Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 01:32 PM JST

PDB ID	:	7EY7
EMDB ID	:	EMD-31321
Title	:	bacteriophage T7 tail complex
Authors	:	Liu, H.R.; Chen, W.Y.
Deposited on	:	2021-05-30
Resolution	:	4.30 Å(reported)

This is a Full wwPDB EM Validation 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:

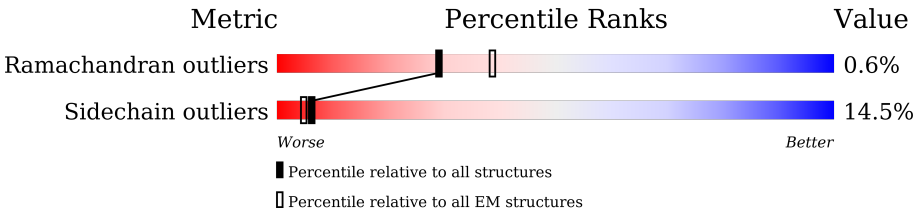
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	a	553	16% · 79%
1	b	553	17% · 79%
1	c	553	17% · 79%
1	d	553	17% · 79%
1	e	553	17% · 79%
1	f	553	17% · 79%
1	g	553	16% · 79%
1	h	553	17% · 79%
1	i	553	17% · 79%

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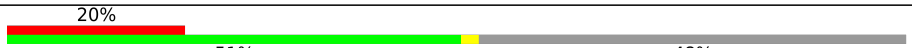
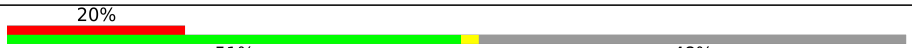
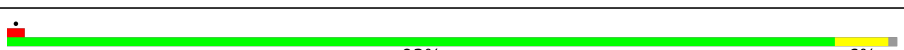
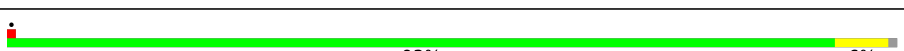
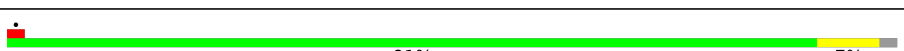
Mol	Chain	Length	Quality of chain
1	j	553	
1	k	553	
1	l	553	
1	m	553	
1	n	553	
1	o	553	
1	p	553	
1	q	553	
1	r	553	
2	s	794	
2	t	794	
2	u	794	
2	v	794	
2	w	794	
2	x	794	
3	A	196	
3	B	196	
3	C	196	
3	D	196	
3	E	196	
3	F	196	
4	M	196	
4	N	196	
4	O	196	
4	P	196	

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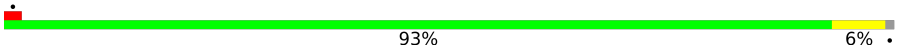
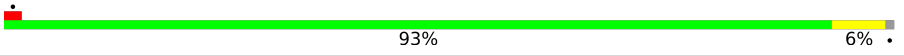
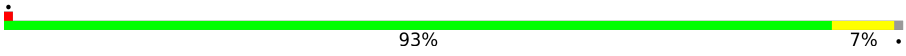
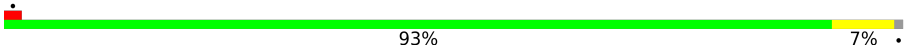
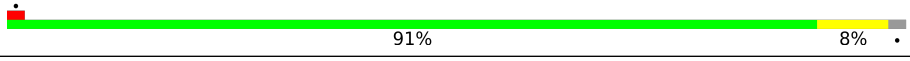
Mol	Chain	Length	Quality of chain
4	Q	196	
4	R	196	
4	S	196	
4	T	196	
4	U	196	
4	V	196	
4	W	196	
4	X	196	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 77574 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 fiber protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	b	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	c	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	d	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	e	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	f	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	g	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	h	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	i	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	j	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	k	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	l	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	m	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	n	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	o	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	p	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
1	q	115	Total	C	N	O	S	0	0
			922	584	160	177	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	r	115	Total	C	N	O	S	0	0
			922	584	160	177	1		

- Molecule 2 is a protein called Tail tubular protein gp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	s	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		
2	t	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		
2	u	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		
2	v	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		
2	w	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		
2	x	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		

- Molecule 3 is a protein called Internal virion protein gp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	102	Total	C	N	O	S	0	0
			787	475	146	160	6		
3	B	102	Total	C	N	O	S	0	0
			787	475	146	160	6		
3	C	102	Total	C	N	O	S	0	0
			787	475	146	160	6		
3	D	102	Total	C	N	O	S	0	0
			787	475	146	160	6		
3	E	102	Total	C	N	O	S	0	0
			787	475	146	160	6		
3	F	102	Total	C	N	O	S	0	0
			787	475	146	160	6		

- Molecule 4 is a protein called Tail tubular protein gp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	195	Total	C	N	O	S	0	0
			1553	965	263	316	9		
4	N	193	Total	C	N	O	S	0	0
			1534	954	258	314	8		

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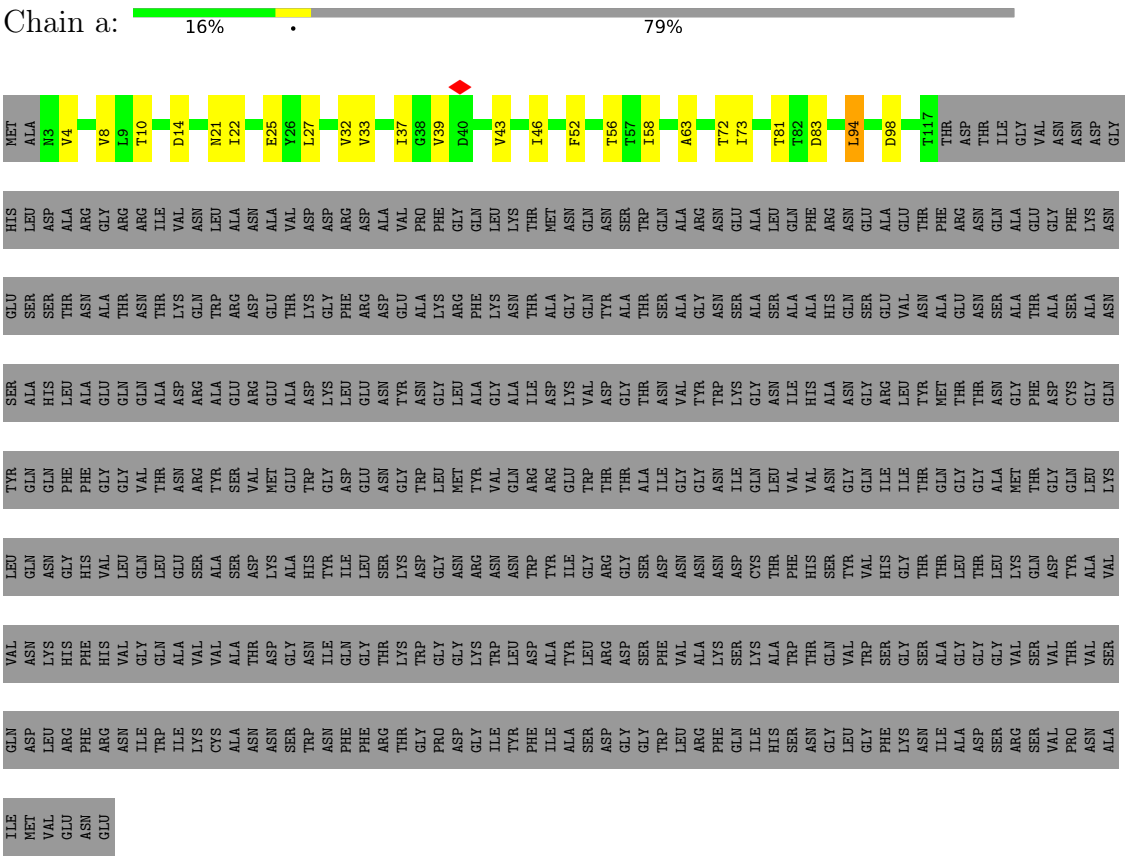
Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	195	Total	C	N	O	S	0	0
			1553	965	263	316	9		
4	P	193	Total	C	N	O	S	0	0
			1534	954	258	314	8		
4	Q	195	Total	C	N	O	S	0	0
			1553	965	263	316	9		
4	R	193	Total	C	N	O	S	0	0
			1534	954	258	314	8		
4	S	195	Total	C	N	O	S	0	0
			1553	965	263	316	9		
4	T	193	Total	C	N	O	S	0	0
			1534	954	258	314	8		
4	U	195	Total	C	N	O	S	0	0
			1553	965	263	316	9		
4	V	193	Total	C	N	O	S	0	0
			1534	954	258	314	8		
4	W	195	Total	C	N	O	S	0	0
			1553	965	263	316	9		
4	X	193	Total	C	N	O	S	0	0
			1534	954	258	314	8		

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.

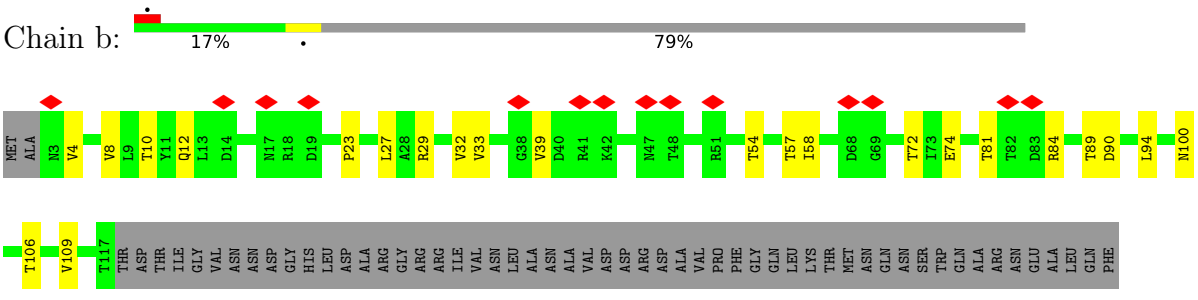
• Molecule 1: Tail fiber protein

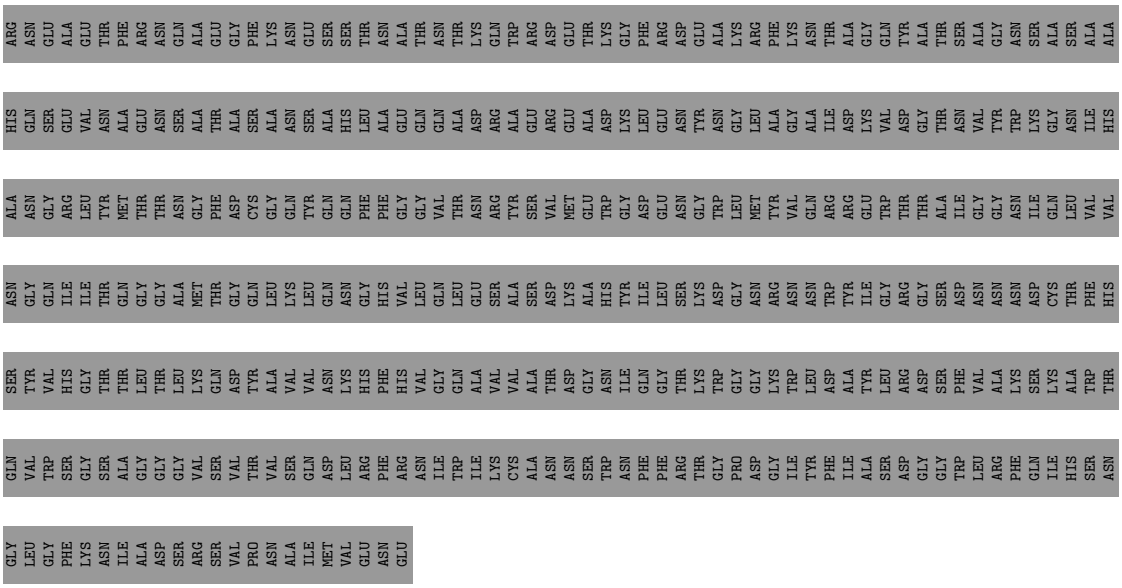
Chain a:



• Molecule 1: Tail fiber protein

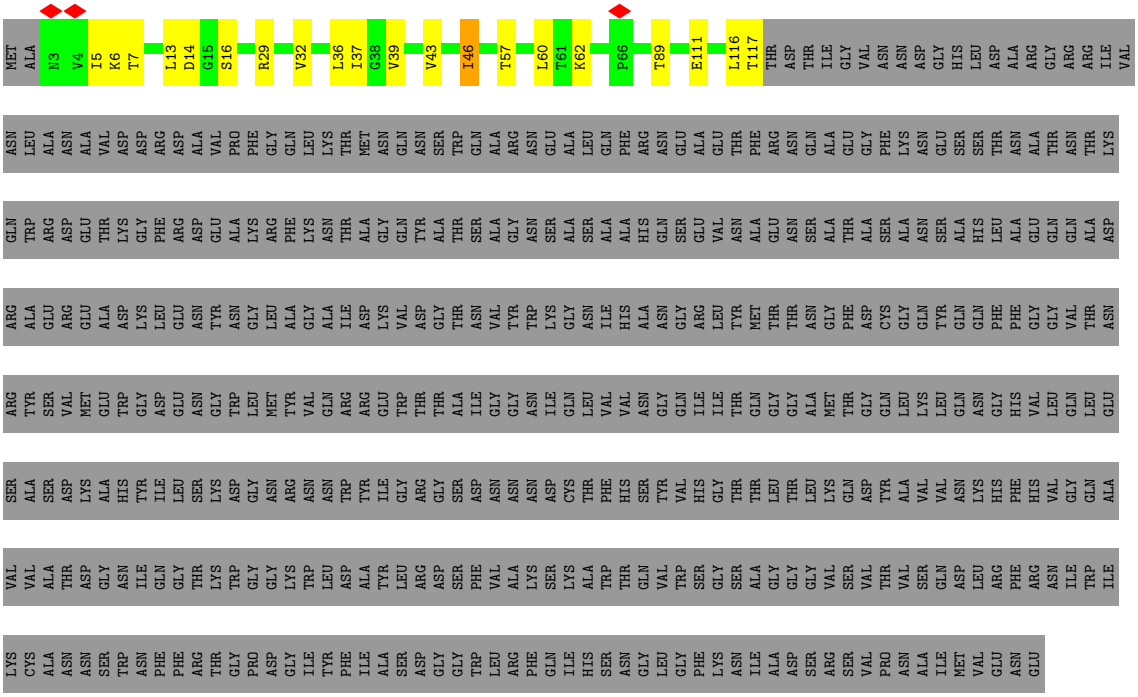
Chain b:





• Molecule 1: Tail fiber protein

Chain c:

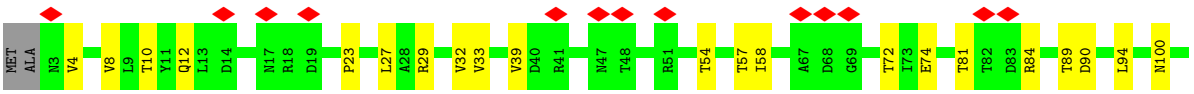


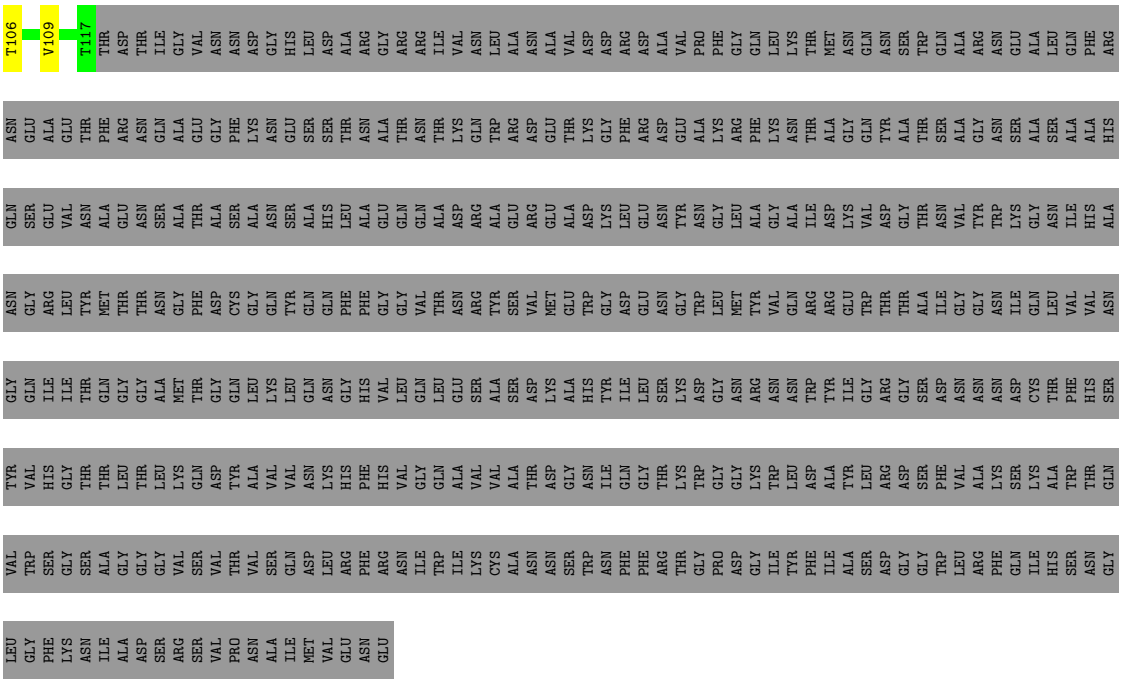
• Molecule 1: Tail fiber protein

Chain d:

• Molecule 1: Tail fiber protein

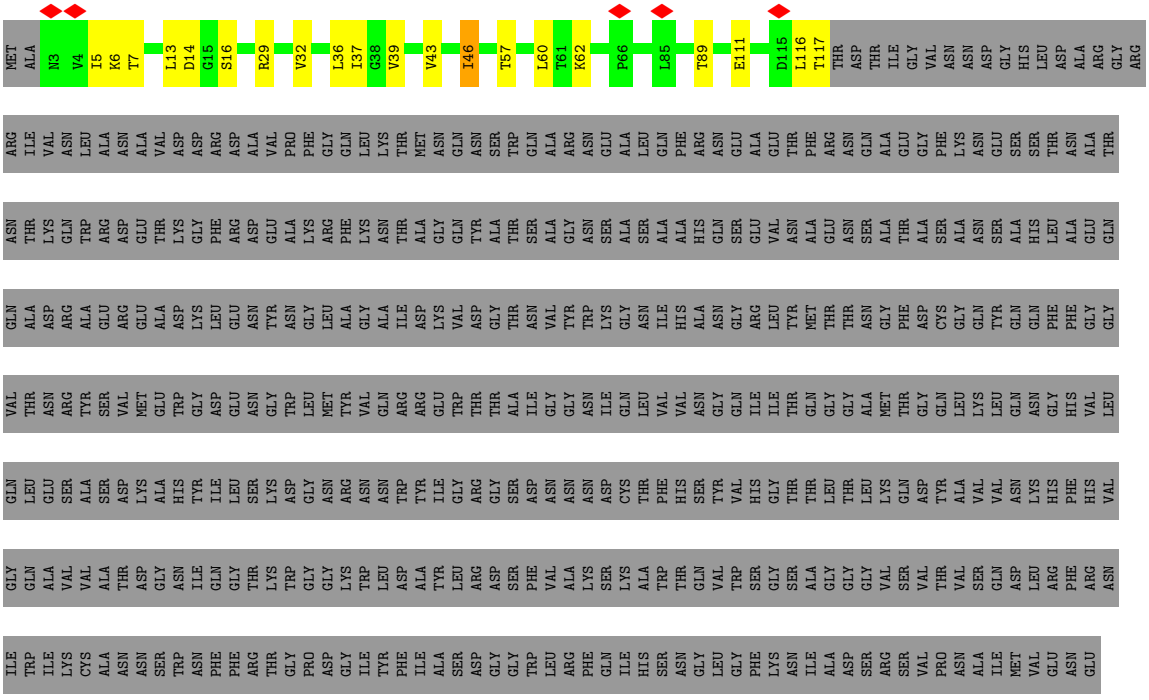
Chain e:





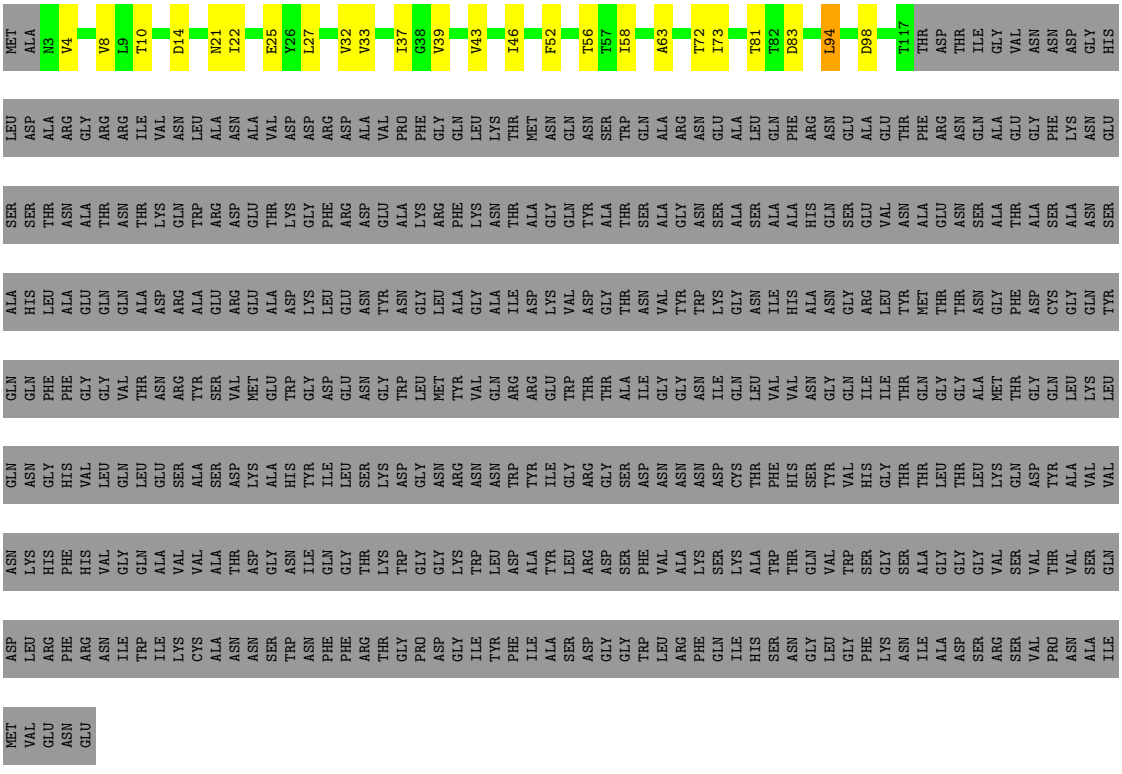
• Molecule 1: Tail fiber protein

Chain f:



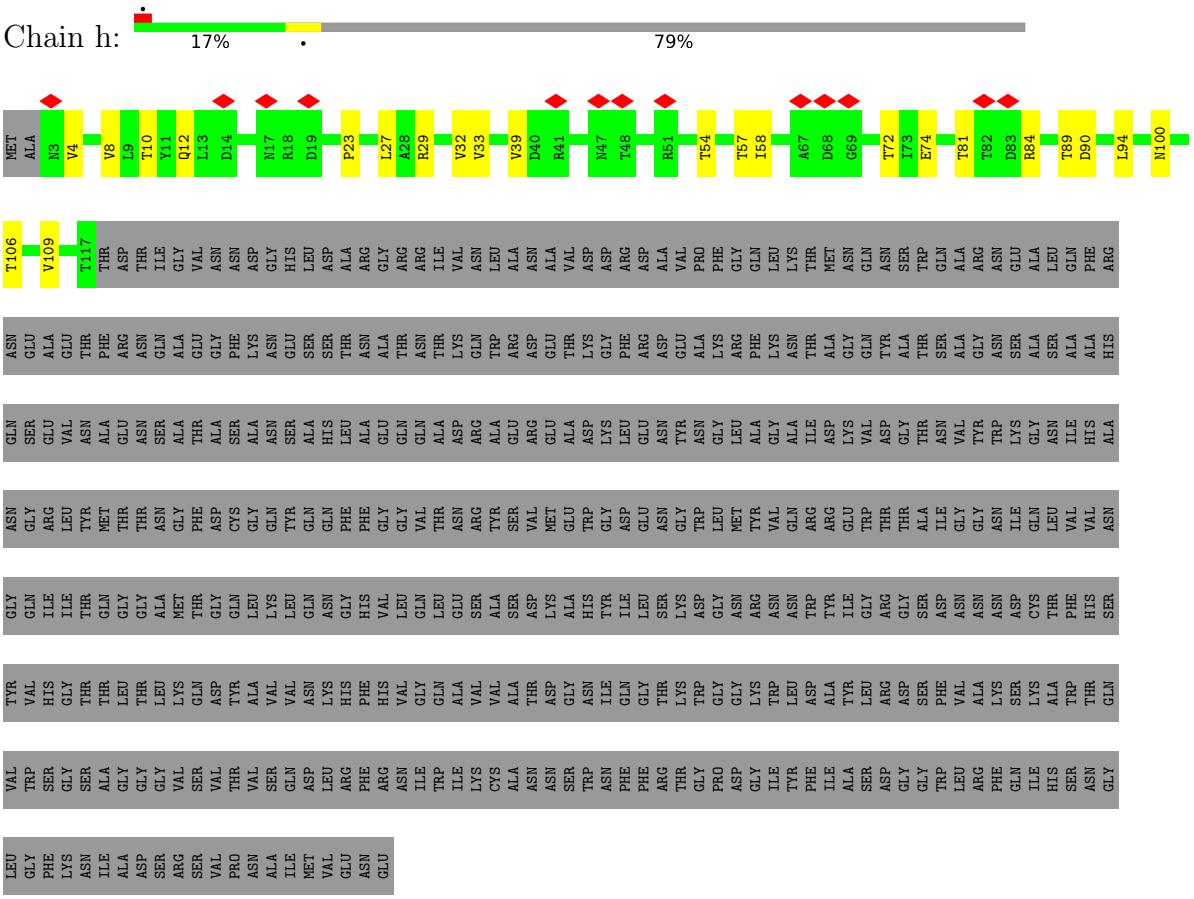
• Molecule 1: Tail fiber protein

Chain g:



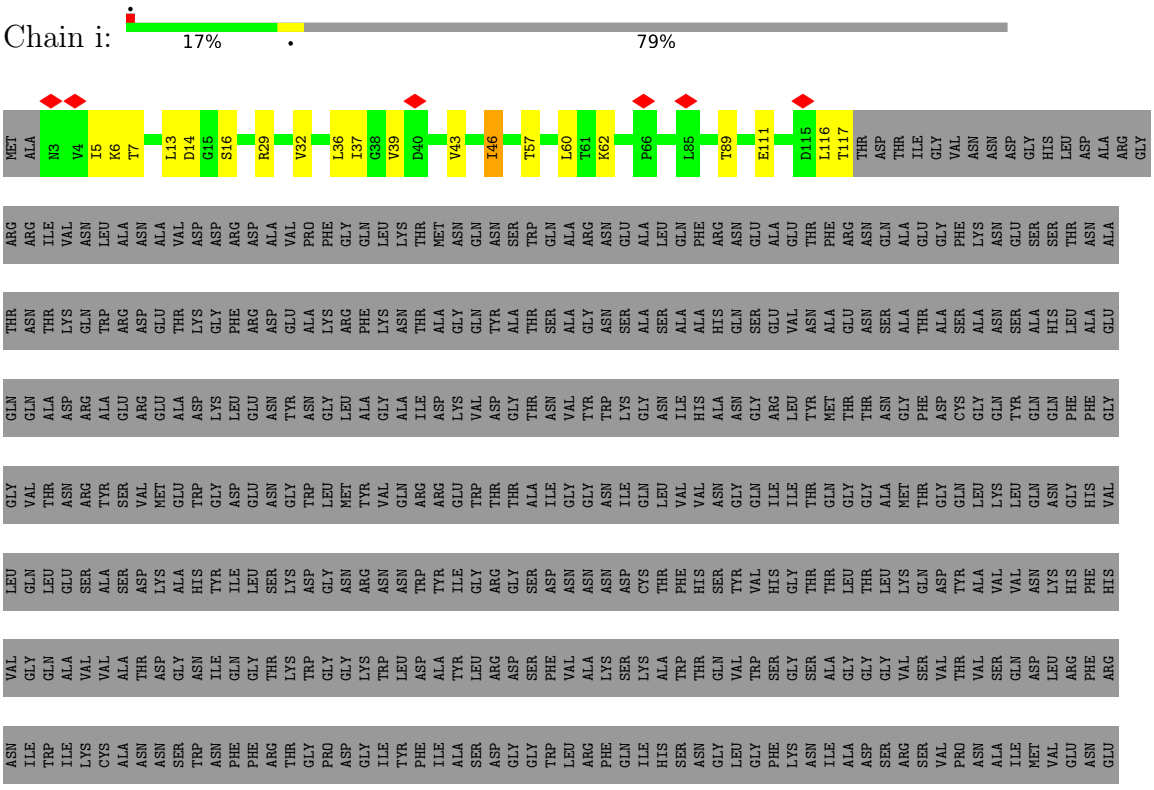
• Molecule 1: Tail fiber protein

Chain h:



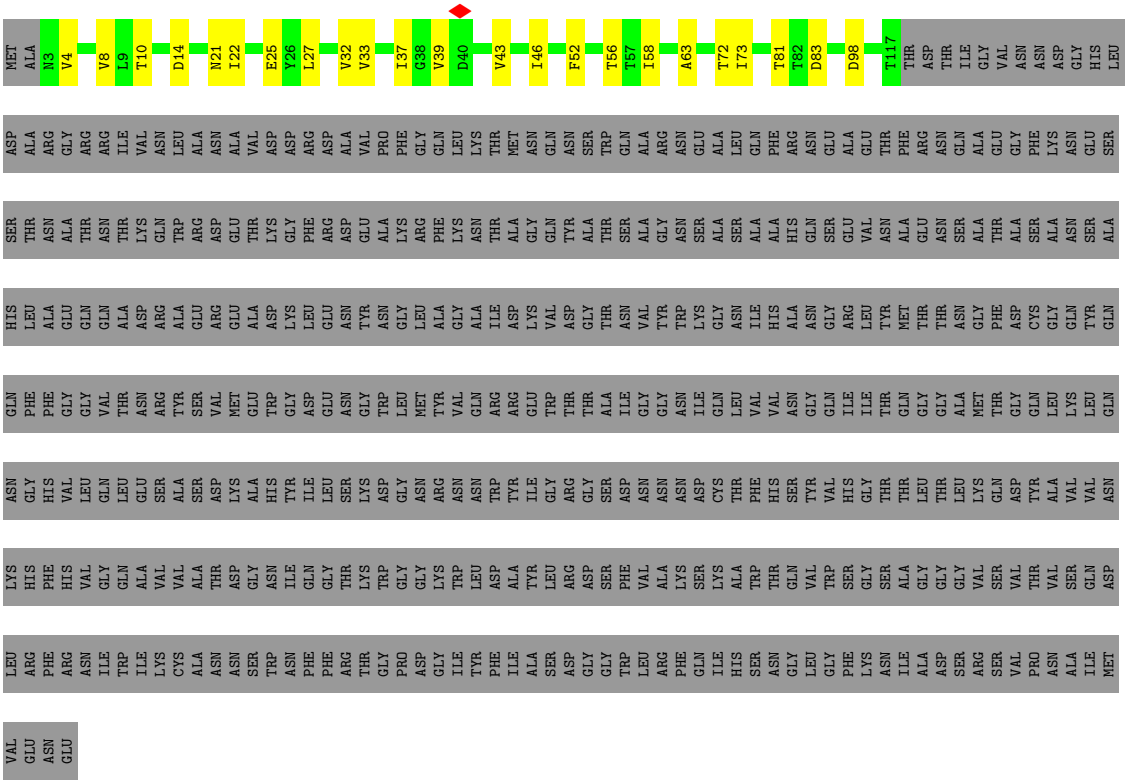
• Molecule 1: Tail fiber protein

Chain i:



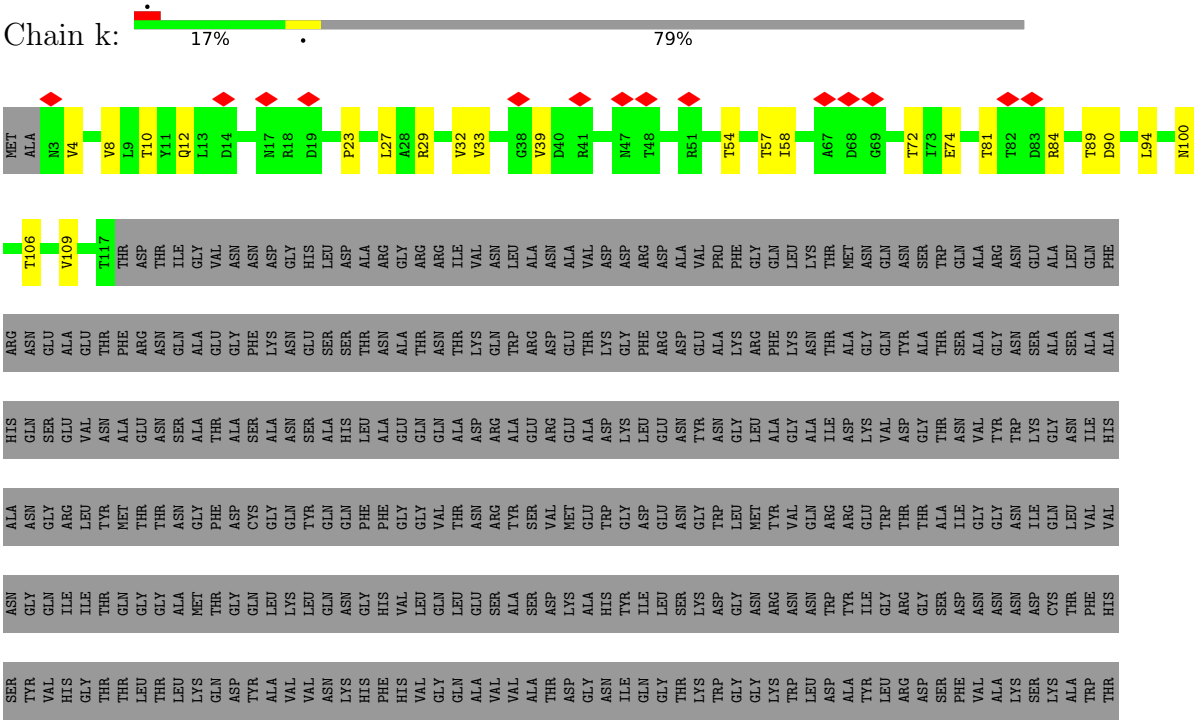
• Molecule 1: Tail fiber protein

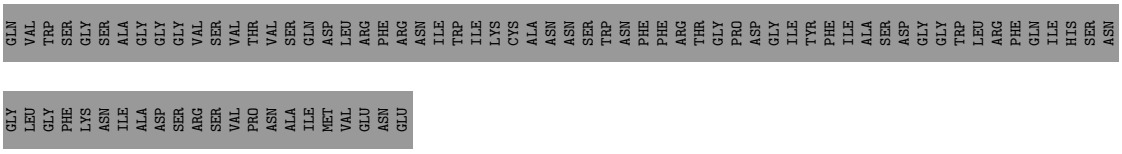
Chain j:



• Molecule 1: Tail fiber protein

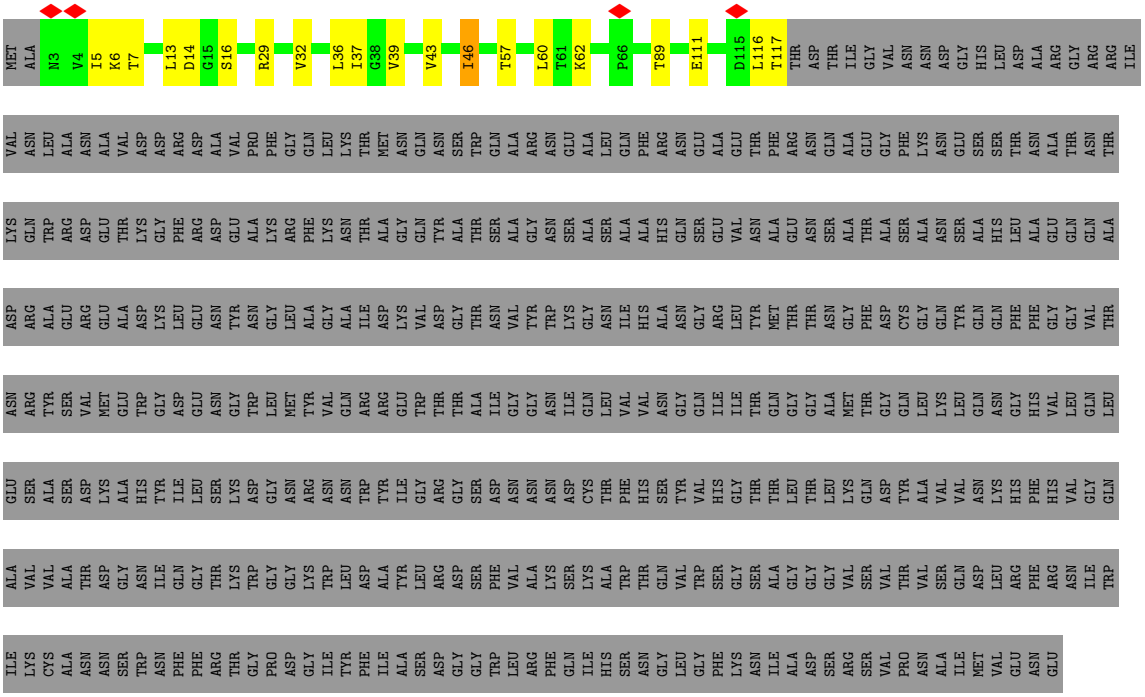
Chain k:





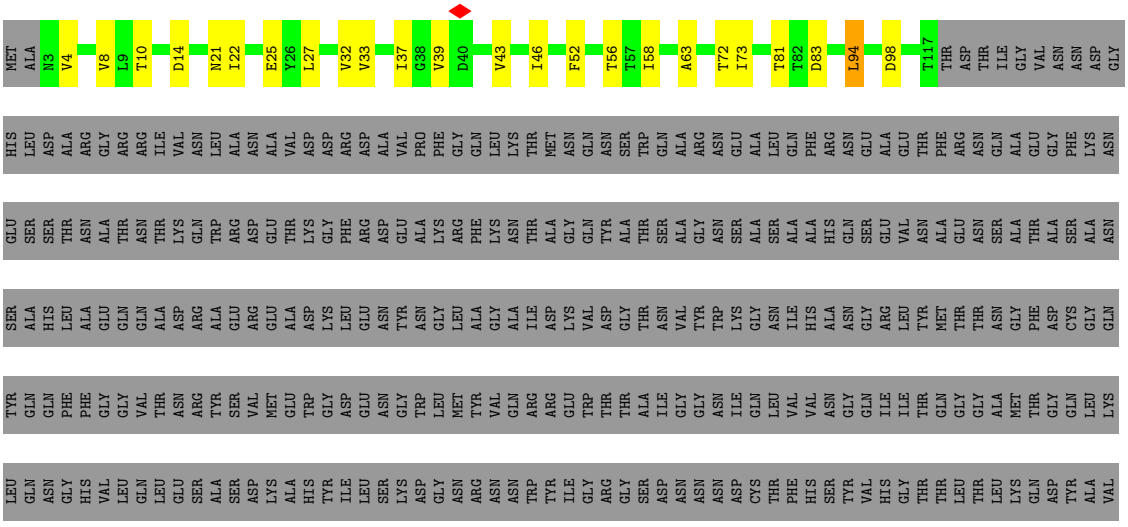
• Molecule 1: Tail fiber protein

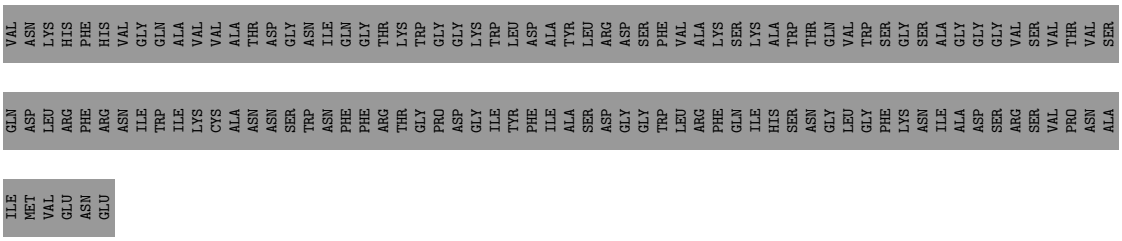
Chain l:



• Molecule 1: Tail fiber protein

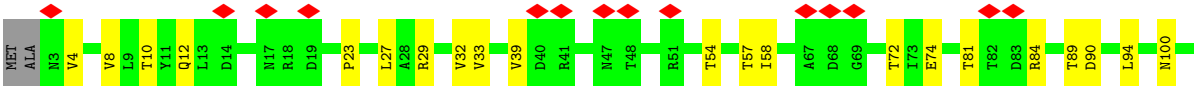
Chain m:





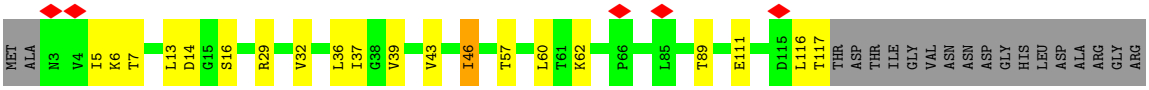
• Molecule 1: Tail fiber protein

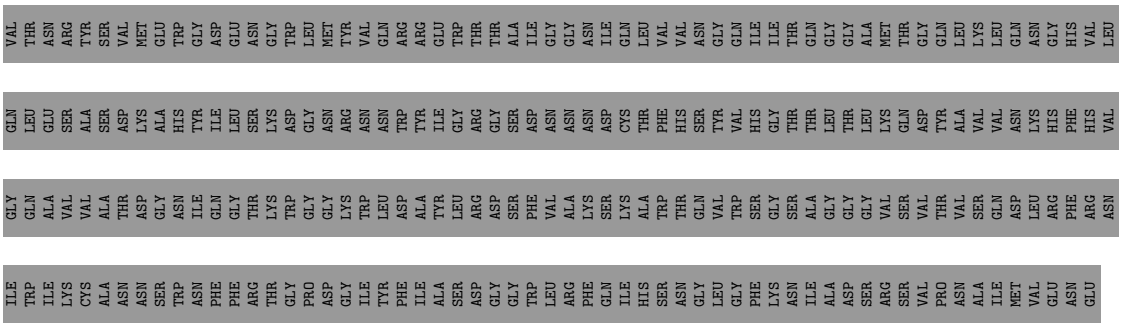
Chain n:



• Molecule 1: Tail fiber protein

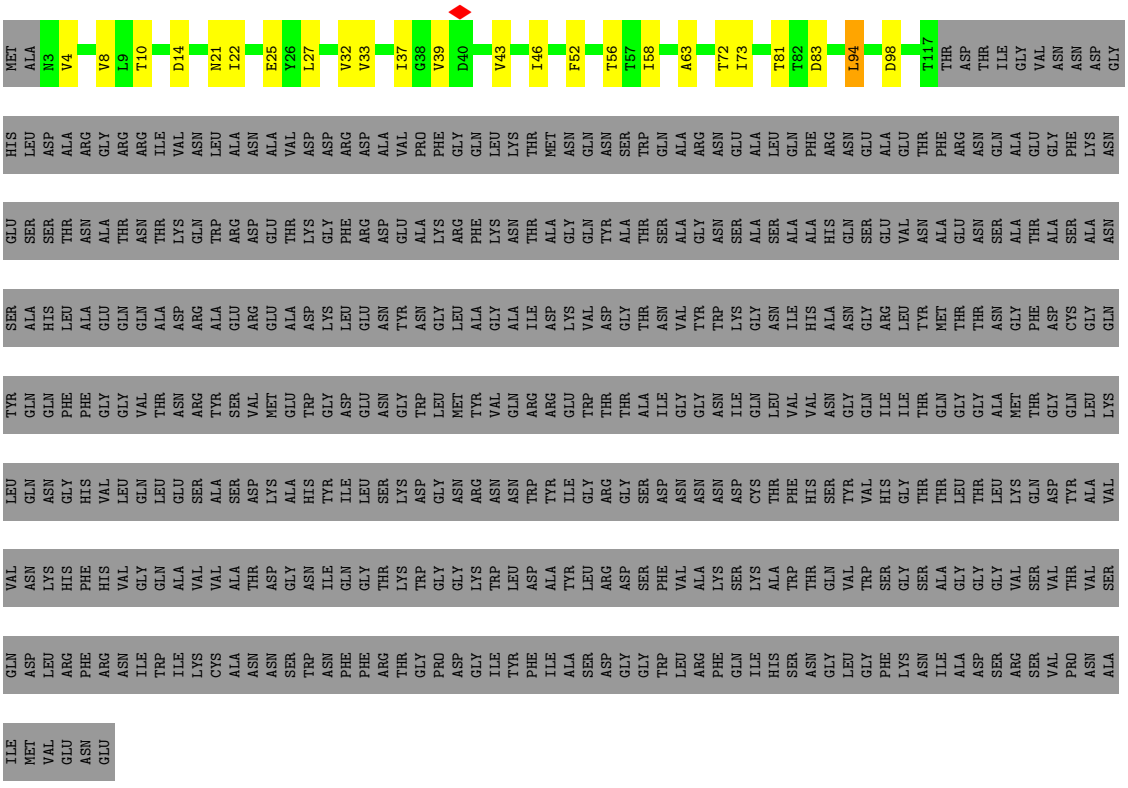
Chain o:





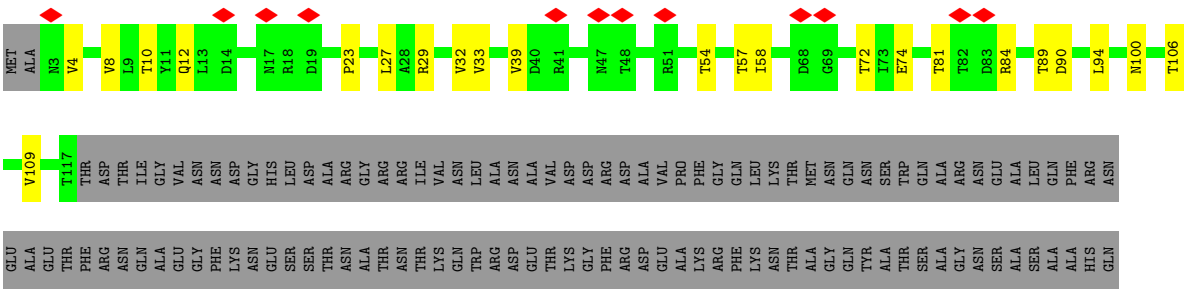
• Molecule 1: Tail fiber protein

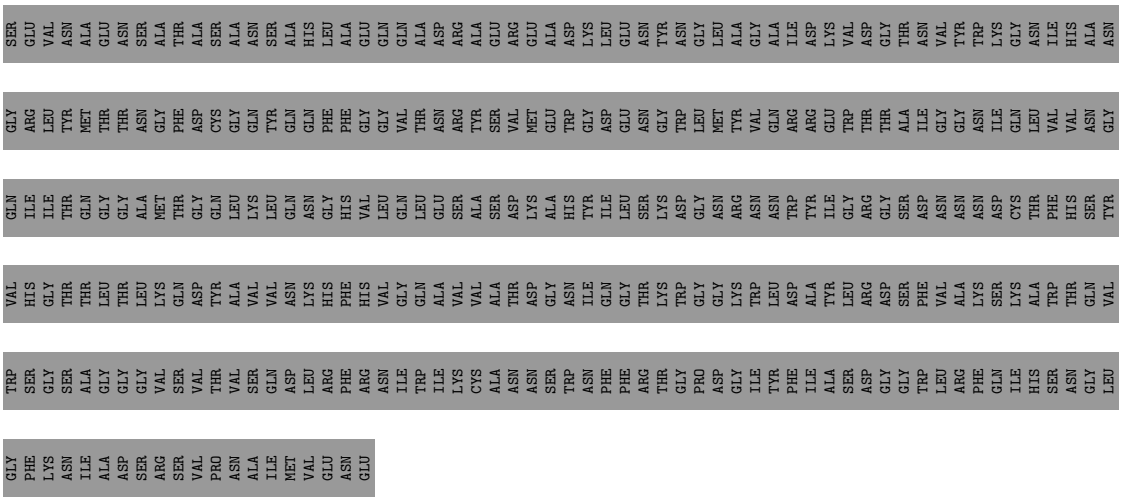
Chain p:



• Molecule 1: Tail fiber protein

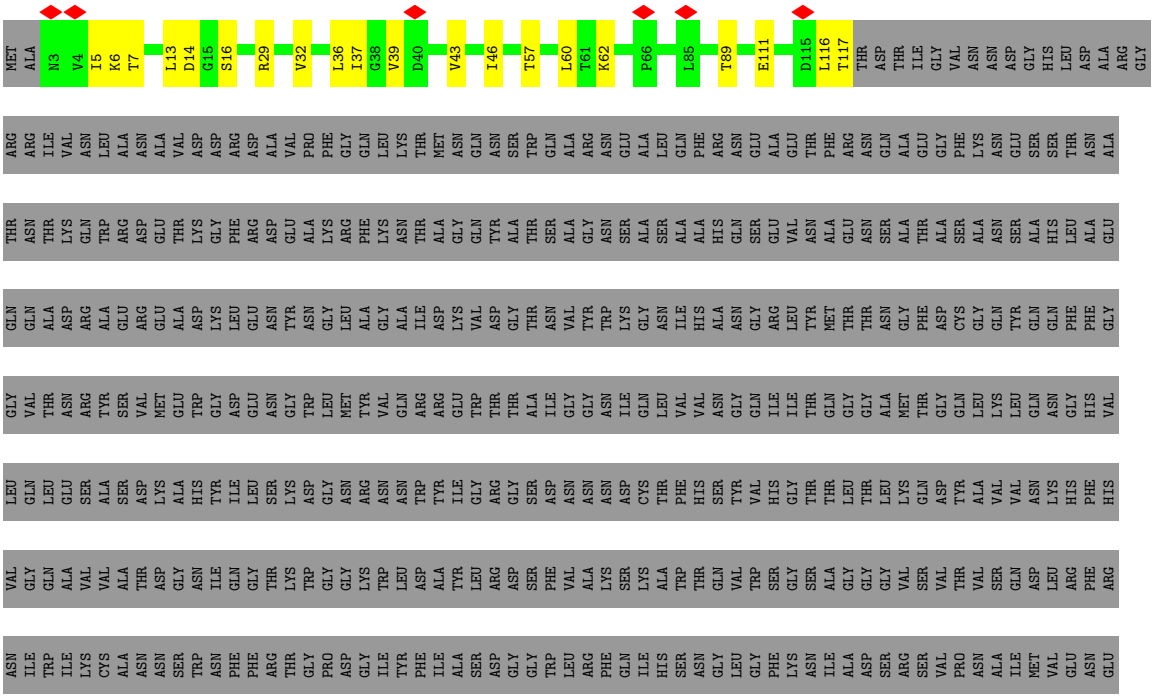
Chain q:





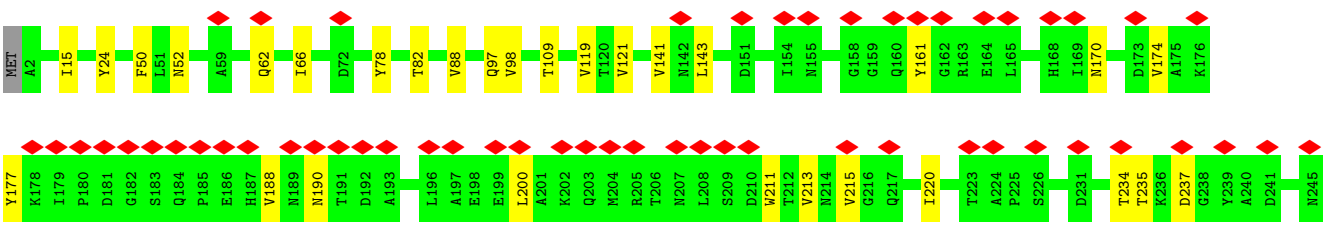
• Molecule 1: Tail fiber protein

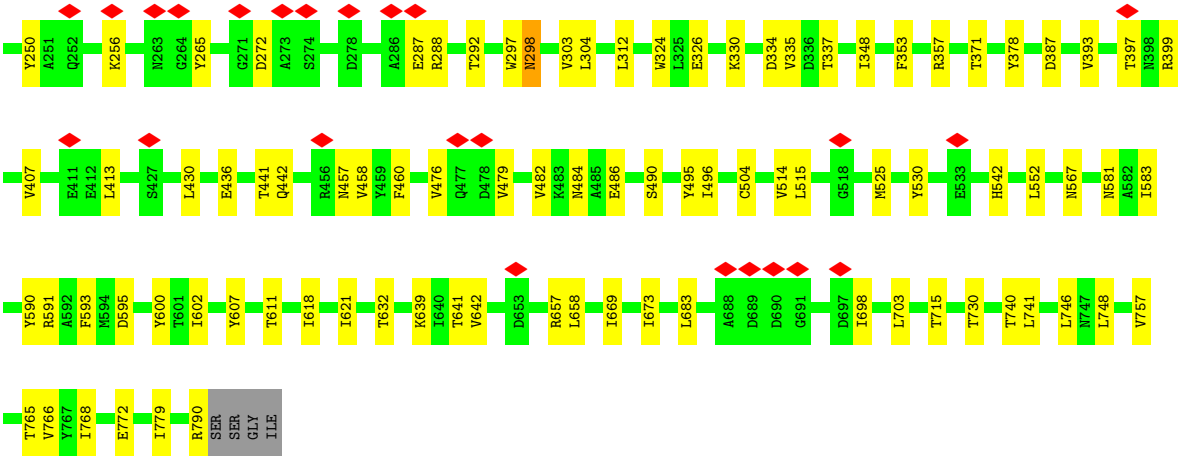
Chain r:



• Molecule 2: Tail tubular protein gp12

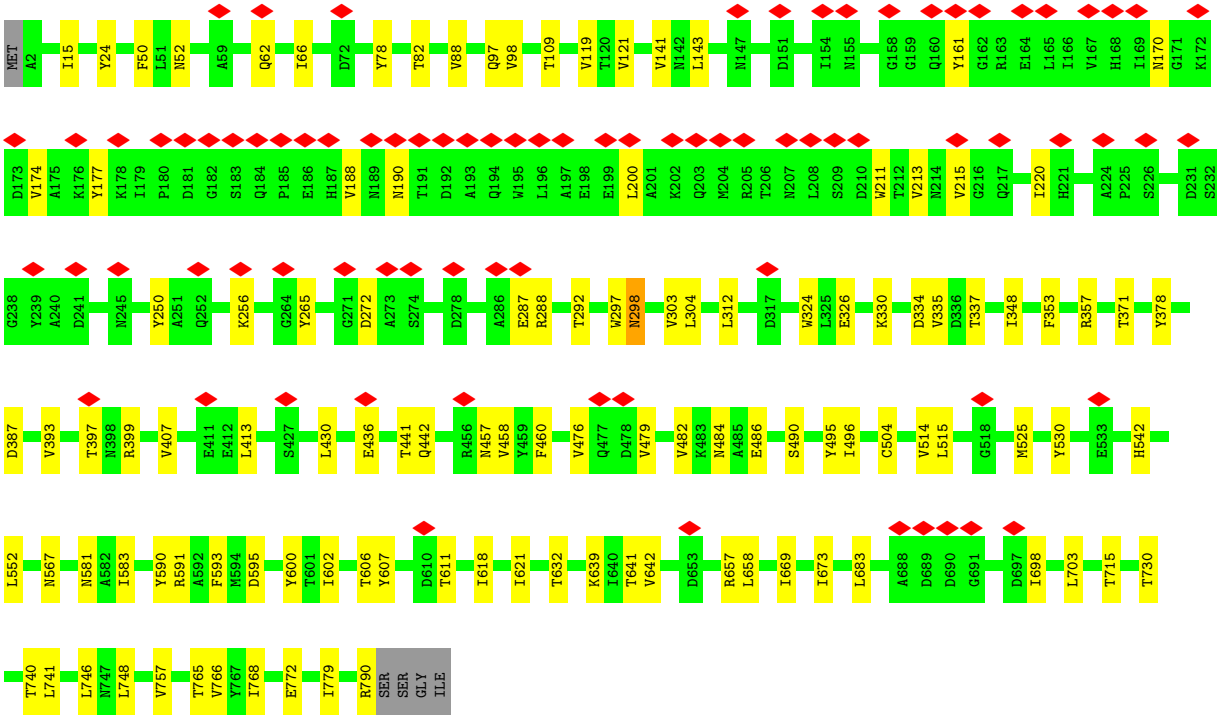
Chain s:





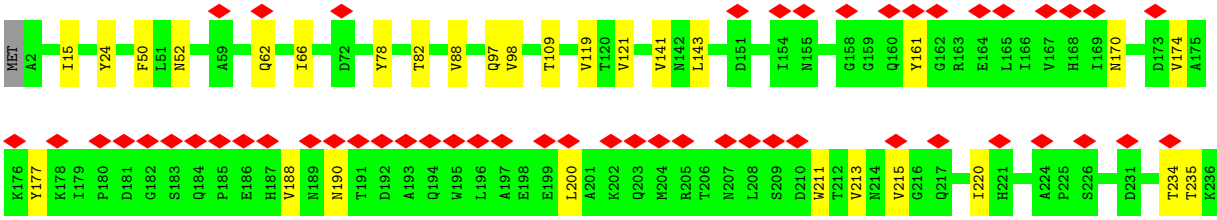
• Molecule 2: Tail tubular protein gp12

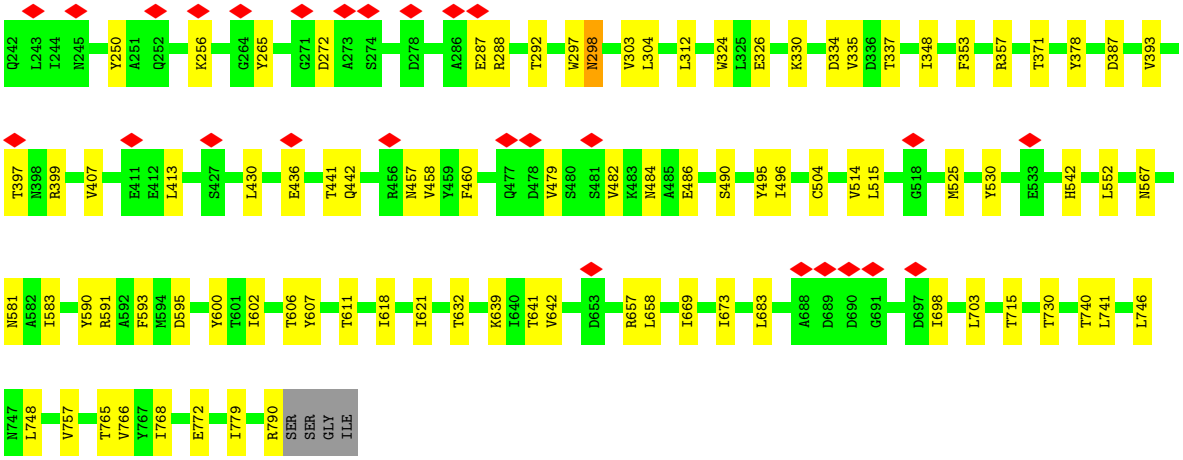
Chain t:



• Molecule 2: Tail tubular protein gp12

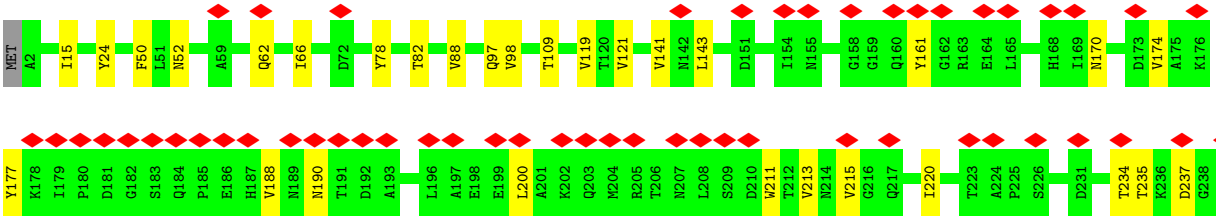
Chain u:





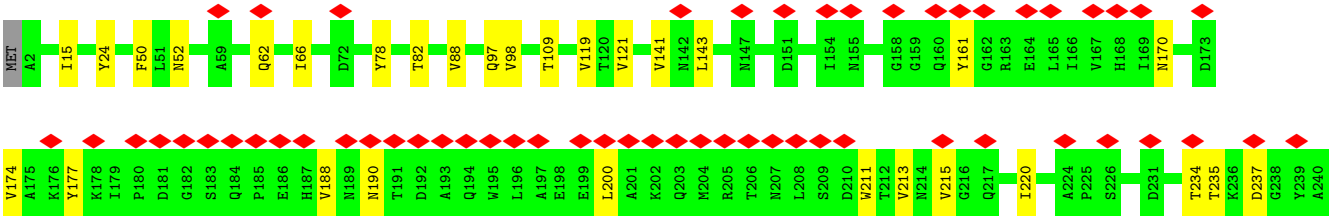
• Molecule 2: Tail tubular protein gp12

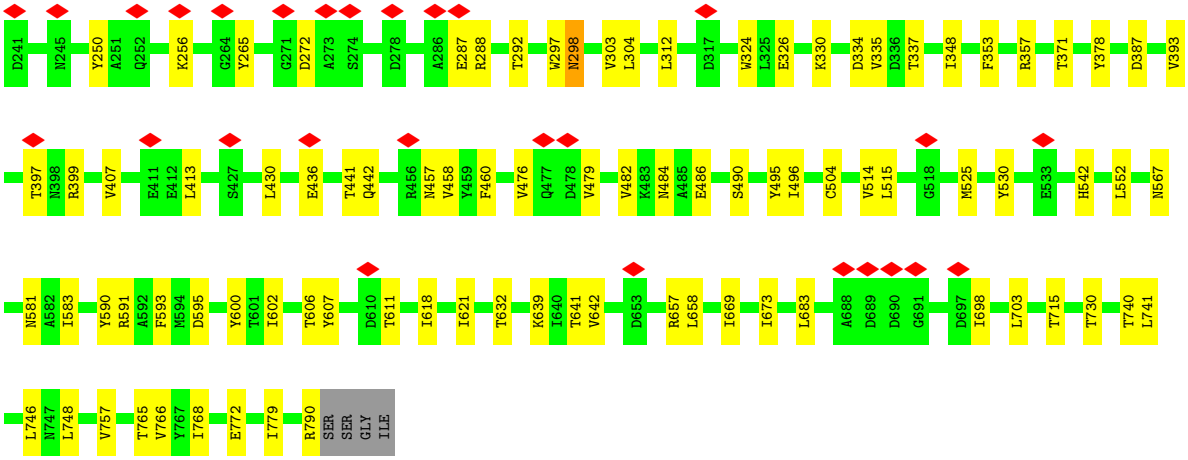
Chain v:



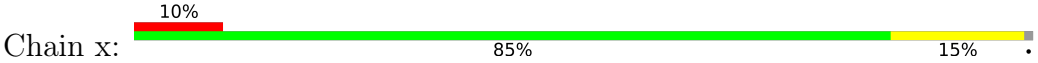
• Molecule 2: Tail tubular protein gp12

Chain w:

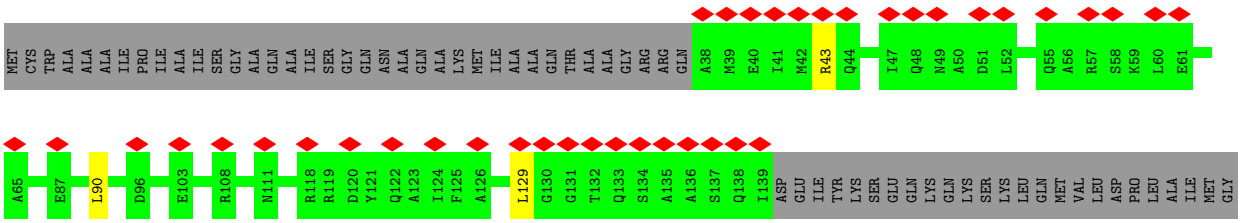




• Molecule 2: Tail tubular protein gp12

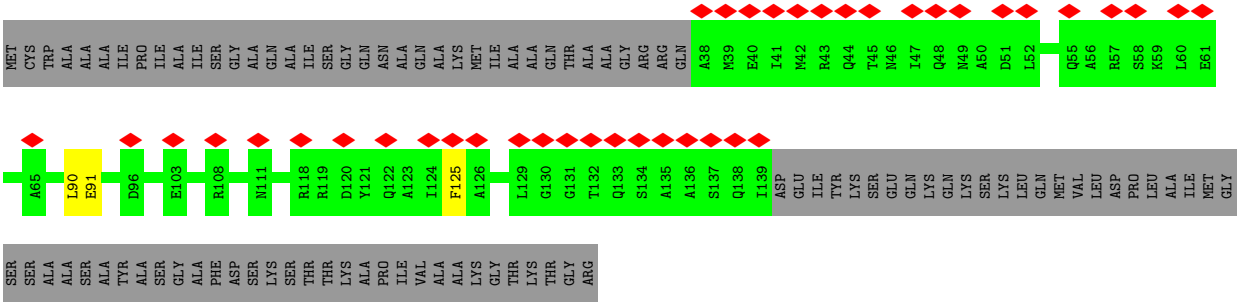


• Molecule 3: Internal virion protein gp14



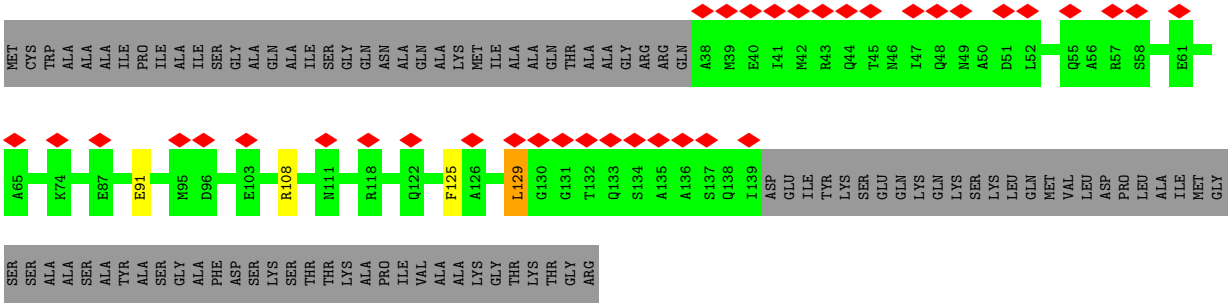
• Molecule 3: Internal virion protein gp14

Chain B:



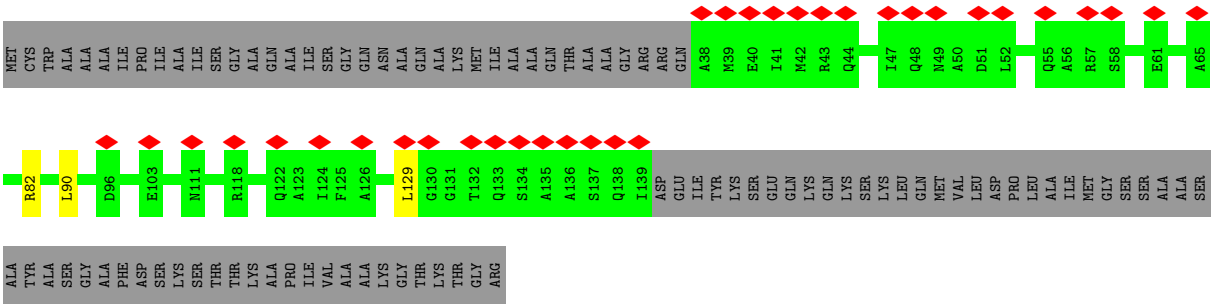
• Molecule 3: Internal virion protein gp14

Chain C:



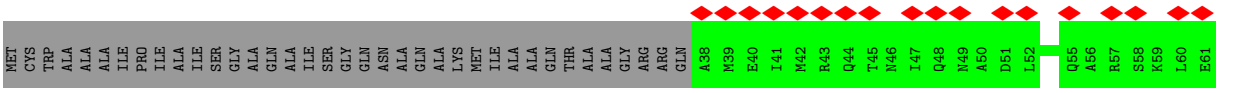
• Molecule 3: Internal virion protein gp14

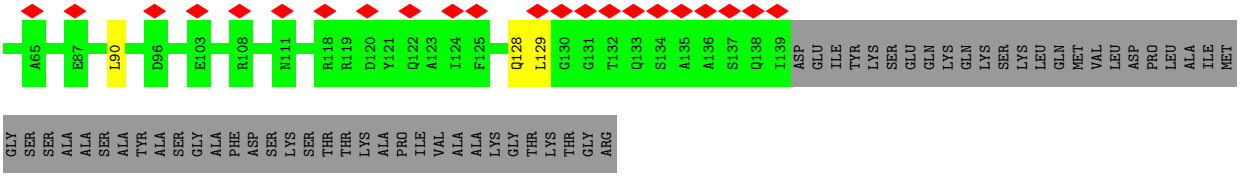
Chain D:



• Molecule 3: Internal virion protein gp14

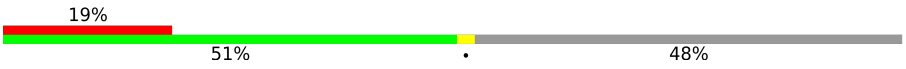
Chain E:

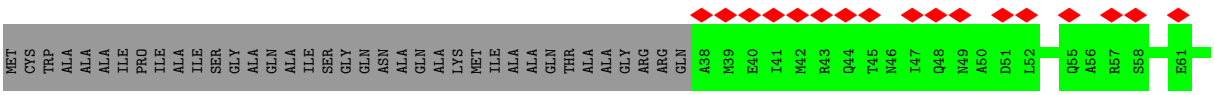


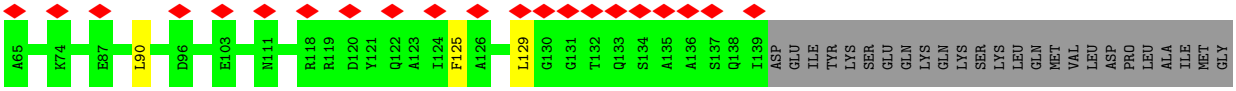


• Molecule 3: Internal virion protein gp14

Chain F:

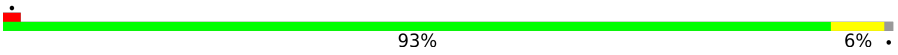


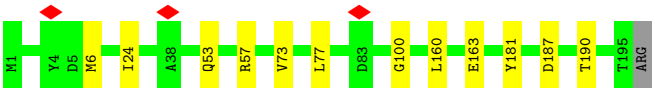




• Molecule 4: Tail tubular protein gp11

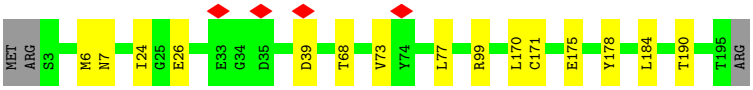
Chain M:





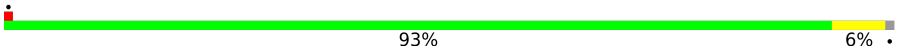
• Molecule 4: Tail tubular protein gp11

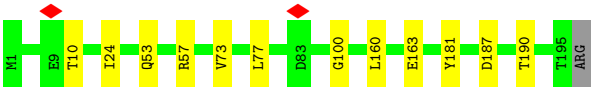
Chain N:



• Molecule 4: Tail tubular protein gp11

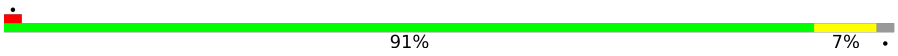
Chain O:

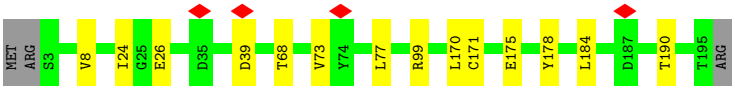




• Molecule 4: Tail tubular protein gp11

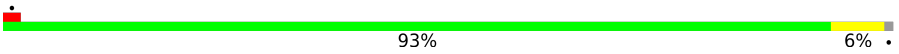
Chain P:

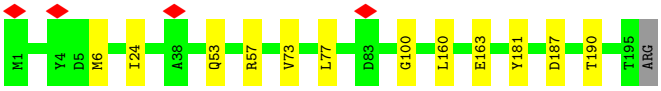




• Molecule 4: Tail tubular protein gp11

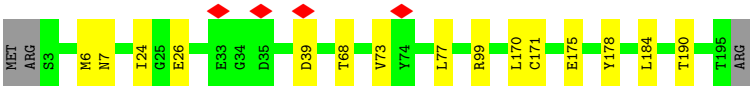
Chain Q:





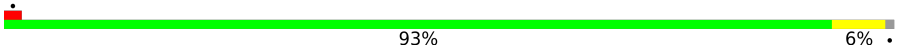
• Molecule 4: Tail tubular protein gp11

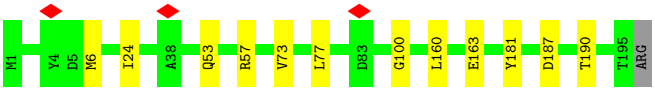
Chain R:



• Molecule 4: Tail tubular protein gp11

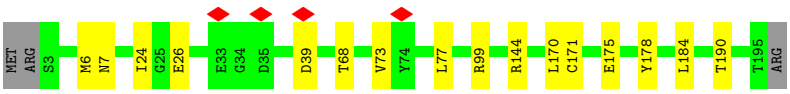
Chain S:





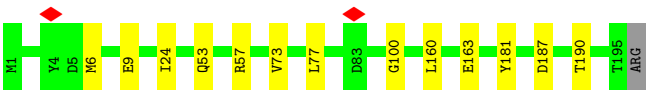
• Molecule 4: Tail tubular protein gp11

Chain T:



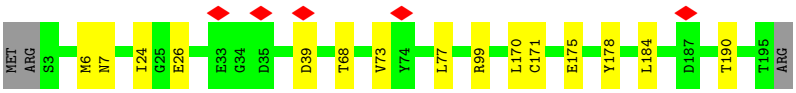
• Molecule 4: Tail tubular protein gp11

Chain U:



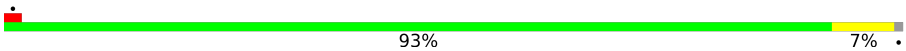
• Molecule 4: Tail tubular protein gp11

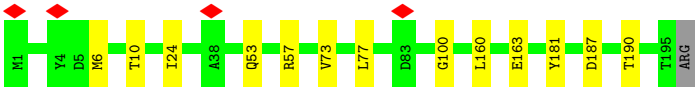
Chain V:



• Molecule 4: Tail tubular protein gp11

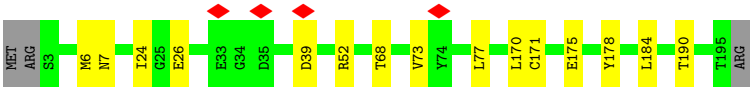
Chain W:





• Molecule 4: Tail tubular protein gp11

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59985	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	43.195	Depositor
Minimum map value	-27.980	Depositor
Average map value	0.013	Depositor
Map value standard deviation	2.048	Depositor
Recommended contour level	8.0	Depositor
Map size (Å)	508.0, 508.0, 508.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.27, 1.27, 1.27	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	a	0.74	0/936	0.94	1/1274 (0.1%)
1	b	0.73	0/936	0.98	0/1274
1	c	0.68	0/936	0.93	0/1274
1	d	0.74	0/936	0.91	0/1274
1	e	0.73	0/936	0.98	0/1274
1	f	0.68	0/936	0.93	0/1274
1	g	0.74	0/936	0.94	1/1274 (0.1%)
1	h	0.73	0/936	0.98	0/1274
1	i	0.68	0/936	0.93	0/1274
1	j	0.74	0/936	0.91	0/1274
1	k	0.73	0/936	0.98	0/1274
1	l	0.68	0/936	0.93	0/1274
1	m	0.74	0/936	0.94	1/1274 (0.1%)
1	n	0.73	0/936	0.98	0/1274
1	o	0.68	0/936	0.94	0/1274
1	p	0.74	0/936	0.94	1/1274 (0.1%)
1	q	0.73	0/936	0.98	0/1274
1	r	0.68	0/936	0.94	0/1274
2	s	0.76	0/6449	0.94	1/8772 (0.0%)
2	t	0.75	0/6449	0.94	1/8772 (0.0%)
2	u	0.76	0/6449	0.94	1/8772 (0.0%)
2	v	0.76	0/6449	0.94	1/8772 (0.0%)
2	w	0.76	0/6449	0.94	1/8772 (0.0%)
2	x	0.76	0/6449	0.94	1/8772 (0.0%)
3	A	0.33	0/790	0.57	2/1056 (0.2%)
3	B	0.31	0/790	0.47	0/1056
3	C	0.33	0/790	0.54	1/1056 (0.1%)
3	D	0.33	0/790	0.53	1/1056 (0.1%)
3	E	0.34	0/790	0.56	0/1056
3	F	0.33	0/790	0.50	0/1056
4	M	0.48	0/1580	0.71	1/2139 (0.0%)
4	N	0.48	0/1561	0.66	1/2115 (0.0%)
4	O	0.48	0/1580	0.68	1/2139 (0.0%)
4	P	0.48	0/1561	0.67	1/2115 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	Q	0.48	0/1580	0.71	1/2139 (0.0%)
4	R	0.49	0/1561	0.68	1/2115 (0.0%)
4	S	0.48	0/1580	0.71	1/2139 (0.0%)
4	T	0.49	0/1561	0.67	1/2115 (0.0%)
4	U	0.48	0/1580	0.71	2/2139 (0.1%)
4	V	0.48	0/1561	0.66	1/2115 (0.0%)
4	W	0.48	0/1580	0.70	1/2139 (0.0%)
4	X	0.49	0/1561	0.66	0/2115
All	All	0.67	0/79128	0.87	26/107424 (0.0%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	m	94	LEU	CA-CB-CG	6.67	130.63	115.30
1	g	94	LEU	CA-CB-CG	6.59	130.46	115.30
1	a	94	LEU	CA-CB-CG	6.57	130.42	115.30
1	p	94	LEU	CA-CB-CG	6.50	130.26	115.30
3	A	129	LEU	CB-CG-CD1	6.05	121.29	111.00
3	A	129	LEU	CA-CB-CG	6.04	129.18	115.30
4	Q	100	GLY	N-CA-C	-5.63	99.04	113.10
4	O	100	GLY	N-CA-C	-5.62	99.04	113.10
4	S	100	GLY	N-CA-C	-5.62	99.06	113.10
4	W	100	GLY	N-CA-C	-5.61	99.07	113.10
4	M	100	GLY	N-CA-C	-5.61	99.09	113.10
4	U	100	GLY	N-CA-C	-5.58	99.15	113.10
2	x	298	ASN	N-CA-C	5.52	125.90	111.00
2	w	298	ASN	N-CA-C	5.51	125.89	111.00
4	V	99	ARG	N-CA-C	-5.51	96.12	111.00
2	s	298	ASN	N-CA-C	5.51	125.87	111.00
2	v	298	ASN	N-CA-C	5.51	125.87	111.00
2	t	298	ASN	N-CA-C	5.49	125.83	111.00
2	u	298	ASN	N-CA-C	5.49	125.83	111.00
4	T	99	ARG	N-CA-C	-5.36	96.52	111.00
4	R	99	ARG	N-CA-C	-5.35	96.56	111.00
4	U	9	GLU	N-CA-C	-5.27	96.77	111.00
3	D	129	LEU	CA-CB-CG	-5.19	103.37	115.30
4	P	99	ARG	N-CA-C	-5.10	97.23	111.00
3	C	129	LEU	CA-CB-CG	5.07	126.97	115.30
4	N	99	ARG	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	113/553 (20%)	102 (90%)	10 (9%)	1 (1%)	17	56
1	b	113/553 (20%)	107 (95%)	4 (4%)	2 (2%)	8	42
1	c	113/553 (20%)	107 (95%)	5 (4%)	1 (1%)	17	56
1	d	113/553 (20%)	102 (90%)	10 (9%)	1 (1%)	17	56
1	e	113/553 (20%)	107 (95%)	4 (4%)	2 (2%)	8	42
1	f	113/553 (20%)	107 (95%)	5 (4%)	1 (1%)	17	56
1	g	113/553 (20%)	102 (90%)	10 (9%)	1 (1%)	17	56
1	h	113/553 (20%)	107 (95%)	4 (4%)	2 (2%)	8	42
1	i	113/553 (20%)	107 (95%)	5 (4%)	1 (1%)	17	56
1	j	113/553 (20%)	102 (90%)	10 (9%)	1 (1%)	17	56
1	k	113/553 (20%)	107 (95%)	4 (4%)	2 (2%)	8	42
1	l	113/553 (20%)	107 (95%)	5 (4%)	1 (1%)	17	56
1	m	113/553 (20%)	102 (90%)	10 (9%)	1 (1%)	17	56
1	n	113/553 (20%)	107 (95%)	4 (4%)	2 (2%)	8	42
1	o	113/553 (20%)	108 (96%)	4 (4%)	1 (1%)	17	56
1	p	113/553 (20%)	102 (90%)	10 (9%)	1 (1%)	17	56
1	q	113/553 (20%)	107 (95%)	4 (4%)	2 (2%)	8	42
1	r	113/553 (20%)	107 (95%)	6 (5%)	0	100	100
2	s	787/794 (99%)	735 (93%)	46 (6%)	6 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	t	787/794 (99%)	735 (93%)	46 (6%)	6 (1%)	19	60
2	u	787/794 (99%)	735 (93%)	46 (6%)	6 (1%)	19	60
2	v	787/794 (99%)	735 (93%)	46 (6%)	6 (1%)	19	60
2	w	787/794 (99%)	734 (93%)	47 (6%)	6 (1%)	19	60
2	x	787/794 (99%)	734 (93%)	47 (6%)	6 (1%)	19	60
3	A	100/196 (51%)	100 (100%)	0	0	100	100
3	B	100/196 (51%)	99 (99%)	1 (1%)	0	100	100
3	C	100/196 (51%)	100 (100%)	0	0	100	100
3	D	100/196 (51%)	99 (99%)	1 (1%)	0	100	100
3	E	100/196 (51%)	100 (100%)	0	0	100	100
3	F	100/196 (51%)	100 (100%)	0	0	100	100
4	M	193/196 (98%)	183 (95%)	10 (5%)	0	100	100
4	N	191/196 (97%)	180 (94%)	11 (6%)	0	100	100
4	O	193/196 (98%)	184 (95%)	9 (5%)	0	100	100
4	P	191/196 (97%)	179 (94%)	11 (6%)	1 (0%)	29	68
4	Q	193/196 (98%)	184 (95%)	9 (5%)	0	100	100
4	R	191/196 (97%)	180 (94%)	11 (6%)	0	100	100
4	S	193/196 (98%)	183 (95%)	10 (5%)	0	100	100
4	T	191/196 (97%)	180 (94%)	11 (6%)	0	100	100
4	U	193/196 (98%)	182 (94%)	11 (6%)	0	100	100
4	V	191/196 (97%)	179 (94%)	12 (6%)	0	100	100
4	W	193/196 (98%)	183 (95%)	10 (5%)	0	100	100
4	X	191/196 (97%)	180 (94%)	11 (6%)	0	100	100
All	All	9660/18246 (53%)	9080 (94%)	520 (5%)	60 (1%)	29	65

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	c	46	ILE
1	f	46	ILE
1	i	46	ILE
1	l	46	ILE
1	o	46	ILE
2	s	62	GLN

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Mol	Chain	Res	Type
2	t	62	GLN
2	u	62	GLN
2	v	62	GLN
2	w	62	GLN
2	x	62	GLN
4	P	8	VAL
1	a	63	ALA
1	d	63	ALA
1	g	63	ALA
1	j	63	ALA
1	m	63	ALA
1	p	63	ALA
2	s	190	ASN
2	s	607	TYR
2	t	190	ASN
2	t	607	TYR
2	u	190	ASN
2	u	607	TYR
2	v	190	ASN
2	v	607	TYR
2	w	190	ASN
2	w	607	TYR
2	x	190	ASN
2	x	607	TYR
2	s	334	ASP
2	s	639	LYS
2	t	334	ASP
2	t	639	LYS
2	u	334	ASP
2	u	639	LYS
2	v	334	ASP
2	v	639	LYS
2	w	334	ASP
2	w	639	LYS
2	x	334	ASP
2	x	639	LYS
1	b	90	ASP
1	e	90	ASP
1	h	90	ASP
1	k	90	ASP
1	n	90	ASP
1	q	90	ASP

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Mol	Chain	Res	Type
1	b	23	PRO
1	e	23	PRO
1	h	23	PRO
1	k	23	PRO
1	n	23	PRO
1	q	23	PRO
2	s	484	ASN
2	t	484	ASN
2	u	484	ASN
2	v	484	ASN
2	w	484	ASN
2	x	484	ASN

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	a	102/451 (23%)	79 (78%)	23 (22%)	1 6
1	b	102/451 (23%)	81 (79%)	21 (21%)	1 7
1	c	102/451 (23%)	82 (80%)	20 (20%)	1 9
1	d	102/451 (23%)	80 (78%)	22 (22%)	1 6
1	e	102/451 (23%)	81 (79%)	21 (21%)	1 7
1	f	102/451 (23%)	82 (80%)	20 (20%)	1 9
1	g	102/451 (23%)	79 (78%)	23 (22%)	1 6
1	h	102/451 (23%)	81 (79%)	21 (21%)	1 7
1	i	102/451 (23%)	82 (80%)	20 (20%)	1 9
1	j	102/451 (23%)	80 (78%)	22 (22%)	1 6
1	k	102/451 (23%)	81 (79%)	21 (21%)	1 7
1	l	102/451 (23%)	82 (80%)	20 (20%)	1 9
1	m	102/451 (23%)	79 (78%)	23 (22%)	1 6
1	n	102/451 (23%)	81 (79%)	21 (21%)	1 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	o	102/451 (23%)	82 (80%)	20 (20%)	1 9
1	p	102/451 (23%)	79 (78%)	23 (22%)	1 6
1	q	102/451 (23%)	81 (79%)	21 (21%)	1 7
1	r	102/451 (23%)	82 (80%)	20 (20%)	1 9
2	s	684/688 (99%)	572 (84%)	112 (16%)	2 14
2	t	684/688 (99%)	571 (84%)	113 (16%)	2 14
2	u	684/688 (99%)	572 (84%)	112 (16%)	2 14
2	v	684/688 (99%)	571 (84%)	113 (16%)	2 14
2	w	684/688 (99%)	571 (84%)	113 (16%)	2 14
2	x	684/688 (99%)	572 (84%)	112 (16%)	2 14
3	A	83/149 (56%)	81 (98%)	2 (2%)	49 69
3	B	83/149 (56%)	80 (96%)	3 (4%)	35 60
3	C	83/149 (56%)	79 (95%)	4 (5%)	25 52
3	D	83/149 (56%)	81 (98%)	2 (2%)	49 69
3	E	83/149 (56%)	80 (96%)	3 (4%)	35 60
3	F	83/149 (56%)	80 (96%)	3 (4%)	35 60
4	M	168/169 (99%)	157 (94%)	11 (6%)	17 44
4	N	166/169 (98%)	152 (92%)	14 (8%)	11 36
4	O	168/169 (99%)	157 (94%)	11 (6%)	17 44
4	P	166/169 (98%)	154 (93%)	12 (7%)	14 41
4	Q	168/169 (99%)	157 (94%)	11 (6%)	17 44
4	R	166/169 (98%)	152 (92%)	14 (8%)	11 36
4	S	168/169 (99%)	157 (94%)	11 (6%)	17 44
4	T	166/169 (98%)	151 (91%)	15 (9%)	9 33
4	U	168/169 (99%)	157 (94%)	11 (6%)	17 44
4	V	166/169 (98%)	152 (92%)	14 (8%)	11 36
4	W	168/169 (99%)	156 (93%)	12 (7%)	14 41
4	X	166/169 (98%)	151 (91%)	15 (9%)	9 33
All	All	8442/15168 (56%)	7217 (86%)	1225 (14%)	6 18

All (1225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	4	VAL
1	a	8	VAL
1	a	10	THR
1	a	14	ASP
1	a	21	ASN
1	a	22	ILE
1	a	25	GLU
1	a	27	LEU
1	a	32	VAL
1	a	33	VAL
1	a	37	ILE
1	a	39	VAL
1	a	43	VAL
1	a	46	ILE
1	a	52	PHE
1	a	56	THR
1	a	58	ILE
1	a	72	THR
1	a	73	ILE
1	a	81	THR
1	a	83	ASP
1	a	94	LEU
1	a	98	ASP
1	b	4	VAL
1	b	8	VAL
1	b	10	THR
1	b	12	GLN
1	b	27	LEU
1	b	29	ARG
1	b	32	VAL
1	b	33	VAL
1	b	39	VAL
1	b	54	THR
1	b	57	THR
1	b	58	ILE
1	b	72	THR
1	b	74	GLU
1	b	81	THR
1	b	84	ARG
1	b	89	THR
1	b	94	LEU
1	b	100	ASN
1	b	106	THR

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Mol	Chain	Res	Type
1	b	109	VAL
1	c	5	ILE
1	c	6	LYS
1	c	7	THR
1	c	13	LEU
1	c	14	ASP
1	c	16	SER
1	c	29	ARG
1	c	32	VAL
1	c	36	LEU
1	c	37	ILE
1	c	39	VAL
1	c	43	VAL
1	c	46	ILE
1	c	57	THR
1	c	60	LEU
1	c	62	LYS
1	c	89	THR
1	c	111	GLU
1	c	116	LEU
1	c	117	THR
1	d	4	VAL
1	d	8	VAL
1	d	10	THR
1	d	14	ASP
1	d	21	ASN
1	d	22	ILE
1	d	25	GLU
1	d	27	LEU
1	d	32	VAL
1	d	33	VAL
1	d	37	ILE
1	d	39	VAL
1	d	43	VAL
1	d	46	ILE
1	d	52	PHE
1	d	56	THR
1	d	58	ILE
1	d	72	THR
1	d	73	ILE
1	d	81	THR
1	d	83	ASP

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Mol	Chain	Res	Type
1	d	98	ASP
1	e	4	VAL
1	e	8	VAL
1	e	10	THR
1	e	12	GLN
1	e	27	LEU
1	e	29	ARG
1	e	32	VAL
1	e	33	VAL
1	e	39	VAL
1	e	54	THR
1	e	57	THR
1	e	58	ILE
1	e	72	THR
1	e	74	GLU
1	e	81	THR
1	e	84	ARG
1	e	89	THR
1	e	94	LEU
1	e	100	ASN
1	e	106	THR
1	e	109	VAL
1	f	5	ILE
1	f	6	LYS
1	f	7	THR
1	f	13	LEU
1	f	14	ASP
1	f	16	SER
1	f	29	ARG
1	f	32	VAL
1	f	36	LEU
1	f	37	ILE
1	f	39	VAL
1	f	43	VAL
1	f	46	ILE
1	f	57	THR
1	f	60	LEU
1	f	62	LYS
1	f	89	THR
1	f	111	GLU
1	f	116	LEU
1	f	117	THR

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Mol	Chain	Res	Type
1	g	4	VAL
1	g	8	VAL
1	g	10	THR
1	g	14	ASP
1	g	21	ASN
1	g	22	ILE
1	g	25	GLU
1	g	27	LEU
1	g	32	VAL
1	g	33	VAL
1	g	37	ILE
1	g	39	VAL
1	g	43	VAL
1	g	46	ILE
1	g	52	PHE
1	g	56	THR
1	g	58	ILE
1	g	72	THR
1	g	73	ILE
1	g	81	THR
1	g	83	ASP
1	g	94	LEU
1	g	98	ASP
1	h	4	VAL
1	h	8	VAL
1	h	10	THR
1	h	12	GLN
1	h	27	LEU
1	h	29	ARG
1	h	32	VAL
1	h	33	VAL
1	h	39	VAL
1	h	54	THR
1	h	57	THR
1	h	58	ILE
1	h	72	THR
1	h	74	GLU
1	h	81	THR
1	h	84	ARG
1	h	89	THR
1	h	94	LEU
1	h	100	ASN

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Mol	Chain	Res	Type
1	h	106	THR
1	h	109	VAL
1	i	5	ILE
1	i	6	LYS
1	i	7	THR
1	i	13	LEU
1	i	14	ASP
1	i	16	SER
1	i	29	ARG
1	i	32	VAL
1	i	36	LEU
1	i	37	ILE
1	i	39	VAL
1	i	43	VAL
1	i	46	ILE
1	i	57	THR
1	i	60	LEU
1	i	62	LYS
1	i	89	THR
1	i	111	GLU
1	i	116	LEU
1	i	117	THR
1	j	4	VAL
1	j	8	VAL
1	j	10	THR
1	j	14	ASP
1	j	21	ASN
1	j	22	ILE
1	j	25	GLU
1	j	27	LEU
1	j	32	VAL
1	j	33	VAL
1	j	37	ILE
1	j	39	VAL
1	j	43	VAL
1	j	46	ILE
1	j	52	PHE
1	j	56	THR
1	j	58	ILE
1	j	72	THR
1	j	73	ILE
1	j	81	THR

