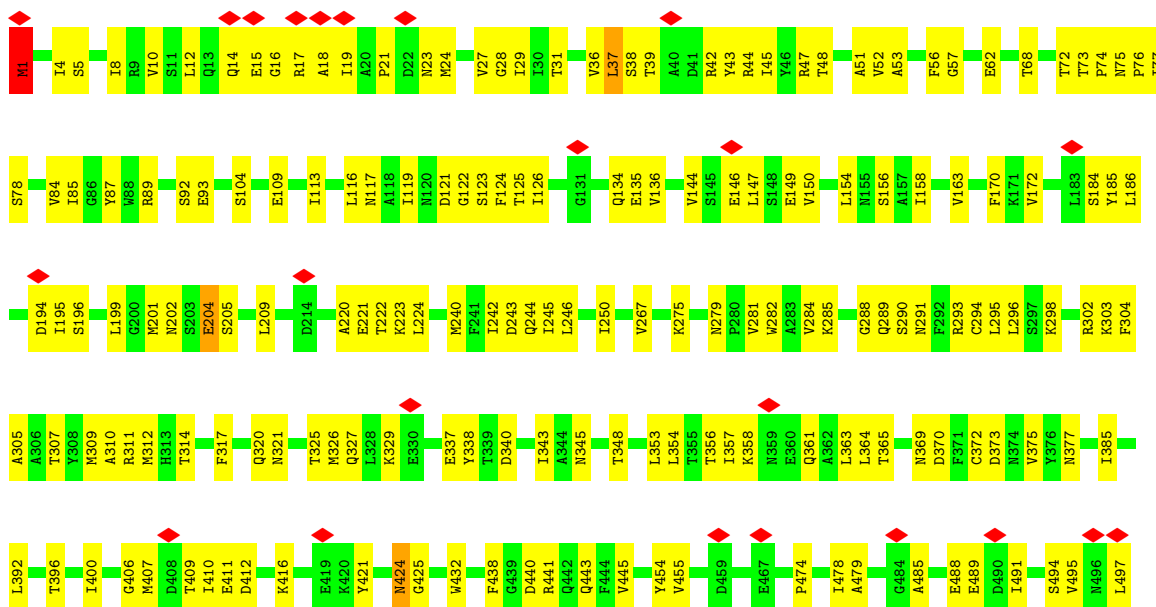


- Molecule 5: baseplate wedge protein, gp16



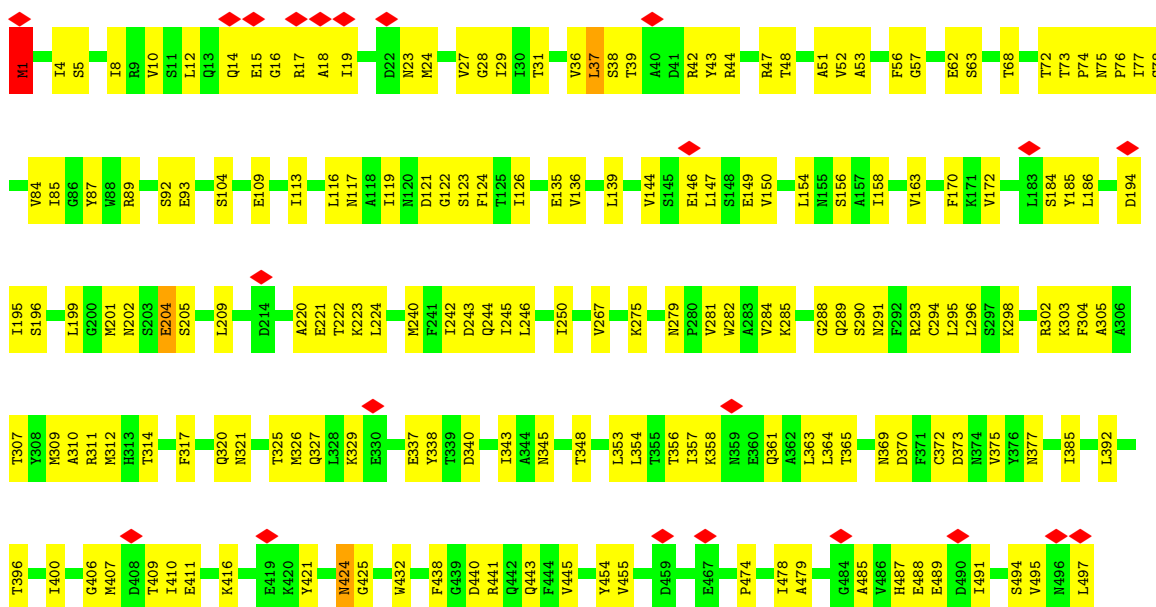
- Molecule 6: tail sheath protein, gp6





- Molecule 6: tail sheath protein, gp6

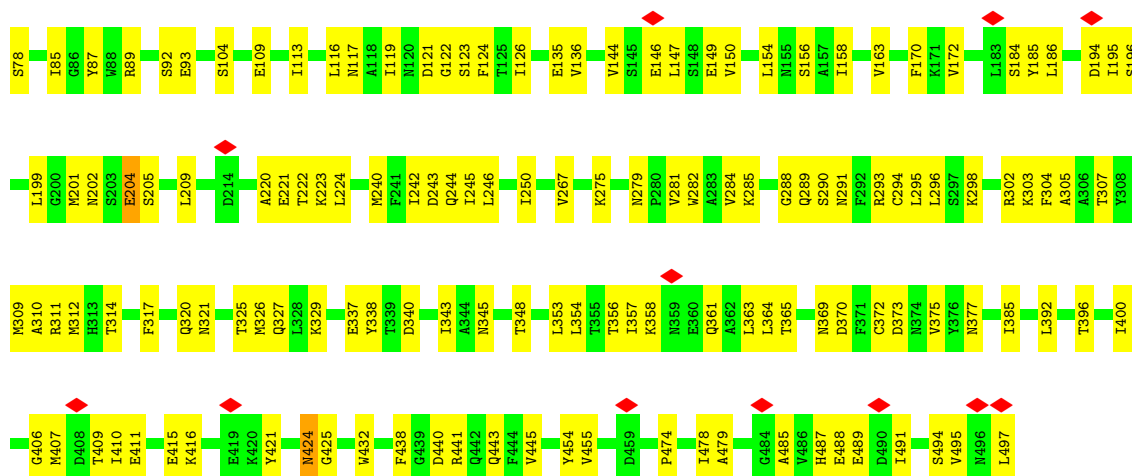
Chain B6: 63% 36%



- Molecule 6: tail sheath protein, gp6

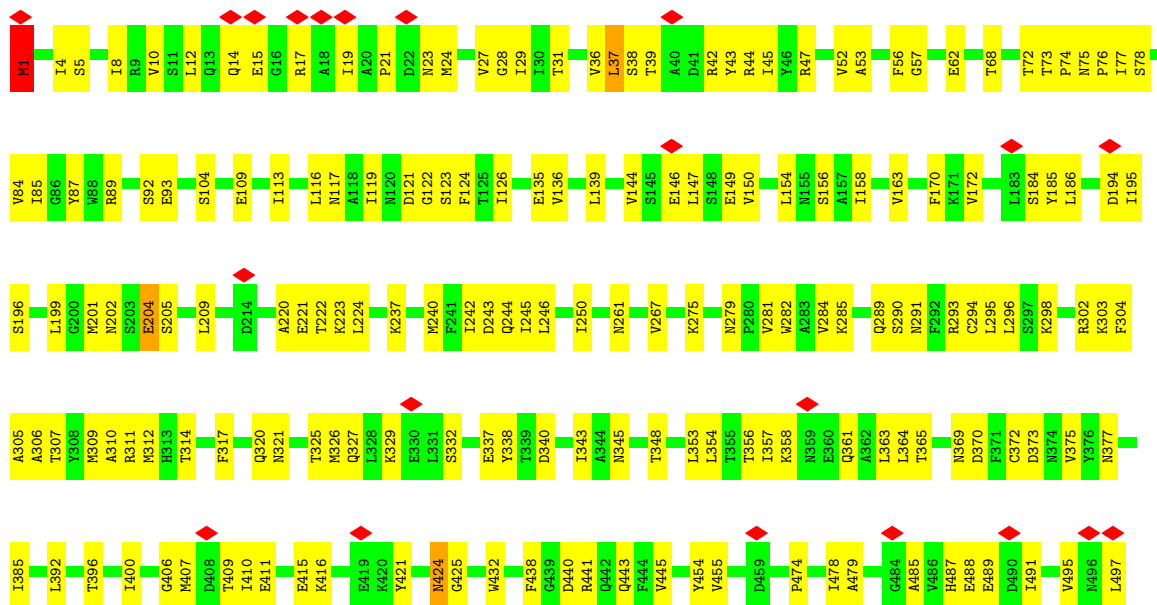
Chain C6: 63% 36%





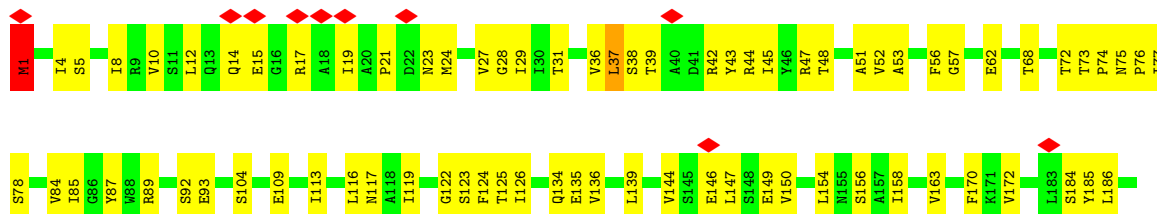
- Molecule 6: tail sheath protein, gp6

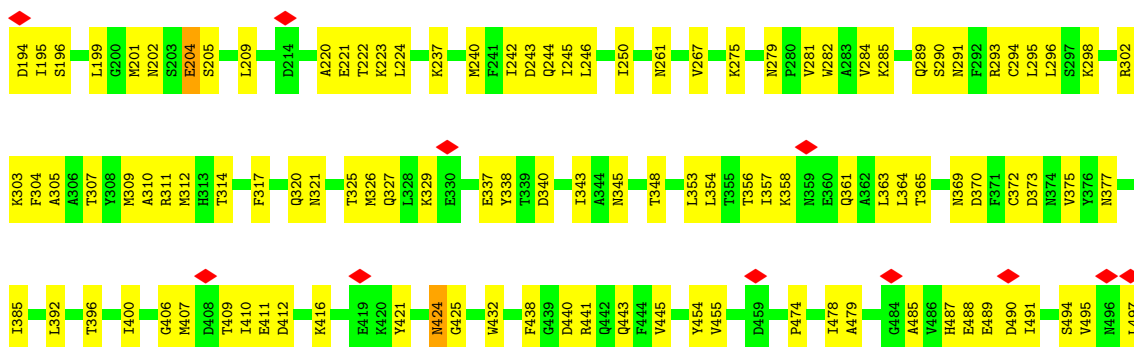
Chain D6: 63% 36% .



