wwPDB EM Validation Summary Report (i)

May 19, 2024 – 06:19 am BST

PDB ID	:	6TUI
EMDB ID	:	EMD-10592
Title	:	Virion of empty GTA particle
Authors	:	Bardy, P.; Fuzik, T.; Hrebik, D.; Pantucek, R.; Beatty, J.T.; Plevka, P.
Deposited on	:	2020-01-07
Resolution	:	10.47 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 (i) 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 (i)) were used in the production of this report:

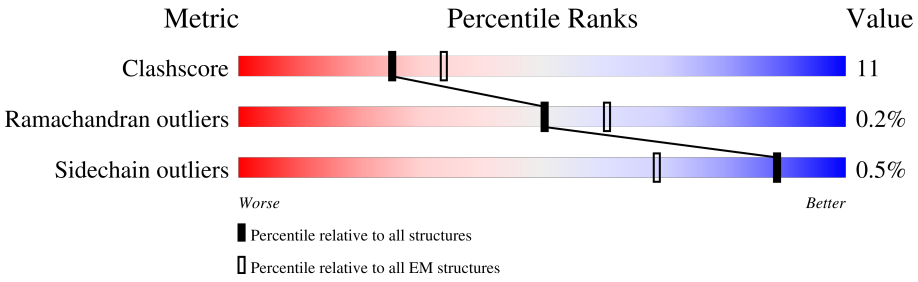
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 10.47 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 <=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	A4	385	60% 16% 24%
1	A5	385	56% 20% 24%
1	B4	385	58% 19% 23%
1	B5	385	50% 20% • 30%
1	C4	385	58% 19% 23%
1	C5	385	62% 15% 23%
1	D4	385	57% 20% 23%
1	E4	385	56% 21% 23%

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Mol	Chain	Length	Quality of chain
1	F4	385	58% 19% 23%
1	G4	385	57% 20% 23%
1	H4	385	52% 23% 24%
1	I4	385	55% 21% 24%
1	J4	385	52% 23% 24%
1	K4	385	52% 23% 24%
1	L4	385	54% 21% 24%
1	M4	385	57% 20% 23%
1	N4	385	57% 20% 23%
1	O4	385	53% 24% 23%
1	P4	385	57% 20% 23%
1	Q4	385	53% 24% 23%
1	R4	385	55% 22% 23%
1	S4	385	55% 21% 24%
1	T4	385	48% 28% 24%
1	U4	385	56% 19% 24%
1	V4	385	55% 21% 24%
1	W4	385	51% 25% 24%
1	X4	385	56% 21% 23%
1	Y4	385	59% 18% 23%
1	Z4	385	59% 18% 23%
2	A1	84	87% 13%
2	A2	84	87% 13%
2	A3	84	82% 18%
2	B2	84	86% 14%

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Mol	Chain	Length	Quality of chain
2	B3	84	88% 12%
2	C2	84	86% 14%
2	C3	84	87% 13%
2	D2	84	83% 17%
2	D3	84	83% 17%
2	E2	84	81% 19%
2	E3	84	82% 18%
3	F2	325	97%
3	F3	325	97%
4	G	137	74% 23%
4	H	137	74% 24%
4	I	137	73% 25%
4	J	137	72% 26%
5	C	197	73% 23%
5	D	197	78% 20%
6	A	396	77% 16% 7%
6	B	396	77% 15% 8%
7	F	135	75% 23%
8	E	112	72% 26%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 84902 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phage major capsid protein, HK97 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C5	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	X4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	Y4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	Z4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	A5	294	Total	C	N	O	S	0	0
			2184	1385	373	420	6		
1	B5	270	Total	C	N	O	S	0	0
			2012	1281	344	381	6		
1	N4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	R4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	M4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	Q4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	O4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	P4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	W4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	U4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	T4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	S4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	K4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	J4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	V4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	L4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	H4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	I4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	A4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	D4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	E4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	F4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	G4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	B4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	C4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	A2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	C2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	B2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	E2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	E3	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	B3	84	Total	C	N	O	S	0	0
			640	403	115	121	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	D3	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	C3	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	A3	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	A1	84	Total	C	N	O	S	0	0
			640	403	115	121	1		

- Molecule 3 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	F2	10	Total	C	N	O	0	0
			62	42	10	10		
3	F3	10	Total	C	N	O	0	0
			62	42	10	10		

- Molecule 4 is a protein called Tail tube protein Rcc01691.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	134	Total	C	N	O	S	0	0
			993	623	167	201	2		
4	I	134	Total	C	N	O	S	0	0
			993	623	167	201	2		
4	J	134	Total	C	N	O	S	0	0
			993	623	167	201	2		
4	G	134	Total	C	N	O	S	0	0
			993	623	167	201	2		

- Molecule 5 is a protein called Adaptor protein Rcc01688.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	192	Total	C	N	O	S	0	0
			1440	926	257	249	8		
5	D	195	Total	C	N	O	S	0	0
			1460	938	260	254	8		

- Molecule 6 is a protein called Portal protein Rcc01684.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	370	Total	C	N	O	S	0	0
			2815	1789	505	508	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	366	Total	C	N	O	S	0	0
			2781	1767	499	502	13		

- Molecule 7 is a protein called Tail terminator protein Rcc01690.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	134	Total	C	N	O	S	0	0
			968	613	174	180	1		

- Molecule 8 is a protein called Stopper protein Rcc01689.

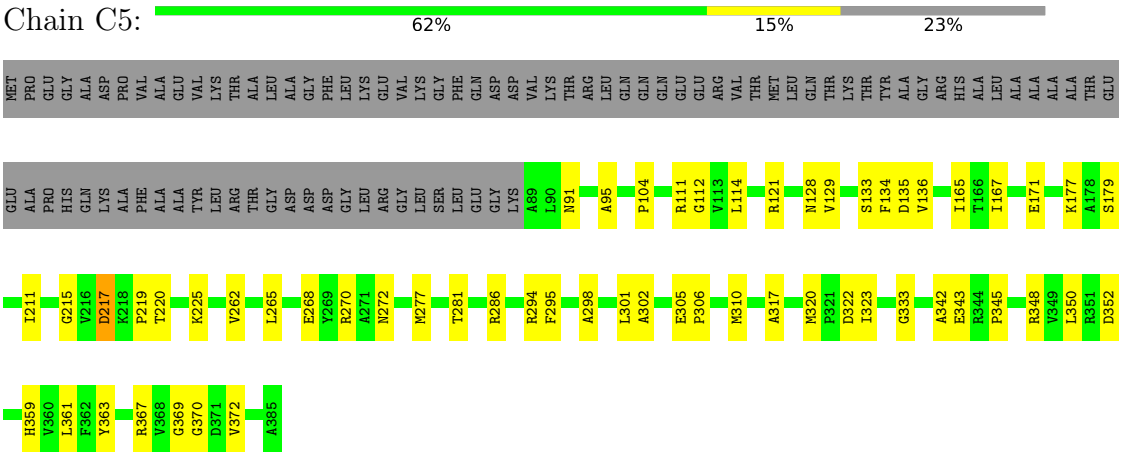
Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	110	Total	C	N	O	S	0	0
			859	536	171	151	1		

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.

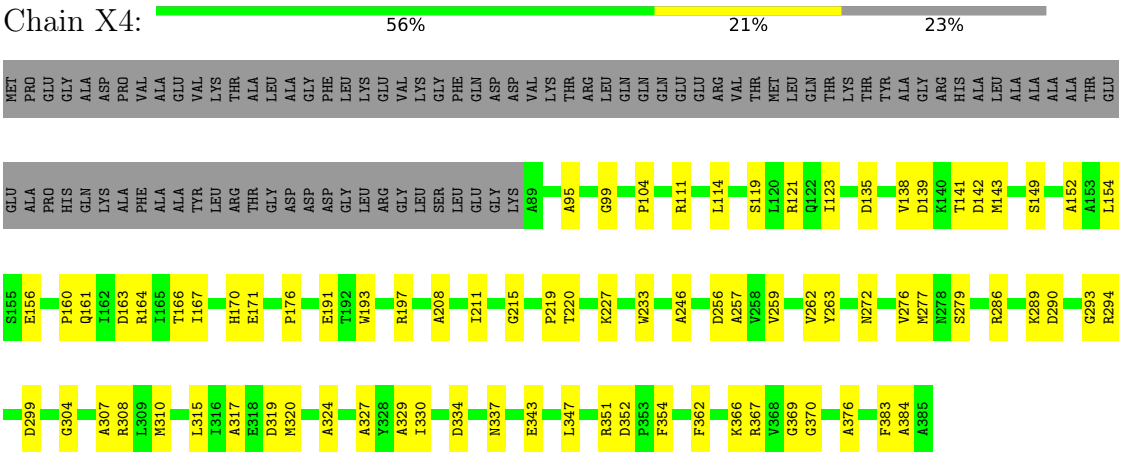
• Molecule 1: Phage major capsid protein, HK97 family

Chain C5:



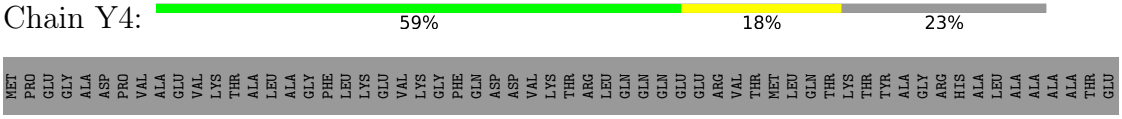
• Molecule 1: Phage major capsid protein, HK97 family

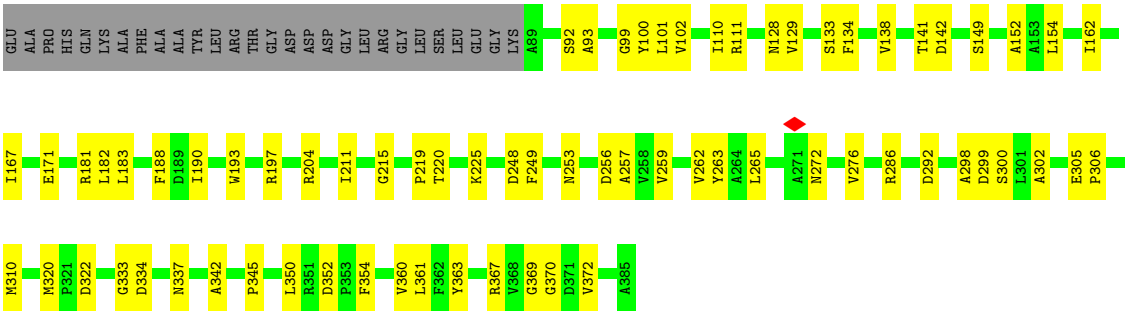
Chain X4:



• Molecule 1: Phage major capsid protein, HK97 family

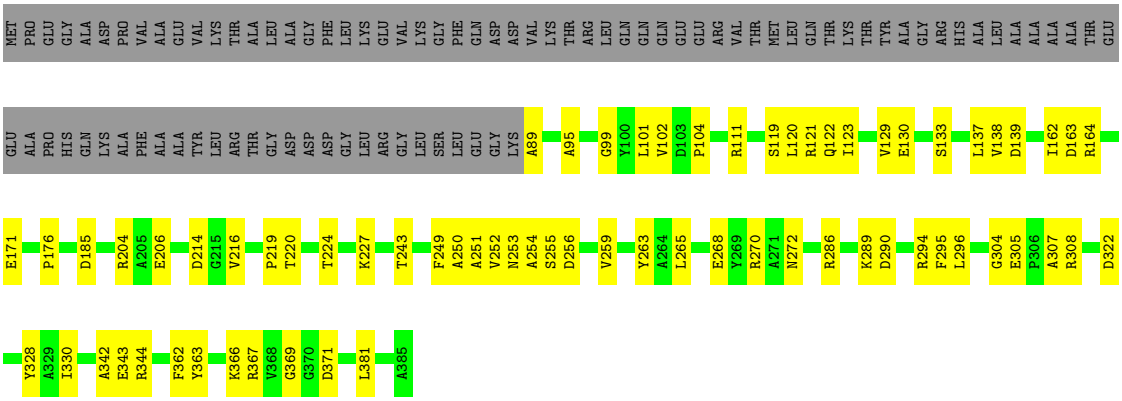
Chain Y4:





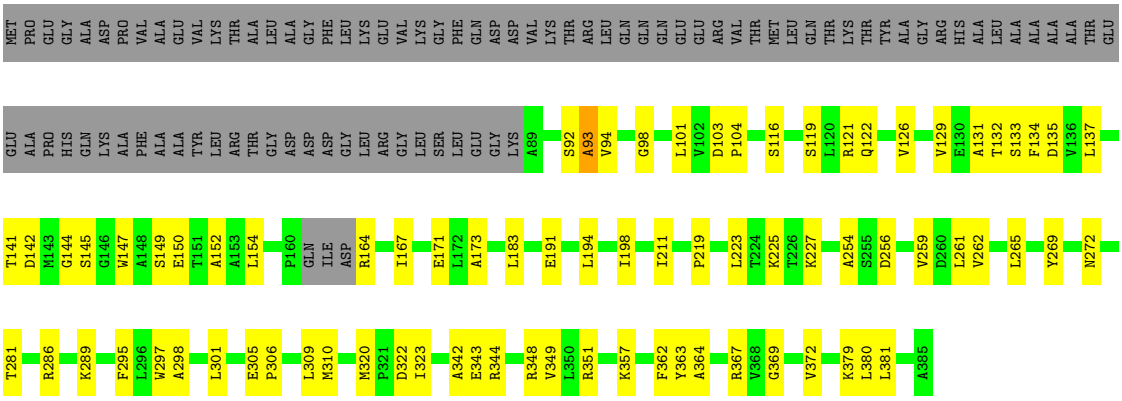
• Molecule 1: Phage major capsid protein, HK97 family

Chain Z4:



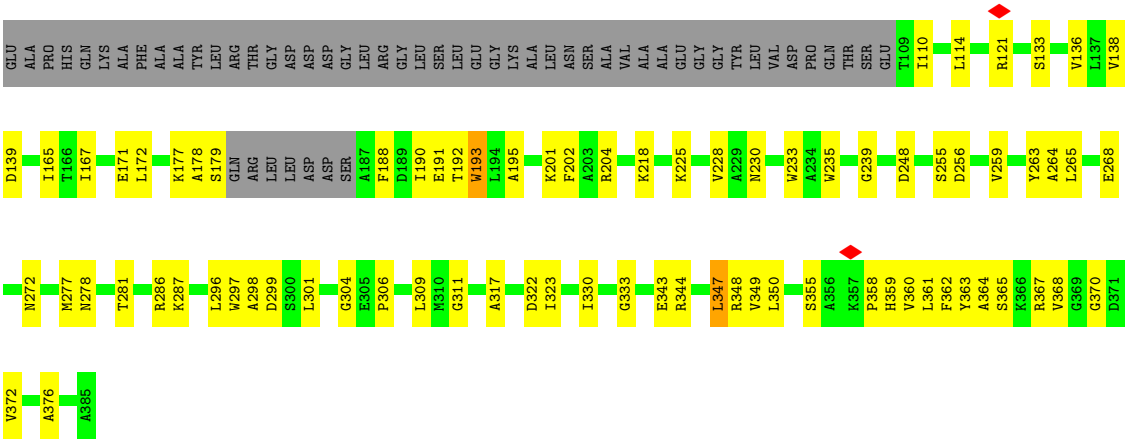
• Molecule 1: Phage major capsid protein, HK97 family

Chain A5:



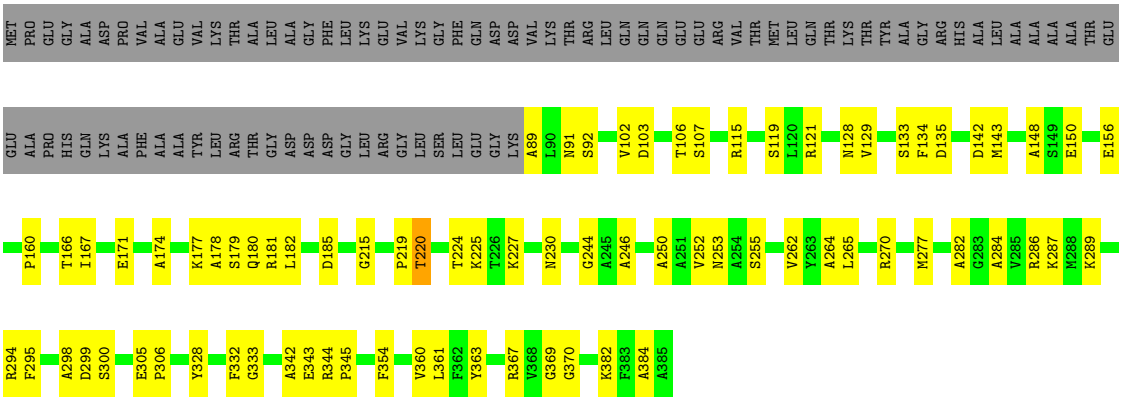
• Molecule 1: Phage major capsid protein, HK97 family

Chain B5:



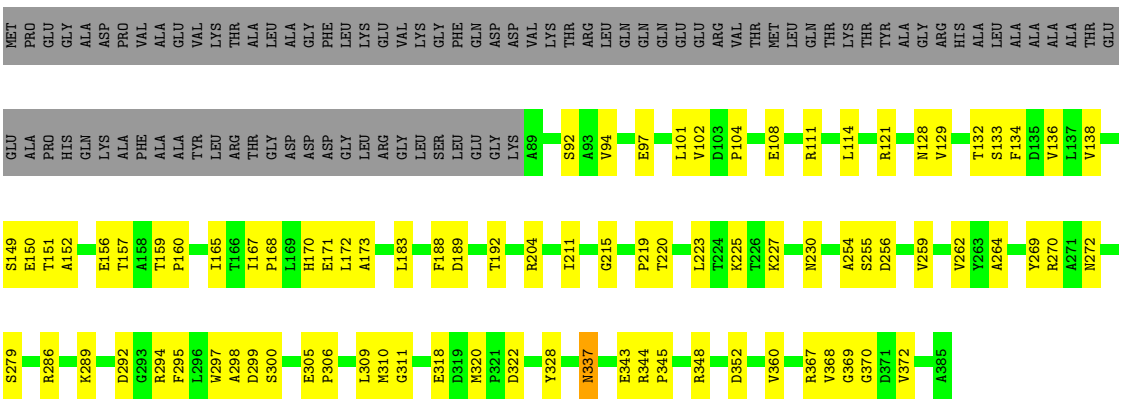
• Molecule 1: Phage major capsid protein, HK97 family

Chain N4:



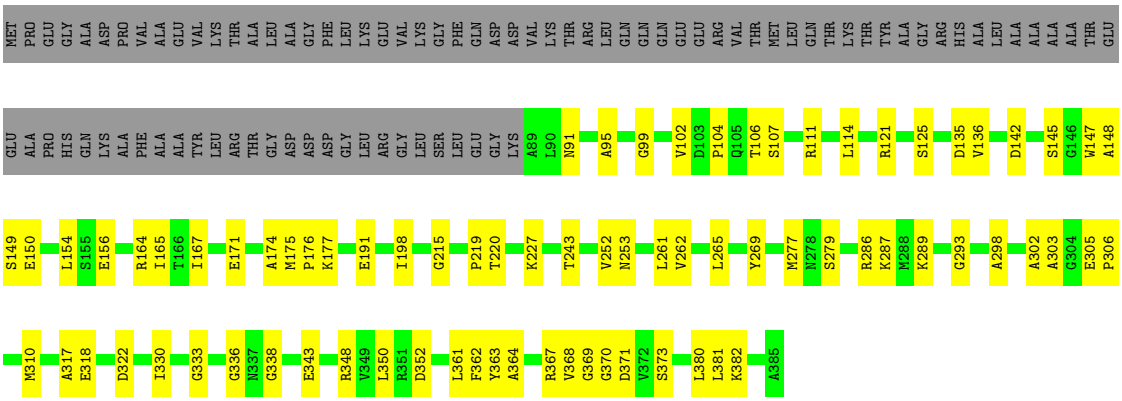
• Molecule 1: Phage major capsid protein, HK97 family

Chain R4:



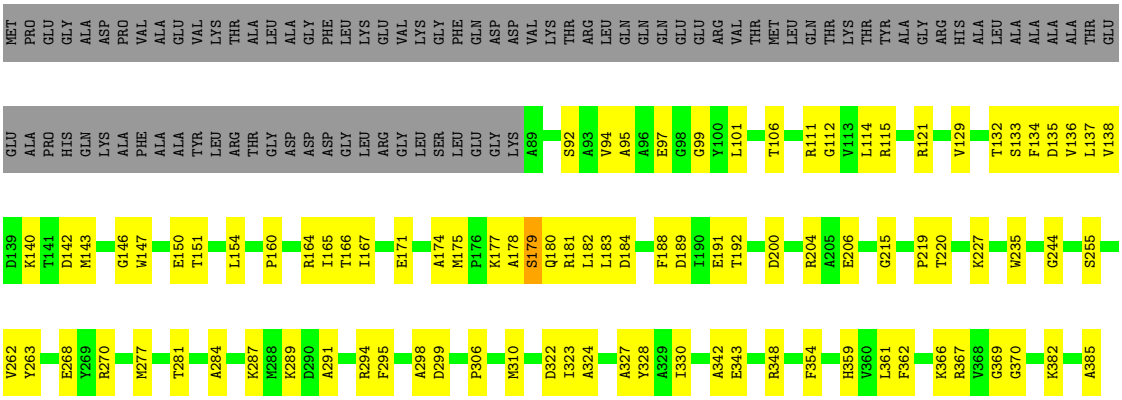
• Molecule 1: Phage major capsid protein, HK97 family

Chain M4:



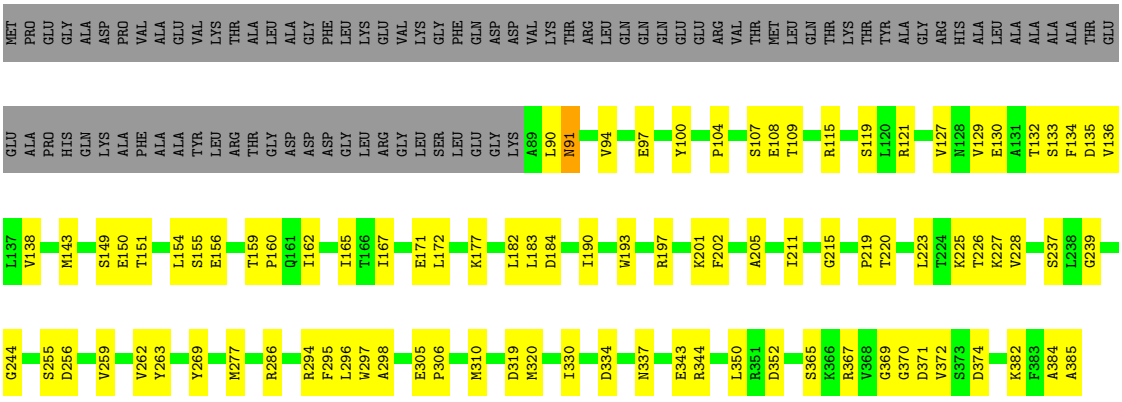
• Molecule 1: Phage major capsid protein, HK97 family

Chain Q4:



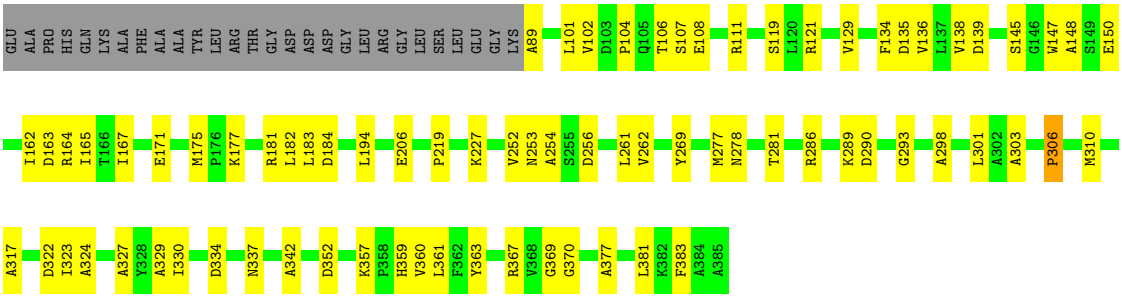
• Molecule 1: Phage major capsid protein, HK97 family

Chain O4:



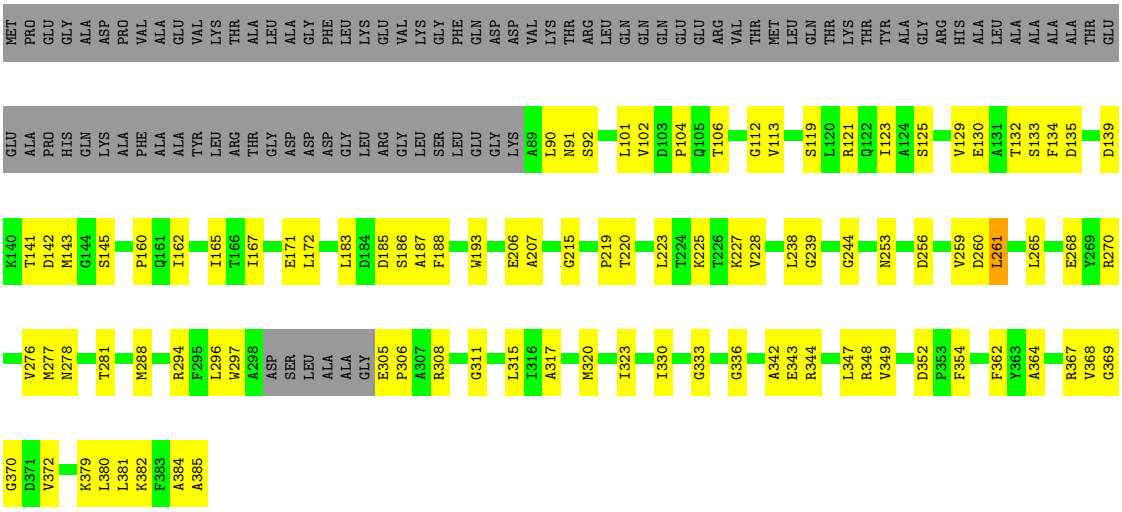
• Molecule 1: Phage major capsid protein, HK97 family

Chain P4:



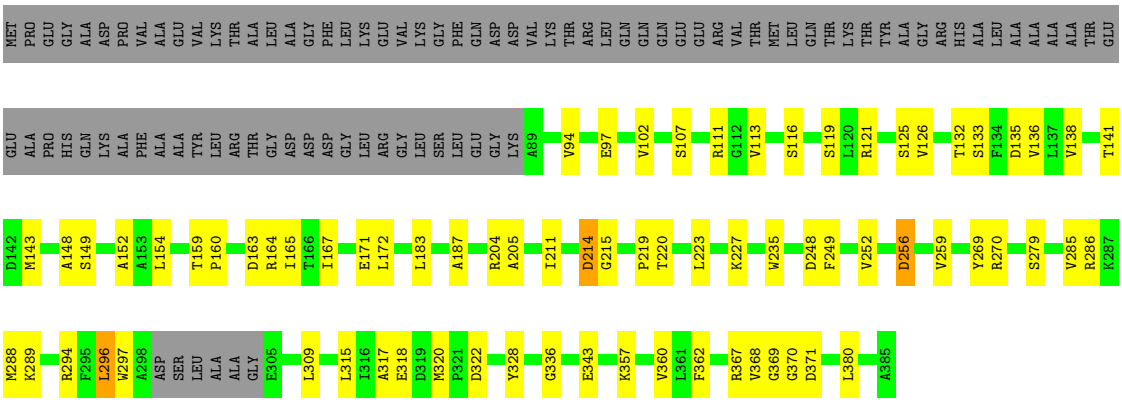
• Molecule 1: Phage major capsid protein, HK97 family

Chain W4:



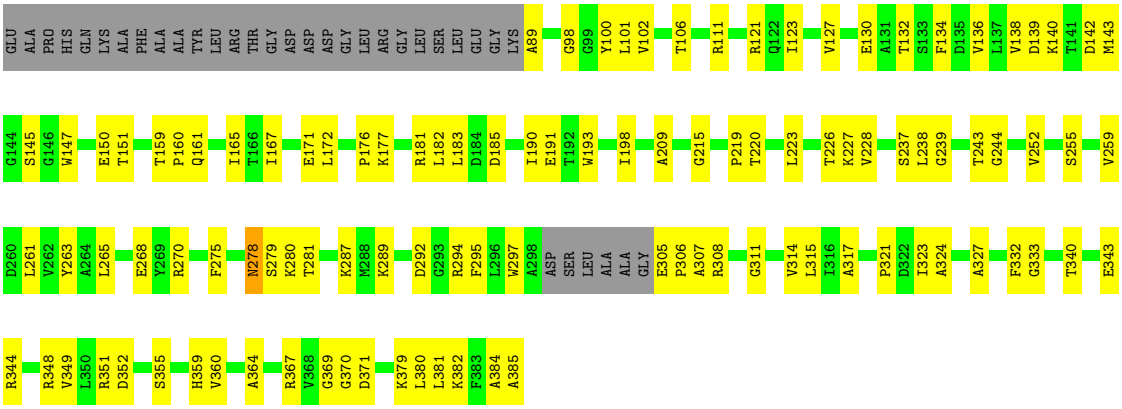
• Molecule 1: Phage major capsid protein, HK97 family

