



wwPDB EM Validation Summary Report ⓘ

Jun 18, 2025 – 02:54 PM JST

PDB ID : 9JZ0 / pdb_00009jz0
EMDB ID : EMD-61911
Title : portal-tail complex of DNA-ejected T7
Authors : Liu, H.R.; Chen, W.Y.
Deposited on : 2024-10-13
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

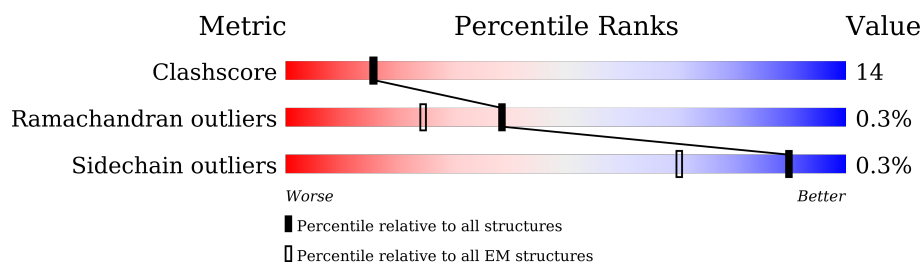
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	196	48% 13% 39%
1	1	196	46% 14% 39%
1	Y	196	41% 19% 39%
1	Z	196	45% 15% 39%
1	y	196	48% 12% 39%
1	z	196	46% 14% 39%
2	2	88	25% 10% 65%
2	3	88	26% 9% 65%
2	4	88	25% 10% 65%












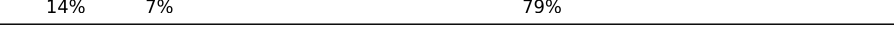







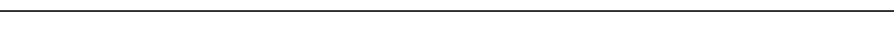

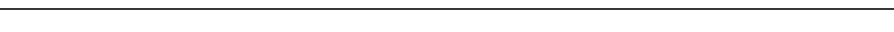
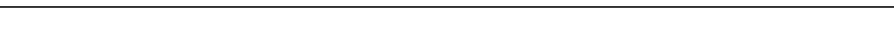


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Mol	Chain	Length	Quality of chain
2	5	88	
2	6	88	
2	7	88	
2	8	88	
2	9	88	
2	AA	88	
2	AB	88	
2	AC	88	
2	AD	88	
3	A	536	
3	B	536	
3	C	536	
3	D	536	
3	E	536	
3	F	536	
3	G	536	
3	H	536	
3	I	536	
3	J	536	
3	K	536	
3	L	536	
4	M	196	
4	N	196	
4	O	196	
4	P	196	


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Mol	Chain	Length	Quality of chain
4	Q	196	 74%26%
4	R	196	 78%21%.
4	S	196	 76%24%
4	T	196	 73%26%.
4	U	196	 72%28%
4	V	196	 72%27%.
4	W	196	 76%24%
4	X	196	 76%23%.
5	a	553	 14%7%79%
5	b	553	 12%9%80%
5	c	553	 12%8%80%
5	d	553	 14%7%79%
5	e	553	 12%8%80%
5	f	553	 12%9%80%
5	g	553	 15%6%79%
5	h	553	 12%8%80%
5	i	553	 14%7%80%
5	j	553	 15%6%79%
5	k	553	 11%9%.80%
5	l	553	 12%8%80%
5	m	553	 15%6%79%
5	n	553	 11%9%80%
5	o	553	 13%8%80%
5	p	553	 15%6%79%
5	q	553	 11%9%80%

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Mol	Chain	Length	Quality of chain
5	r	553	 12% 8% 80%
6	s	794	 57% 42% .
6	t	794	 56% 43% ..
6	u	794	 57% 42% ..
6	v	794	 56% 43% ...
6	w	794	 57% 41% ..
6	x	794	 56% 42% ...

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 122376 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 Internal virion protein gp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	119	Total	C	N	O	S	0	0
			920	556	172	185	7		
1	1	119	Total	C	N	O	S	0	0
			920	556	172	185	7		
1	Y	119	Total	C	N	O	S	0	0
			920	556	172	185	7		
1	Z	119	Total	C	N	O	S	0	0
			920	556	172	185	7		
1	y	119	Total	C	N	O	S	0	0
			920	556	172	185	7		
1	z	119	Total	C	N	O	S	0	0
			920	556	172	185	7		

- Molecule 2 is a protein called Protein 6.7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	31	Total	C	N	O	S	0	0
			231	139	38	53	1		
2	3	31	Total	C	N	O	S	0	0
			231	139	38	53	1		
2	4	31	Total	C	N	O	S	0	0
			231	139	38	53	1		
2	5	31	Total	C	N	O	S	0	0
			231	139	38	53	1		
2	6	31	Total	C	N	O	S	0	0
			231	139	38	53	1		
2	7	31	Total	C	N	O	S	0	0
			231	139	38	53	1		
2	8	49	Total	C	N	O	S	0	0
			368	219	64	84	1		
2	9	49	Total	C	N	O	S	0	0
			368	219	64	84	1		
2	AA	49	Total	C	N	O	S	0	0
			368	219	64	84	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	49	Total	C	N	O	S	0	0
			368	219	64	84	1		
2	AC	49	Total	C	N	O	S	0	0
			368	219	64	84	1		
2	AD	49	Total	C	N	O	S	0	0
			368	219	64	84	1		

- Molecule 3 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	429	Total	C	N	O	S	0	0
			3363	2120	562	667	14		
3	B	431	Total	C	N	O	S	0	0
			3378	2128	567	669	14		
3	C	429	Total	C	N	O	S	0	0
			3363	2120	562	667	14		
3	D	431	Total	C	N	O	S	0	0
			3378	2128	567	669	14		
3	E	429	Total	C	N	O	S	0	0
			3363	2120	562	667	14		
3	F	431	Total	C	N	O	S	0	0
			3378	2128	567	669	14		
3	G	429	Total	C	N	O	S	0	0
			3363	2120	562	667	14		
3	H	431	Total	C	N	O	S	0	0
			3378	2128	567	669	14		
3	I	429	Total	C	N	O	S	0	0
			3363	2120	562	667	14		
3	J	431	Total	C	N	O	S	0	0
			3378	2128	567	669	14		
3	K	429	Total	C	N	O	S	0	0
			3363	2120	562	667	14		
3	L	431	Total	C	N	O	S	0	0
			3378	2128	567	669	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
4	N	194	Total	C	N	O	S	0	0
			1546	960	262	316	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
4	P	194	Total	C	N	O	S	0	0
			1546	960	262	316	8		
4	Q	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
4	R	194	Total	C	N	O	S	0	0
			1546	960	262	316	8		
4	S	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
4	T	194	Total	C	N	O	S	0	0
			1546	960	262	316	8		
4	U	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
4	V	194	Total	C	N	O	S	0	0
			1546	960	262	316	8		
4	W	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
4	X	194	Total	C	N	O	S	0	0
			1546	960	262	316	8		

- Molecule 5 is a protein called Tail fiber protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
5	b	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	c	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	d	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
5	e	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	f	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	g	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
5	h	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	i	113	Total	C	N	O	S	0	0
			907	575	157	174	1		

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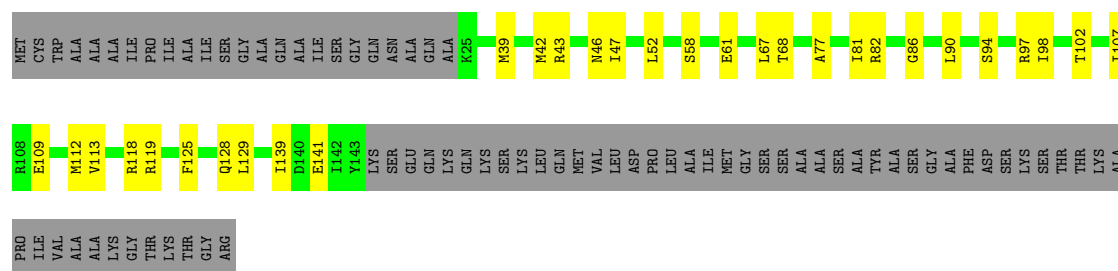
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	j	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
5	k	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	l	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	m	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
5	n	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	o	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	p	115	Total	C	N	O	S	0	0
			922	584	160	177	1		
5	q	113	Total	C	N	O	S	0	0
			907	575	157	174	1		
5	r	113	Total	C	N	O	S	0	0
			907	575	157	174	1		

- Molecule 6 is a protein called Tail tubular protein gp12.