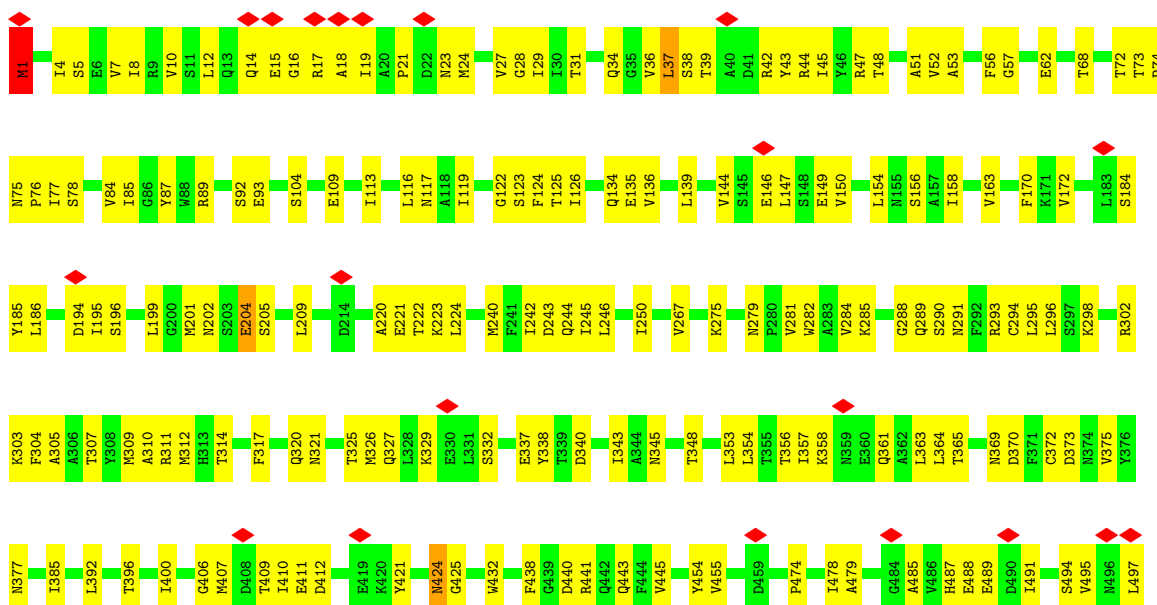
- Molecule 6: tail sheath protein, gp6

Chain E6: 63% 37% .

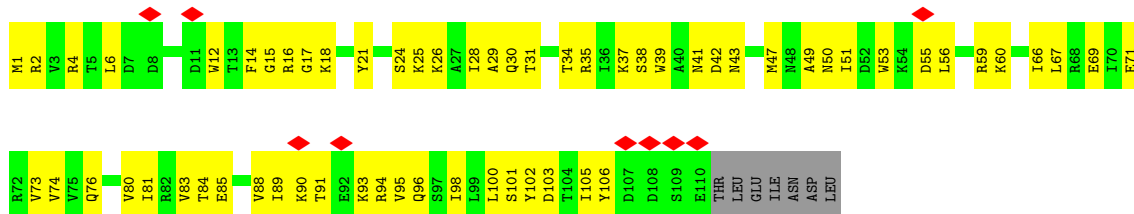




- Molecule 6: tail sheath protein, gp6

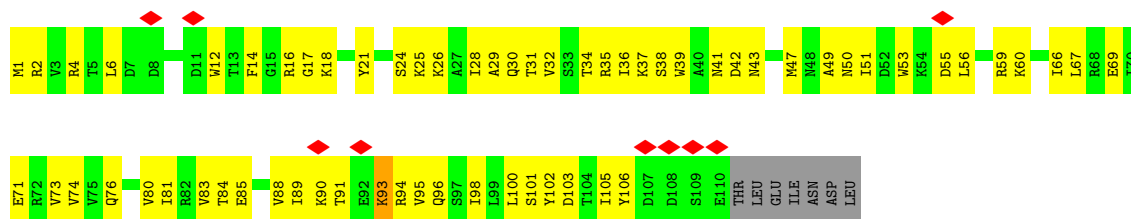


- Molecule 7: tail sheath initiator protein, gp15

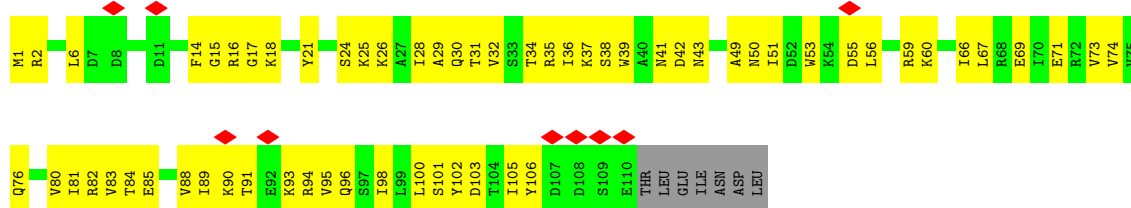


- Molecule 7: tail sheath initiator protein, gp15

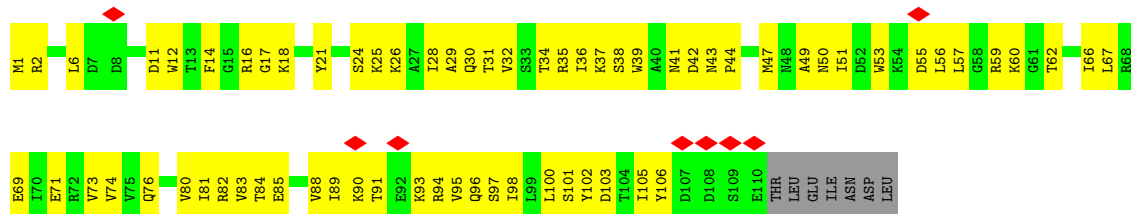




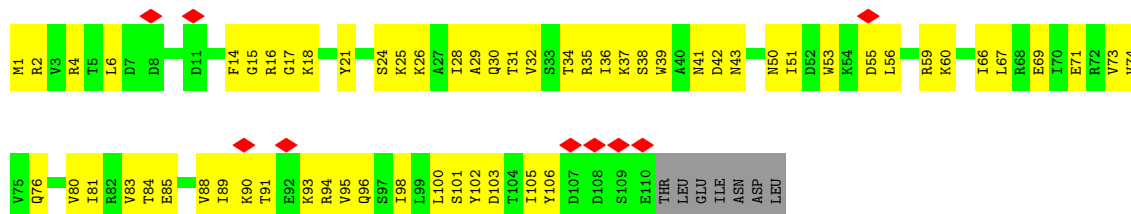
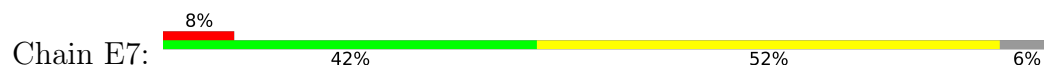
- Molecule 7: tail sheath initiator protein, gp15