Chain U4:



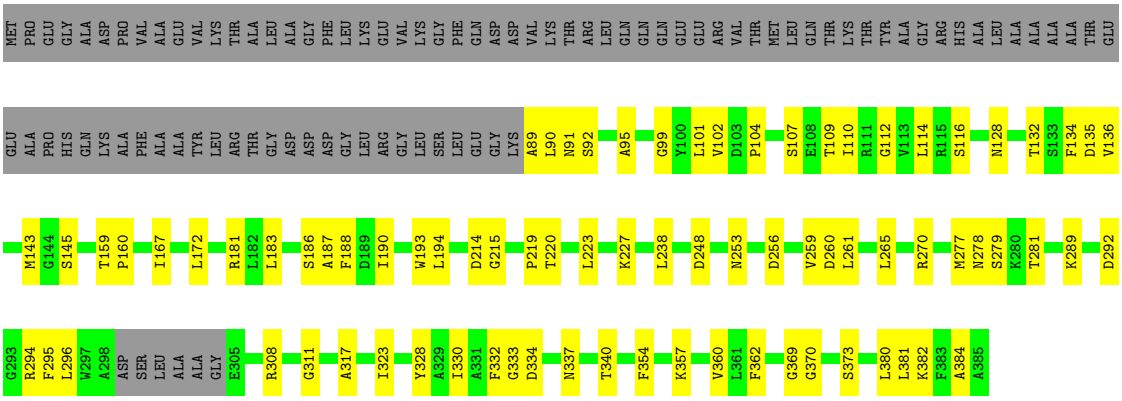
• Molecule 1: Phage major capsid protein, HK97 family

Chain T4:



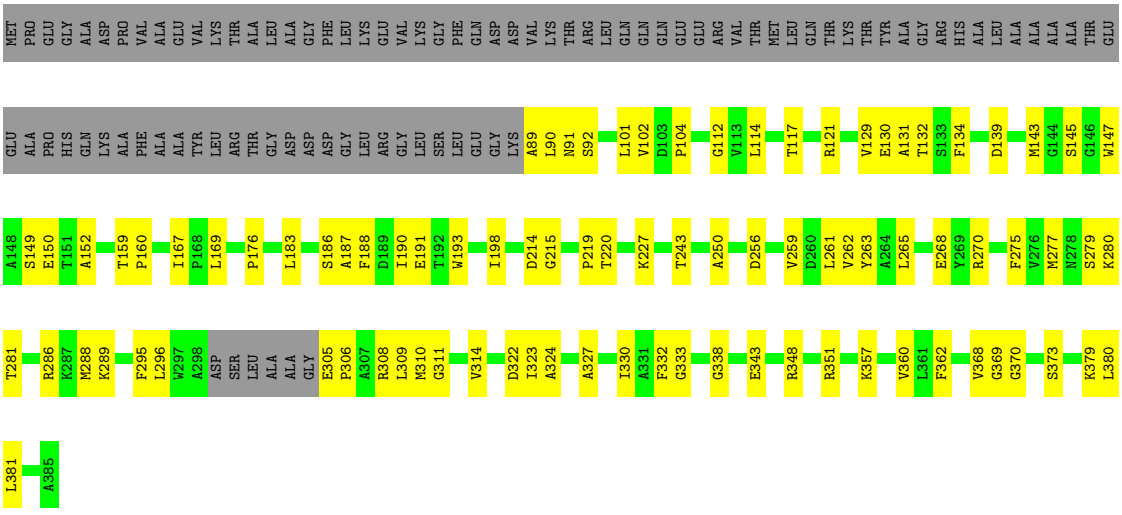
• Molecule 1: Phage major capsid protein, HK97 family

Chain S4:



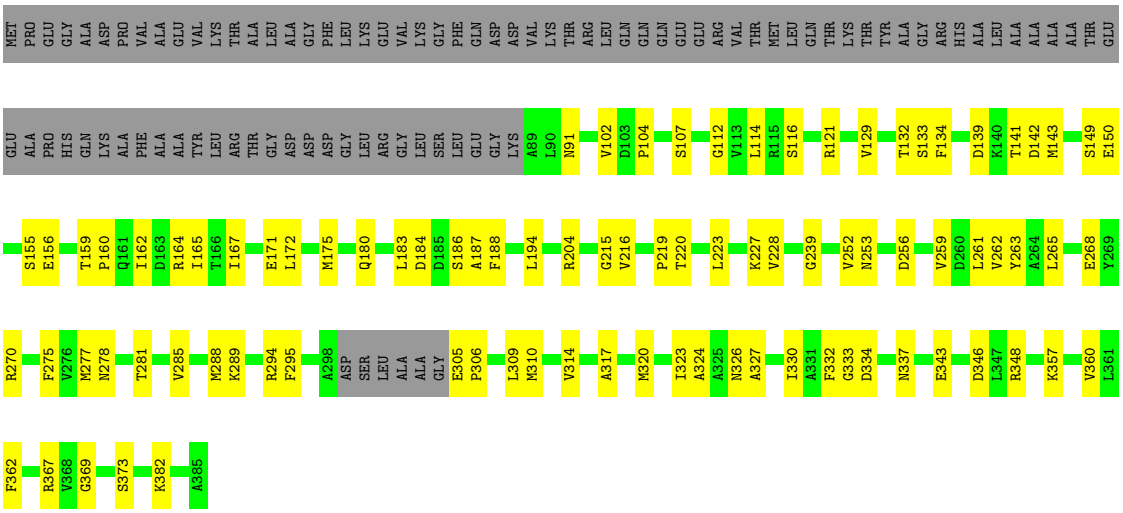
• Molecule 1: Phage major capsid protein, HK97 family

Chain K4:



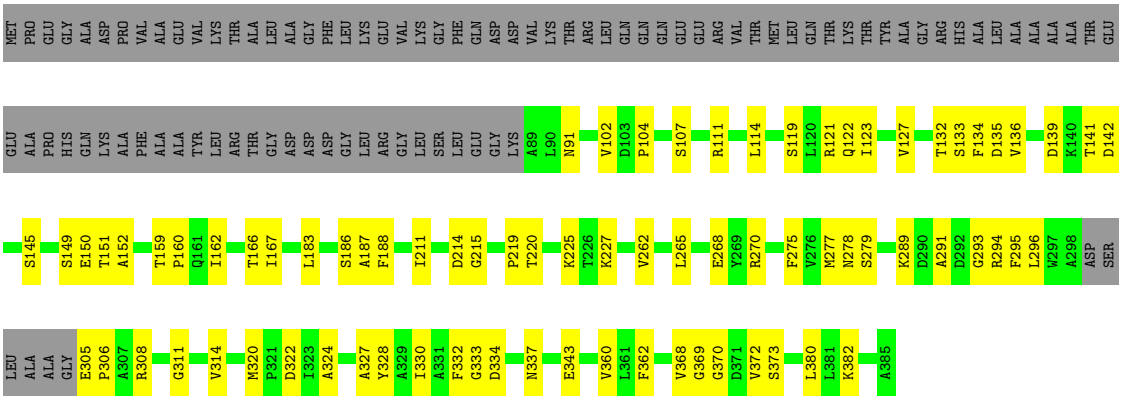
• Molecule 1: Phage major capsid protein, HK97 family

Chain J4:



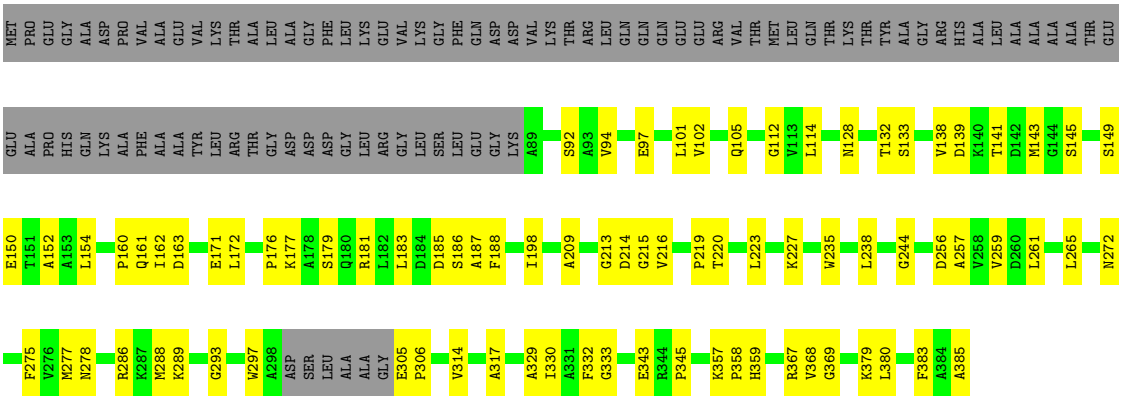
• Molecule 1: Phage major capsid protein, HK97 family

Chain V4:



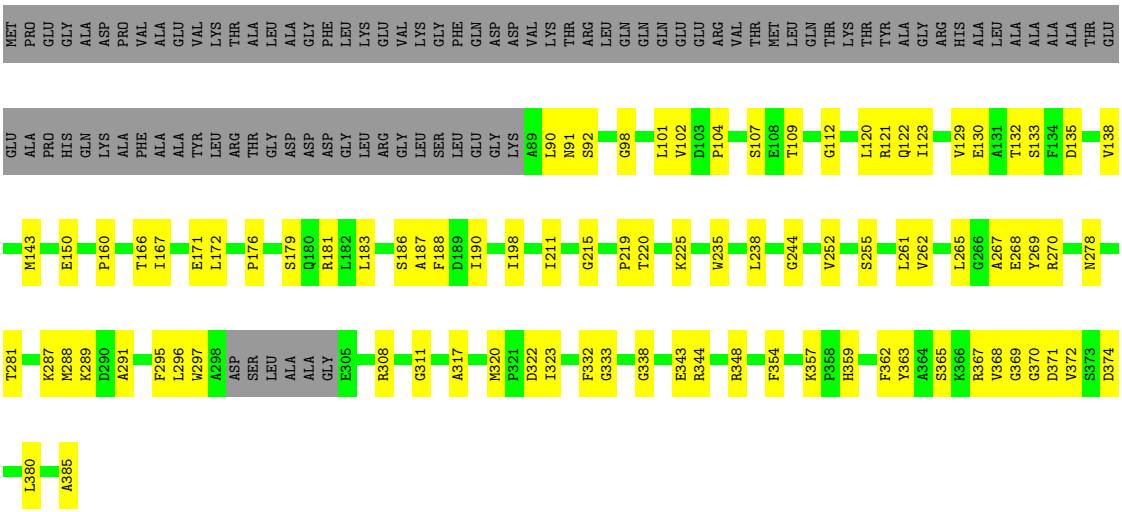
• Molecule 1: Phage major capsid protein, HK97 family

Chain L4:



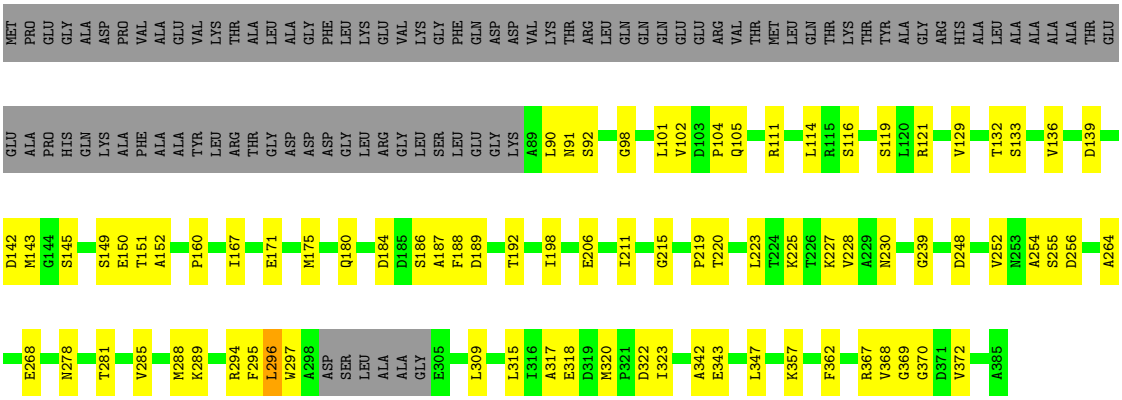
• Molecule 1: Phage major capsid protein, HK97 family

Chain H4:



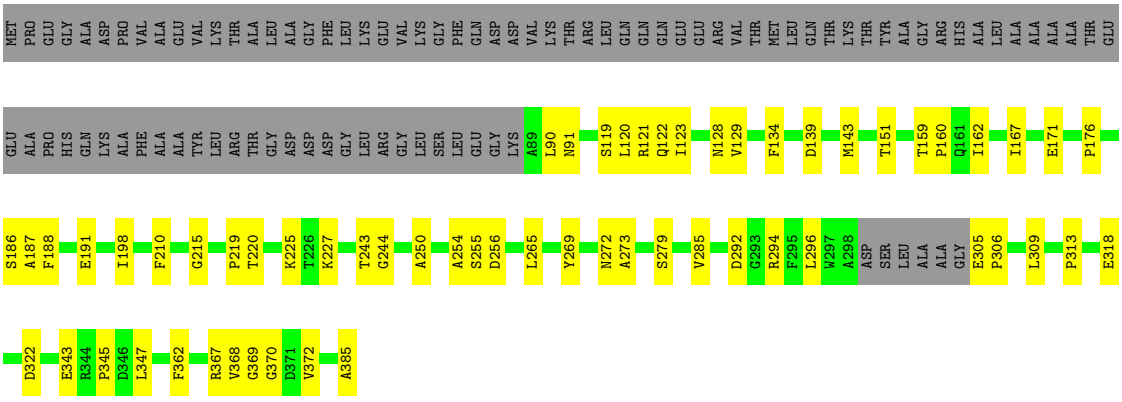
• Molecule 1: Phage major capsid protein, HK97 family

Chain I4:



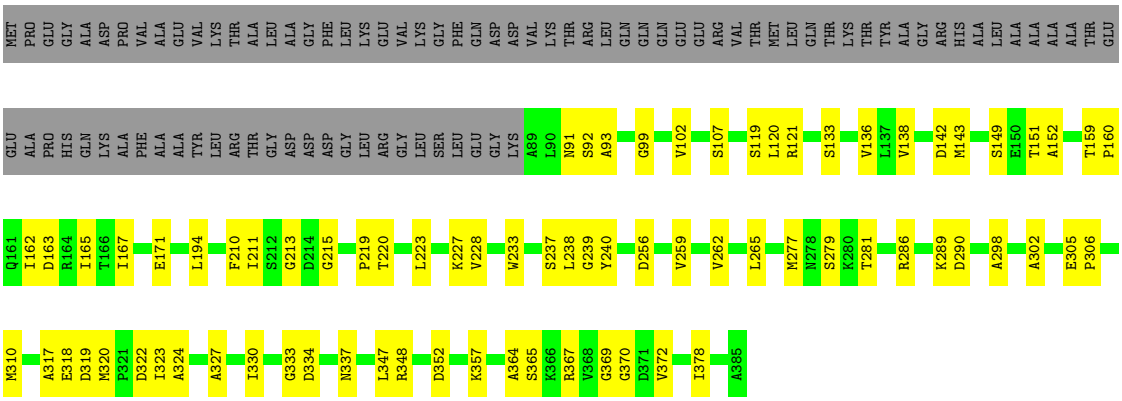
• Molecule 1: Phage major capsid protein, HK97 family

Chain A4:



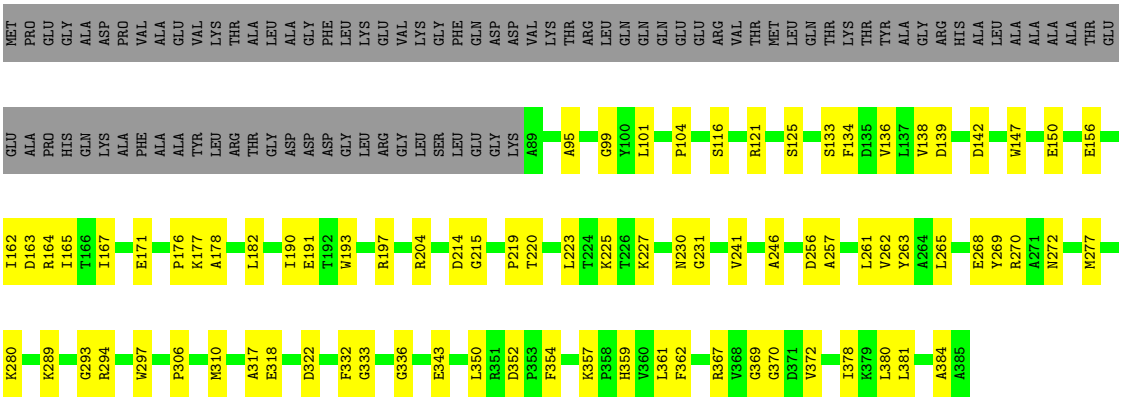
• Molecule 1: Phage major capsid protein, HK97 family

Chain D4:



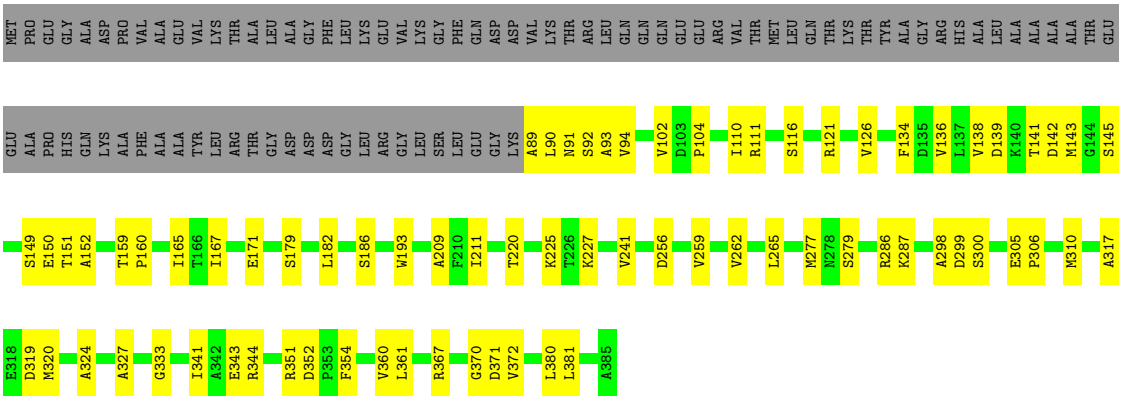
• Molecule 1: Phage major capsid protein, HK97 family

Chain E4:



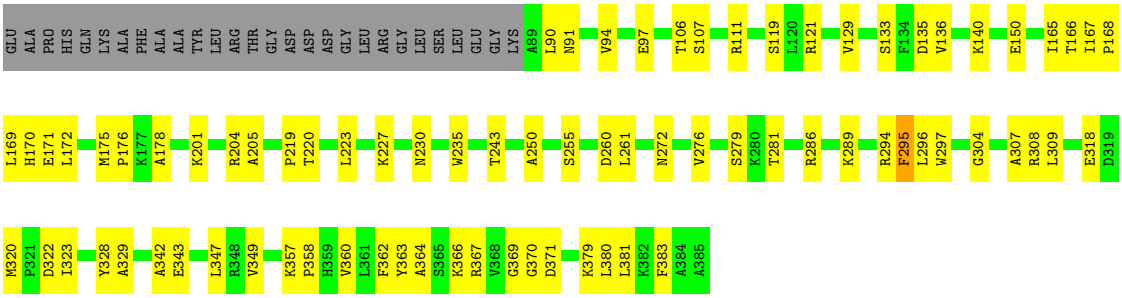
• Molecule 1: Phage major capsid protein, HK97 family

Chain F4:



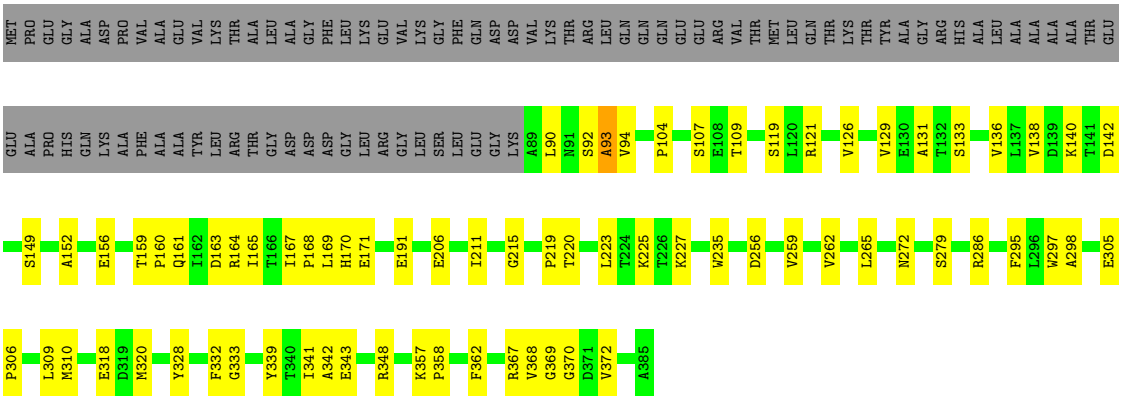
• Molecule 1: Phage major capsid protein, HK97 family

Chain G4:



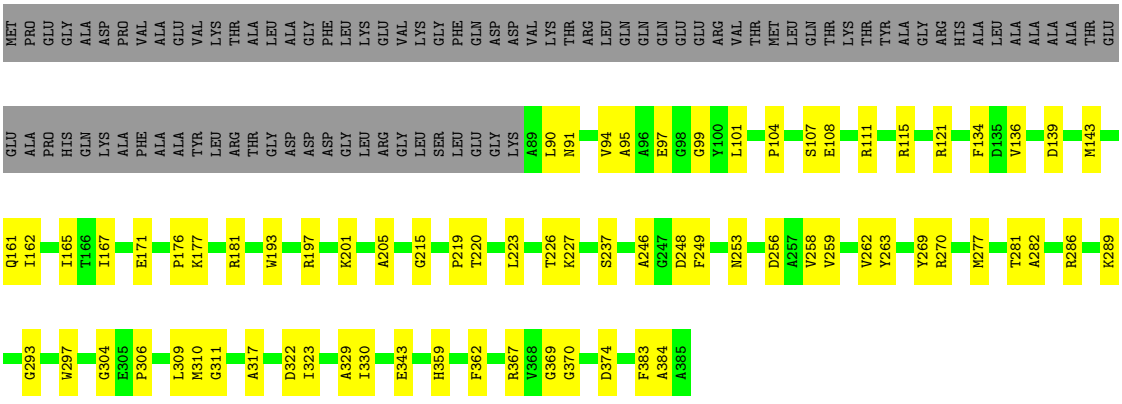
• Molecule 1: Phage major capsid protein, HK97 family

Chain B4:



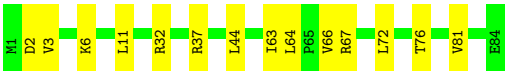
• Molecule 1: Phage major capsid protein, HK97 family

Chain C4:



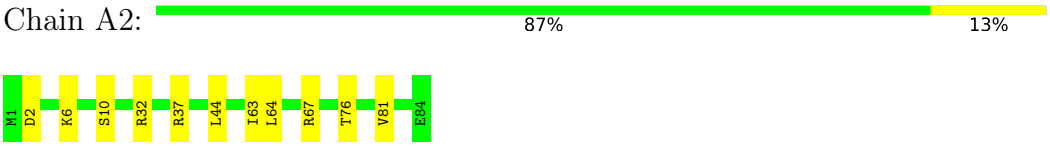
• Molecule 2: Uncharacterized protein

Chain D2:



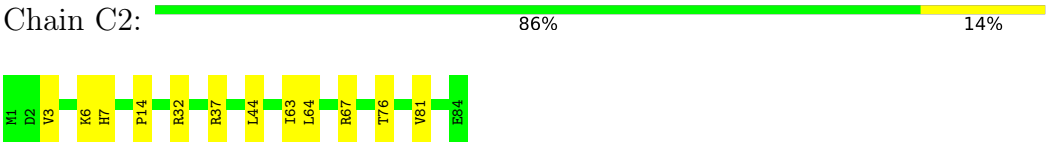
• Molecule 2: Uncharacterized protein

Chain A2:



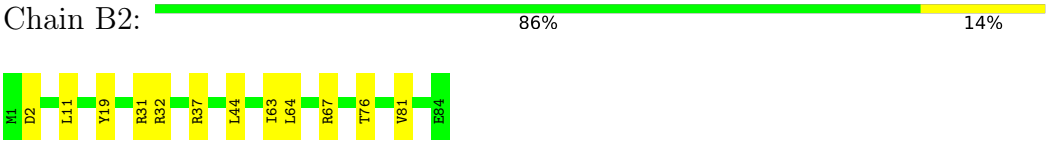
• Molecule 2: Uncharacterized protein

Chain C2:



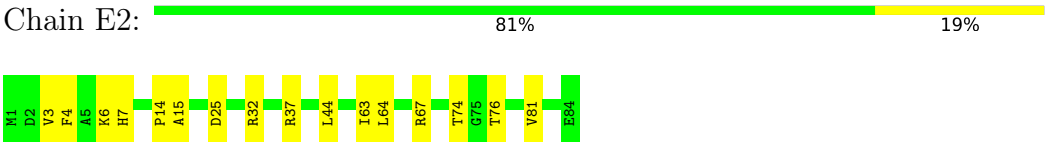
• Molecule 2: Uncharacterized protein

Chain B2:



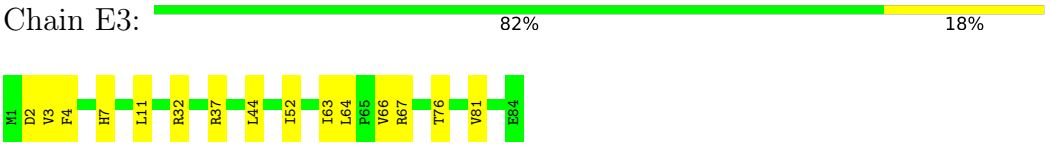
• Molecule 2: Uncharacterized protein

Chain E2:



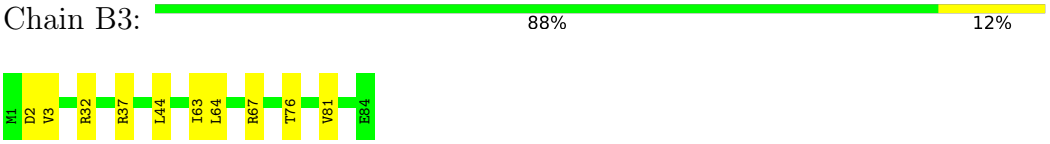
• Molecule 2: Uncharacterized protein

Chain E3:



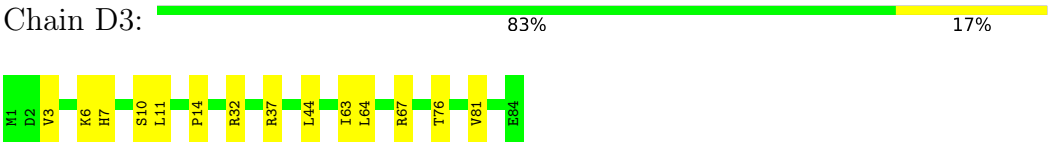
• Molecule 2: Uncharacterized protein

Chain B3:



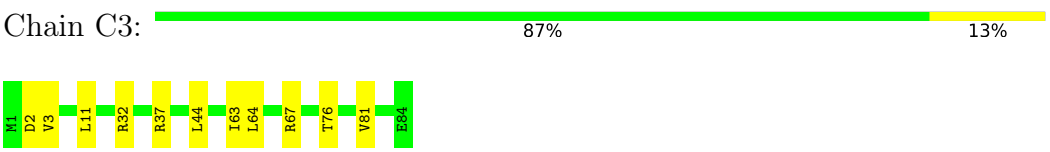
• Molecule 2: Uncharacterized protein

Chain D3:



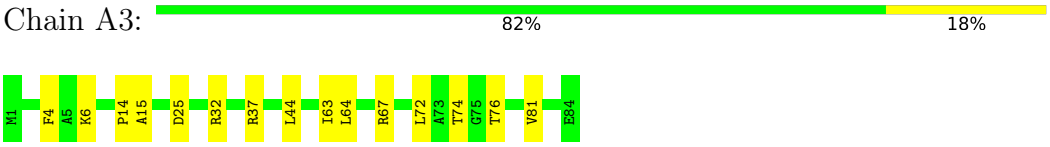
• Molecule 2: Uncharacterized protein

Chain C3:



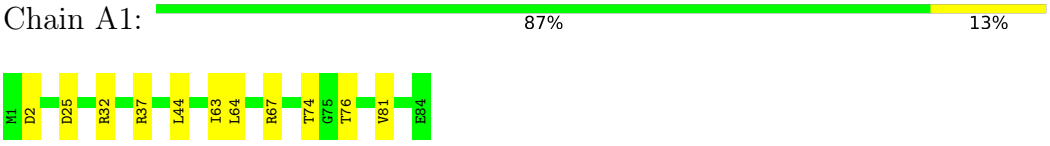
• Molecule 2: Uncharacterized protein

Chain A3:



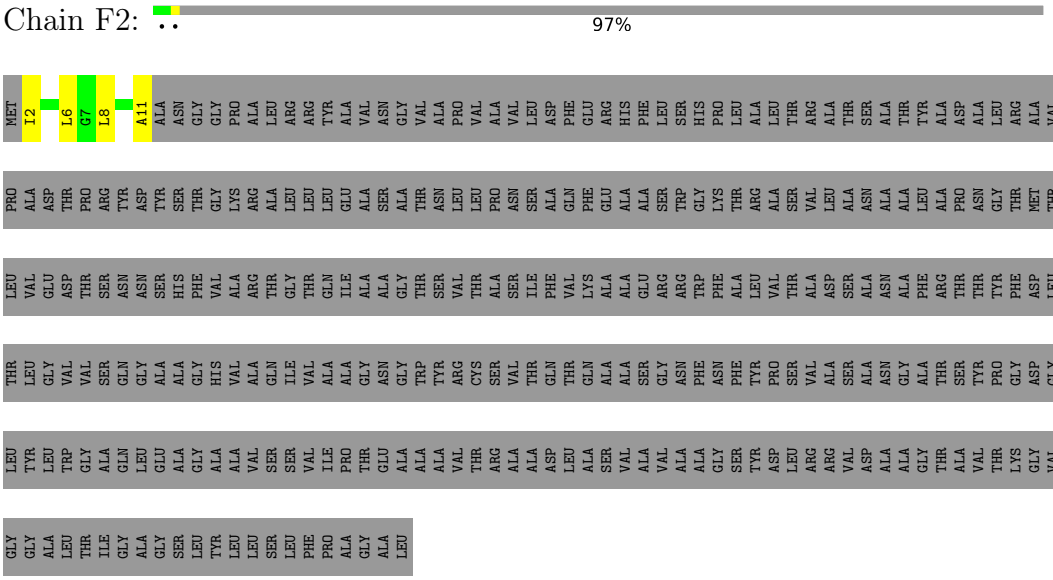
• Molecule 2: Uncharacterized protein

Chain A1:



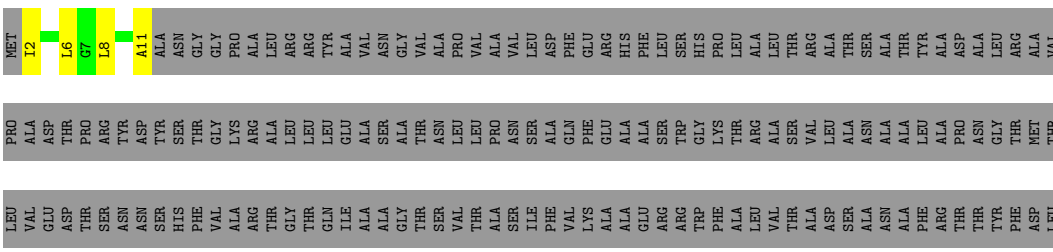
• Molecule 3: Uncharacterized protein

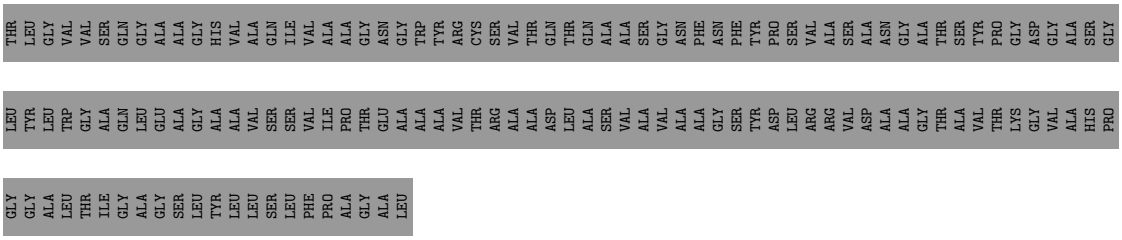
Chain F2:



• Molecule 3: Uncharacterized protein

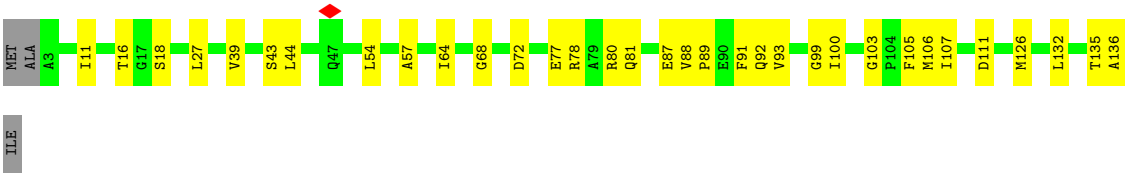
Chain F3:





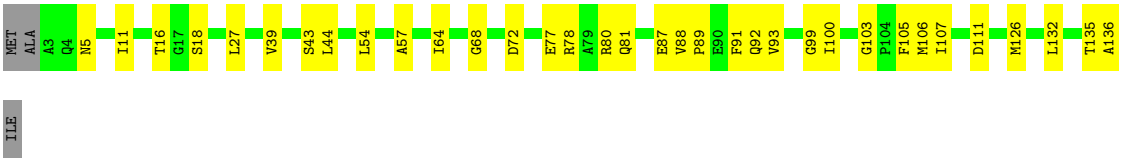
• Molecule 4: Tail tube protein Rcc01691

Chain H:



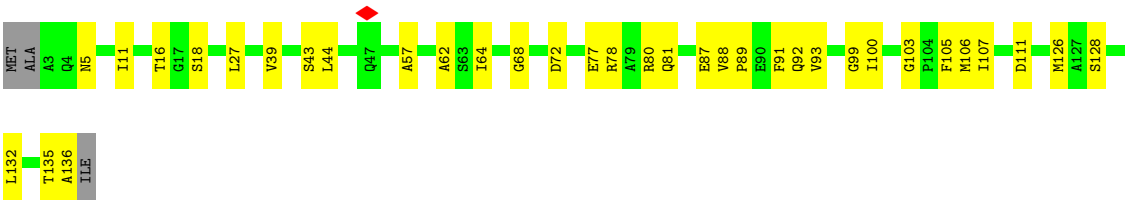
• Molecule 4: Tail tube protein Rcc01691

Chain I:



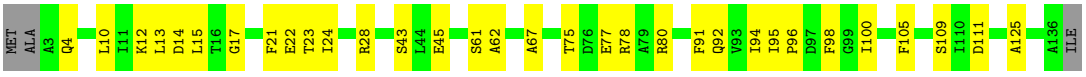
• Molecule 4: Tail tube protein Rcc01691

Chain J:



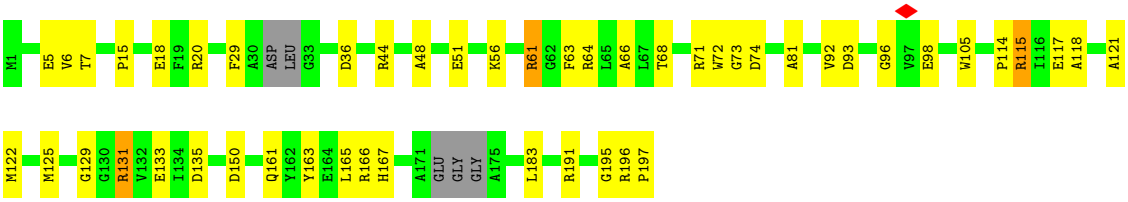
• Molecule 4: Tail tube protein Rcc01691

Chain G:



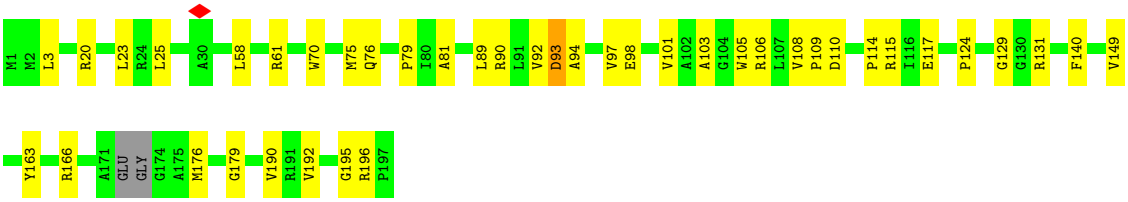
• Molecule 5: Adaptor protein Rcc01688

Chain C:



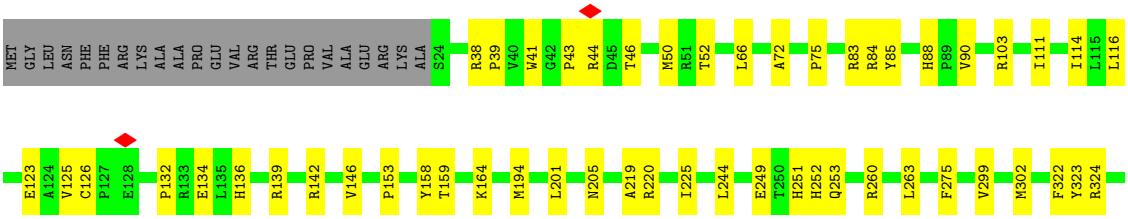
• Molecule 5: Adaptor protein Rcc01688

Chain D:



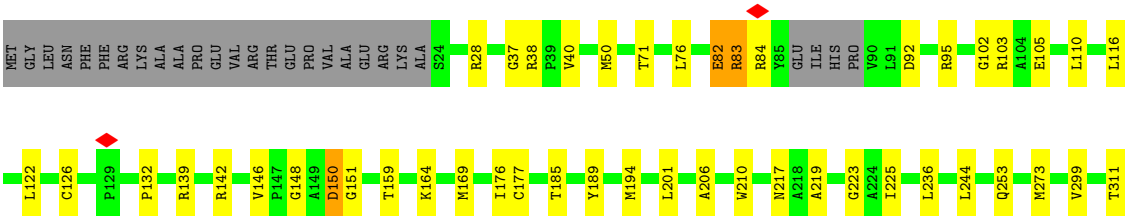
• Molecule 6: Portal protein Rcc01684

Chain A:



• Molecule 6: Portal protein Rcc01684

Chain B:

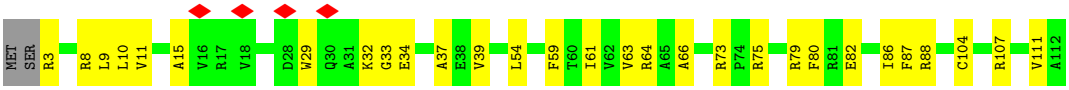


• Molecule 7: Tail terminator protein Rcc01690

Chain F:

• Molecule 8: Stopper protein Rcc01689

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	6277	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42.75	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	1530.72, 1530.72, 1530.72	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.252, 4.252, 4.252	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	A4	0.47	0/2216	0.59	0/3012
1	A5	0.41	0/2227	0.55	0/3027
1	B4	0.48	0/2253	0.56	0/3064
1	B5	0.45	0/2053	0.62	0/2789
1	C4	0.46	0/2253	0.53	0/3064
1	C5	0.45	0/2253	0.54	0/3064
1	D4	0.45	0/2253	0.53	0/3064
1	E4	0.45	0/2253	0.52	0/3064
1	F4	0.46	0/2253	0.54	0/3064
1	G4	0.47	0/2253	0.58	0/3064
1	H4	0.44	0/2216	0.52	0/3012
1	I4	0.45	0/2216	0.59	1/3012 (0.0%)
1	J4	0.43	0/2216	0.52	0/3012
1	K4	0.43	0/2216	0.53	0/3012
1	L4	0.43	0/2216	0.52	0/3012
1	M4	0.44	0/2253	0.54	0/3064
1	N4	0.44	0/2253	0.55	0/3064
1	O4	0.43	0/2253	0.53	0/3064
1	P4	0.45	0/2253	0.53	0/3064
1	Q4	0.45	0/2253	0.53	0/3064
1	R4	0.44	0/2253	0.55	0/3064
1	S4	0.42	0/2216	0.53	0/3012
1	T4	0.45	0/2216	0.52	0/3012
1	U4	0.44	0/2216	0.58	1/3012 (0.0%)
1	V4	0.42	0/2216	0.53	0/3012
1	W4	0.43	0/2216	0.53	0/3012
1	X4	0.44	0/2253	0.53	0/3064
1	Y4	0.44	0/2253	0.53	0/3064
1	Z4	0.43	0/2253	0.59	0/3064
2	A1	0.43	0/652	0.68	1/892 (0.1%)
2	A2	0.43	0/652	0.68	1/892 (0.1%)
2	A3	0.43	0/652	0.68	1/892 (0.1%)
2	B2	0.43	0/652	0.68	1/892 (0.1%)
2	B3	0.43	0/652	0.68	1/892 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	C2	0.43	0/652	0.68	1/892 (0.1%)
2	C3	0.43	0/652	0.68	1/892 (0.1%)
2	D2	0.43	0/652	0.68	1/892 (0.1%)
2	D3	0.43	0/652	0.68	1/892 (0.1%)
2	E2	0.43	0/652	0.68	1/892 (0.1%)
2	E3	0.43	0/652	0.68	1/892 (0.1%)
3	F2	0.40	0/61	1.46	2/81 (2.5%)
3	F3	0.40	0/61	1.46	2/81 (2.5%)
4	G	0.37	0/1009	0.65	0/1363
4	H	0.52	0/1009	0.71	0/1363
4	I	0.52	0/1009	0.72	0/1363
4	J	0.52	0/1009	0.72	0/1363
5	C	0.42	0/1471	0.71	1/2003 (0.0%)
5	D	0.45	1/1492 (0.1%)	0.74	1/2033 (0.0%)
6	A	0.41	0/2889	0.63	2/3934 (0.1%)
6	B	0.41	0/2852	0.64	3/3881 (0.1%)
7	F	0.43	0/982	0.69	0/1337
8	E	0.45	0/875	0.61	0/1182
All	All	0.44	1/86595 (0.0%)	0.58	24/117768 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	109	PRO	N-CD	5.26	1.55	1.47

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F2	8	LEU	CA-CB-CG	6.74	130.80	115.30
3	F3	8	LEU	CA-CB-CG	6.72	130.76	115.30
1	I4	296	LEU	CA-CB-CG	6.57	130.41	115.30
6	B	219	ALA	C-N-CA	-6.24	106.11	121.70
6	B	356	LEU	CA-CB-CG	6.07	129.27	115.30

There are no chirality outliers.