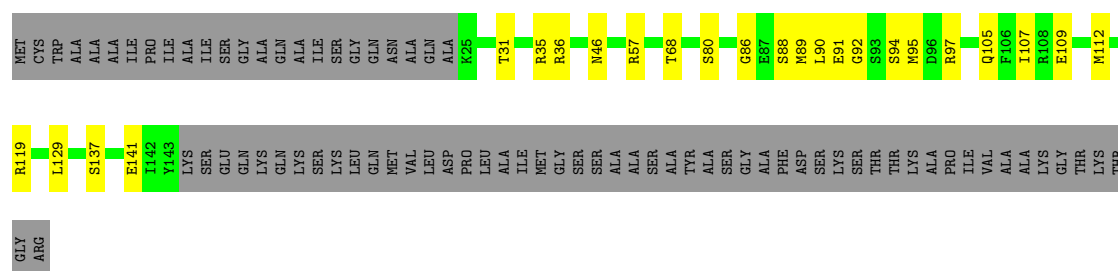
Mol	Chain	Residues	Atoms					AltConf	Trace
6	s	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		
6	t	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		
6	u	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		
6	v	789	Total	C	N	O	S	0	0
			6289	3989	1083	1202	15		
6	w	789	Total	C	N	O	S	0	0
			6289	3989	1083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

Chain Z:  45% 15% 39%



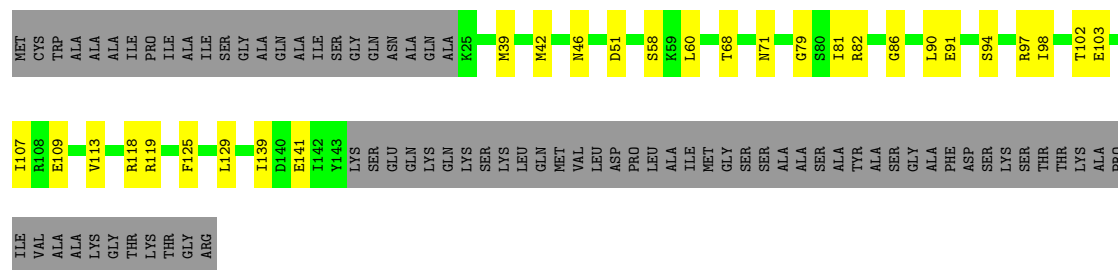
• Molecule 1: Internal virion protein gp14

Chain y:  48% 12% 39%



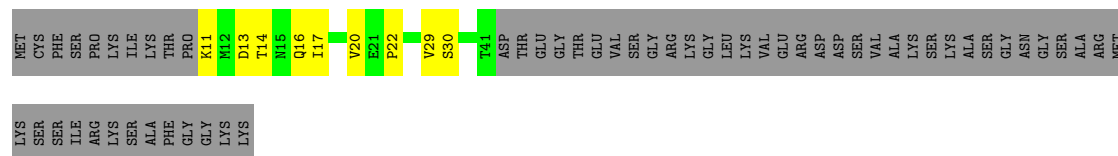
• Molecule 1: Internal virion protein gp14