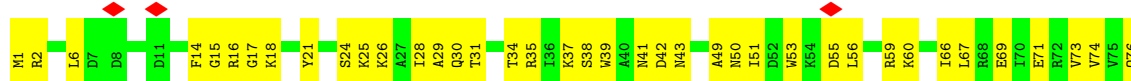
- Molecule 7: tail sheath initiator protein, gp15



- Molecule 7: tail sheath initiator protein, gp15



- Molecule 7: tail sheath initiator protein, gp15





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16068	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-16 (4k x 4k)	Depositor
Maximum map value	13.778	Depositor
Minimum map value	-10.260	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.584	Depositor
Recommended contour level	2.4	Depositor
Map size (\AA)	414.72, 414.72, 414.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.81, 0.81, 0.81	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	A1	0.52	0/1108	0.54	0/1505
1	B1	0.52	0/1108	0.54	0/1505
1	C1	0.52	0/1108	0.54	0/1505
1	D1	0.52	0/1108	0.54	0/1505
1	E1	0.52	0/1108	0.54	0/1505
1	F1	0.52	0/1108	0.54	0/1505
2	A2	0.49	0/1444	0.58	0/1959
2	B2	0.48	0/1444	0.58	0/1959
2	C2	0.49	0/1444	0.58	0/1959
2	D2	0.49	0/1444	0.58	0/1959
2	E2	0.49	0/1444	0.58	0/1959
2	F2	0.49	0/1444	0.58	0/1959
3	A3	0.53	0/1973	0.55	0/2668
3	B3	0.53	0/1973	0.55	0/2668
3	C3	0.53	0/1973	0.55	0/2668
3	D3	0.53	0/1973	0.55	0/2668
3	E3	0.53	0/1973	0.55	0/2668
3	F3	0.53	0/1973	0.55	0/2668
4	A4	0.56	0/989	0.63	0/1346
4	B4	0.56	0/989	0.62	0/1346
4	C4	0.55	0/989	0.62	0/1346
4	D4	0.56	0/989	0.62	0/1346
4	E4	0.56	0/989	0.62	0/1346
4	F4	0.55	0/989	0.62	0/1346
5	A5	0.47	1/3152 (0.0%)	0.64	4/4298 (0.1%)
5	B5	0.41	0/3154	0.59	1/4301 (0.0%)
5	C5	0.48	2/3152 (0.1%)	0.59	2/4298 (0.0%)
5	D5	0.41	0/3154	0.61	4/4301 (0.1%)
5	E5	0.48	1/3152 (0.0%)	0.63	4/4298 (0.1%)
5	F5	0.42	0/3154	0.60	4/4301 (0.1%)
5	G5	0.46	1/3152 (0.0%)	0.62	3/4298 (0.1%)
5	H5	0.43	2/3154 (0.1%)	0.61	3/4301 (0.1%)
5	I5	0.46	0/3152	0.59	2/4298 (0.0%)
5	J5	0.41	0/3154	0.60	3/4301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	K5	0.47	1/3152 (0.0%)	0.62	4/4298 (0.1%)
5	L5	0.42	0/3154	0.62	6/4301 (0.1%)
6	A6	0.48	0/3772	0.56	2/5134 (0.0%)
6	B6	0.47	0/3772	0.56	2/5134 (0.0%)
6	C6	0.47	0/3772	0.56	2/5134 (0.0%)
6	D6	0.48	0/3772	0.56	2/5134 (0.0%)
6	E6	0.47	0/3772	0.56	2/5134 (0.0%)
6	F6	0.47	0/3772	0.56	2/5134 (0.0%)
7	A7	0.53	0/893	0.63	0/1207
7	B7	0.53	0/893	0.63	0/1207
7	C7	0.53	0/893	0.63	0/1207
7	D7	0.53	0/893	0.63	0/1207
7	E7	0.53	0/893	0.63	0/1207
7	F7	0.53	0/893	0.63	0/1207
All	All	0.48	8/98910 (0.0%)	0.59	52/134508 (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	A3	0	1
3	B3	0	1
3	C3	0	1
3	D3	0	1
3	E3	0	1
3	F3	0	1
5	H5	0	1
All	All	0	7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C5	39	GLU	CG-CD	-6.40	1.42	1.51
5	E5	39	GLU	CG-CD	-6.24	1.42	1.51
5	H5	321	LYS	CD-CE	-5.90	1.36	1.51
5	H5	321	LYS	CB-CG	-5.51	1.37	1.52
5	A5	45	ARG	CG-CD	-5.15	1.39	1.51

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H5	321	LYS	CB-CG-CD	-9.91	85.83	111.60
5	A5	45	ARG	NE-CZ-NH1	9.58	125.09	120.30
5	A5	381	ARG	NE-CZ-NH2	-8.98	115.81	120.30
5	G5	381	ARG	NE-CZ-NH2	-8.80	115.90	120.30
5	L5	45	ARG	CB-CG-CD	-8.61	89.22	111.60

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A3	103	GLN	Peptide
3	B3	103	GLN	Peptide
3	C3	103	GLN	Peptide
3	D3	103	GLN	Peptide
3	E3	103	GLN	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	A1	1091	0	1069	56	0
1	B1	1091	0	1069	58	0
1	C1	1091	0	1069	61	0
1	D1	1091	0	1069	60	0
1	E1	1091	0	1069	62	0
1	F1	1091	0	1069	60	0
2	A2	1416	0	1406	86	0
2	B2	1416	0	1406	93	0
2	C2	1416	0	1406	90	0
2	D2	1416	0	1406	102	0
2	E2	1416	0	1406	92	0
2	F2	1416	0	1406	91	0
3	A3	1944	0	1902	122	0
3	B3	1944	0	1902	111	0
3	C3	1944	0	1902	125	0
3	D3	1944	0	1902	123	0
3	E3	1944	0	1902	127	0
3	F3	1944	0	1902	121	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A4	965	0	931	68	0
4	B4	965	0	931	66	0
4	C4	965	0	931	68	0
4	D4	965	0	931	68	0
4	E4	965	0	931	65	0
4	F4	965	0	931	66	0
5	A5	3101	0	3001	221	0
5	B5	3103	0	3008	186	0
5	C5	3101	0	3001	209	0
5	D5	3103	0	3008	200	0
5	E5	3101	0	3001	209	0
5	F5	3103	0	3008	195	0
5	G5	3101	0	3001	207	0
5	H5	3103	0	3008	191	0
5	I5	3101	0	3001	215	0
5	J5	3103	0	3008	193	0
5	K5	3101	0	3001	214	0
5	L5	3103	0	3008	200	0
6	A6	3721	0	3660	165	0
6	B6	3721	0	3660	164	0
6	C6	3721	0	3660	162	0
6	D6	3721	0	3660	163	0
6	E6	3721	0	3660	169	0
6	F6	3721	0	3660	166	0
7	A7	883	0	892	78	0
7	B7	883	0	892	80	0
7	C7	883	0	892	77	0
7	D7	883	0	892	92	0
7	E7	883	0	892	73	0
7	F7	883	0	892	68	0
All	All	97344	0	95214	4823	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 25.