There are no planarity outliers.

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	A4	2173	0	2142	38	0
1	A5	2184	0	2152	85	0
1	B4	2209	0	2176	51	0
1	B5	2012	0	1990	107	0
1	C4	2209	0	2176	51	0
1	C5	2209	0	2176	44	0
1	D4	2209	0	2176	58	0
1	E4	2209	0	2176	64	0
1	F4	2209	0	2176	60	0
1	G4	2209	0	2176	52	0
1	H4	2173	0	2142	72	0
1	I4	2173	0	2142	69	0
1	J4	2173	0	2142	70	0
1	K4	2173	0	2142	66	0
1	L4	2173	0	2142	64	0
1	M4	2209	0	2176	63	0
1	N4	2209	0	2176	64	0
1	O4	2209	0	2176	66	0
1	P4	2209	0	2176	73	0
1	Q4	2209	0	2176	75	0
1	R4	2209	0	2176	67	0
1	S4	2173	0	2142	65	0
1	T4	2173	0	2142	82	0
1	U4	2173	0	2142	65	0
1	V4	2173	0	2142	68	0
1	W4	2173	0	2142	78	0
1	X4	2209	0	2176	60	0
1	Y4	2209	0	2176	58	0
1	Z4	2209	0	2176	61	0
2	A1	640	0	653	8	0
2	A2	640	0	653	11	0
2	A3	640	0	653	13	0
2	B2	640	0	653	9	0
2	B3	640	0	653	9	0
2	C2	640	0	653	14	0
2	C3	640	0	653	9	0
2	D2	640	0	653	15	0
2	D3	640	0	653	14	0
2	E2	640	0	653	15	0
2	E3	640	0	653	15	0
3	F2	62	0	73	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F3	62	0	73	1	0
4	G	993	0	957	22	0
4	H	993	0	957	19	0
4	I	993	0	957	20	0
4	J	993	0	957	20	0
5	C	1440	0	1472	71	0
5	D	1460	0	1493	45	0
6	A	2815	0	2788	46	0
6	B	2781	0	2756	50	0
7	F	968	0	987	30	0
8	E	859	0	861	18	0
All	All	84902	0	84034	1939	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 11.

The worst 5 of 1939 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)
1:B5:358:PRO:HG3	5:C:73:GLY:CA	1.56	1.35
1:B5:358:PRO:CG	5:C:73:GLY:N	1.91	1.32
1:B5:358:PRO:CG	5:C:73:GLY:H	1.44	1.30
1:B5:358:PRO:HG3	5:C:73:GLY:N	0.96	1.28
1:B5:358:PRO:CG	5:C:73:GLY:CA	2.19	1.18

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	A4	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	41 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A5	290/385 (75%)	259 (89%)	29 (10%)	2 (1%)	22	63
1	B4	295/385 (77%)	260 (88%)	34 (12%)	1 (0%)	41	77
1	B5	266/385 (69%)	227 (85%)	38 (14%)	1 (0%)	34	72
1	C4	295/385 (77%)	262 (89%)	33 (11%)	0	100	100
1	C5	295/385 (77%)	265 (90%)	30 (10%)	0	100	100
1	D4	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	41	77
1	E4	295/385 (77%)	267 (90%)	28 (10%)	0	100	100
1	F4	295/385 (77%)	265 (90%)	30 (10%)	0	100	100
1	G4	295/385 (77%)	259 (88%)	35 (12%)	1 (0%)	41	77
1	H4	287/385 (74%)	254 (88%)	32 (11%)	1 (0%)	41	77
1	I4	287/385 (74%)	261 (91%)	25 (9%)	1 (0%)	41	77
1	J4	287/385 (74%)	249 (87%)	37 (13%)	1 (0%)	41	77
1	K4	287/385 (74%)	257 (90%)	29 (10%)	1 (0%)	41	77
1	L4	287/385 (74%)	256 (89%)	30 (10%)	1 (0%)	41	77
1	M4	295/385 (77%)	257 (87%)	38 (13%)	0	100	100
1	N4	295/385 (77%)	259 (88%)	35 (12%)	1 (0%)	41	77
1	O4	295/385 (77%)	256 (87%)	38 (13%)	1 (0%)	41	77
1	P4	295/385 (77%)	249 (84%)	45 (15%)	1 (0%)	41	77
1	Q4	295/385 (77%)	259 (88%)	35 (12%)	1 (0%)	41	77
1	R4	295/385 (77%)	254 (86%)	40 (14%)	1 (0%)	41	77
1	S4	287/385 (74%)	253 (88%)	33 (12%)	1 (0%)	41	77
1	T4	287/385 (74%)	261 (91%)	26 (9%)	0	100	100
1	U4	287/385 (74%)	257 (90%)	29 (10%)	1 (0%)	41	77
1	V4	287/385 (74%)	256 (89%)	30 (10%)	1 (0%)	41	77
1	W4	287/385 (74%)	253 (88%)	33 (12%)	1 (0%)	41	77
1	X4	295/385 (77%)	265 (90%)	30 (10%)	0	100	100
1	Y4	295/385 (77%)	265 (90%)	30 (10%)	0	100	100
1	Z4	295/385 (77%)	257 (87%)	38 (13%)	0	100	100
2	A1	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	A2	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	A3	82/84 (98%)	76 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B2	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	B3	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	C2	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	C3	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	D2	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	D3	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	E2	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	E3	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
3	F2	8/325 (2%)	5 (62%)	3 (38%)	0	100	100
3	F3	8/325 (2%)	5 (62%)	3 (38%)	0	100	100
4	G	132/137 (96%)	116 (88%)	16 (12%)	0	100	100
4	H	132/137 (96%)	118 (89%)	14 (11%)	0	100	100
4	I	132/137 (96%)	118 (89%)	14 (11%)	0	100	100
4	J	132/137 (96%)	118 (89%)	14 (11%)	0	100	100
5	C	186/197 (94%)	158 (85%)	27 (14%)	1 (0%)	29	69
5	D	191/197 (97%)	161 (84%)	30 (16%)	0	100	100
6	A	368/396 (93%)	330 (90%)	37 (10%)	1 (0%)	41	77
6	B	362/396 (91%)	325 (90%)	37 (10%)	0	100	100
7	F	132/135 (98%)	115 (87%)	17 (13%)	0	100	100
8	E	108/112 (96%)	97 (90%)	11 (10%)	0	100	100
All	All	11226/14720 (76%)	9966 (89%)	1237 (11%)	23 (0%)	50	81

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P4	306	PRO
1	J4	187	ALA
1	V4	187	ALA
1	L4	187	ALA
1	A5	132	THR

5.3.2 Protein sidechains (i)

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	A4	215/284 (76%)	214 (100%)	1 (0%)	88 93
1	A5	215/284 (76%)	214 (100%)	1 (0%)	88 93
1	B4	218/284 (77%)	217 (100%)	1 (0%)	88 93
1	B5	197/284 (69%)	196 (100%)	1 (0%)	88 93
1	C4	218/284 (77%)	217 (100%)	1 (0%)	88 93
1	C5	218/284 (77%)	217 (100%)	1 (0%)	88 93
1	D4	218/284 (77%)	218 (100%)	0	100 100
1	E4	218/284 (77%)	218 (100%)	0	100 100
1	F4	218/284 (77%)	218 (100%)	0	100 100
1	G4	218/284 (77%)	217 (100%)	1 (0%)	88 93
1	H4	215/284 (76%)	215 (100%)	0	100 100
1	I4	215/284 (76%)	215 (100%)	0	100 100
1	J4	215/284 (76%)	215 (100%)	0	100 100
1	K4	215/284 (76%)	215 (100%)	0	100 100
1	L4	215/284 (76%)	214 (100%)	1 (0%)	88 93
1	M4	218/284 (77%)	217 (100%)	1 (0%)	88 93
1	N4	218/284 (77%)	216 (99%)	2 (1%)	78 87
1	O4	218/284 (77%)	216 (99%)	2 (1%)	78 87
1	P4	218/284 (77%)	217 (100%)	1 (0%)	88 93
1	Q4	218/284 (77%)	217 (100%)	1 (0%)	88 93
1	R4	218/284 (77%)	216 (99%)	2 (1%)	78 87
1	S4	215/284 (76%)	215 (100%)	0	100 100
1	T4	215/284 (76%)	214 (100%)	1 (0%)	88 93
1	U4	215/284 (76%)	213 (99%)	2 (1%)	78 87
1	V4	215/284 (76%)	215 (100%)	0	100 100
1	W4	215/284 (76%)	214 (100%)	1 (0%)	88 93
1	X4	218/284 (77%)	218 (100%)	0	100 100
1	Y4	218/284 (77%)	217 (100%)	1 (0%)	88 93
1	Z4	218/284 (77%)	218 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A1	69/69 (100%)	69 (100%)	0	100	100
2	A2	69/69 (100%)	69 (100%)	0	100	100
2	A3	69/69 (100%)	69 (100%)	0	100	100
2	B2	69/69 (100%)	69 (100%)	0	100	100
2	B3	69/69 (100%)	69 (100%)	0	100	100
2	C2	69/69 (100%)	69 (100%)	0	100	100
2	C3	69/69 (100%)	69 (100%)	0	100	100
2	D2	69/69 (100%)	69 (100%)	0	100	100
2	D3	69/69 (100%)	69 (100%)	0	100	100
2	E2	69/69 (100%)	69 (100%)	0	100	100
2	E3	69/69 (100%)	69 (100%)	0	100	100
3	F2	5/224 (2%)	5 (100%)	0	100	100
3	F3	5/224 (2%)	5 (100%)	0	100	100
4	G	101/103 (98%)	101 (100%)	0	100	100
4	H	101/103 (98%)	101 (100%)	0	100	100
4	I	101/103 (98%)	101 (100%)	0	100	100
4	J	101/103 (98%)	101 (100%)	0	100	100
5	C	138/141 (98%)	133 (96%)	5 (4%)	35	59
5	D	140/141 (99%)	137 (98%)	3 (2%)	53	72
6	A	283/302 (94%)	279 (99%)	4 (1%)	67	80
6	B	279/302 (92%)	275 (99%)	4 (1%)	67	80
7	F	91/92 (99%)	87 (96%)	4 (4%)	28	53
8	E	83/85 (98%)	81 (98%)	2 (2%)	49	69
All	All	8452/10918 (77%)	8408 (100%)	44 (0%)	89	93

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	A	84	ARG
5	D	61	ARG
6	A	333	ARG
6	B	83	ARG
5	D	93	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	A2	7	HIS
2	E3	7	HIS
7	F	10	GLN
2	E2	7	HIS
2	D3	7	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

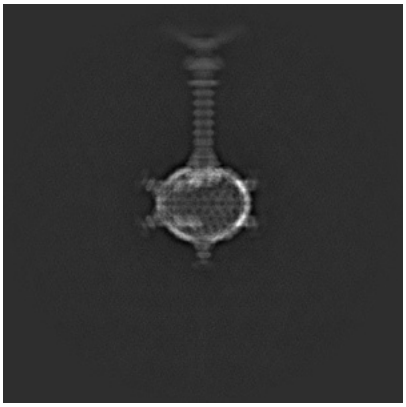
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10592. These allow visual inspection of the internal detail of the map and identification of artifacts.

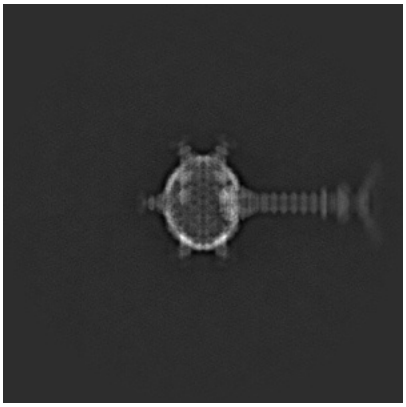
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

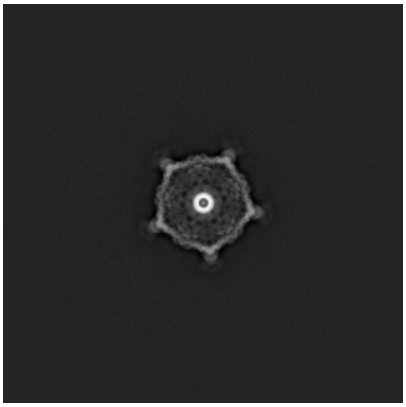
6.1.1 Primary map



X



Y

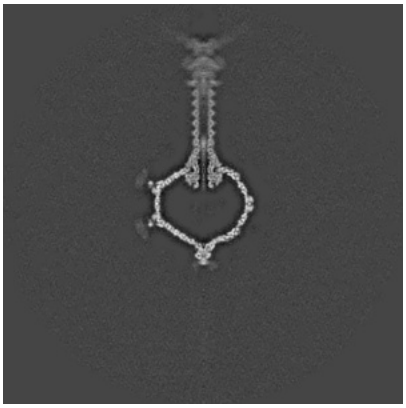


Z

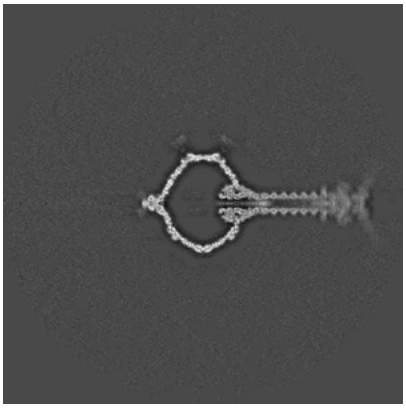
The images above show the map projected in three orthogonal directions.