Chain z:  46% 14% 39%



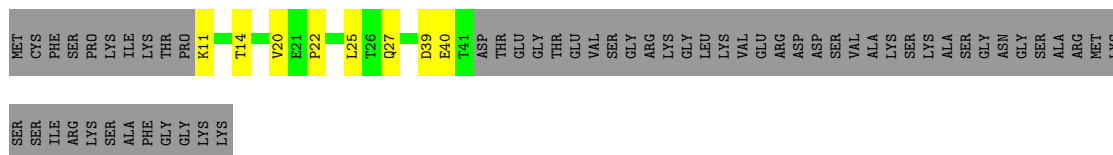
• Molecule 2: Protein 6.7

Chain 2:  25% 10% 65%



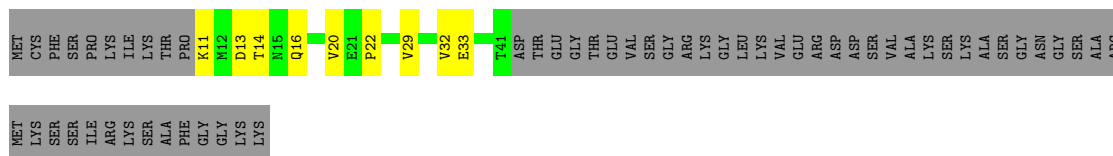
• Molecule 2: Protein 6.7

Chain 3:  26% 9% 65%



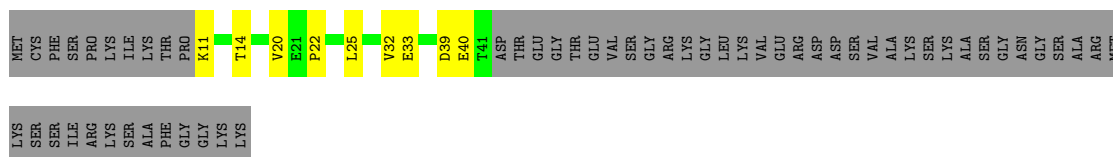
- Molecule 2: Protein 6.7

Chain 4: 25% 10% 65%



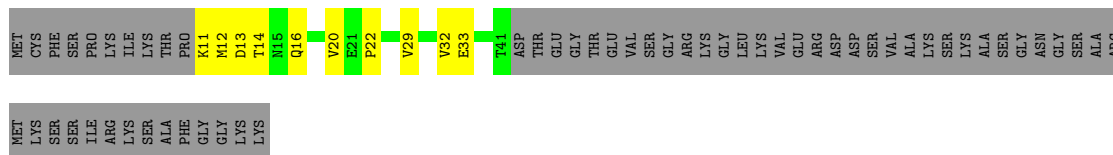
- Molecule 2: Protein 6.7

Chain 5: 25% 10% 65%



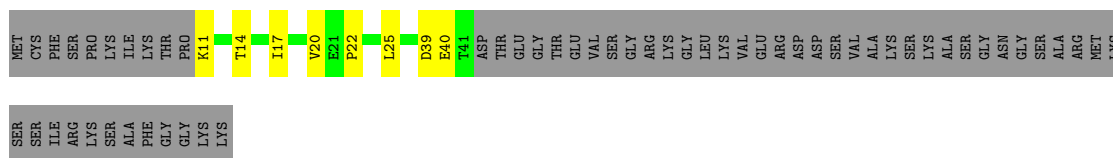
- Molecule 2: Protein 6.7

Chain 6: 24% 11% 65%



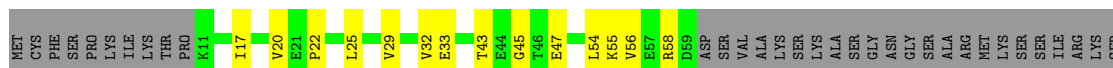
- Molecule 2: Protein 6.7

Chain 7: 26% 9% 65%



- Molecule 2: Protein 6.7

Chain 8: 40% 16% 44%



ALA
PHE
GLY
GLY
LYS
LYS

• Molecule 2: Protein 6.7



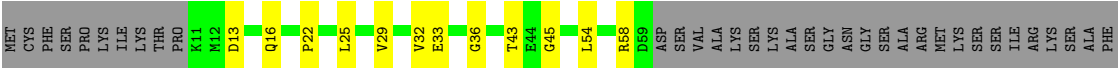
PHE
GLY
GLY
LYS

• Molecule 2: Protein 6.7



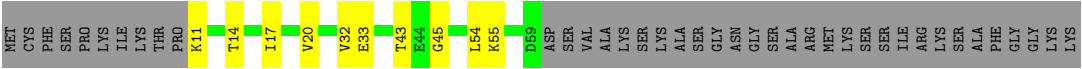
GLY
LYS
LYS

• Molecule 2: Protein 6.7

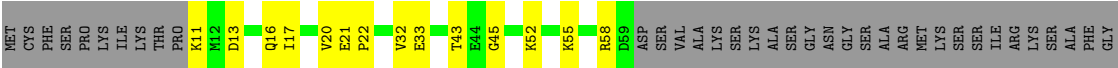


GLY
GLY
LYS
LYS

• Molecule 2: Protein 6.7



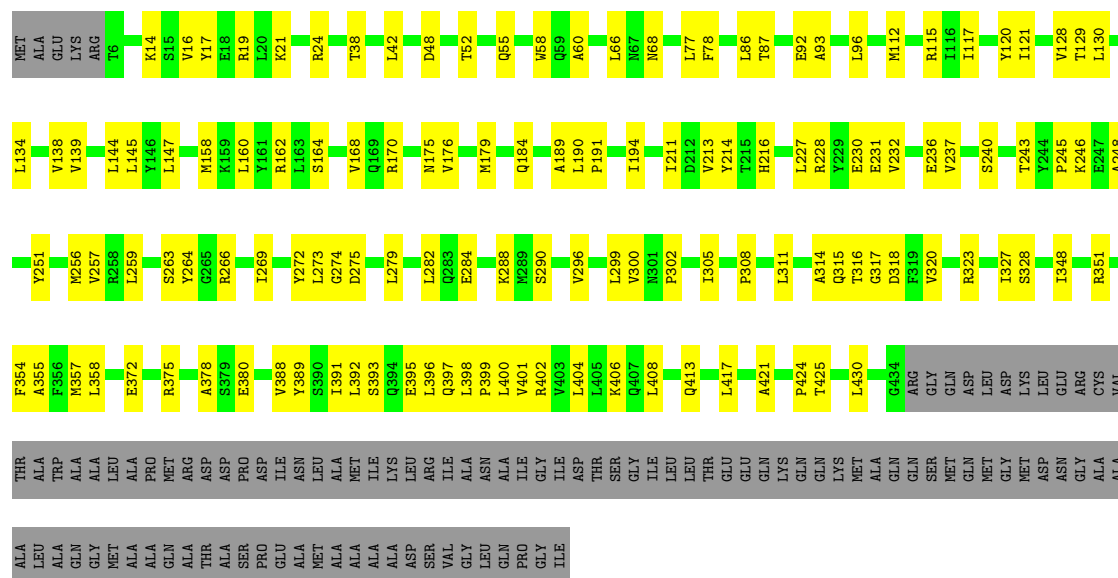
• Molecule 2: Protein 6.7



GLY
LYS
LYS

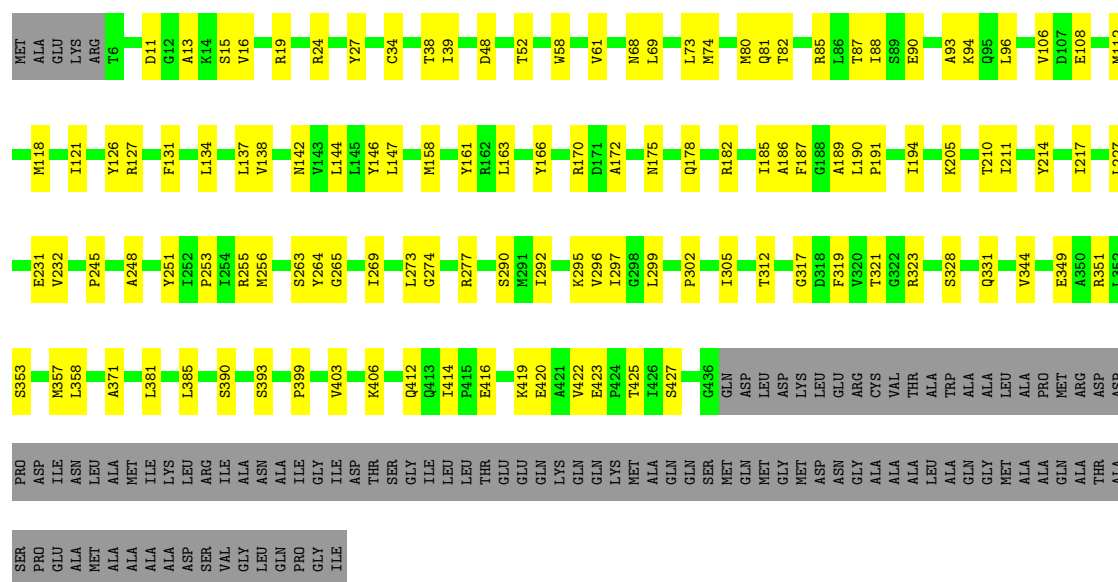
• Molecule 3: Portal protein





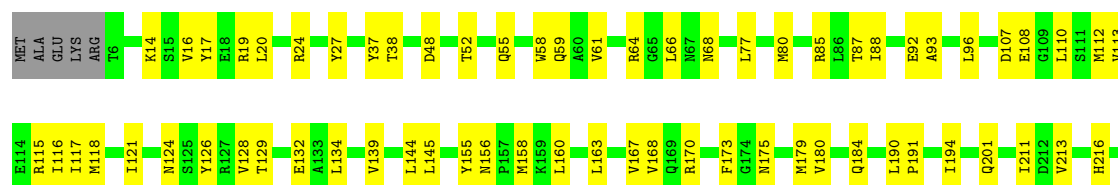
• Molecule 3: Portal protein

Chain B: 58% 22% 20%

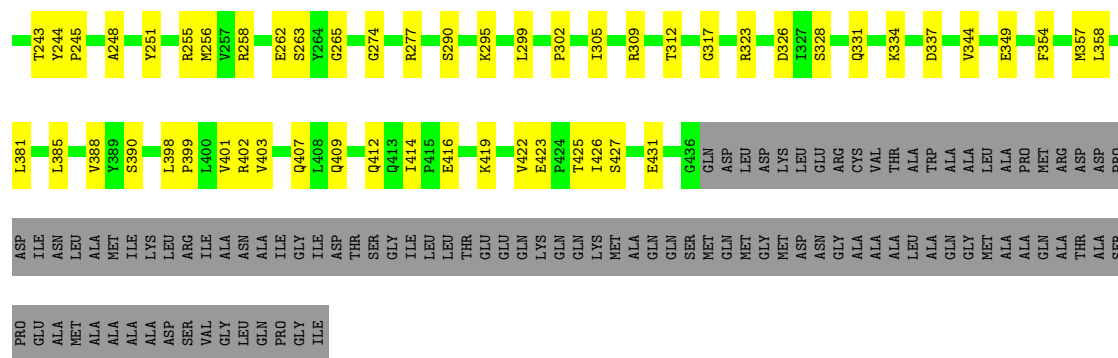


• Molecule 3: Portal protein

Chain C: 54% 26% 20%

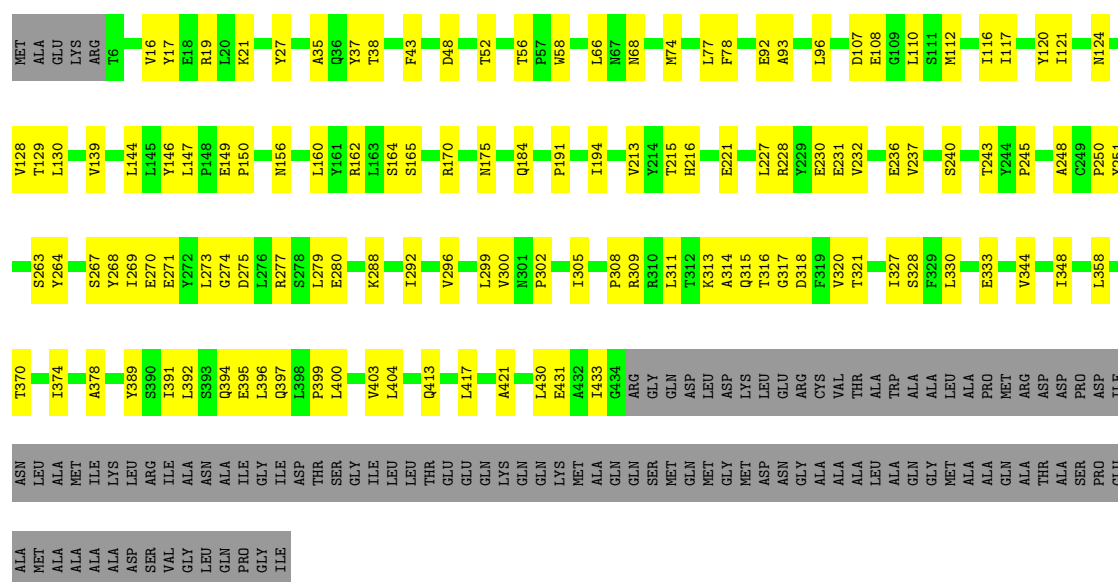






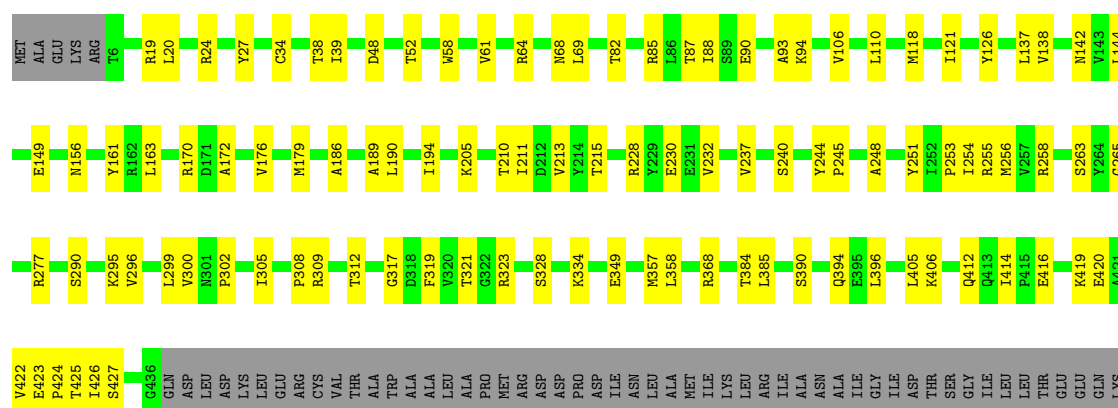
• Molecule 3: Portal protein

Chain K: 57% 23% 20%

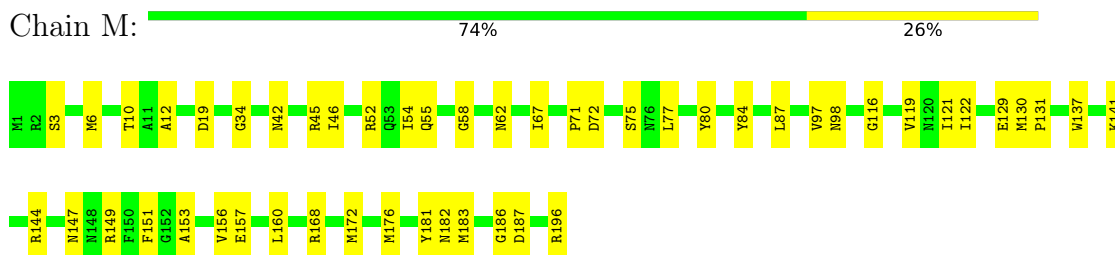


• Molecule 3: Portal protein