The worst 5 of 4823 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)
3:E3:106:GLN:HE22	5:G5:143:LEU:HA	1.29	0.98
5:H5:320:GLN:HE22	5:H5:403:PRO:HA	1.31	0.96
3:B3:106:GLN:HE22	5:A5:143:LEU:HA	1.29	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A4:71:ASN:HD21	5:B5:90:PRO:HA	1.28	0.95
2:C2:30:ILE:HD13	5:E5:52:LEU:HD11	1.48	0.95

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	A1	140/143 (98%)	133 (95%)	7 (5%)	0	100	100
1	B1	140/143 (98%)	133 (95%)	7 (5%)	0	100	100
1	C1	140/143 (98%)	133 (95%)	7 (5%)	0	100	100
1	D1	140/143 (98%)	133 (95%)	7 (5%)	0	100	100
1	E1	140/143 (98%)	133 (95%)	7 (5%)	0	100	100
1	F1	140/143 (98%)	132 (94%)	8 (6%)	0	100	100
2	A2	169/242 (70%)	156 (92%)	13 (8%)	0	100	100
2	B2	169/242 (70%)	155 (92%)	14 (8%)	0	100	100
2	C2	169/242 (70%)	155 (92%)	14 (8%)	0	100	100
2	D2	169/242 (70%)	156 (92%)	13 (8%)	0	100	100
2	E2	169/242 (70%)	155 (92%)	14 (8%)	0	100	100
2	F2	169/242 (70%)	156 (92%)	13 (8%)	0	100	100
3	A3	248/250 (99%)	214 (86%)	34 (14%)	0	100	100
3	B3	248/250 (99%)	214 (86%)	34 (14%)	0	100	100
3	C3	248/250 (99%)	214 (86%)	34 (14%)	0	100	100
3	D3	248/250 (99%)	214 (86%)	34 (14%)	0	100	100
3	E3	248/250 (99%)	214 (86%)	34 (14%)	0	100	100
3	F3	248/250 (99%)	214 (86%)	34 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A4	116/118 (98%)	101 (87%)	15 (13%)	0	100	100
4	B4	116/118 (98%)	101 (87%)	15 (13%)	0	100	100
4	C4	116/118 (98%)	101 (87%)	15 (13%)	0	100	100
4	D4	116/118 (98%)	101 (87%)	15 (13%)	0	100	100
4	E4	116/118 (98%)	101 (87%)	15 (13%)	0	100	100
4	F4	116/118 (98%)	101 (87%)	15 (13%)	0	100	100
5	A5	402/404 (100%)	360 (90%)	42 (10%)	0	100	100
5	B5	402/404 (100%)	355 (88%)	47 (12%)	0	100	100
5	C5	402/404 (100%)	358 (89%)	44 (11%)	0	100	100
5	D5	402/404 (100%)	360 (90%)	42 (10%)	0	100	100
5	E5	402/404 (100%)	359 (89%)	43 (11%)	0	100	100
5	F5	402/404 (100%)	356 (89%)	46 (11%)	0	100	100
5	G5	402/404 (100%)	361 (90%)	41 (10%)	0	100	100
5	H5	402/404 (100%)	355 (88%)	47 (12%)	0	100	100
5	I5	402/404 (100%)	359 (89%)	43 (11%)	0	100	100
5	J5	402/404 (100%)	358 (89%)	44 (11%)	0	100	100
5	K5	402/404 (100%)	359 (89%)	43 (11%)	0	100	100
5	L5	402/404 (100%)	356 (89%)	46 (11%)	0	100	100
6	A6	495/497 (100%)	441 (89%)	54 (11%)	0	100	100
6	B6	495/497 (100%)	441 (89%)	54 (11%)	0	100	100
6	C6	495/497 (100%)	441 (89%)	54 (11%)	0	100	100
6	D6	495/497 (100%)	441 (89%)	54 (11%)	0	100	100
6	E6	495/497 (100%)	441 (89%)	54 (11%)	0	100	100
6	F6	495/497 (100%)	441 (89%)	54 (11%)	0	100	100
7	A7	108/117 (92%)	87 (81%)	21 (19%)	0	100	100
7	B7	108/117 (92%)	87 (81%)	21 (19%)	0	100	100
7	C7	108/117 (92%)	87 (81%)	21 (19%)	0	100	100
7	D7	108/117 (92%)	87 (81%)	21 (19%)	0	100	100
7	E7	108/117 (92%)	87 (81%)	21 (19%)	0	100	100
7	F7	108/117 (92%)	87 (81%)	21 (19%)	0	100	100
All	All	12480/13050 (96%)	11084 (89%)	1396 (11%)	0	100	100

There are no Ramachandran outliers to report.

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	A1	124/125 (99%)	123 (99%)	1 (1%)	81	93
1	B1	124/125 (99%)	123 (99%)	1 (1%)	81	93
1	C1	124/125 (99%)	123 (99%)	1 (1%)	81	93
1	D1	124/125 (99%)	123 (99%)	1 (1%)	81	93
1	E1	124/125 (99%)	123 (99%)	1 (1%)	81	93
1	F1	124/125 (99%)	123 (99%)	1 (1%)	81	93
2	A2	156/211 (74%)	152 (97%)	4 (3%)	46	76
2	B2	156/211 (74%)	152 (97%)	4 (3%)	46	76
2	C2	156/211 (74%)	152 (97%)	4 (3%)	46	76
2	D2	156/211 (74%)	152 (97%)	4 (3%)	46	76
2	E2	156/211 (74%)	152 (97%)	4 (3%)	46	76
2	F2	156/211 (74%)	152 (97%)	4 (3%)	46	76
3	A3	220/220 (100%)	220 (100%)	0	100	100
3	B3	220/220 (100%)	220 (100%)	0	100	100
3	C3	220/220 (100%)	219 (100%)	1 (0%)	88	95
3	D3	220/220 (100%)	220 (100%)	0	100	100
3	E3	220/220 (100%)	220 (100%)	0	100	100
3	F3	220/220 (100%)	220 (100%)	0	100	100
4	A4	106/106 (100%)	105 (99%)	1 (1%)	78	91
4	B4	106/106 (100%)	105 (99%)	1 (1%)	78	91
4	C4	106/106 (100%)	105 (99%)	1 (1%)	78	91
4	D4	106/106 (100%)	105 (99%)	1 (1%)	78	91
4	E4	106/106 (100%)	105 (99%)	1 (1%)	78	91
4	F4	106/106 (100%)	105 (99%)	1 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A5	352/353 (100%)	351 (100%)	1 (0%)	92	96
5	B5	353/353 (100%)	353 (100%)	0	100	100
5	C5	352/353 (100%)	350 (99%)	2 (1%)	86	94
5	D5	353/353 (100%)	353 (100%)	0	100	100
5	E5	352/353 (100%)	351 (100%)	1 (0%)	92	96
5	F5	353/353 (100%)	353 (100%)	0	100	100
5	G5	352/353 (100%)	352 (100%)	0	100	100
5	H5	353/353 (100%)	353 (100%)	0	100	100
5	I5	352/353 (100%)	351 (100%)	1 (0%)	92	96
5	J5	353/353 (100%)	353 (100%)	0	100	100
5	K5	352/353 (100%)	351 (100%)	1 (0%)	92	96
5	L5	353/353 (100%)	353 (100%)	0	100	100
6	A6	407/407 (100%)	402 (99%)	5 (1%)	71	88
6	B6	407/407 (100%)	402 (99%)	5 (1%)	71	88
6	C6	407/407 (100%)	402 (99%)	5 (1%)	71	88
6	D6	407/407 (100%)	402 (99%)	5 (1%)	71	88
6	E6	407/407 (100%)	402 (99%)	5 (1%)	71	88
6	F6	407/407 (100%)	402 (99%)	5 (1%)	71	88
7	A7	98/105 (93%)	96 (98%)	2 (2%)	55	80
7	B7	98/105 (93%)	96 (98%)	2 (2%)	55	80
7	C7	98/105 (93%)	96 (98%)	2 (2%)	55	80
7	D7	98/105 (93%)	96 (98%)	2 (2%)	55	80
7	E7	98/105 (93%)	96 (98%)	2 (2%)	55	80
7	F7	98/105 (93%)	96 (98%)	2 (2%)	55	80
All	All	10896/11280 (97%)	10811 (99%)	85 (1%)	82	93

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	C6	424	ASN
6	F6	204	GLU
6	D6	37	LEU
6	E6	156	SER
7	B7	93	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
5	F5	13	ASN
5	H5	320	GLN
5	F5	78	GLN
5	G5	218	GLN
5	I5	364	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

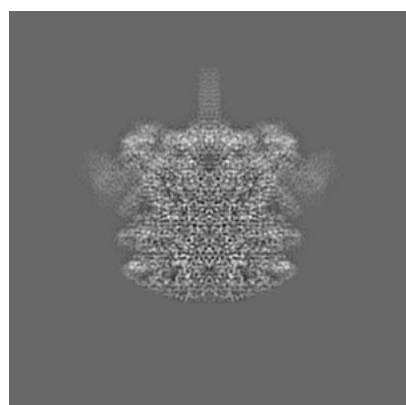
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22873. These allow visual inspection of the internal detail of the map and identification of artifacts.