6.2 Central slices

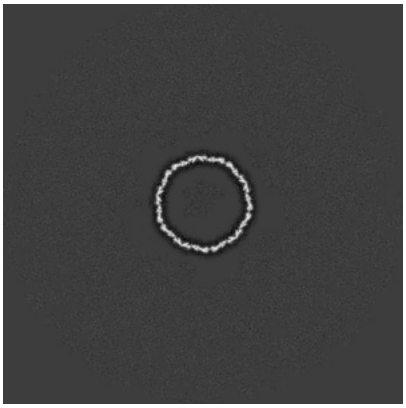
6.2.1 Primary map



X Index: 180



Y Index: 180

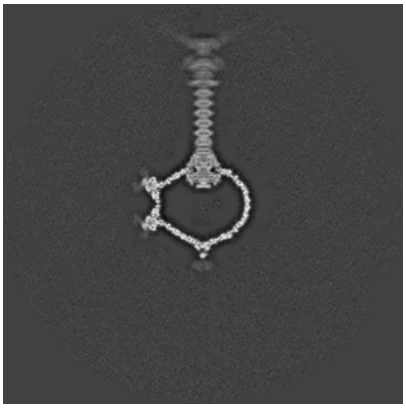


Z Index: 180

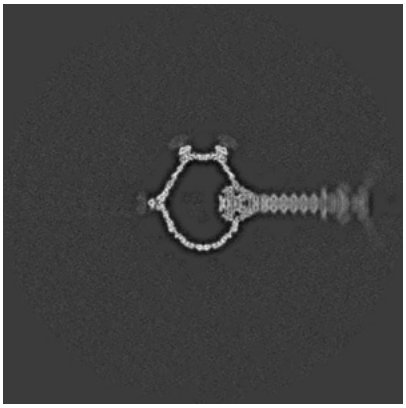
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

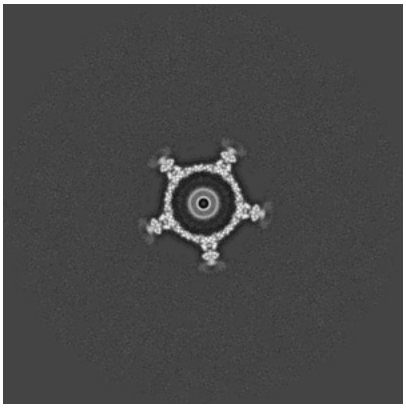
6.3.1 Primary map



X Index: 186



Y Index: 175

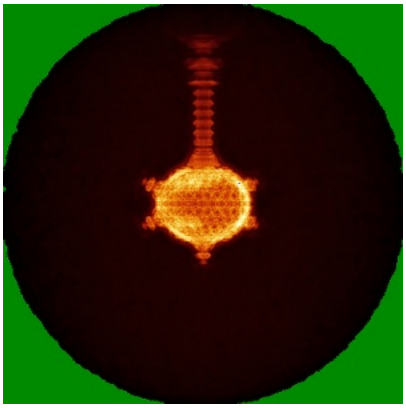


Z Index: 199

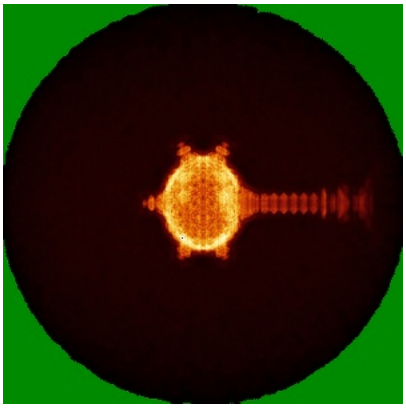
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

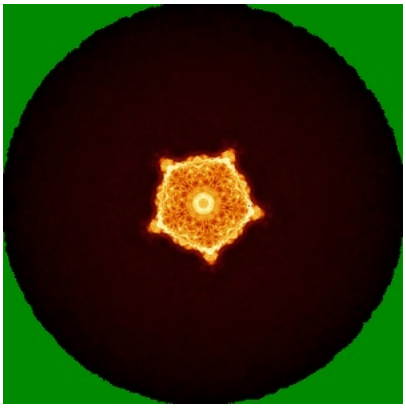
6.4.1 Primary map



X



Y

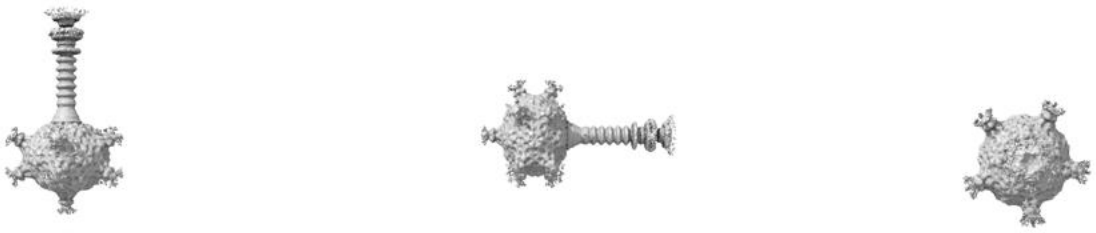


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

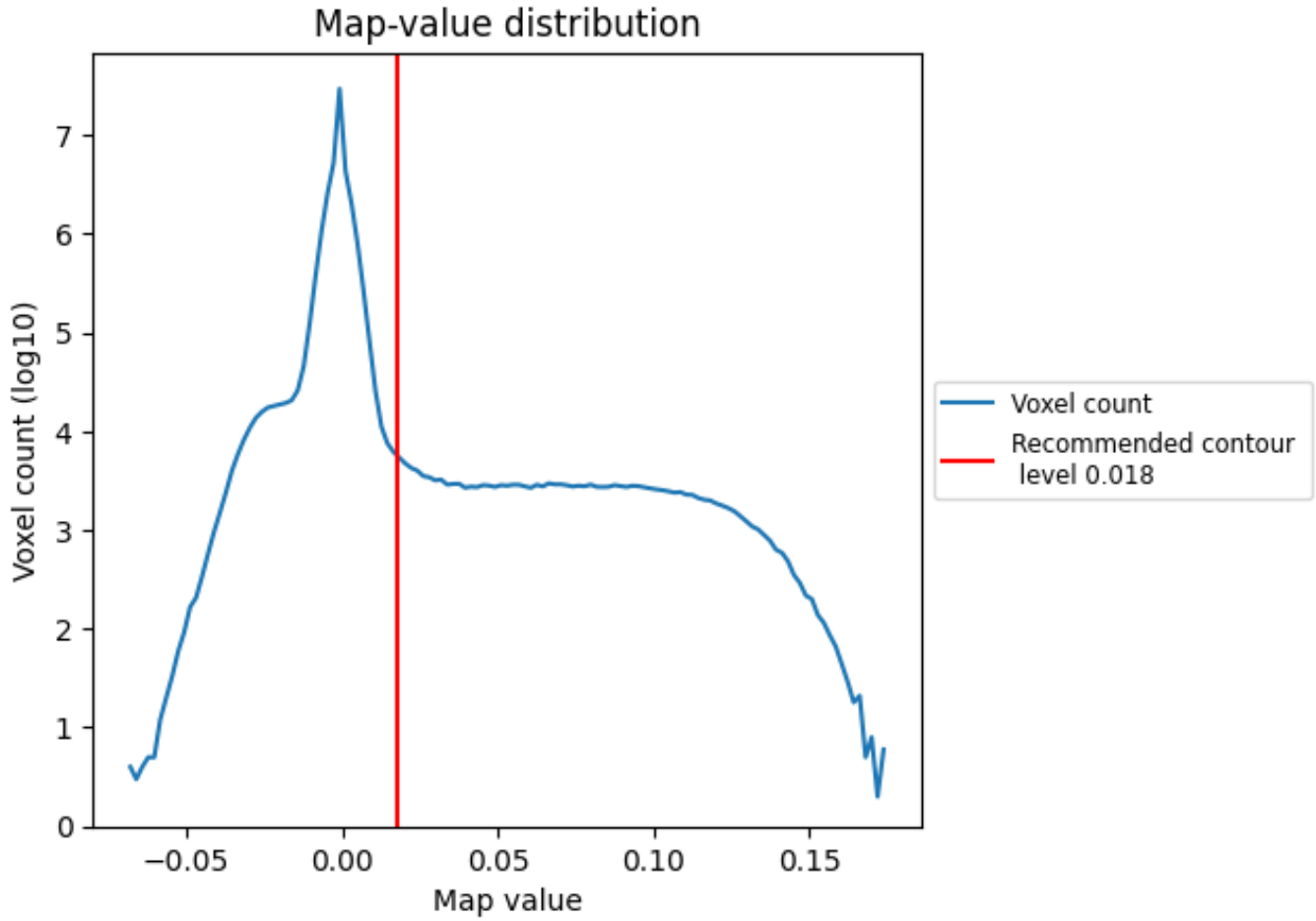
6.6 Mask visualisation (i)

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

7 Map analysis

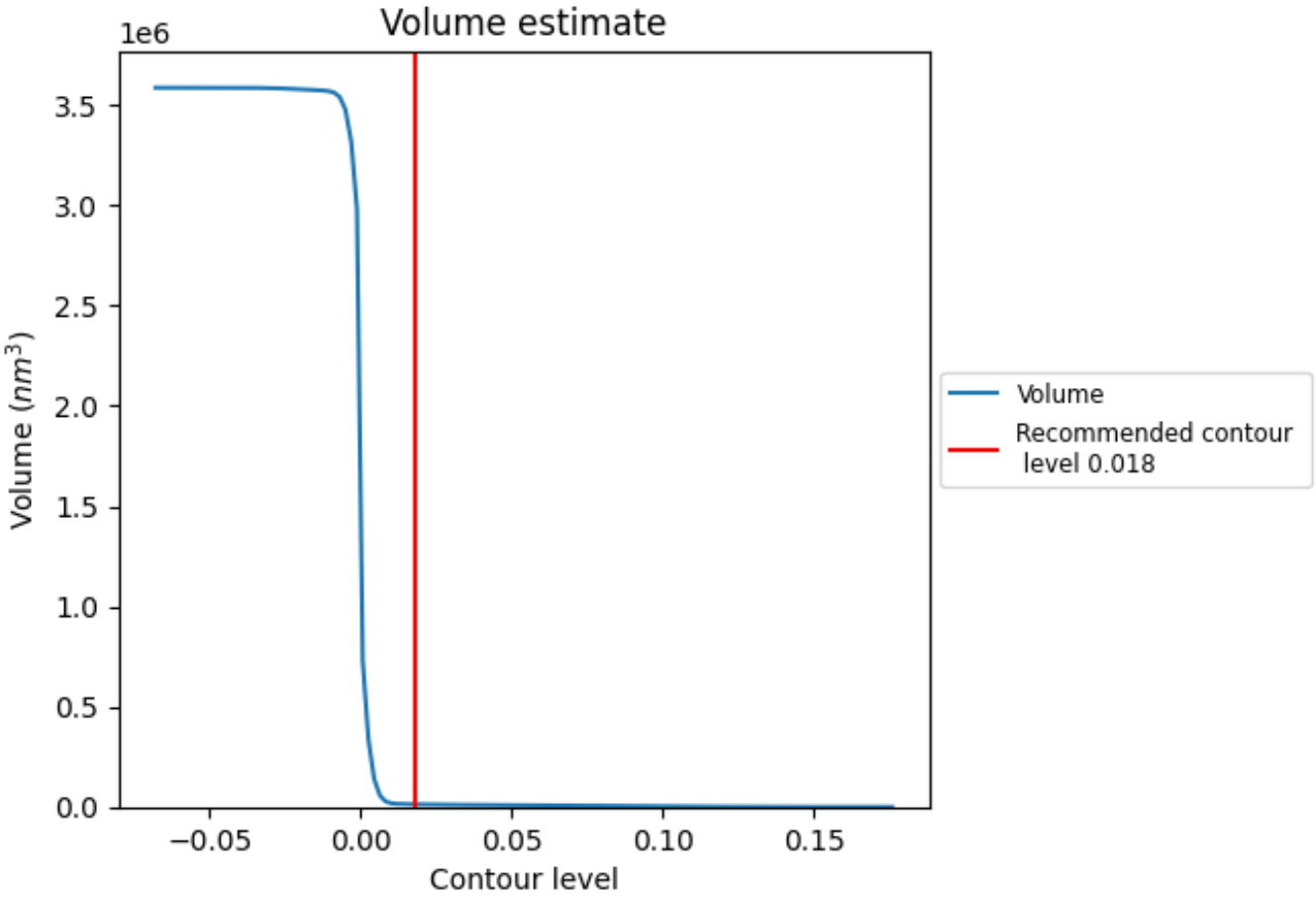
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

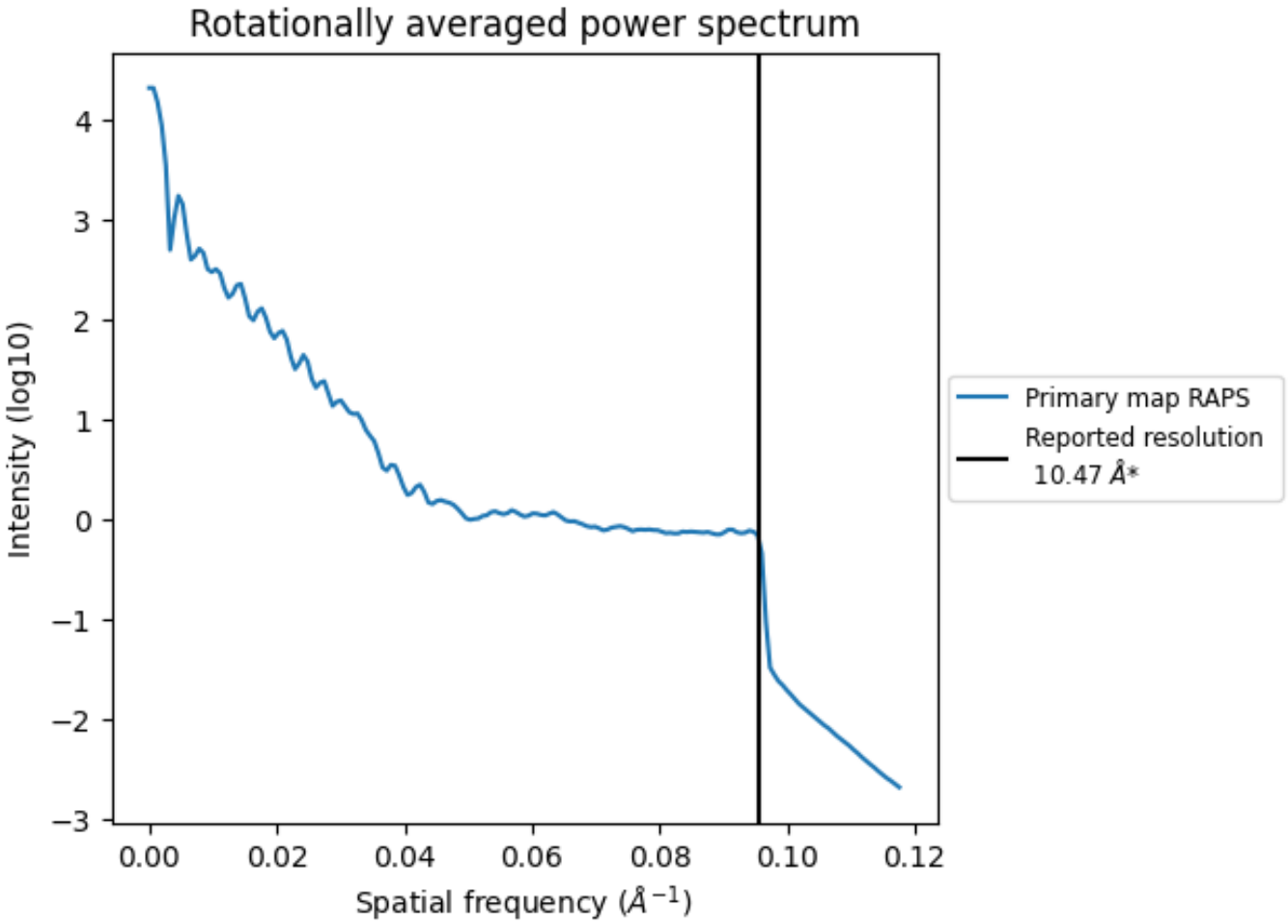
7.2 Volume estimate (i)