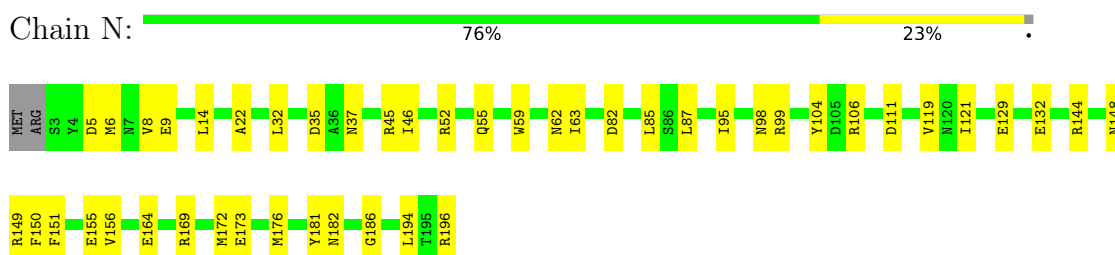
Chain L: 61% 19% 20%



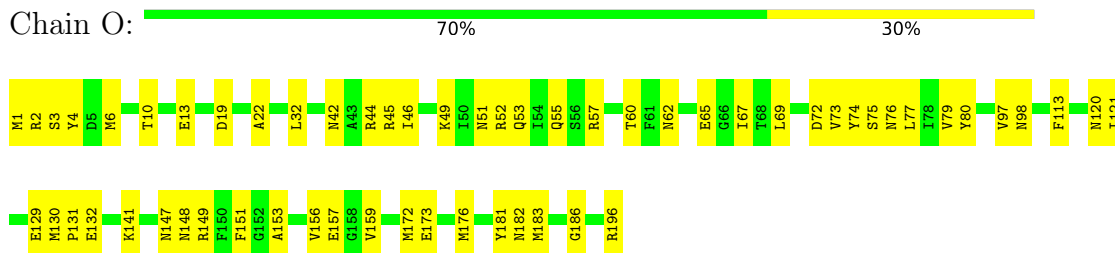
- Molecule 4: Tail tubular protein gp11



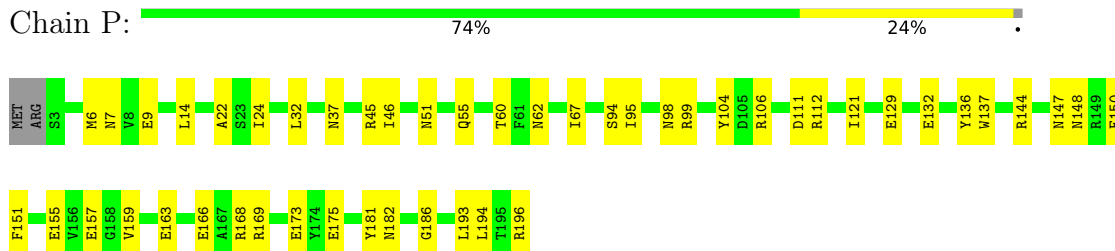
- Molecule 4: Tail tubular protein gp11



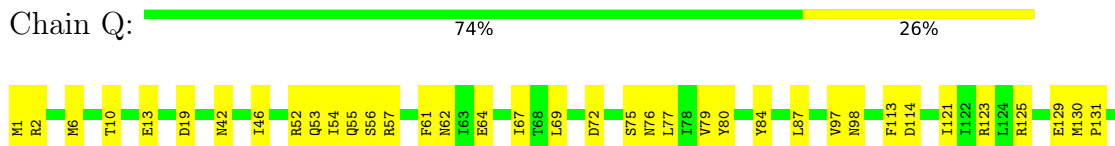
- Molecule 4: Tail tubular protein gp11

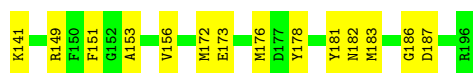


- Molecule 4: Tail tubular protein gp11

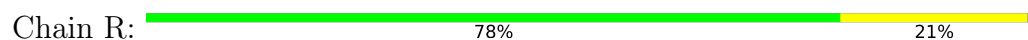


- Molecule 4: Tail tubular protein gp11





- Molecule 4: Tail tubular protein gp11



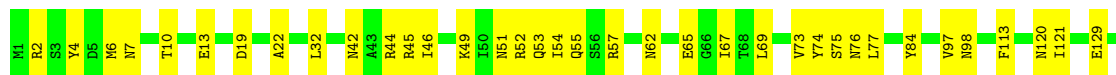
- Molecule 4: Tail tubular protein gp11



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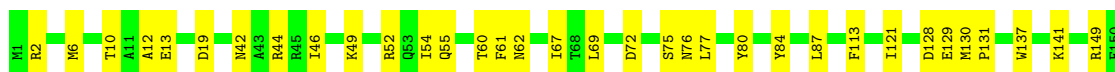
- Molecule 4: Tail tubular protein gp11





• Molecule 4: Tail tubular protein gp11

Chain W: 76% 24%



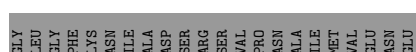
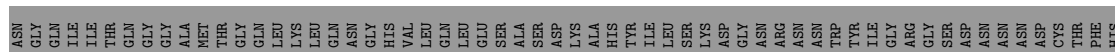
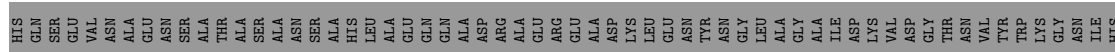
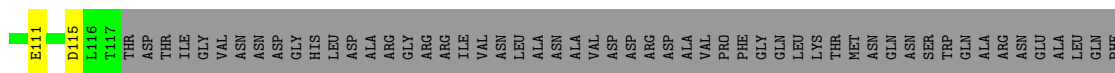
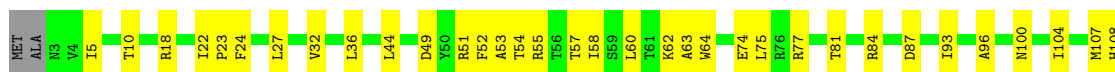
• Molecule 4: Tail tubular protein gp11

Chain X: 76% 23%



• Molecule 5: Tail fiber protein

Chain a: 14% 7% 79%



- Molecule 5: Tail fiber protein

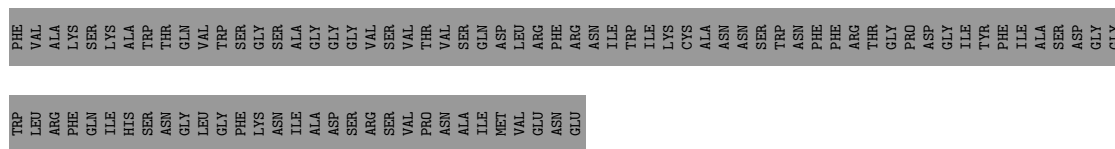
Chain b:  12% 9% 80%

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- Molecule 5: Tail fiber protein

Chain c:  12% 8% 80%

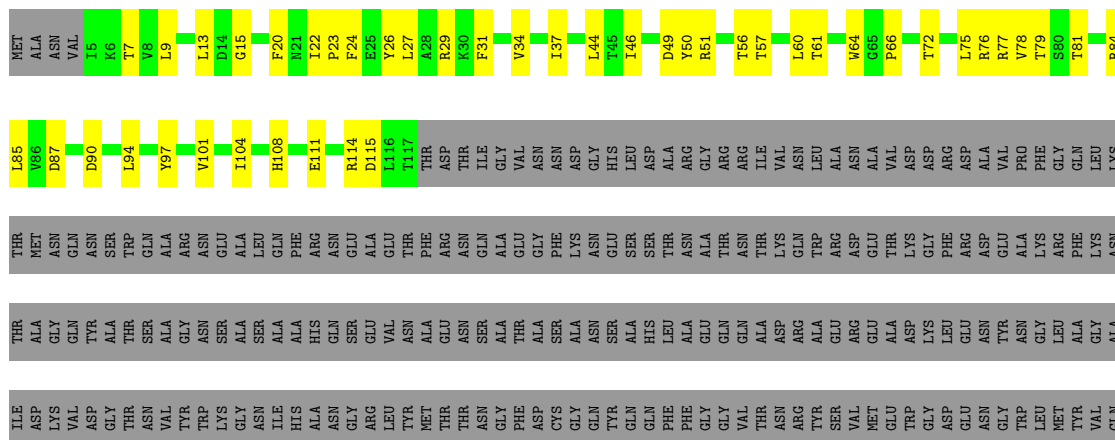
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- Molecule 5: Tail fiber protein



- Molecule 5: Tail fiber protein



[illegible]