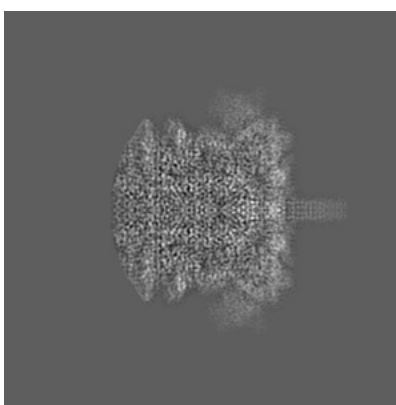
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

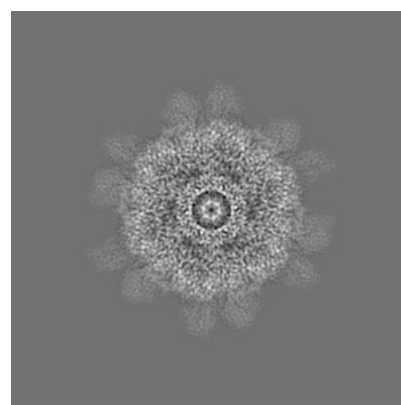
6.1.1 Primary map



X



Y

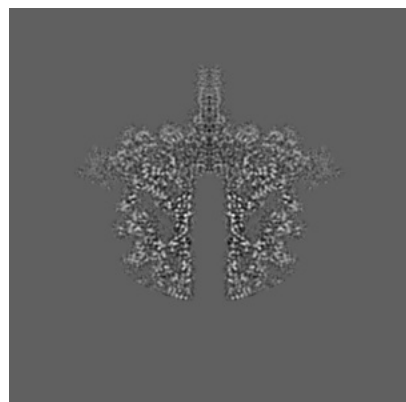


Z

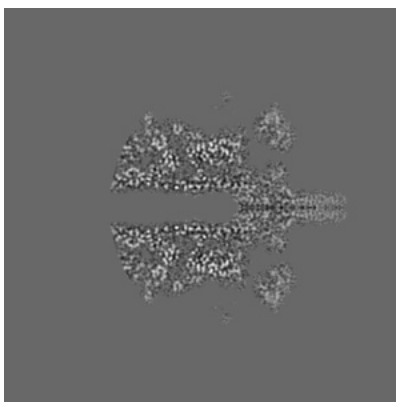
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

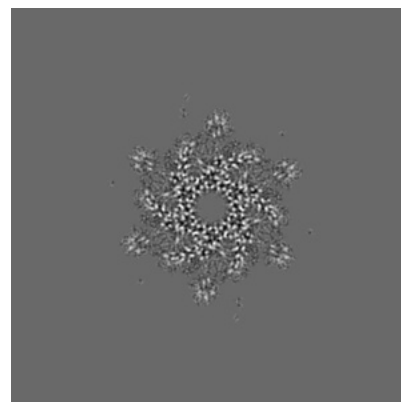
6.2.1 Primary map



X Index: 256



Y Index: 256

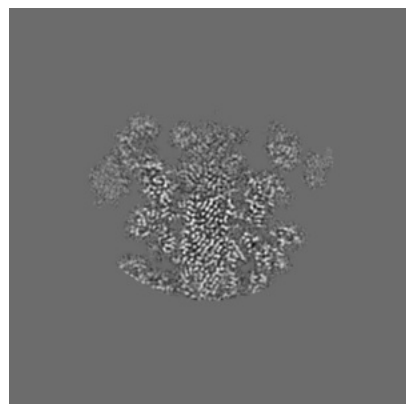


Z Index: 256

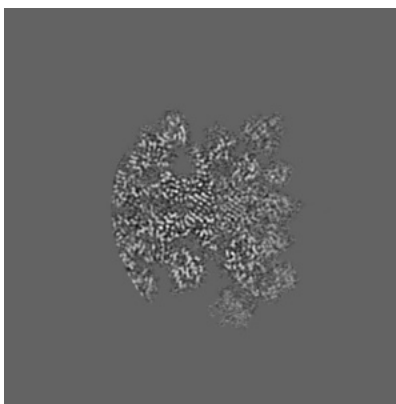
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

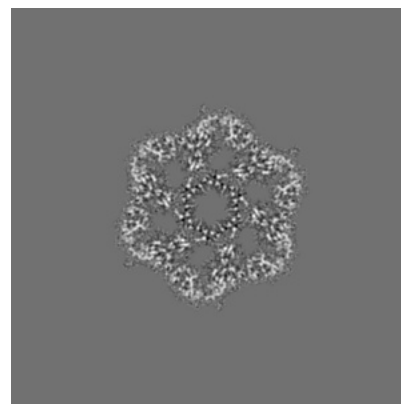
6.3.1 Primary map



X Index: 285



Y Index: 280

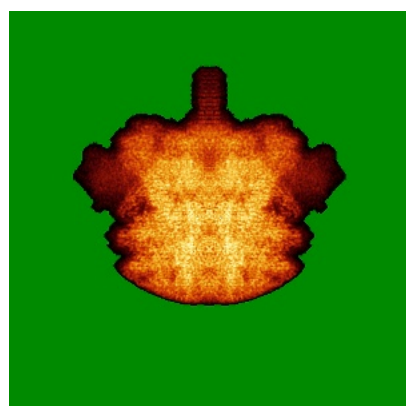


Z Index: 224

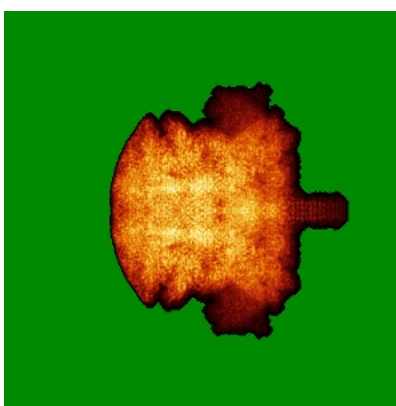
The images above show the largest variance slices of the map in three orthogonal directions.

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

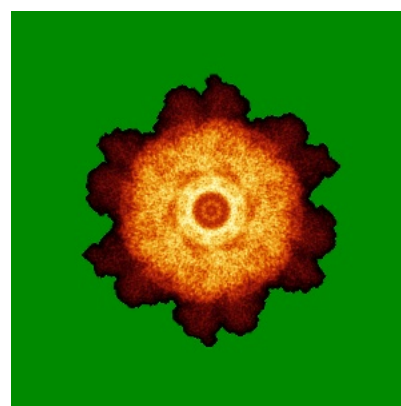
6.4.1 Primary map



X



Y

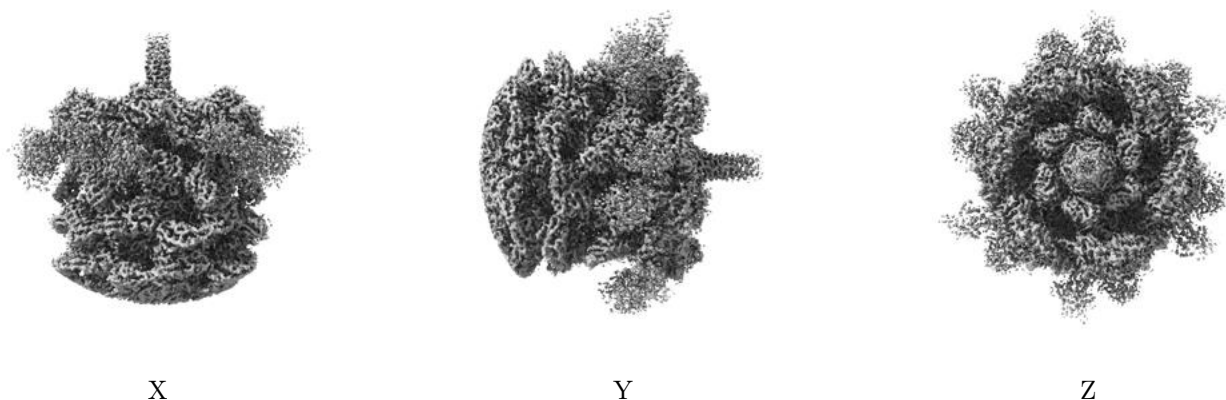


Z

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 2.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