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Mol	Chain	Res	Type
1	j	83	ASP
1	j	98	ASP
1	k	4	VAL
1	k	8	VAL
1	k	10	THR
1	k	12	GLN
1	k	27	LEU
1	k	29	ARG
1	k	32	VAL
1	k	33	VAL
1	k	39	VAL
1	k	54	THR
1	k	57	THR
1	k	58	ILE
1	k	72	THR
1	k	74	GLU
1	k	81	THR
1	k	84	ARG
1	k	89	THR
1	k	94	LEU
1	k	100	ASN
1	k	106	THR
1	k	109	VAL
1	l	5	ILE
1	l	6	LYS
1	l	7	THR
1	l	13	LEU
1	l	14	ASP
1	l	16	SER
1	l	29	ARG
1	l	32	VAL
1	l	36	LEU
1	l	37	ILE
1	l	39	VAL
1	l	43	VAL
1	l	46	ILE
1	l	57	THR
1	l	60	LEU
1	l	62	LYS
1	l	89	THR
1	l	111	GLU
1	l	116	LEU

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Mol	Chain	Res	Type
1	l	117	THR
1	m	4	VAL
1	m	8	VAL
1	m	10	THR
1	m	14	ASP
1	m	21	ASN
1	m	22	ILE
1	m	25	GLU
1	m	27	LEU
1	m	32	VAL
1	m	33	VAL
1	m	37	ILE
1	m	39	VAL
1	m	43	VAL
1	m	46	ILE
1	m	52	PHE
1	m	56	THR
1	m	58	ILE
1	m	72	THR
1	m	73	ILE
1	m	81	THR
1	m	83	ASP
1	m	94	LEU
1	m	98	ASP
1	n	4	VAL
1	n	8	VAL
1	n	10	THR
1	n	12	GLN
1	n	27	LEU
1	n	29	ARG
1	n	32	VAL
1	n	33	VAL
1	n	39	VAL
1	n	54	THR
1	n	57	THR
1	n	58	ILE
1	n	72	THR
1	n	74	GLU
1	n	81	THR
1	n	84	ARG
1	n	89	THR
1	n	94	LEU

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Mol	Chain	Res	Type
1	n	100	ASN
1	n	106	THR
1	n	109	VAL
1	o	5	ILE
1	o	6	LYS
1	o	7	THR
1	o	13	LEU
1	o	14	ASP
1	o	16	SER
1	o	29	ARG
1	o	32	VAL
1	o	36	LEU
1	o	37	ILE
1	o	39	VAL
1	o	43	VAL
1	o	46	ILE
1	o	57	THR
1	o	60	LEU
1	o	62	LYS
1	o	89	THR
1	o	111	GLU
1	o	116	LEU
1	o	117	THR
1	p	4	VAL
1	p	8	VAL
1	p	10	THR
1	p	14	ASP
1	p	21	ASN
1	p	22	ILE
1	p	25	GLU
1	p	27	LEU
1	p	32	VAL
1	p	33	VAL
1	p	37	ILE
1	p	39	VAL
1	p	43	VAL
1	p	46	ILE
1	p	52	PHE
1	p	56	THR
1	p	58	ILE
1	p	72	THR
1	p	73	ILE

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Mol	Chain	Res	Type
1	p	81	THR
1	p	83	ASP
1	p	94	LEU
1	p	98	ASP
1	q	4	VAL
1	q	8	VAL
1	q	10	THR
1	q	12	GLN
1	q	27	LEU
1	q	29	ARG
1	q	32	VAL
1	q	33	VAL
1	q	39	VAL
1	q	54	THR
1	q	57	THR
1	q	58	ILE
1	q	72	THR
1	q	74	GLU
1	q	81	THR
1	q	84	ARG
1	q	89	THR
1	q	94	LEU
1	q	100	ASN
1	q	106	THR
1	q	109	VAL
1	r	5	ILE
1	r	6	LYS
1	r	7	THR
1	r	13	LEU
1	r	14	ASP
1	r	16	SER
1	r	29	ARG
1	r	32	VAL
1	r	36	LEU
1	r	37	ILE
1	r	39	VAL
1	r	43	VAL
1	r	46	ILE
1	r	57	THR
1	r	60	LEU
1	r	62	LYS
1	r	89	THR

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Mol	Chain	Res	Type
1	r	111	GLU
1	r	116	LEU
1	r	117	THR
2	s	15	ILE
2	s	24	TYR
2	s	50	PHE
2	s	52	ASN
2	s	66	ILE
2	s	78	TYR
2	s	82	THR
2	s	88	VAL
2	s	97	GLN
2	s	98	VAL
2	s	109	THR
2	s	119	VAL
2	s	121	VAL
2	s	141	VAL
2	s	143	LEU
2	s	161	TYR
2	s	170	ASN
2	s	174	VAL
2	s	177	TYR
2	s	188	VAL
2	s	200	LEU
2	s	211	TRP
2	s	213	VAL
2	s	215	VAL
2	s	220	ILE
2	s	234	THR
2	s	235	THR
2	s	237	ASP
2	s	250	TYR
2	s	256	LYS
2	s	265	TYR
2	s	272	ASP
2	s	287	GLU
2	s	288	ARG
2	s	292	THR
2	s	297	TRP
2	s	298	ASN
2	s	303	VAL
2	s	304	LEU

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Mol	Chain	Res	Type
2	s	312	LEU
2	s	324	TRP
2	s	326	GLU
2	s	330	LYS
2	s	335	VAL
2	s	337	THR
2	s	348	ILE
2	s	353	PHE
2	s	357	ARG
2	s	371	THR
2	s	378	TYR
2	s	387	ASP
2	s	393	VAL
2	s	397	THR
2	s	399	ARG
2	s	407	VAL
2	s	413	LEU
2	s	430	LEU
2	s	436	GLU
2	s	441	THR
2	s	442	GLN
2	s	457	ASN
2	s	458	VAL
2	s	460	PHE
2	s	476	VAL
2	s	479	VAL
2	s	482	VAL
2	s	486	GLU
2	s	490	SER
2	s	495	TYR
2	s	496	ILE
2	s	504	CYS
2	s	514	VAL
2	s	515	LEU
2	s	525	MET
2	s	530	TYR
2	s	542	HIS
2	s	552	LEU
2	s	567	ASN
2	s	581	ASN
2	s	583	ILE
2	s	590	TYR

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Mol	Chain	Res	Type
2	s	591	ARG
2	s	593	PHE
2	s	595	ASP
2	s	600	TYR
2	s	602	ILE
2	s	611	THR
2	s	618	ILE
2	s	621	ILE
2	s	632	THR
2	s	641	THR
2	s	642	VAL
2	s	657	ARG
2	s	658	LEU
2	s	669	ILE
2	s	673	ILE
2	s	683	LEU
2	s	698	ILE
2	s	703	LEU
2	s	715	THR
2	s	730	THR
2	s	740	THR
2	s	741	LEU
2	s	746	LEU
2	s	748	LEU
2	s	757	VAL
2	s	765	THR
2	s	766	VAL
2	s	768	ILE
2	s	772	GLU
2	s	779	ILE
2	s	790	ARG
2	t	15	ILE
2	t	24	TYR
2	t	50	PHE
2	t	52	ASN
2	t	66	ILE
2	t	78	TYR
2	t	82	THR
2	t	88	VAL
2	t	97	GLN
2	t	98	VAL
2	t	109	THR

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Mol	Chain	Res	Type
2	t	119	VAL
2	t	121	VAL
2	t	141	VAL
2	t	143	LEU
2	t	161	TYR
2	t	170	ASN
2	t	174	VAL
2	t	177	TYR
2	t	188	VAL
2	t	200	LEU
2	t	211	TRP
2	t	213	VAL
2	t	215	VAL
2	t	220	ILE
2	t	234	THR
2	t	235	THR
2	t	237	ASP
2	t	250	TYR
2	t	256	LYS
2	t	265	TYR
2	t	272	ASP
2	t	287	GLU
2	t	288	ARG
2	t	292	THR
2	t	297	TRP
2	t	298	ASN
2	t	303	VAL
2	t	304	LEU
2	t	312	LEU
2	t	324	TRP
2	t	326	GLU
2	t	330	LYS
2	t	335	VAL
2	t	337	THR
2	t	348	ILE
2	t	353	PHE
2	t	357	ARG
2	t	371	THR
2	t	378	TYR
2	t	387	ASP
2	t	393	VAL
2	t	397	THR

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Mol	Chain	Res	Type
2	t	399	ARG
2	t	407	VAL
2	t	413	LEU
2	t	430	LEU
2	t	436	GLU
2	t	441	THR
2	t	442	GLN
2	t	457	ASN
2	t	458	VAL
2	t	460	PHE
2	t	476	VAL
2	t	479	VAL
2	t	482	VAL
2	t	486	GLU
2	t	490	SER
2	t	495	TYR
2	t	496	ILE
2	t	504	CYS
2	t	514	VAL
2	t	515	LEU
2	t	525	MET
2	t	530	TYR
2	t	542	HIS
2	t	552	LEU
2	t	567	ASN
2	t	581	ASN
2	t	583	ILE
2	t	590	TYR
2	t	591	ARG
2	t	593	PHE
2	t	595	ASP
2	t	600	TYR
2	t	602	ILE
2	t	606	THR
2	t	611	THR
2	t	618	ILE
2	t	621	ILE
2	t	632	THR
2	t	641	THR
2	t	642	VAL
2	t	657	ARG
2	t	658	LEU

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Mol	Chain	Res	Type
2	t	669	ILE
2	t	673	ILE
2	t	683	LEU
2	t	698	ILE
2	t	703	LEU
2	t	715	THR
2	t	730	THR
2	t	740	THR
2	t	741	LEU
2	t	746	LEU
2	t	748	LEU
2	t	757	VAL
2	t	765	THR
2	t	766	VAL
2	t	768	ILE
2	t	772	GLU
2	t	779	ILE
2	t	790	ARG
2	u	15	ILE
2	u	24	TYR
2	u	50	PHE
2	u	52	ASN
2	u	66	ILE
2	u	78	TYR
2	u	82	THR
2	u	88	VAL
2	u	97	GLN
2	u	98	VAL
2	u	109	THR
2	u	119	VAL
2	u	121	VAL
2	u	141	VAL
2	u	143	LEU
2	u	161	TYR
2	u	170	ASN
2	u	174	VAL
2	u	177	TYR
2	u	188	VAL
2	u	200	LEU
2	u	211	TRP
2	u	213	VAL
2	u	215	VAL

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Mol	Chain	Res	Type
2	u	220	ILE
2	u	234	THR
2	u	235	THR
2	u	237	ASP
2	u	250	TYR
2	u	256	LYS
2	u	265	TYR
2	u	272	ASP
2	u	287	GLU
2	u	288	ARG
2	u	292	THR
2	u	297	TRP
2	u	298	ASN
2	u	303	VAL
2	u	304	LEU
2	u	312	LEU
2	u	324	TRP
2	u	326	GLU
2	u	330	LYS
2	u	335	VAL
2	u	337	THR
2	u	348	ILE
2	u	353	PHE
2	u	357	ARG
2	u	371	THR
2	u	378	TYR
2	u	387	ASP
2	u	393	VAL
2	u	397	THR
2	u	399	ARG
2	u	407	VAL
2	u	413	LEU
2	u	430	LEU
2	u	436	GLU
2	u	441	THR
2	u	442	GLN
2	u	457	ASN
2	u	458	VAL
2	u	460	PHE
2	u	479	VAL
2	u	482	VAL
2	u	486	GLU

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Mol	Chain	Res	Type
2	u	490	SER
2	u	495	TYR
2	u	496	ILE
2	u	504	CYS
2	u	514	VAL
2	u	515	LEU
2	u	525	MET
2	u	530	TYR
2	u	542	HIS
2	u	552	LEU
2	u	567	ASN
2	u	581	ASN
2	u	583	ILE
2	u	590	TYR
2	u	591	ARG
2	u	593	PHE
2	u	595	ASP
2	u	600	TYR
2	u	602	ILE
2	u	606	THR
2	u	611	THR
2	u	618	ILE
2	u	621	ILE
2	u	632	THR
2	u	641	THR
2	u	642	VAL
2	u	657	ARG
2	u	658	LEU
2	u	669	ILE
2	u	673	ILE
2	u	683	LEU
2	u	698	ILE
2	u	703	LEU
2	u	715	THR
2	u	730	THR
2	u	740	THR
2	u	741	LEU
2	u	746	LEU
2	u	748	LEU
2	u	757	VAL
2	u	765	THR
2	u	766	VAL

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Mol	Chain	Res	Type
2	u	768	ILE
2	u	772	GLU
2	u	779	ILE
2	u	790	ARG
2	v	15	ILE
2	v	24	TYR
2	v	50	PHE
2	v	52	ASN
2	v	66	ILE
2	v	78	TYR
2	v	82	THR
2	v	88	VAL
2	v	97	GLN
2	v	98	VAL
2	v	109	THR
2	v	119	VAL
2	v	121	VAL
2	v	141	VAL
2	v	143	LEU
2	v	161	TYR
2	v	170	ASN
2	v	174	VAL
2	v	177	TYR
2	v	188	VAL
2	v	200	LEU
2	v	211	TRP
2	v	213	VAL
2	v	215	VAL
2	v	220	ILE
2	v	234	THR
2	v	235	THR
2	v	237	ASP
2	v	250	TYR
2	v	256	LYS
2	v	265	TYR
2	v	272	ASP
2	v	287	GLU
2	v	288	ARG
2	v	292	THR
2	v	297	TRP
2	v	298	ASN
2	v	303	VAL

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Mol	Chain	Res	Type
2	v	304	LEU
2	v	312	LEU
2	v	324	TRP
2	v	326	GLU
2	v	330	LYS
2	v	335	VAL
2	v	337	THR
2	v	348	ILE
2	v	353	PHE
2	v	357	ARG
2	v	371	THR
2	v	378	TYR
2	v	387	ASP
2	v	393	VAL
2	v	397	THR
2	v	399	ARG
2	v	407	VAL
2	v	413	LEU
2	v	430	LEU
2	v	436	GLU
2	v	441	THR
2	v	442	GLN
2	v	457	ASN
2	v	458	VAL
2	v	460	PHE
2	v	476	VAL
2	v	479	VAL
2	v	482	VAL
2	v	486	GLU
2	v	490	SER
2	v	495	TYR
2	v	496	ILE
2	v	504	CYS
2	v	514	VAL
2	v	515	LEU
2	v	525	MET
2	v	530	TYR
2	v	542	HIS
2	v	552	LEU
2	v	567	ASN
2	v	581	ASN
2	v	583	ILE

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Mol	Chain	Res	Type
2	v	590	TYR
2	v	591	ARG
2	v	593	PHE
2	v	595	ASP
2	v	600	TYR
2	v	602	ILE
2	v	606	THR
2	v	611	THR
2	v	618	ILE
2	v	621	ILE
2	v	632	THR
2	v	641	THR
2	v	642	VAL
2	v	657	ARG
2	v	658	LEU
2	v	669	ILE
2	v	673	ILE
2	v	683	LEU
2	v	698	ILE
2	v	703	LEU
2	v	715	THR
2	v	730	THR
2	v	740	THR
2	v	741	LEU
2	v	746	LEU
2	v	748	LEU
2	v	757	VAL
2	v	765	THR
2	v	766	VAL
2	v	768	ILE
2	v	772	GLU
2	v	779	ILE
2	v	790	ARG
2	w	15	ILE
2	w	24	TYR
2	w	50	PHE
2	w	52	ASN
2	w	66	ILE
2	w	78	TYR
2	w	82	THR
2	w	88	VAL
2	w	97	GLN

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Mol	Chain	Res	Type
2	w	98	VAL
2	w	109	THR
2	w	119	VAL
2	w	121	VAL
2	w	141	VAL
2	w	143	LEU
2	w	161	TYR
2	w	170	ASN
2	w	174	VAL
2	w	177	TYR
2	w	188	VAL
2	w	200	LEU
2	w	211	TRP
2	w	213	VAL
2	w	215	VAL
2	w	220	ILE
2	w	234	THR
2	w	235	THR
2	w	237	ASP
2	w	250	TYR
2	w	256	LYS
2	w	265	TYR
2	w	272	ASP
2	w	287	GLU
2	w	288	ARG
2	w	292	THR
2	w	297	TRP
2	w	298	ASN
2	w	303	VAL
2	w	304	LEU
2	w	312	LEU
2	w	324	TRP
2	w	326	GLU
2	w	330	LYS
2	w	335	VAL
2	w	337	THR
2	w	348	ILE
2	w	353	PHE
2	w	357	ARG
2	w	371	THR
2	w	378	TYR
2	w	387	ASP

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Mol	Chain	Res	Type
2	w	393	VAL
2	w	397	THR
2	w	399	ARG
2	w	407	VAL
2	w	413	LEU
2	w	430	LEU
2	w	436	GLU
2	w	441	THR
2	w	442	GLN
2	w	457	ASN
2	w	458	VAL
2	w	460	PHE
2	w	476	VAL
2	w	479	VAL
2	w	482	VAL
2	w	486	GLU
2	w	490	SER
2	w	495	TYR
2	w	496	ILE
2	w	504	CYS
2	w	514	VAL
2	w	515	LEU
2	w	525	MET
2	w	530	TYR
2	w	542	HIS
2	w	552	LEU
2	w	567	ASN
2	w	581	ASN
2	w	583	ILE
2	w	590	TYR
2	w	591	ARG
2	w	593	PHE
2	w	595	ASP
2	w	600	TYR
2	w	602	ILE
2	w	606	THR
2	w	611	THR
2	w	618	ILE
2	w	621	ILE
2	w	632	THR
2	w	641	THR
2	w	642	VAL

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Mol	Chain	Res	Type
2	w	657	ARG
2	w	658	LEU
2	w	669	ILE
2	w	673	ILE
2	w	683	LEU
2	w	698	ILE
2	w	703	LEU
2	w	715	THR
2	w	730	THR
2	w	740	THR
2	w	741	LEU
2	w	746	LEU
2	w	748	LEU
2	w	757	VAL
2	w	765	THR
2	w	766	VAL
2	w	768	ILE
2	w	772	GLU
2	w	779	ILE
2	w	790	ARG
2	x	15	ILE
2	x	24	TYR
2	x	50	PHE
2	x	52	ASN
2	x	66	ILE
2	x	78	TYR
2	x	82	THR
2	x	88	VAL
2	x	97	GLN
2	x	98	VAL
2	x	109	THR
2	x	119	VAL
2	x	121	VAL
2	x	141	VAL
2	x	143	LEU
2	x	161	TYR
2	x	170	ASN
2	x	174	VAL
2	x	177	TYR
2	x	188	VAL
2	x	200	LEU
2	x	211	TRP

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Mol	Chain	Res	Type
2	x	213	VAL
2	x	215	VAL
2	x	220	ILE
2	x	234	THR
2	x	235	THR
2	x	237	ASP
2	x	250	TYR
2	x	256	LYS
2	x	265	TYR
2	x	272	ASP
2	x	287	GLU
2	x	288	ARG
2	x	292	THR
2	x	297	TRP
2	x	298	ASN
2	x	303	VAL
2	x	304	LEU
2	x	312	LEU
2	x	324	TRP
2	x	326	GLU
2	x	330	LYS
2	x	335	VAL
2	x	337	THR
2	x	348	ILE
2	x	353	PHE
2	x	357	ARG
2	x	371	THR
2	x	378	TYR
2	x	387	ASP
2	x	393	VAL
2	x	397	THR
2	x	399	ARG
2	x	407	VAL
2	x	413	LEU
2	x	430	LEU
2	x	436	GLU
2	x	441	THR
2	x	442	GLN
2	x	457	ASN
2	x	458	VAL
2	x	460	PHE
2	x	476	VAL