- Molecule 5: Tail fiber protein

Chain f: 12% 9% 80%

ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR	TRP	ARG	ASP	TRP	ILE	ALA	TYR
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- Molecule 5: Tail fiber protein

Chain g:  15% 6% 79%

ALA	D115	MET
GLU	L116	ALA
THR	T117	R3
PHE	THR	V4
ARG	ASP	I5
ASN	THR	
GLN	ILE	L9
ALA	GLY	T10
GLU	VAL	
GLY	ASN	L13
PHE	ASN	
LYS	ASP	R17
ASN	GLY	R18
GLU	HIS	
SER	LEU	N21
THR	ASP	I22
SER	ALA	P23
ASN	ARG	F24
ALA	GLY	E25
THR	ARG	
ASN	ARG	V32
THR	ILE	V33
LYS	VAL	V34
GLN	ASN	V35
TRP	LEU	L36
ARG	ALA	
ASP	ASN	D40
GLU	ALA	
THR	VAL	L44
LYS	ASP	
GLY	ASP	D49
PHE	ARG	
ASP	ASP	T54
ASP	ALA	
GLU	VAL	T57
ALA	PRO	
LYS	PHE	E74
ARG	GLY	L75
PHE	GLN	R76
LYS	LEU	R77
ASN	LYS	
THR	THR	T81
ALA	MET	
GLY	ASN	T93
GLN	GLN	L94
TYR	ASN	R95
ALA	SER	A96
THR	TRP	
SER	GLN	N100
ALA	ALA	
GLY	ARG	I104
ASN	ASN	O105
SER	GLU	T106
ALA	ALA	H107
SER	LEU	H108
ALA	GLN	V109
ALA	PHE	
HIS	ARG	E112
GLN	ASN	H113
PER	GLU	F114

- Molecule 5: Tail fiber protein

[illegible]

- Molecule 5: Tail fiber protein

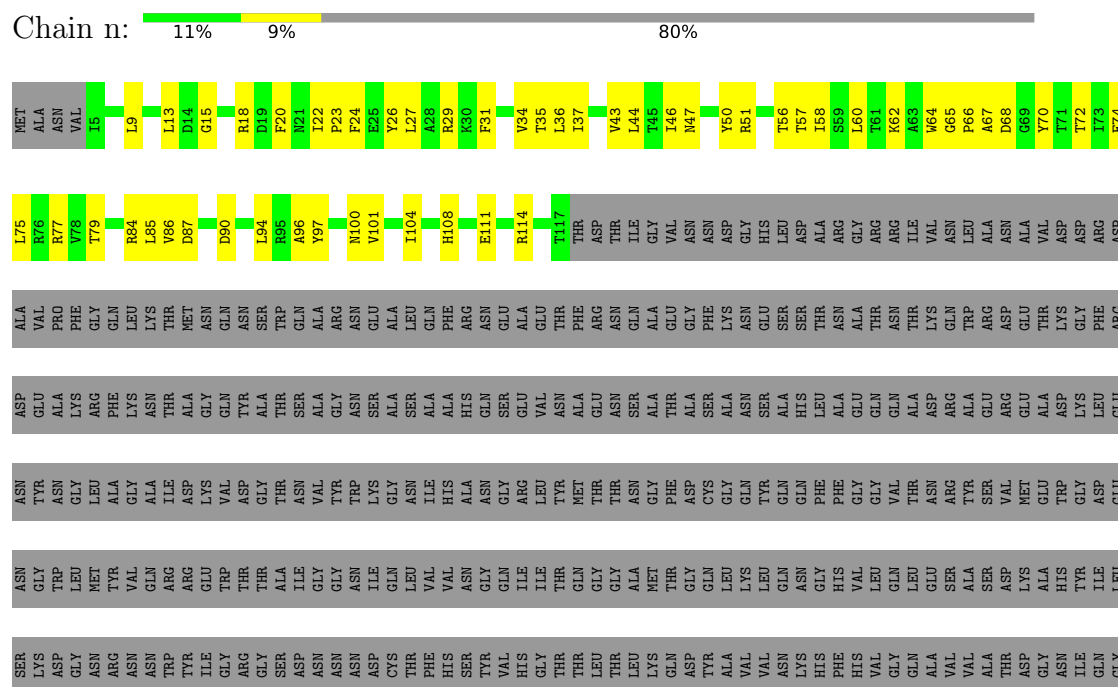


MET	ALA	ASN	VAL	I5	K6	T7	V8	R18	D19	F20	N21	F24	E25	V38	D40	R41	L44	T45	I46	N47	T48	Y50	R51	F52	A53	S59	K62	G69	E74	L75	R76	R77	T81	R84	S92	I93	L94	R95	D98	V101	T104
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● Molecule 5: Tail fiber protein



● Molecule 5: Tail fiber protein



[illegible]

- Molecule 5: Tail fiber protein



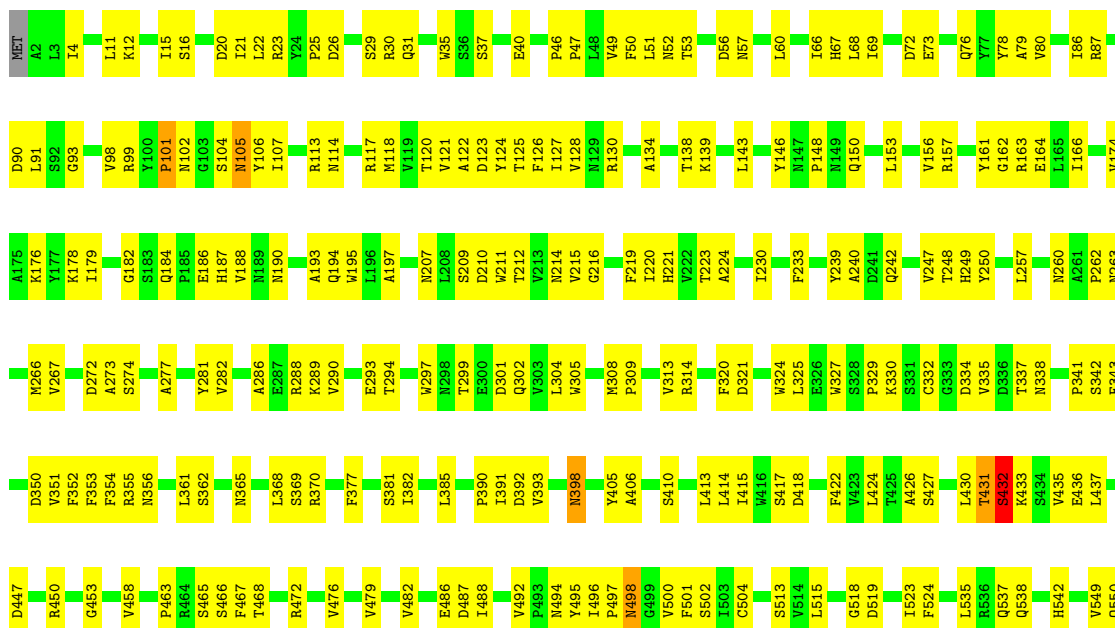
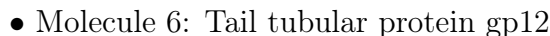
LEU	ARG	ALA	VAL	ASN	GLY	VAL	ALA	ALA	193	MET
PHE	GLN	LYS	ALA	ASN	GLY	TRP	GLN	ARG	V101	ALA
ILE	ILE	LYS	LYS	CYS	GLN	GLY	ALA	GLU	I104	ASN
HIS	SER	ALA	ALA	THR	LEU	ASN	SER	LEU	M107	K6
ASN	THR	TRP	TRP	PHE	VAL	ILE	ALA	GLN	H108	T7
GLN	GLN	GLN	GLN	HIS	VAL	VAL	ALA	PHE	V109	V8
LEU	GLY	VAL	VAL	SER	GLY	ASN	HIS	ALA	A110	Y11
PHE	PHE	TRP	TRP	VAL	GLY	GLY	SER	ASN	E111	Q12
LYS	LYS	GLY	GLY	HIS	ILE	ARG	GLU	ALA	E112	L13
ASN	ASN	SER	SER	GLY	ILE	LEU	VAL	GLU	T117	D14
ILE	ILE	ALA	ALA	THR	GLN	TYR	THR	THR	THR	G15
ALA	ALA	GLY	GLY	LEU	GLN	THR	GLU	PHE	ASP	R18
ASP	GLY	GLY	GLY	THR	GLY	THR	GLU	ARG	THR	D19
SER	GLY	GLY	GLY	LEU	ALA	ASN	SER	GLN	ILE	F20
ARG	ARG	VAL	VAL	LYS	MET	GLY	ALA	ALA	GLY	N21
SER	SER	VAL	VAL	GLN	THR	PHE	ALA	VAL	VAL	F24
VAL	VAL	VAL	THR	ASP	GLY	ASP	ALA	GLY	ASN	Y34
PRO	PRO	THR	THR	TYR	GLN	CYS	SER	PHE	ASN	T36
ASN	ASN	VAL	VAL	ALA	LEU	GLY	ALA	LYS	ASP	L36
ALA	ALA	SER	SER	VAL	LYS	GLN	ASN	ASN	GLY	L44
ILE	ILE	GLN	GLN	VAL	LEU	TYR	SER	GLU	HIS	Y60
MET	MET	ASP	ASP	ASN	GLN	GLN	SER	GLU	LEU	Y60
VAL	VAL	LEU	LEU	LYS	GLY	PHE	HIS	SER	ASP	A53
GLU	GLU	ARG	ARG	HIS	GLY	PHE	LEU	THR	ALA	T54
ASN	ASN	PHE	PHE	PHE	VAL	GLY	ALA	ALA	GLY	Y60
GLU	GLU	ARG	ASN	HIS	VAL	GLY	GLN	THR	ARG	Y60
ASN	ASN	ILE	ILE	VAL	LEU	GLY	GLN	ASN	ARG	Y60
ASN	ASN	TRP	TRP	GLN	GLY	VAL	GLN	ASN	ILE	T54
ASN	ASN	ILE	ILE	ALA	LEU	ASN	ASP	LYS	VAL	T54
CYS	CYS	LYS	LYS	VAL	SER	ARG	ARG	GLN	ASN	T57
ALA	ALA	GLY	GLY	VAL	VAL	TRP	ALA	TRP	LEU	I58
ALA	ALA	VAL	VAL	ALA	SER	SER	GLU	ARG	ALA	S59
ASN	ASN	THR	THR	THR	ASP	VAL	ARG	ASP	ASN	L60
SER	SER	ASN	ASN	ASP	LYS	MET	GLU	GLU	ALA	T61
TRP	TRP	GLY	GLY	GLY	ALA	GLU	ALA	THR	VAL	K62
ASN	ASN	ASN	ASN	HIS	HIS	TRP	ASP	LYS	ASP	A63
ILE	ILE	ILE	ILE	ILE	TYR	GLY	LYS	GLY	ASP	Y64
PHE	PHE	GLN	GLN	GLY	ILE	ASP	LEU	PHE	ARG	G65
ARG	ARG	PHE	PHE	GLY	LEU	GLU	GLU	ARG	ASP	P66
THR	THR	THR	THR	THR	SER	ASN	ASN	ASP	ALA	A67
GLY	GLY	GLY	GLY	LYS	LYS	GLY	TYR	GLU	VAL	D68
PRO	PRO	PRO	PRO	GLY	ASP	TRP	ASN	ALA	PRO	G69
ASP	ASP	ASP	ASP	GLY	GLY	LEU	GLY	LYS	PHE	Y70
GLY	GLY	GLY	GLY	GLY	ASN	MET	LEU	ARG	GLY	Y70
ILE	ILE	ILE	ILE	ARG	ASN	TYR	ALA	PHE	GLN	L75
TYR	TYR	ILE	TYR	ASN	ASN	VAL	GLY	LYS	LEU	R76
PHE	PHE	TYR	THR	LEU	GLN	ARG	ILE	THR	THR	R77
ILE	ILE	THR	THR	ASP	TRP	ARG	ASP	ALA	MET	Y76
ALA	ALA	ALA	TYR	ALA	TYR	GLU	GLY	GLN	ASN	T79
SER	SER	SER	SER	ARG	GLY	TRP	VAL	GLN	THR	S80
ASP	ASP	ASP	THR	THR	ARG	THR	ASP	TYR	ALA	T81
GLY	GLY	GLY	GLY	ASP	GLY	THR	GLY	SER	ASN	G81
GLY	GLY	GLY	THR	SER	SER	THR	THR	THR	THR	S82