The volume at the recommended contour level is 13130 nm^3; this corresponds to an approximate mass of 11861 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)

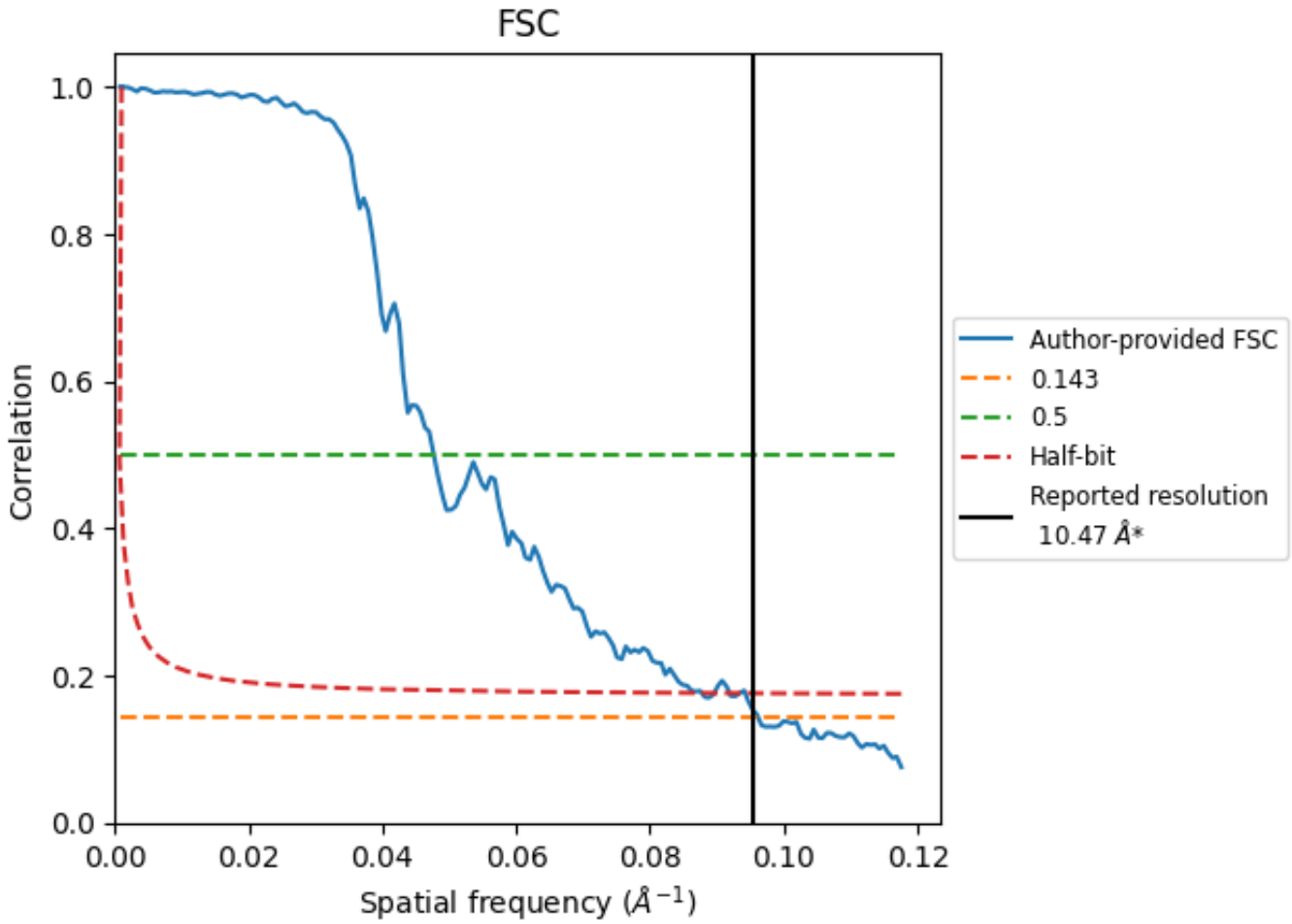


*Reported resolution corresponds to spatial frequency of 0.096 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.096 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.47	-	-
Author-provided FSC curve	10.40	20.96	11.39
Unmasked-calculated*	-	-	-

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

9 Map-model fit

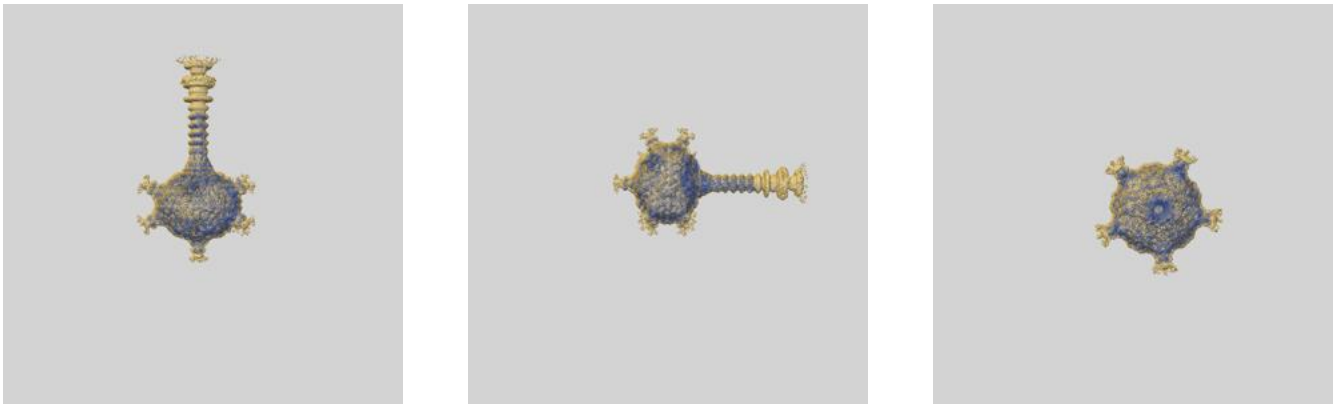
This section contains information regarding the fit between EMDB map EMD-10592 and PDB model 6TUI. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

9.1.1 Map-model overlay

X Y Z

9.1.2 Map-model assembly overlay



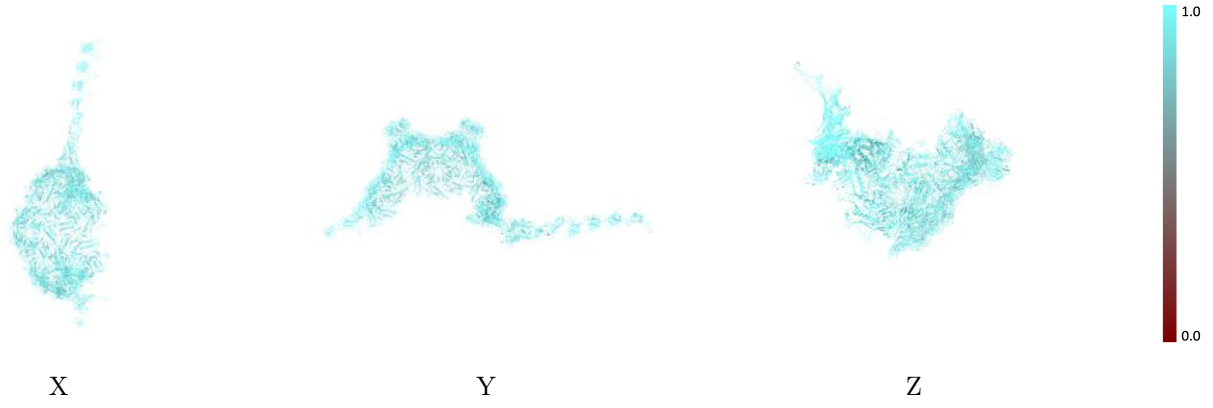
X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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

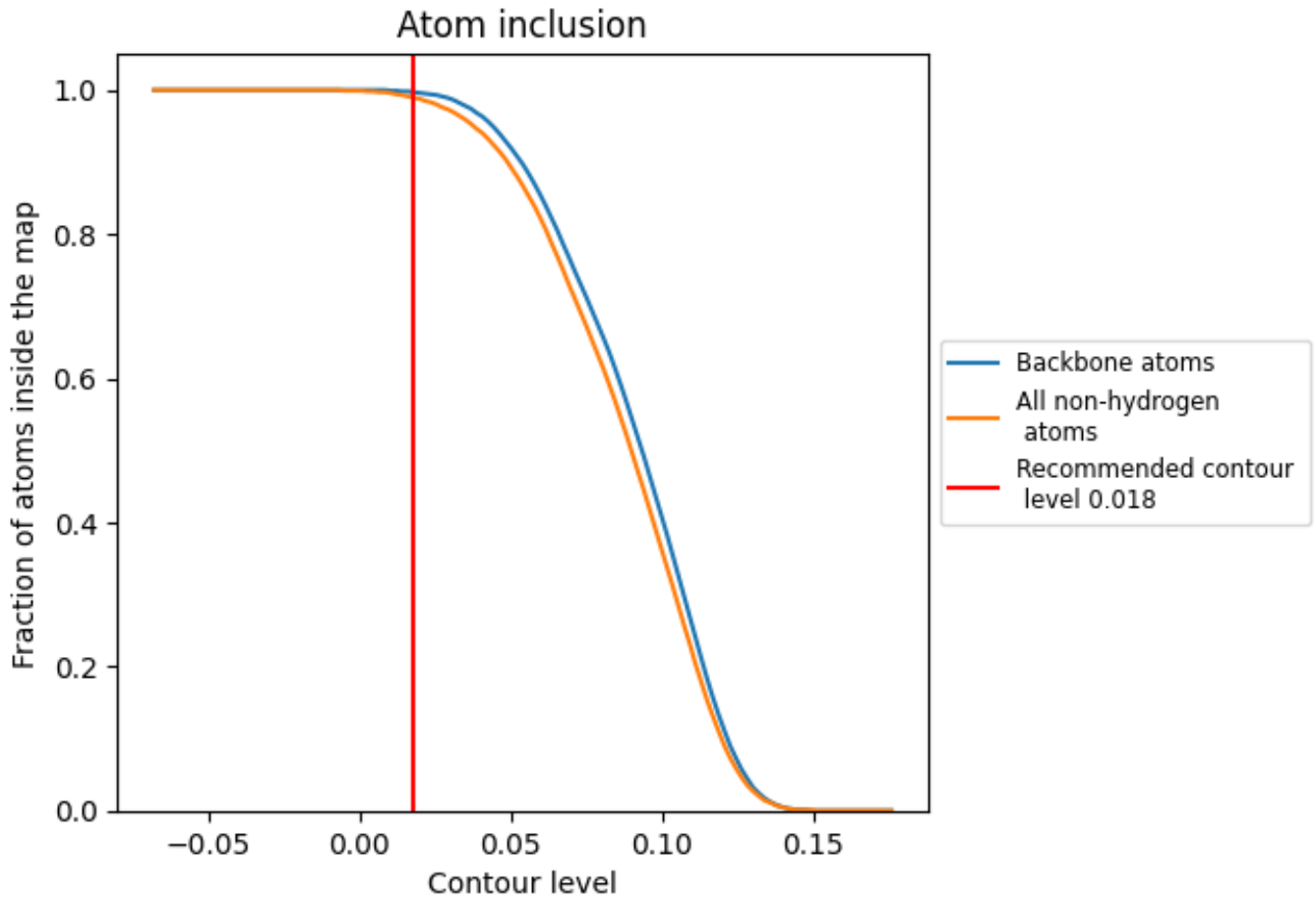
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9890	0.0800
A	0.9750	0.0660
A1	0.9980	0.0980
A2	1.0000	0.0930
A3	1.0000	0.0770
A4	0.9920	0.0930
A5	0.9900	0.0750
B	0.9810	0.0660
B2	1.0000	0.0890
B3	1.0000	0.0880
B4	0.9880	0.0800
B5	0.9750	0.0810
C	0.9820	0.0560
C2	1.0000	0.0930
C3	0.9940	0.0790
C4	0.9950	0.0860
C5	0.9890	0.0760
D	0.9790	0.0480
D2	0.9970	0.0820
D3	0.9970	0.0950
D4	0.9910	0.0820
E	0.9490	0.0500
E2	0.9980	0.0860
E3	0.9950	0.0770
E4	0.9910	0.0840
F	0.9820	0.0710
F2	1.0000	-0.0400
F3	1.0000	-0.0130
F4	0.9870	0.0850
G	0.9770	0.0770
G4	0.9900	0.0840
H	0.9840	0.0780
H4	0.9900	0.0800
I	0.9910	0.0780
I4	0.9930	0.0770

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Chain	Atom inclusion	Q-score
J	0.9890	0.0870
J4	0.9910	0.0820
K4	0.9910	0.0720
L4	0.9900	0.0830
M4	0.9870	0.0840
N4	0.9890	0.0850
O4	0.9930	0.0820
P4	0.9910	0.0870
Q4	0.9920	0.0830
R4	0.9910	0.0840
S4	0.9900	0.0800
T4	0.9950	0.0820
U4	0.9950	0.0780
V4	0.9950	0.0840
W4	0.9930	0.0780
X4	0.9890	0.0910
Y4	0.9890	0.0820
Z4	0.9900	0.0840