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Mol	Chain	Res	Type
2	x	479	VAL
2	x	482	VAL
2	x	486	GLU
2	x	490	SER
2	x	495	TYR
2	x	496	ILE
2	x	504	CYS
2	x	514	VAL
2	x	515	LEU
2	x	525	MET
2	x	530	TYR
2	x	542	HIS
2	x	552	LEU
2	x	567	ASN
2	x	581	ASN
2	x	583	ILE
2	x	590	TYR
2	x	591	ARG
2	x	593	PHE
2	x	595	ASP
2	x	600	TYR
2	x	602	ILE
2	x	611	THR
2	x	618	ILE
2	x	621	ILE
2	x	632	THR
2	x	641	THR
2	x	642	VAL
2	x	657	ARG
2	x	658	LEU
2	x	669	ILE
2	x	673	ILE
2	x	683	LEU
2	x	698	ILE
2	x	703	LEU
2	x	715	THR
2	x	730	THR
2	x	740	THR
2	x	741	LEU
2	x	746	LEU
2	x	748	LEU
2	x	757	VAL

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Mol	Chain	Res	Type
2	x	765	THR
2	x	766	VAL
2	x	768	ILE
2	x	772	GLU
2	x	779	ILE
2	x	790	ARG
3	A	43	ARG
3	A	90	LEU
3	B	90	LEU
3	B	91	GLU
3	B	125	PHE
3	C	91	GLU
3	C	108	ARG
3	C	125	PHE
3	C	129	LEU
3	D	82	ARG
3	D	90	LEU
3	E	90	LEU
3	E	128	GLN
3	E	129	LEU
3	F	90	LEU
3	F	125	PHE
3	F	129	LEU
4	M	6	MET
4	M	24	ILE
4	M	53	GLN
4	M	57	ARG
4	M	73	VAL
4	M	77	LEU
4	M	160	LEU
4	M	163	GLU
4	M	181	TYR
4	M	187	ASP
4	M	190	THR
4	N	6	MET
4	N	7	ASN
4	N	24	ILE
4	N	26	GLU
4	N	39	ASP
4	N	68	THR
4	N	73	VAL
4	N	77	LEU

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Mol	Chain	Res	Type
4	N	170	LEU
4	N	171	CYS
4	N	175	GLU
4	N	178	TYR
4	N	184	LEU
4	N	190	THR
4	O	10	THR
4	O	24	ILE
4	O	53	GLN
4	O	57	ARG
4	O	73	VAL
4	O	77	LEU
4	O	160	LEU
4	O	163	GLU
4	O	181	TYR
4	O	187	ASP
4	O	190	THR
4	P	24	ILE
4	P	26	GLU
4	P	39	ASP
4	P	68	THR
4	P	73	VAL
4	P	77	LEU
4	P	170	LEU
4	P	171	CYS
4	P	175	GLU
4	P	178	TYR
4	P	184	LEU
4	P	190	THR
4	Q	6	MET
4	Q	24	ILE
4	Q	53	GLN
4	Q	57	ARG
4	Q	73	VAL
4	Q	77	LEU
4	Q	160	LEU
4	Q	163	GLU
4	Q	181	TYR
4	Q	187	ASP
4	Q	190	THR
4	R	6	MET
4	R	7	ASN

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Mol	Chain	Res	Type
4	R	24	ILE
4	R	26	GLU
4	R	39	ASP
4	R	68	THR
4	R	73	VAL
4	R	77	LEU
4	R	170	LEU
4	R	171	CYS
4	R	175	GLU
4	R	178	TYR
4	R	184	LEU
4	R	190	THR
4	S	6	MET
4	S	24	ILE
4	S	53	GLN
4	S	57	ARG
4	S	73	VAL
4	S	77	LEU
4	S	160	LEU
4	S	163	GLU
4	S	181	TYR
4	S	187	ASP
4	S	190	THR
4	T	6	MET
4	T	7	ASN
4	T	24	ILE
4	T	26	GLU
4	T	39	ASP
4	T	68	THR
4	T	73	VAL
4	T	77	LEU
4	T	144	ARG
4	T	170	LEU
4	T	171	CYS
4	T	175	GLU
4	T	178	TYR
4	T	184	LEU
4	T	190	THR
4	U	6	MET
4	U	24	ILE
4	U	53	GLN
4	U	57	ARG

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Mol	Chain	Res	Type
4	U	73	VAL
4	U	77	LEU
4	U	160	LEU
4	U	163	GLU
4	U	181	TYR
4	U	187	ASP
4	U	190	THR
4	V	6	MET
4	V	7	ASN
4	V	24	ILE
4	V	26	GLU
4	V	39	ASP
4	V	68	THR
4	V	73	VAL
4	V	77	LEU
4	V	170	LEU
4	V	171	CYS
4	V	175	GLU
4	V	178	TYR
4	V	184	LEU
4	V	190	THR
4	W	6	MET
4	W	10	THR
4	W	24	ILE
4	W	53	GLN
4	W	57	ARG
4	W	73	VAL
4	W	77	LEU
4	W	160	LEU
4	W	163	GLU
4	W	181	TYR
4	W	187	ASP
4	W	190	THR
4	X	6	MET
4	X	7	ASN
4	X	24	ILE
4	X	26	GLU
4	X	39	ASP
4	X	52	ARG
4	X	68	THR
4	X	73	VAL
4	X	77	LEU

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Mol	Chain	Res	Type
4	X	170	LEU
4	X	171	CYS
4	X	175	GLU
4	X	178	TYR
4	X	184	LEU
4	X	190	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (182) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	3	ASN
1	a	108	HIS
1	b	12	GLN
1	c	3	ASN
1	c	100	ASN
1	d	3	ASN
1	d	108	HIS
1	e	12	GLN
1	f	3	ASN
1	f	100	ASN
1	g	3	ASN
1	g	108	HIS
1	h	12	GLN
1	i	3	ASN
1	i	100	ASN
1	j	3	ASN
1	j	108	HIS
1	k	12	GLN
1	l	3	ASN
1	l	100	ASN
1	m	3	ASN
1	m	108	HIS
1	n	12	GLN
1	o	3	ASN
1	o	100	ASN
1	p	3	ASN
1	p	108	HIS
1	q	12	GLN
1	r	3	ASN
1	r	100	ASN
2	s	52	ASN
2	s	97	GLN

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Mol	Chain	Res	Type
2	s	137	ASN
2	s	147	ASN
2	s	170	ASN
2	s	184	GLN
2	s	229	GLN
2	s	319	ASN
2	s	384	ASN
2	s	494	ASN
2	s	538	GLN
2	s	567	ASN
2	s	581	ASN
2	s	651	ASN
2	s	723	GLN
2	s	726	ASN
2	t	52	ASN
2	t	97	GLN
2	t	137	ASN
2	t	147	ASN
2	t	170	ASN
2	t	184	GLN
2	t	229	GLN
2	t	242	GLN
2	t	319	ASN
2	t	356	ASN
2	t	494	ASN
2	t	538	GLN
2	t	567	ASN
2	t	581	ASN
2	t	651	ASN
2	t	723	GLN
2	t	726	ASN
2	u	52	ASN
2	u	97	GLN
2	u	137	ASN
2	u	147	ASN
2	u	170	ASN
2	u	184	GLN
2	u	229	GLN
2	u	319	ASN
2	u	384	ASN
2	u	494	ASN
2	u	538	GLN

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Mol	Chain	Res	Type
2	u	567	ASN
2	u	581	ASN
2	u	651	ASN
2	u	723	GLN
2	u	726	ASN
2	v	52	ASN
2	v	97	GLN
2	v	137	ASN
2	v	147	ASN
2	v	170	ASN
2	v	184	GLN
2	v	229	GLN
2	v	319	ASN
2	v	384	ASN
2	v	494	ASN
2	v	538	GLN
2	v	567	ASN
2	v	581	ASN
2	v	651	ASN
2	v	723	GLN
2	v	726	ASN
2	w	52	ASN
2	w	97	GLN
2	w	137	ASN
2	w	147	ASN
2	w	170	ASN
2	w	184	GLN
2	w	229	GLN
2	w	319	ASN
2	w	384	ASN
2	w	494	ASN
2	w	538	GLN
2	w	567	ASN
2	w	581	ASN
2	w	651	ASN
2	w	723	GLN
2	w	726	ASN
2	x	52	ASN
2	x	97	GLN
2	x	137	ASN
2	x	147	ASN
2	x	170	ASN

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Mol	Chain	Res	Type
2	x	184	GLN
2	x	229	GLN
2	x	319	ASN
2	x	384	ASN
2	x	494	ASN
2	x	538	GLN
2	x	567	ASN
2	x	581	ASN
2	x	651	ASN
2	x	723	GLN
2	x	726	ASN
3	A	44	GLN
3	A	138	GLN
3	B	44	GLN
3	B	138	GLN
3	C	44	GLN
3	C	138	GLN
3	D	44	GLN
3	D	138	GLN
3	E	44	GLN
3	E	138	GLN
3	F	44	GLN
3	F	138	GLN
4	M	53	GLN
4	M	76	ASN
4	N	51	ASN
4	N	55	GLN
4	N	76	ASN
4	N	109	GLN
4	N	147	ASN
4	O	53	GLN
4	O	76	ASN
4	P	7	ASN
4	P	51	ASN
4	P	55	GLN
4	P	76	ASN
4	P	109	GLN
4	P	147	ASN
4	Q	53	GLN
4	Q	76	ASN
4	R	51	ASN
4	R	55	GLN

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Mol	Chain	Res	Type
4	R	76	ASN
4	R	109	GLN
4	R	147	ASN
4	S	53	GLN
4	S	76	ASN
4	T	51	ASN
4	T	55	GLN
4	T	76	ASN
4	T	109	GLN
4	T	147	ASN
4	U	53	GLN
4	U	76	ASN
4	V	51	ASN
4	V	55	GLN
4	V	76	ASN
4	V	109	GLN
4	V	147	ASN
4	W	53	GLN
4	W	76	ASN
4	X	51	ASN
4	X	55	GLN
4	X	76	ASN
4	X	109	GLN
4	X	147	ASN

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

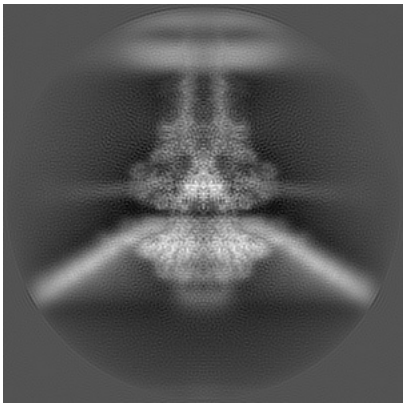
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31321. These allow visual inspection of the internal detail of the map and identification of artifacts.

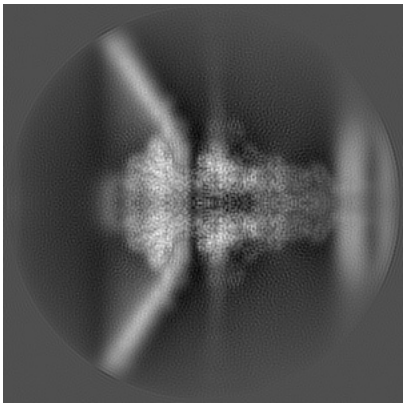
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

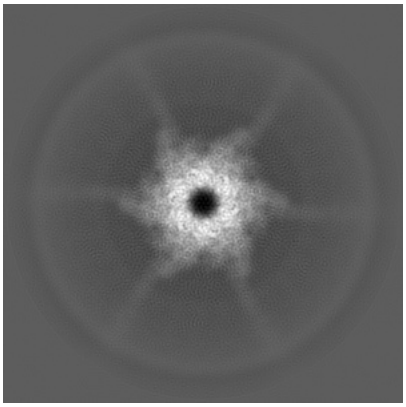
6.1.1 Primary map



X



Y

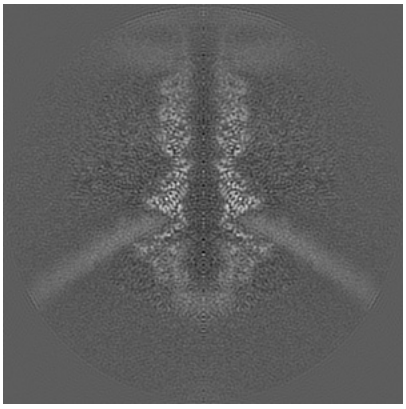


Z

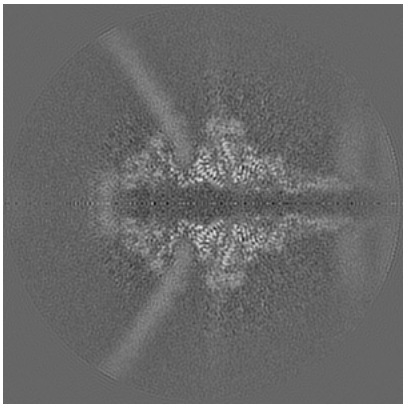
The images above show the map projected in three orthogonal directions.

6.2 Central slices

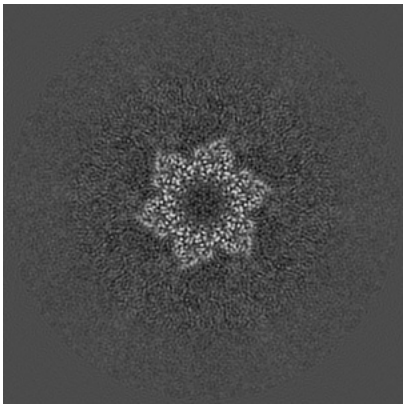
6.2.1 Primary map



X Index: 200



Y Index: 200

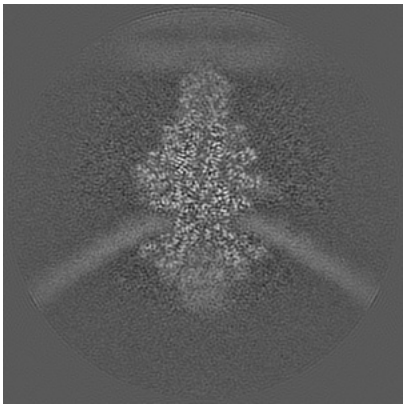


Z Index: 200

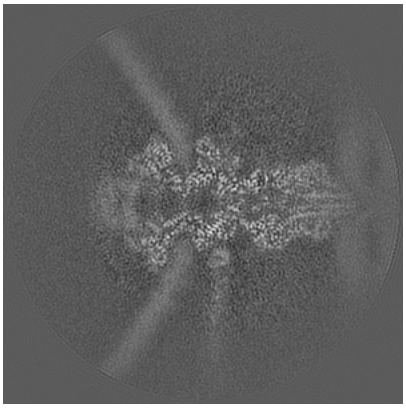
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

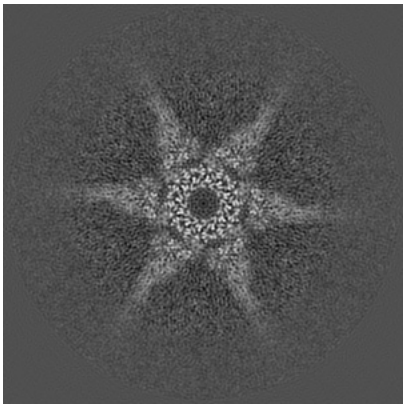
6.3.1 Primary map



X Index: 177



Y Index: 216

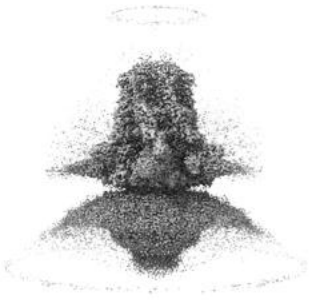


Z Index: 217

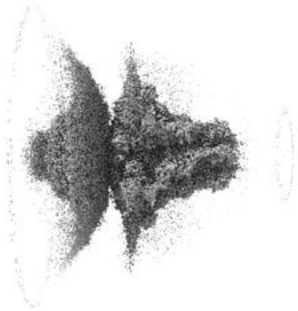
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

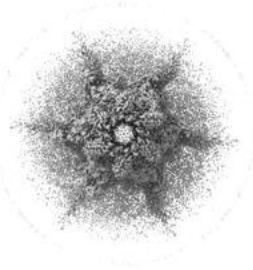
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

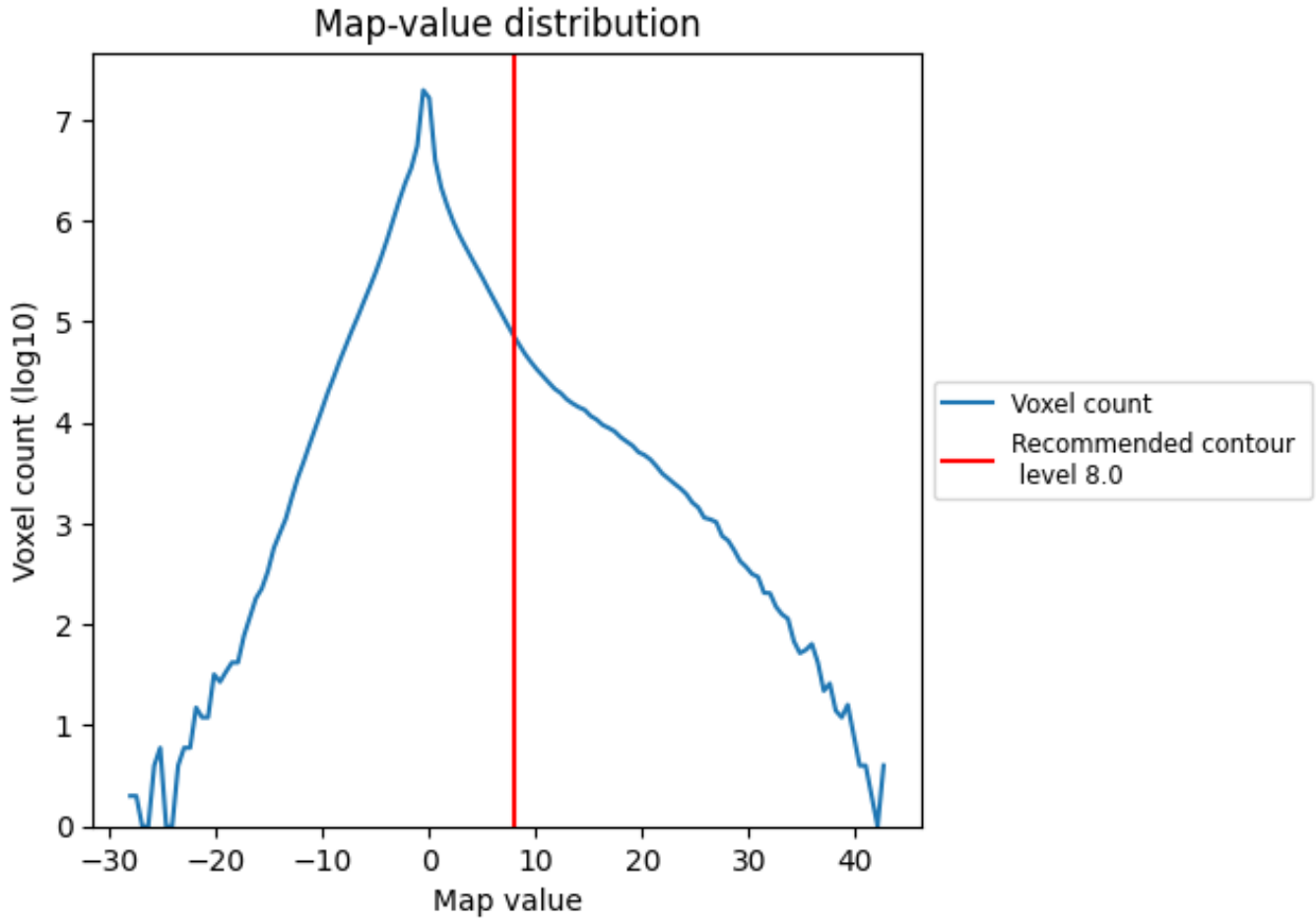
6.5 Mask visualisation (i)