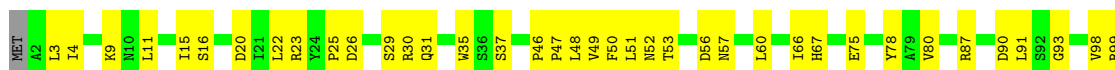
- Molecule 5: Tail fiber protein

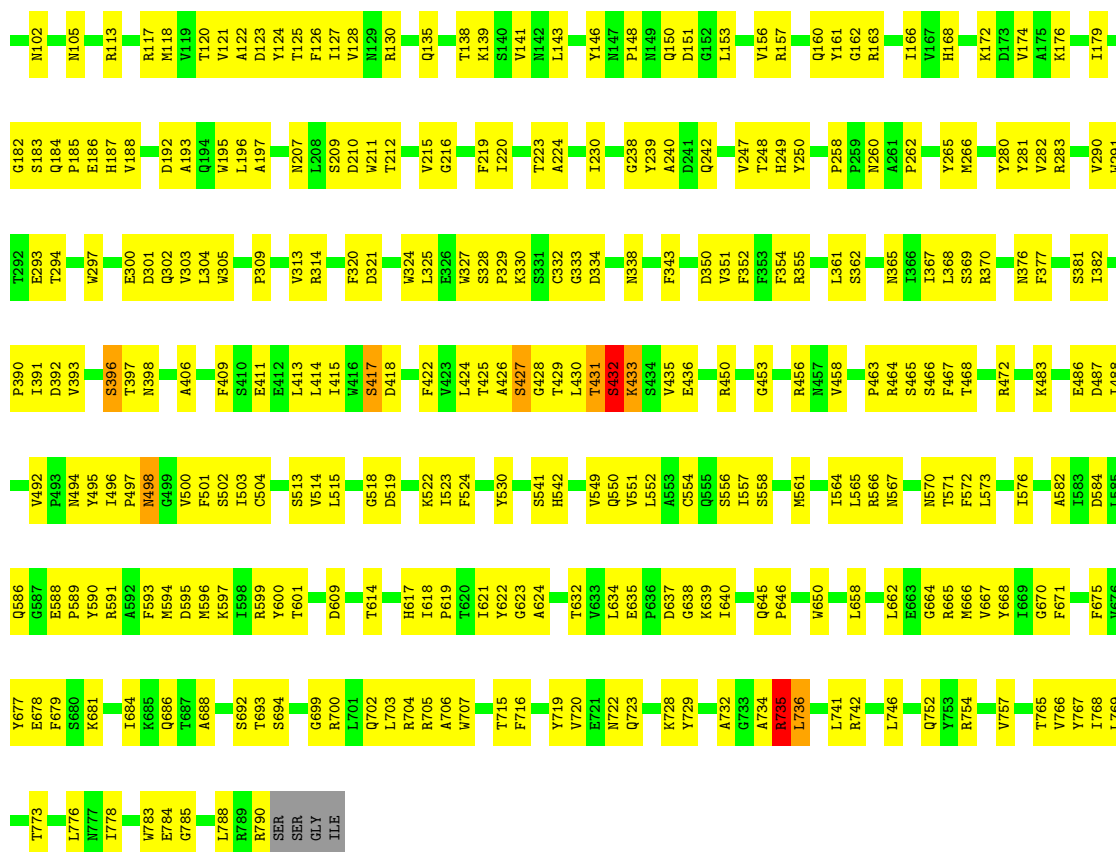
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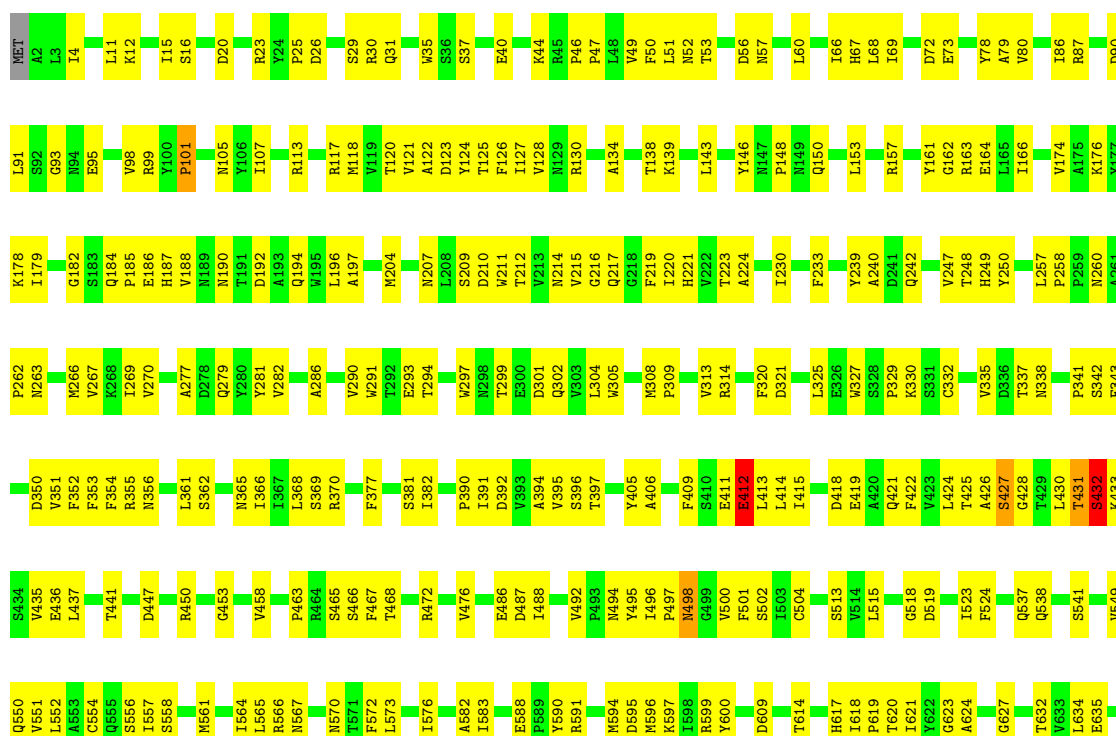