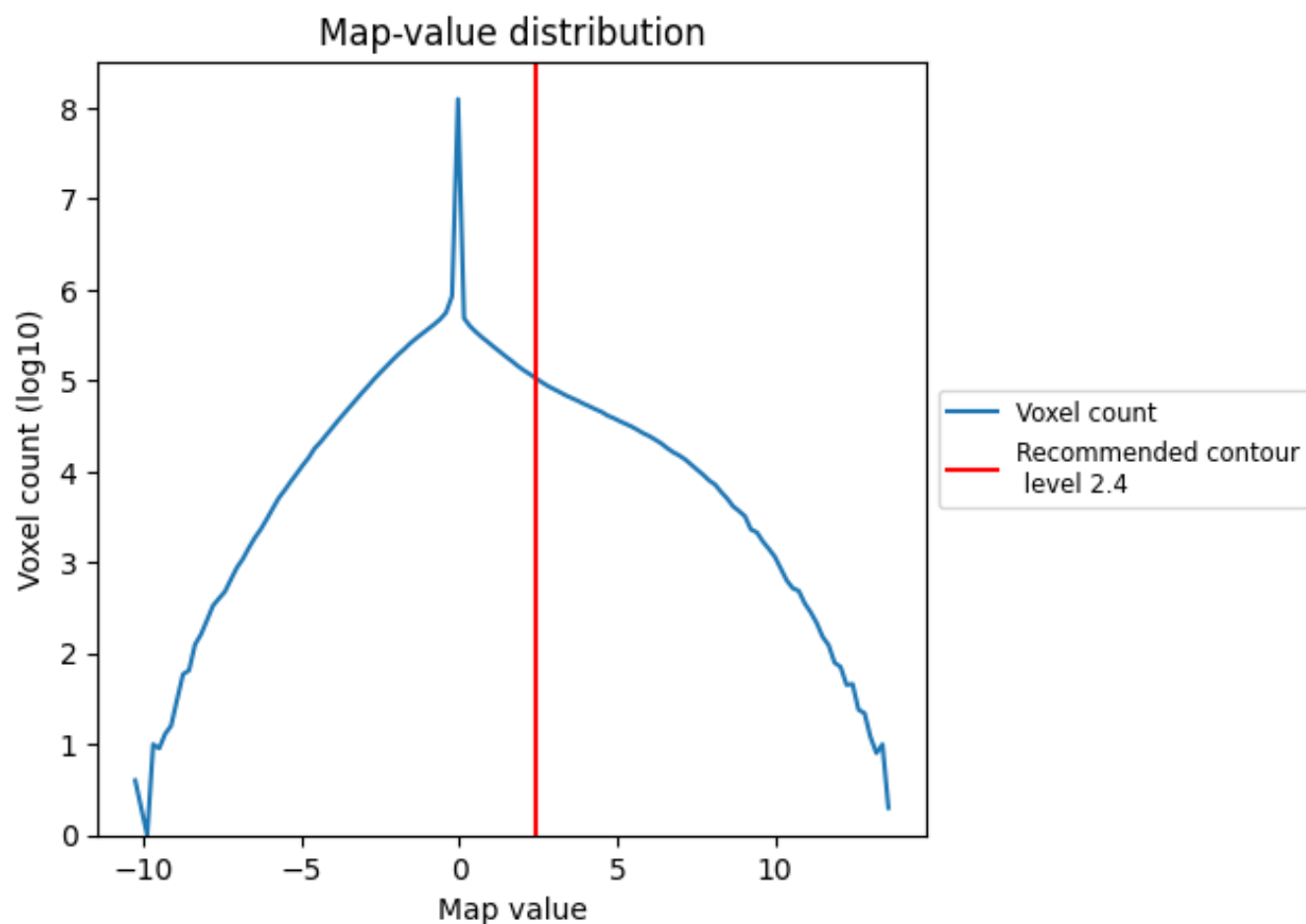
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

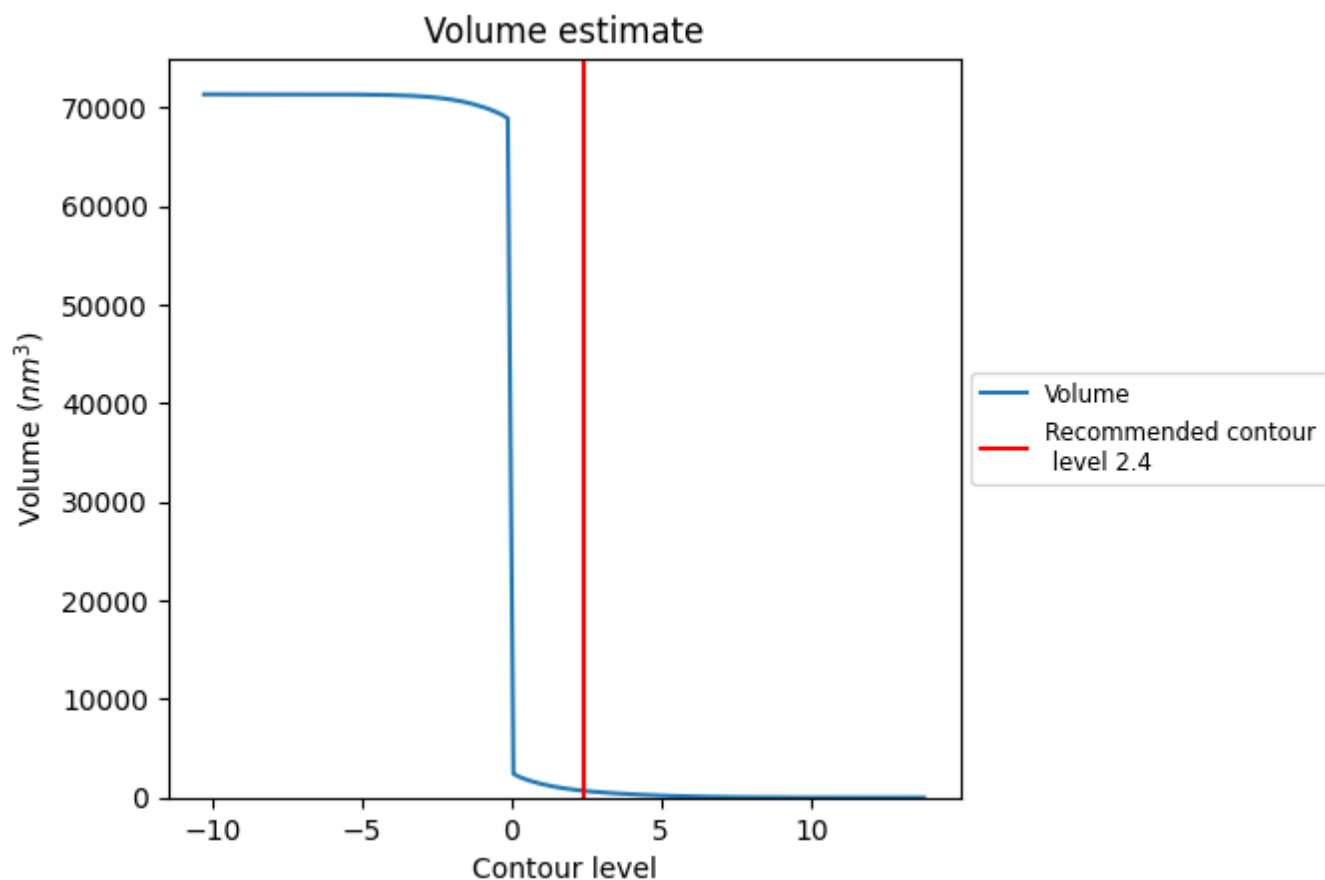
This section contains the results of statistical analysis of the map.

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.