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

7 Map analysis

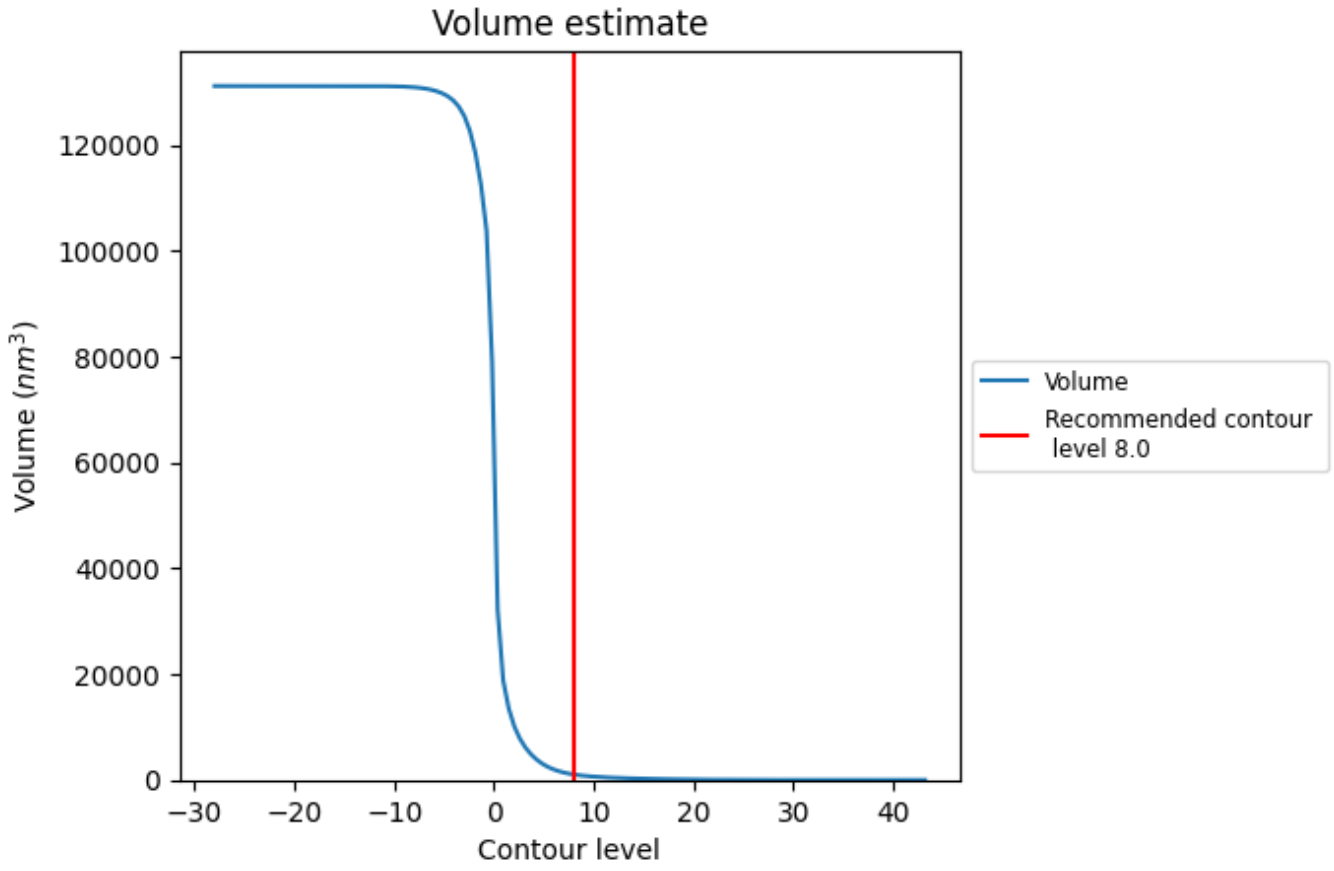
This section contains the results of statistical analysis of the map.

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.

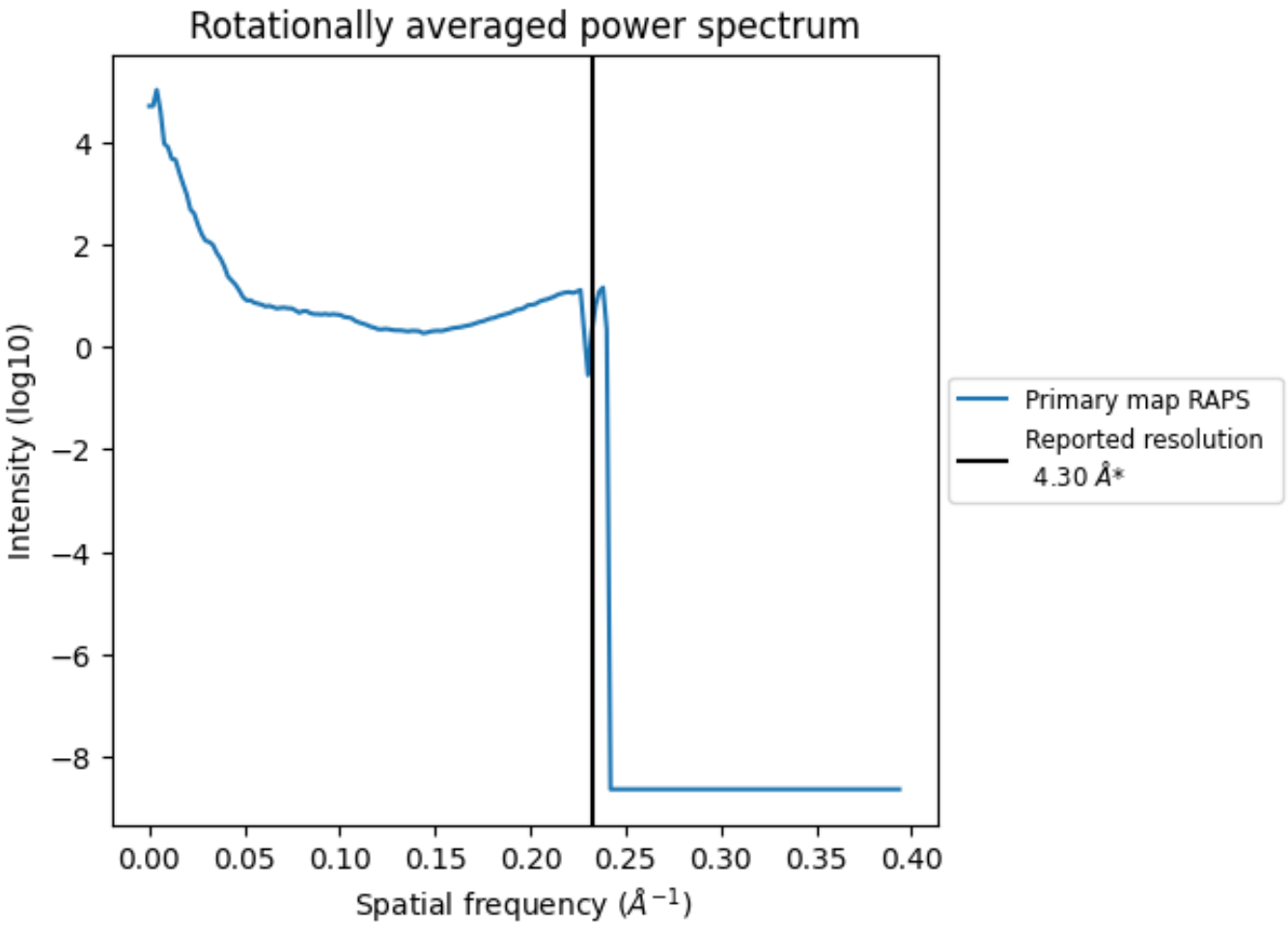
7.2 Volume estimate



The volume at the recommended contour level is 1038 nm^3; this corresponds to an approximate mass of 938 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 0.233 Å^{-1}

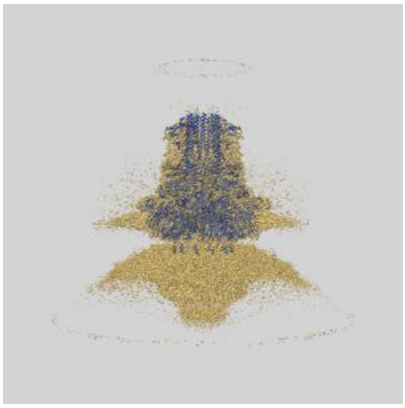
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

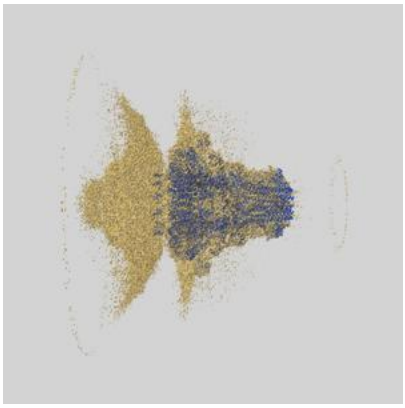
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31321 and PDB model 7EY7. Per-residue inclusion information can be found in section 3 on page 8.

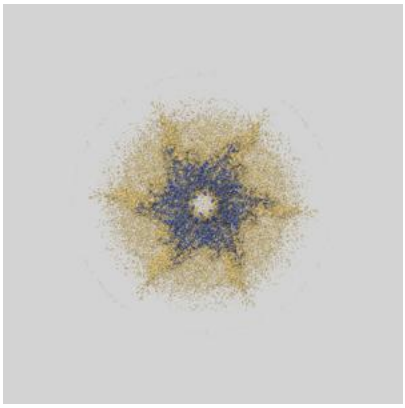
9.1 Map-model overlay



X



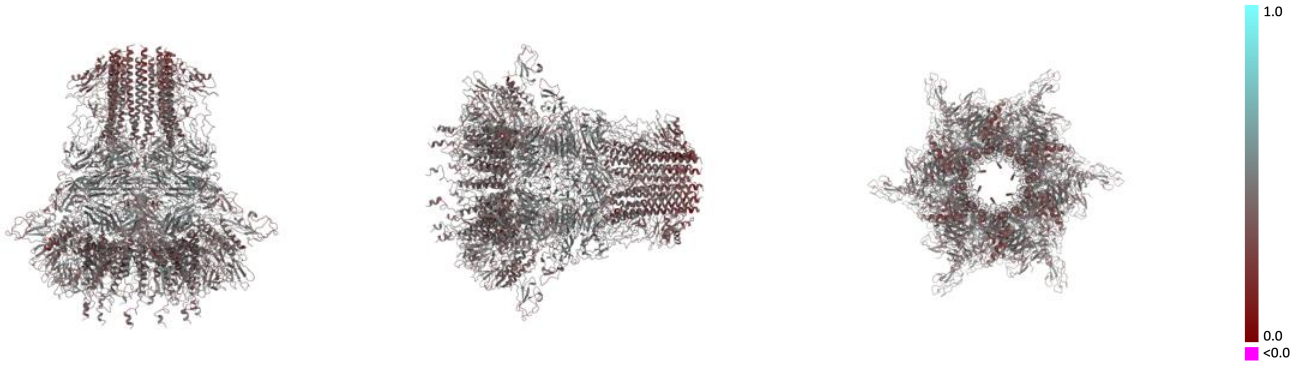
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

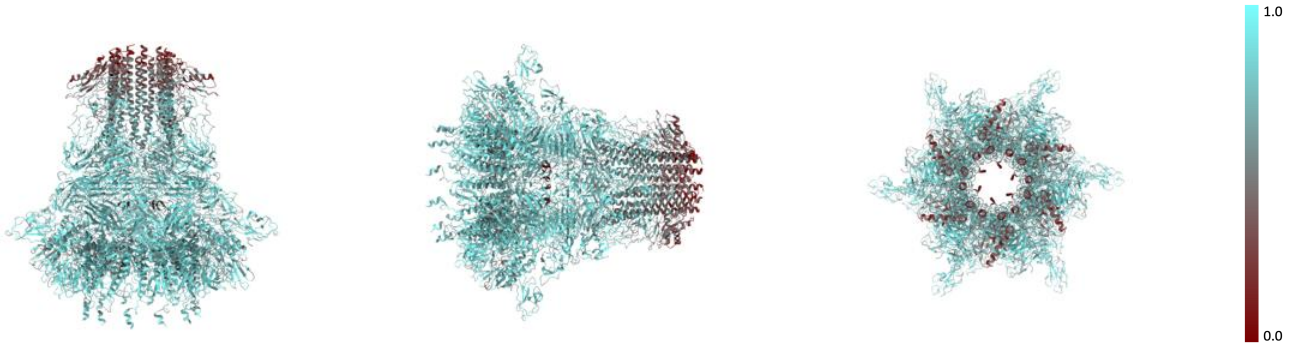
9.2 Q-score mapped to coordinate model



X Y Z

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.

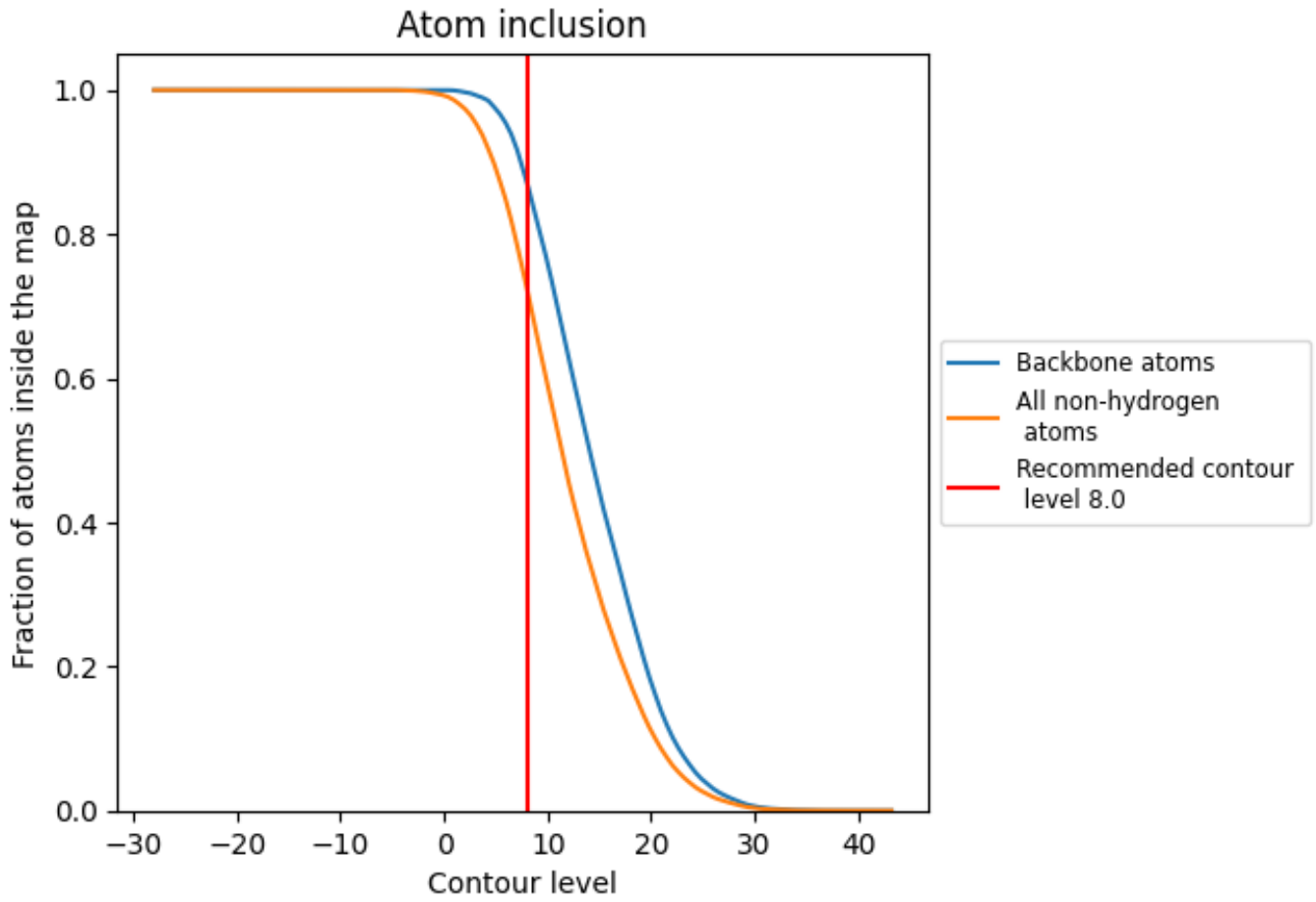
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (8.0).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 72% 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 (8.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7247	0.4200
A	0.5176	0.3430
B	0.5150	0.3450
C	0.5189	0.3450
D	0.5397	0.3540
E	0.5163	0.3450
F	0.5202	0.3530
M	0.7661	0.4190
N	0.7755	0.4130
O	0.7647	0.4190
P	0.7741	0.4120
Q	0.7641	0.4180
R	0.7802	0.4130
S	0.7674	0.4180
T	0.7768	0.4150
U	0.7647	0.4190
V	0.7721	0.4150
W	0.7641	0.4190
X	0.7842	0.4130
a	0.7991	0.4370
b	0.6942	0.4050
c	0.7589	0.4100
d	0.7924	0.4330
e	0.6886	0.4000
f	0.7533	0.4070
g	0.7935	0.4360
h	0.6931	0.4020
i	0.7511	0.4080
j	0.7969	0.4400
k	0.6886	0.4040
l	0.7567	0.4110
m	0.7946	0.4370
n	0.6853	0.4000
o	0.7511	0.4050
p	0.7924	0.4370

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Chain	Atom inclusion	Q-score
q	0.6942	0.4040
r	0.7522	0.4050
s	0.7190	0.4340
t	0.7173	0.4310
u	0.7165	0.4320
v	0.7190	0.4340
w	0.7194	0.4320
x	0.7165	0.4320