• Molecule 6: Tail tubular protein gp12

Chain x: 56% 42%



G638	K639	I640	F643	E644	Q645	P646	G649	P654	W655	L656	R657	L658	L662	E663	G664	R665	Y668	F671	F675	V676	Y677	E678	K681	I684	A688	S692	T693	S694	T695	G699	R700	L701	Q702	L703	R704	R705	A706	W707	G714	T715	F716	D717	I718	Y719	V720	E721
N722	Q723	Y729	A734	R735	L736	G737	S738	N739	T740	L741	R742	R745	L746	Q752	Y753	R754	V757	T765	Y766	Y767	I768	L769	S770	T773	T774	P775	L776	N777	I778	I779	W783	E784	G785	L788	R789	R790	SER	SER	GLY	ILE						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23461	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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	0	0.14	0/924	0.30	0/1235
1	1	0.15	0/924	0.34	0/1235
1	Y	0.16	0/924	0.32	0/1235
1	Z	0.15	0/924	0.32	0/1235
1	y	0.15	0/924	0.32	0/1235
1	z	0.17	0/924	0.31	0/1235
2	2	0.17	0/233	0.36	0/315
2	3	0.17	0/233	0.34	0/315
2	4	0.16	0/233	0.35	0/315
2	5	0.18	0/233	0.35	0/315
2	6	0.16	0/233	0.36	0/315
2	7	0.17	0/233	0.36	0/315
2	8	0.20	0/370	0.38	0/497
2	9	0.17	0/370	0.36	0/497
2	AA	0.16	0/370	0.33	0/497
2	AB	0.16	0/370	0.40	0/497
2	AC	0.14	0/370	0.33	0/497
2	AD	0.14	0/370	0.33	0/497
3	A	0.15	0/3419	0.35	0/4632
3	B	0.15	0/3434	0.32	0/4651
3	C	0.15	0/3419	0.34	0/4632
3	D	0.16	0/3434	0.34	1/4651 (0.0%)
3	E	0.15	0/3419	0.35	0/4632
3	F	0.14	0/3434	0.31	0/4651
3	G	0.15	0/3419	0.35	0/4632
3	H	0.14	0/3434	0.31	0/4651
3	I	0.15	0/3419	0.34	0/4632
3	J	0.14	0/3434	0.31	0/4651
3	K	0.14	0/3419	0.34	0/4632
3	L	0.14	0/3434	0.31	0/4651
4	M	0.20	0/1592	0.35	0/2153
4	N	0.20	0/1573	0.35	0/2129
4	O	0.19	0/1592	0.33	0/2153
4	P	0.19	0/1573	0.35	0/2129

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	Q	0.19	0/1592	0.35	0/2153
4	R	0.19	0/1573	0.35	0/2129
4	S	0.20	0/1592	0.35	0/2153
4	T	0.22	0/1573	0.37	0/2129
4	U	0.19	0/1592	0.35	0/2153
4	V	0.20	0/1573	0.35	0/2129
4	W	0.19	0/1592	0.34	0/2153
4	X	0.19	0/1573	0.35	0/2129
5	a	0.18	0/936	0.36	0/1274
5	b	0.19	0/921	0.46	0/1253
5	c	0.19	0/921	0.45	0/1253
5	d	0.18	0/936	0.35	0/1274
5	e	0.20	0/921	0.41	0/1253
5	f	0.18	0/921	0.42	0/1253
5	g	0.18	0/936	0.35	0/1274
5	h	0.17	0/921	0.41	1/1253 (0.1%)
5	i	0.18	0/921	0.39	0/1253
5	j	0.18	0/936	0.32	0/1274
5	k	0.20	0/921	0.54	2/1253 (0.2%)
5	l	0.17	0/921	0.40	0/1253
5	m	0.19	0/936	0.35	0/1274
5	n	0.22	0/921	0.55	1/1253 (0.1%)
5	o	0.20	0/921	0.46	1/1253 (0.1%)
5	p	0.21	0/936	0.39	0/1274
5	q	0.18	0/921	0.40	0/1253
5	r	0.23	0/921	0.54	4/1253 (0.3%)
6	s	0.32	0/6449	0.58	8/8772 (0.1%)
6	t	0.29	0/6449	0.55	5/8772 (0.1%)
6	u	0.30	0/6449	0.55	4/8772 (0.0%)
6	v	0.30	0/6449	0.59	12/8772 (0.1%)
6	w	0.31	0/6449	0.57	7/8772 (0.1%)
6	x	0.32	0/6449	0.59	10/8772 (0.1%)
All	All	0.22	0/124632	0.43	56/168984 (0.0%)

There are no bond length outliers.

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	v	736	LEU	N-CA-C	9.92	122.10	111.28
6	x	736	LEU	N-CA-C	8.98	121.07	111.28
6	x	105	ASN	N-CA-C	-8.61	102.53	113.72
6	s	12	LYS	N-CA-C	-8.22	102.28	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	w	105	ASN	N-CA-C	-7.91	103.44	113.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	920	0	919	25	0
1	1	920	0	919	23	0
1	Y	920	0	919	37	0
1	Z	920	0	919	30	0
1	y	920	0	919	20	0
1	z	920	0	919	33	0
2	2	231	0	217	9	0
2	3	231	0	217	9	0
2	4	231	0	217	10	0
2	5	231	0	217	9	0
2	6	231	0	217	8	0
2	7	231	0	217	8	0
2	8	368	0	352	19	0
2	9	368	0	352	12	0
2	AA	368	0	352	10	0
2	AB	368	0	352	15	0
2	AC	368	0	352	11	0
2	AD	368	0	352	17	0
3	A	3363	0	3347	95	0
3	B	3378	0	3363	96	0
3	C	3363	0	3347	97	0
3	D	3378	0	3363	87	0
3	E	3363	0	3347	84	0
3	F	3378	0	3363	82	0
3	G	3363	0	3347	91	0
3	H	3378	0	3363	77	0
3	I	3363	0	3347	100	0
3	J	3378	0	3363	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	3363	0	3347	83	0
3	L	3378	0	3363	74	0
4	M	1565	0	1485	41	0
4	N	1546	0	1460	44	0
4	O	1565	0	1485	55	0
4	P	1546	0	1460	45	0
4	Q	1565	0	1485	42	0
4	R	1546	0	1460	34	0
4	S	1565	0	1485	46	0
4	T	1546	0	1460	45	0
4	U	1565	0	1485	47	0
4	V	1546	0	1460	49	0
4	W	1565	0	1485	42	0
4	X	1546	0	1460	38	0
5	a	922	0	931	30	0
5	b	907	0	916	36	0
5	c	907	0	916	35	0
5	d	922	0	931	35	0
5	e	907	0	916	36	0
5	f	907	0	916	40	0
5	g	922	0	931	31	0
5	h	907	0	916	28	0
5	i	907	0	916	31	0
5	j	922	0	931	27	0
5	k	907	0	916	41	0
5	l	907	0	916	33	0
5	m	922	0	931	33	0
5	n	907	0	916	41	0
5	o	907	0	916	30	0
5	p	922	0	931	29	0
5	q	907	0	916	39	0
5	r	907	0	916	35	0
6	s	6289	0	6051	261	0
6	t	6289	0	6051	262	0
6	u	6289	0	6051	250	0
6	v	6289	0	6051	266	0
6	w	6289	0	6051	263	0
6	x	6289	0	6051	257	0
All	All	122376	0	119742	3482	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 14.

The worst 5 of 3482 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)
5:o:18:ARG:HH22	5:o:63:ALA:HB2	1.35	0.91
6:s:570:ASN:HD21	6:s:624:ALA:HB3	1.39	0.88
6:u:570:ASN:HD21	6:u:624:ALA:HB3	1.38	0.85
6:w:570:ASN:HD21	6:w:624:ALA:HB3	1.40	0.85
6:v:570:ASN:HD21	6:v:624:ALA:HB3	1.39	0.85