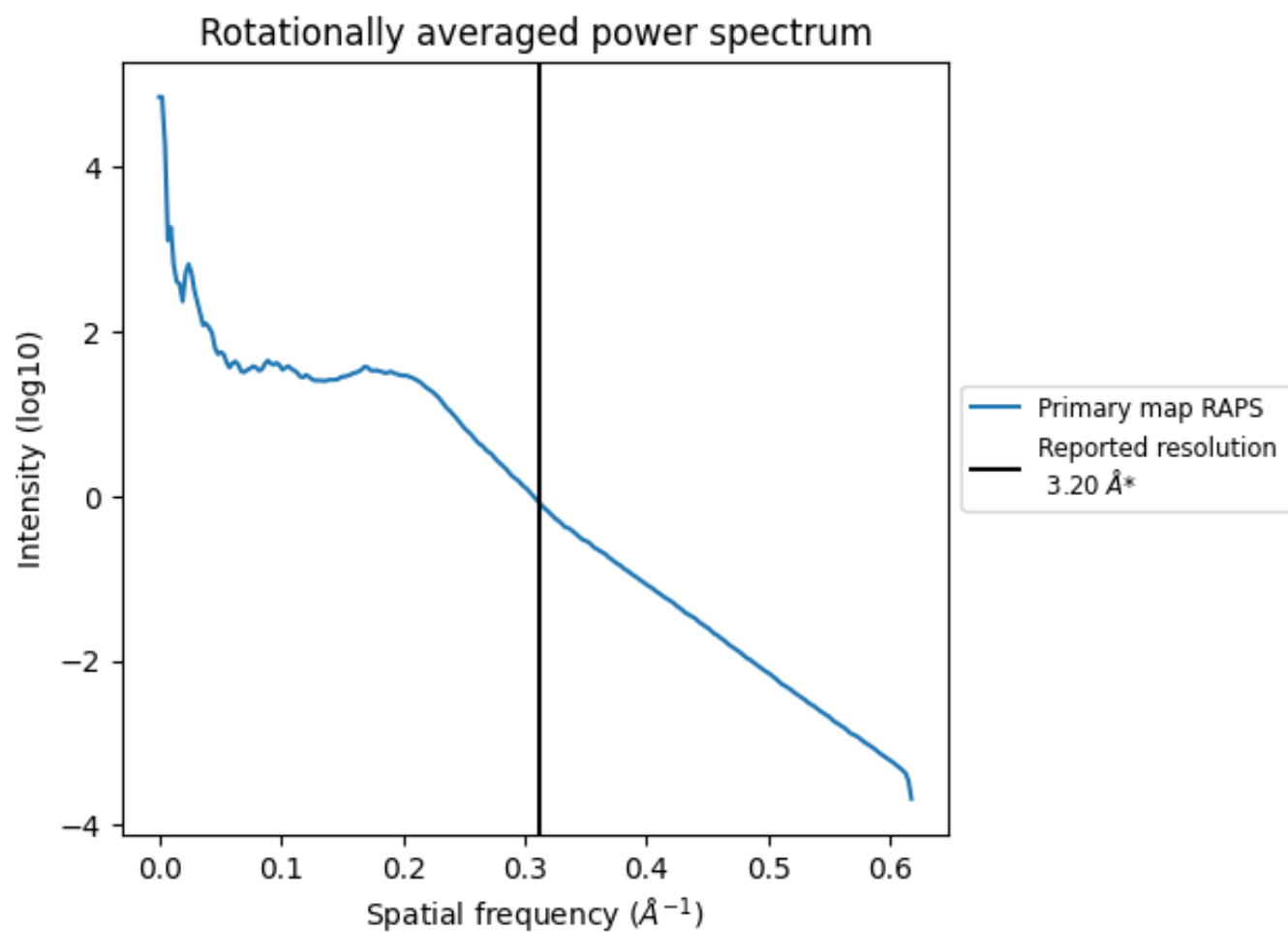
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 692 nm³; this corresponds to an approximate mass of 625 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 ⓘ

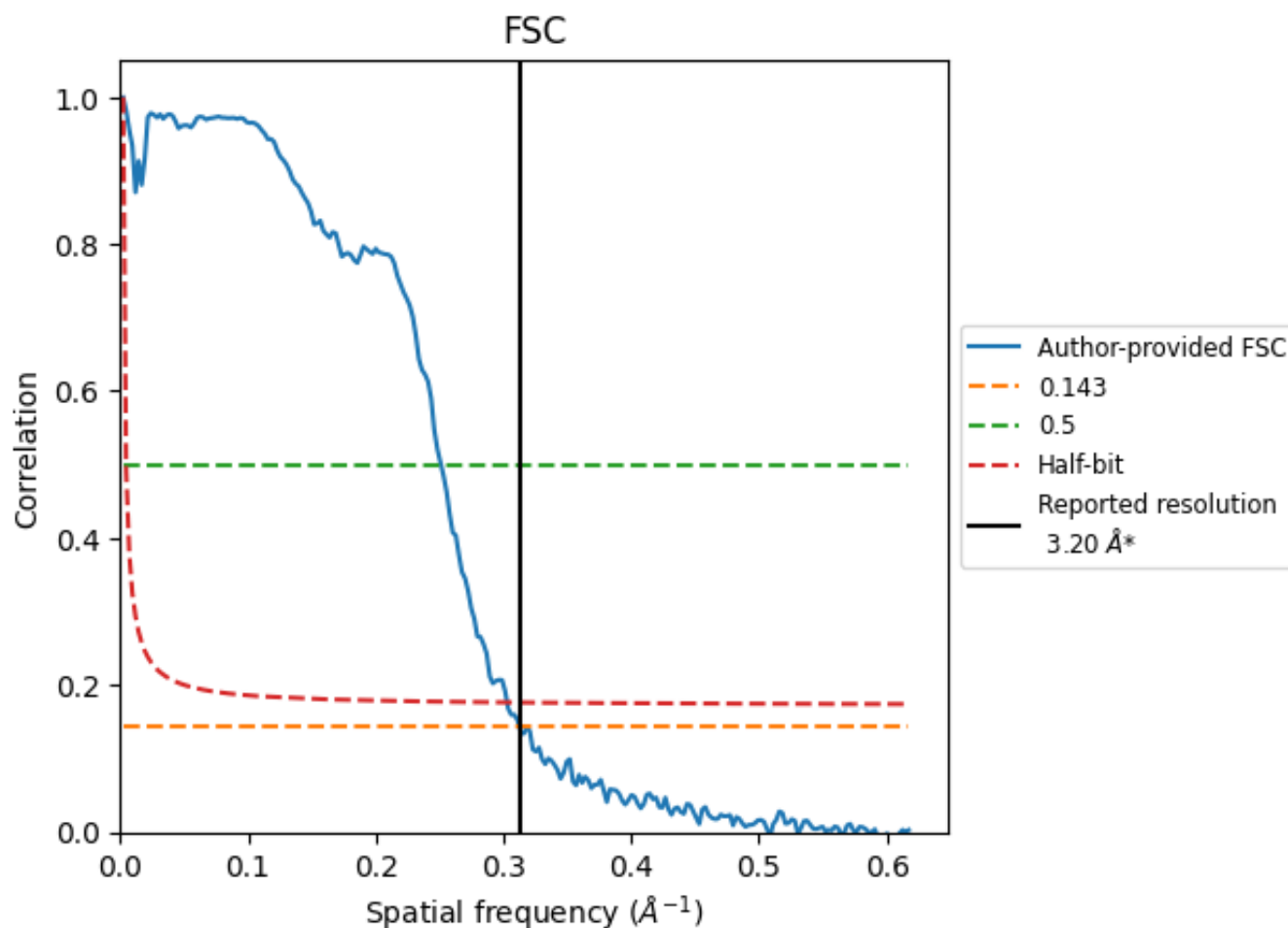


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

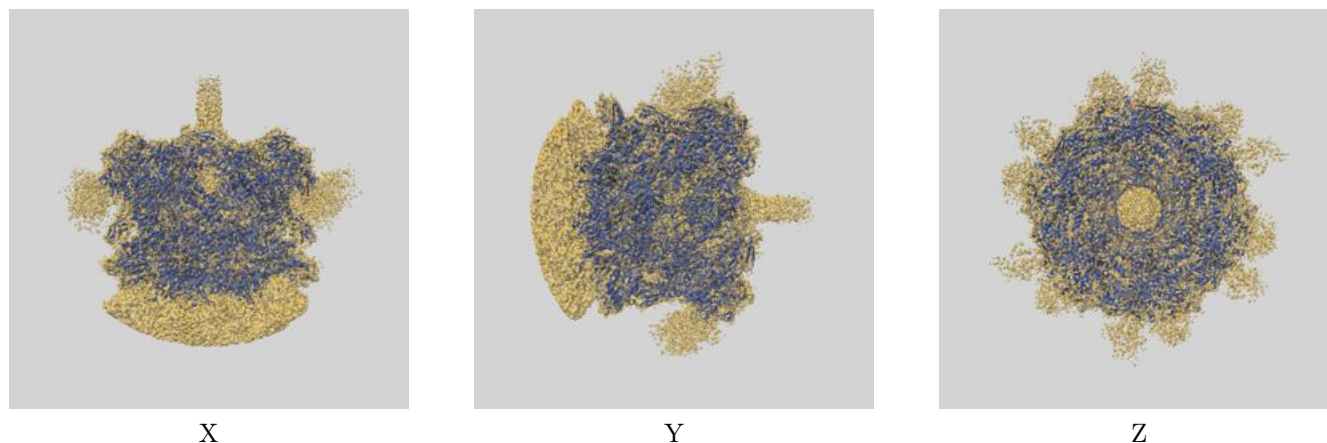
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.98	3.30
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