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	0	117/196 (60%)	115 (98%)	2 (2%)	0	100	100
1	1	117/196 (60%)	116 (99%)	1 (1%)	0	100	100
1	Y	117/196 (60%)	115 (98%)	2 (2%)	0	100	100
1	Z	117/196 (60%)	115 (98%)	2 (2%)	0	100	100
1	y	117/196 (60%)	115 (98%)	2 (2%)	0	100	100
1	z	117/196 (60%)	116 (99%)	1 (1%)	0	100	100
2	2	29/88 (33%)	25 (86%)	4 (14%)	0	100	100
2	3	29/88 (33%)	26 (90%)	3 (10%)	0	100	100
2	4	29/88 (33%)	23 (79%)	6 (21%)	0	100	100
2	5	29/88 (33%)	25 (86%)	4 (14%)	0	100	100
2	6	29/88 (33%)	23 (79%)	6 (21%)	0	100	100
2	7	29/88 (33%)	24 (83%)	5 (17%)	0	100	100
2	8	47/88 (53%)	45 (96%)	2 (4%)	0	100	100
2	9	47/88 (53%)	45 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AA	47/88 (53%)	45 (96%)	2 (4%)	0	100	100
2	AB	47/88 (53%)	45 (96%)	2 (4%)	0	100	100
2	AC	47/88 (53%)	44 (94%)	3 (6%)	0	100	100
2	AD	47/88 (53%)	44 (94%)	3 (6%)	0	100	100
3	A	427/536 (80%)	419 (98%)	8 (2%)	0	100	100
3	B	429/536 (80%)	422 (98%)	7 (2%)	0	100	100
3	C	427/536 (80%)	416 (97%)	11 (3%)	0	100	100
3	D	429/536 (80%)	422 (98%)	7 (2%)	0	100	100
3	E	427/536 (80%)	417 (98%)	10 (2%)	0	100	100
3	F	429/536 (80%)	422 (98%)	7 (2%)	0	100	100
3	G	427/536 (80%)	418 (98%)	9 (2%)	0	100	100
3	H	429/536 (80%)	423 (99%)	6 (1%)	0	100	100
3	I	427/536 (80%)	414 (97%)	13 (3%)	0	100	100
3	J	429/536 (80%)	425 (99%)	4 (1%)	0	100	100
3	K	427/536 (80%)	417 (98%)	10 (2%)	0	100	100
3	L	429/536 (80%)	423 (99%)	6 (1%)	0	100	100
4	M	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
4	N	192/196 (98%)	185 (96%)	7 (4%)	0	100	100
4	O	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
4	P	192/196 (98%)	185 (96%)	7 (4%)	0	100	100
4	Q	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
4	R	192/196 (98%)	187 (97%)	5 (3%)	0	100	100
4	S	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
4	T	192/196 (98%)	185 (96%)	7 (4%)	0	100	100
4	U	194/196 (99%)	191 (98%)	3 (2%)	0	100	100
4	V	192/196 (98%)	184 (96%)	8 (4%)	0	100	100
4	W	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
4	X	192/196 (98%)	186 (97%)	6 (3%)	0	100	100
5	a	113/553 (20%)	107 (95%)	6 (5%)	0	100	100
5	b	111/553 (20%)	106 (96%)	5 (4%)	0	100	100
5	c	111/553 (20%)	105 (95%)	5 (4%)	1 (1%)	14	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	d	113/553 (20%)	108 (96%)	5 (4%)	0	100	100
5	e	111/553 (20%)	103 (93%)	7 (6%)	1 (1%)	14	49
5	f	111/553 (20%)	106 (96%)	5 (4%)	0	100	100
5	g	113/553 (20%)	110 (97%)	3 (3%)	0	100	100
5	h	111/553 (20%)	105 (95%)	4 (4%)	2 (2%)	7	35
5	i	111/553 (20%)	107 (96%)	4 (4%)	0	100	100
5	j	113/553 (20%)	109 (96%)	4 (4%)	0	100	100
5	k	111/553 (20%)	104 (94%)	5 (4%)	2 (2%)	7	35
5	l	111/553 (20%)	107 (96%)	4 (4%)	0	100	100
5	m	113/553 (20%)	109 (96%)	4 (4%)	0	100	100
5	n	111/553 (20%)	103 (93%)	8 (7%)	0	100	100
5	o	111/553 (20%)	108 (97%)	3 (3%)	0	100	100
5	p	113/553 (20%)	107 (95%)	5 (4%)	1 (1%)	14	49
5	q	111/553 (20%)	106 (96%)	5 (4%)	0	100	100
5	r	111/553 (20%)	106 (96%)	5 (4%)	0	100	100
6	s	787/794 (99%)	701 (89%)	80 (10%)	6 (1%)	16	51
6	t	787/794 (99%)	702 (89%)	78 (10%)	7 (1%)	14	49
6	u	787/794 (99%)	699 (89%)	80 (10%)	8 (1%)	13	46
6	v	787/794 (99%)	699 (89%)	79 (10%)	9 (1%)	12	45
6	w	787/794 (99%)	699 (89%)	83 (10%)	5 (1%)	22	56
6	x	787/794 (99%)	702 (89%)	80 (10%)	5 (1%)	22	56
All	All	15342/25734 (60%)	14513 (95%)	782 (5%)	47 (0%)	38	68

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	c	68	ASP
6	s	432	SER
6	s	498	ASN
6	s	735	ARG
6	t	498	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	95/149 (64%)	95 (100%)	0	100	100
1	1	95/149 (64%)	95 (100%)	0	100	100
1	Y	95/149 (64%)	95 (100%)	0	100	100
1	Z	95/149 (64%)	95 (100%)	0	100	100
1	y	95/149 (64%)	95 (100%)	0	100	100
1	z	95/149 (64%)	95 (100%)	0	100	100
2	2	27/73 (37%)	27 (100%)	0	100	100
2	3	27/73 (37%)	27 (100%)	0	100	100
2	4	27/73 (37%)	27 (100%)	0	100	100
2	5	27/73 (37%)	27 (100%)	0	100	100
2	6	27/73 (37%)	27 (100%)	0	100	100
2	7	27/73 (37%)	27 (100%)	0	100	100
2	8	42/73 (58%)	42 (100%)	0	100	100
2	9	42/73 (58%)	42 (100%)	0	100	100
2	AA	42/73 (58%)	42 (100%)	0	100	100
2	AB	42/73 (58%)	42 (100%)	0	100	100
2	AC	42/73 (58%)	42 (100%)	0	100	100
2	AD	42/73 (58%)	42 (100%)	0	100	100
3	A	365/442 (83%)	365 (100%)	0	100	100
3	B	366/442 (83%)	366 (100%)	0	100	100
3	C	365/442 (83%)	365 (100%)	0	100	100
3	D	366/442 (83%)	366 (100%)	0	100	100
3	E	365/442 (83%)	365 (100%)	0	100	100
3	F	366/442 (83%)	366 (100%)	0	100	100
3	G	365/442 (83%)	365 (100%)	0	100	100
3	H	366/442 (83%)	366 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	365/442 (83%)	365 (100%)	0	100	100
3	J	366/442 (83%)	366 (100%)	0	100	100
3	K	365/442 (83%)	365 (100%)	0	100	100
3	L	366/442 (83%)	366 (100%)	0	100	100
4	M	169/169 (100%)	169 (100%)	0	100	100
4	N	167/169 (99%)	167 (100%)	0	100	100
4	O	169/169 (100%)	169 (100%)	0	100	100
4	P	167/169 (99%)	167 (100%)	0	100	100
4	Q	169/169 (100%)	169 (100%)	0	100	100
4	R	167/169 (99%)	167 (100%)	0	100	100
4	S	169/169 (100%)	169 (100%)	0	100	100
4	T	167/169 (99%)	167 (100%)	0	100	100
4	U	169/169 (100%)	169 (100%)	0	100	100
4	V	167/169 (99%)	167 (100%)	0	100	100
4	W	169/169 (100%)	169 (100%)	0	100	100
4	X	167/169 (99%)	167 (100%)	0	100	100
5	a	102/451 (23%)	102 (100%)	0	100	100
5	b	100/451 (22%)	99 (99%)	1 (1%)	73	84
5	c	100/451 (22%)	100 (100%)	0	100	100
5	d	102/451 (23%)	102 (100%)	0	100	100
5	e	100/451 (22%)	100 (100%)	0	100	100
5	f	100/451 (22%)	99 (99%)	1 (1%)	73	84
5	g	102/451 (23%)	102 (100%)	0	100	100
5	h	100/451 (22%)	99 (99%)	1 (1%)	73	84
5	i	100/451 (22%)	100 (100%)	0	100	100
5	j	102/451 (23%)	102 (100%)	0	100	100
5	k	100/451 (22%)	99 (99%)	1 (1%)	73	84
5	l	100/451 (22%)	99 (99%)	1 (1%)	73	84
5	m	102/451 (23%)	102 (100%)	0	100	100
5	n	100/451 (22%)	99 (99%)	1 (1%)	73	84
5	o	100/451 (22%)	99 (99%)	1 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	p	102/451 (23%)	102 (100%)	0	100	100
5	q	100/451 (22%)	100 (100%)	0	100	100
5	r	100/451 (22%)	99 (99%)	1 (1%)	73	84
6	s	684/688 (99%)	677 (99%)	7 (1%)	73	84
6	t	684/688 (99%)	678 (99%)	6 (1%)	75	86
6	u	684/688 (99%)	683 (100%)	1 (0%)	92	97
6	v	684/688 (99%)	681 (100%)	3 (0%)	89	95
6	w	684/688 (99%)	678 (99%)	6 (1%)	75	86
6	x	684/688 (99%)	675 (99%)	9 (1%)	65	81
All	All	13302/21348 (62%)	13262 (100%)	40 (0%)	90	96

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	w	433	LYS
6	x	419	GLU
6	w	735	ARG
6	x	397	THR
6	x	538	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
6	u	538	GLN
6	x	338	ASN
6	u	645	GLN
6	v	645	GLN
1	y	49	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.