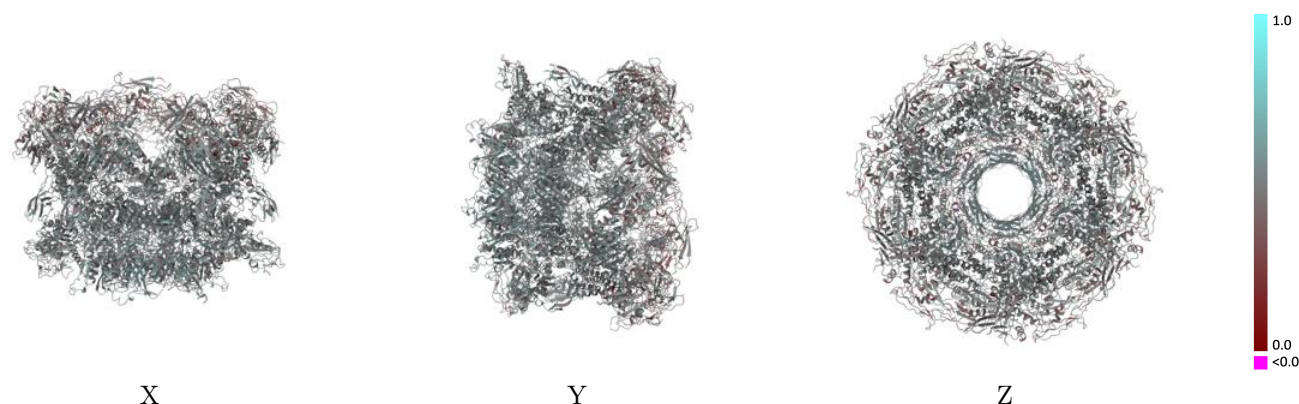
This section contains information regarding the fit between EMDB map EMD-22873 and PDB model 7KH1. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



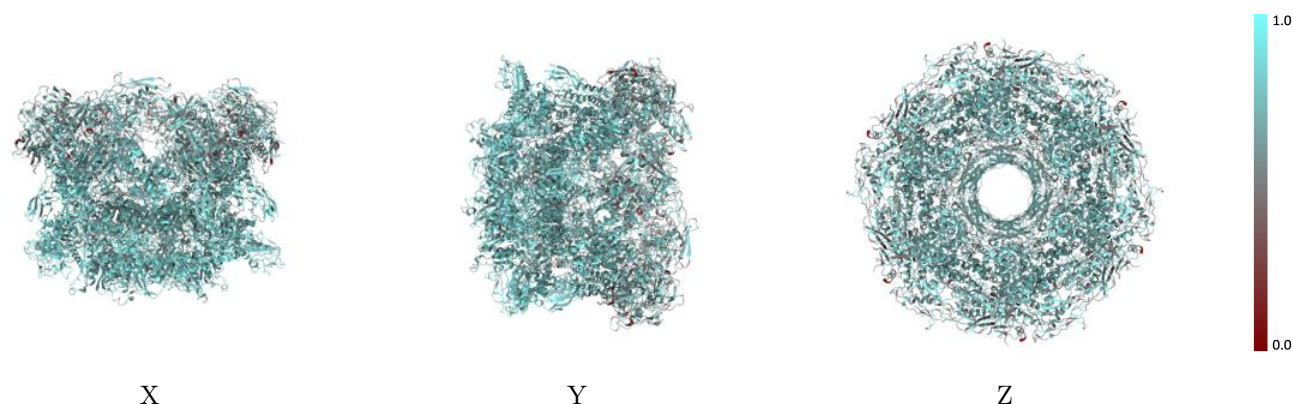
The images above show the 3D surface view of the map at the recommended contour level 2.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



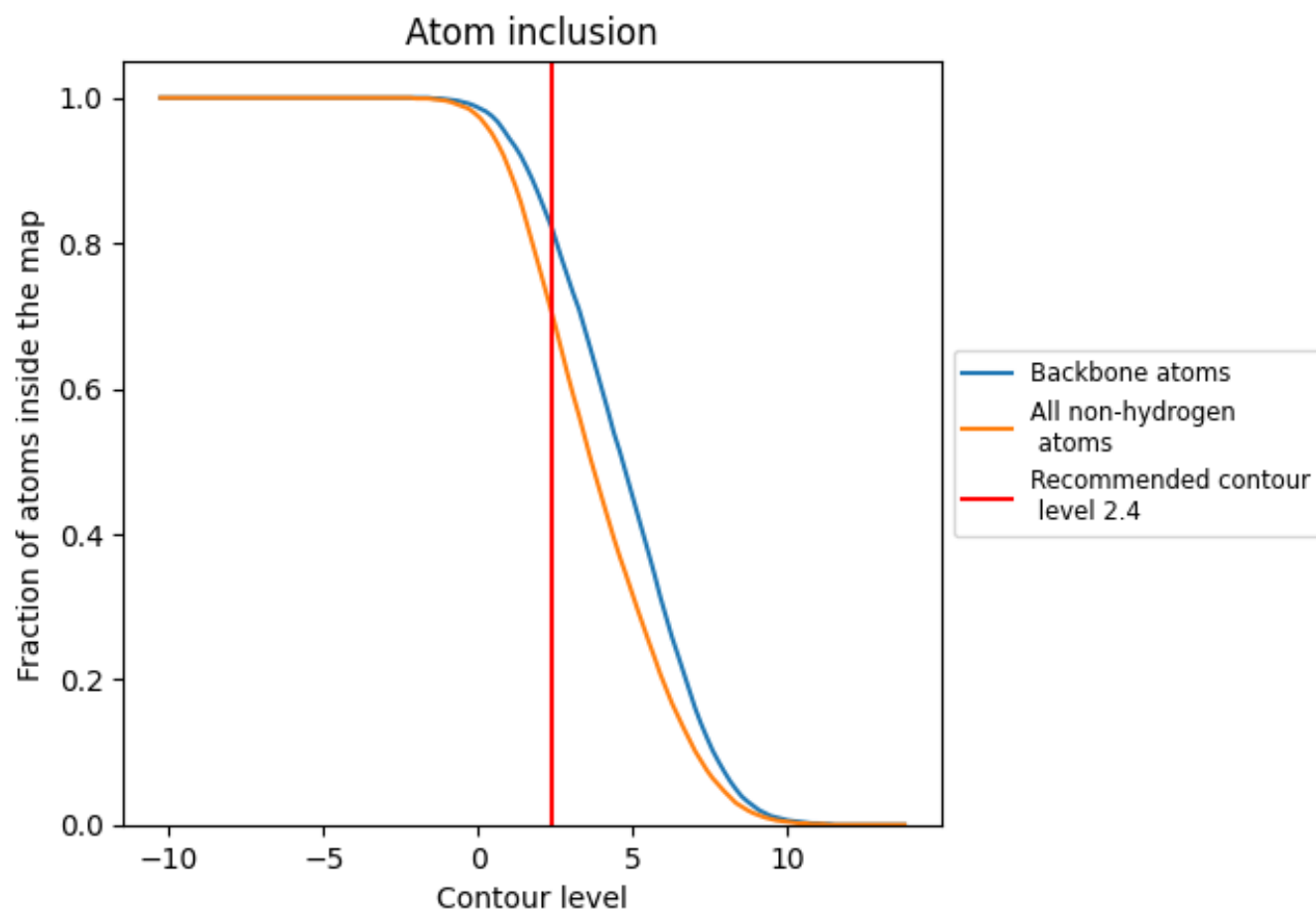
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





























The table lists the average atom inclusion at the recommended contour level (2.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7020	 0.4930
A1	 0.7700	 0.5370
A2	 0.6420	 0.4680
A3	 0.7160	 0.5170
A4	 0.7590	 0.5200
A5	 0.6740	 0.4760
A6	 0.7440	 0.5030
A7	 0.7190	 0.5160
B1	 0.7760	 0.5390
B2	 0.6440	 0.4690
B3	 0.7060	 0.5170
B4	 0.7620	 0.5230
B5	 0.6510	 0.4630
B6	 0.7470	 0.5040
B7	 0.7220	 0.5160
C1	 0.7630	 0.5380
C2	 0.6390	 0.4700
C3	 0.7150	 0.5160
C4	 0.7590	 0.5240
C5	 0.6720	 0.4760
C6	 0.7460	 0.5040
C7	 0.7250	 0.5160
D1	 0.7720	 0.5380
D2	 0.6370	 0.4690
D3	 0.7150	 0.5170
D4	 0.7600	 0.5230
D5	 0.6470	 0.4620
D6	 0.7440	 0.5040
D7	 0.7260	 0.5170
E1	 0.7670	 0.5380
E2	 0.6440	 0.4690
E3	 0.7060	 0.5190
E4	 0.7620	 0.5220
E5	 0.6720	 0.4750
E6	 0.7460	 0.5030



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Chain	Atom inclusion	Q-score
E7	 0.7260	 0.5140
F1	 0.7690	 0.5370
F2	 0.6410	 0.4670
F3	 0.7170	 0.5170
F4	 0.7600	 0.5220
F5	 0.6520	 0.4650
F6	 0.7450	 0.5030
F7	 0.7230	 0.5140
G5	 0.6760	 0.4770
H5	 0.6510	 0.4640
I5	 0.6730	 0.4740
J5	 0.6450	 0.4620
K5	 0.6720	 0.4750
L5	 0.6510	 0.4630