



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 15, 2018 – 11:49 AM EST

PDB ID : 3J2N
EMDB ID: : EMD-1086
Title : The X-ray structure of the gp15 hexamer and the model of the gp18 protein
fitted into the cryo-EM reconstruction of the contracted T4 tail
Authors : Fokine, A.; Zhang, Z.; Kanamaru, S.; Bowman, V.D.; Aksyuk, A.; Arisaka, F.;
Rao, V.B.; Rossmann, M.G.
Deposited on : 2012-11-10
Resolution : 16.00 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

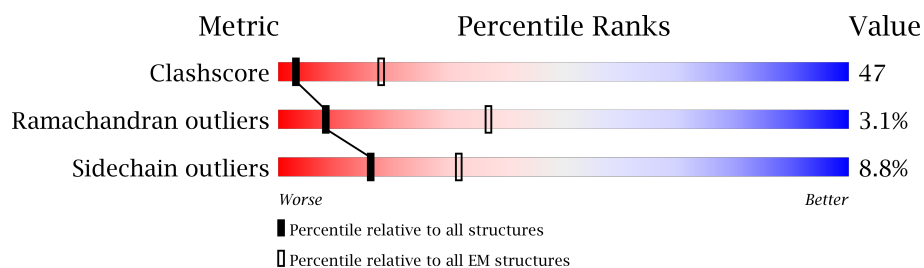
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 16.00 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	A	272	
1	B	272	
1	C	272	
1	D	272	
1	E	272	
1	F	272	
2	U	659	
2	V	659	
2	W	659	

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Mol	Chain	Length	Quality of chain
2	X	659	 34% 49% 9% 8%
2	Y	659	 34% 50% 9% 8%
2	Z	659	 33% 50% 9% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 38334 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 connector protein Gp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	211	Total	C	N	O	S	0	0
			1742	1123	283	328	8		
1	B	211	Total	C	N	O	S	0	0
			1742	1123	283	328	8		
1	C	211	Total	C	N	O	S	0	0
			1742	1123	283	328	8		
1	D	211	Total	C	N	O	S	0	0
			1742	1123	283	328	8		
1	E	211	Total	C	N	O	S	0	0
			1742	1123	283	328	8		
1	F	211	Total	C	N	O	S	0	0
			1742	1123	283	328	8		

- Molecule 2 is a protein called Tail sheath protein Gp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	609	Total	C	N	O	S	0	0
			4647	2929	785	923	10		
2	V	609	Total	C	N	O	S	0	0
			4647	2929	785	923	10		
2	W	609	Total	C	N	O	S	0	0
			4647	2929	785	923	10		
2	X	609	Total	C	N	O	S	0	0
			4647	2929	785	923	10		
2	Y	609	Total	C	N	O	S	0	0
			4647	2929	785	923	10		
2	Z	609	Total	C	N	O	S	0	0
			4647	2929	785	923	10		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	100	GLU	ASP	SEE REMARK 999	UNP P13332
U	148	ALA	GLY	SEE REMARK 999	UNP P13332

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Chain	Residue	Modelled	Actual	Comment	Reference
U	150	ILE	ASN	SEE REMARK 999	UNP P13332
U	151	ILE	TYR	SEE REMARK 999	UNP P13332
U	301	GLY	GLU	SEE REMARK 999	UNP P13332
U	399	VAL	ALA	SEE REMARK 999	UNP P13332
U	454	TYR	HIS	SEE REMARK 999	UNP P13332
U	510	PRO	ARG	ENGINEERED MUTATION	UNP P13332
V	100	GLU	ASP	SEE REMARK 999	UNP P13332
V	148	ALA	GLY	SEE REMARK 999	UNP P13332
V	150	ILE	ASN	SEE REMARK 999	UNP P13332
V	151	ILE	TYR	SEE REMARK 999	UNP P13332
V	301	GLY	GLU	SEE REMARK 999	UNP P13332
V	399	VAL	ALA	SEE REMARK 999	UNP P13332
V	454	TYR	HIS	SEE REMARK 999	UNP P13332
V	510	PRO	ARG	ENGINEERED MUTATION	UNP P13332
W	100	GLU	ASP	SEE REMARK 999	UNP P13332
W	148	ALA	GLY	SEE REMARK 999	UNP P13332
W	150	ILE	ASN	SEE REMARK 999	UNP P13332
W	151	ILE	TYR	SEE REMARK 999	UNP P13332
W	301	GLY	GLU	SEE REMARK 999	UNP P13332
W	399	VAL	ALA	SEE REMARK 999	UNP P13332
W	454	TYR	HIS	SEE REMARK 999	UNP P13332
W	510	PRO	ARG	ENGINEERED MUTATION	UNP P13332
X	100	GLU	ASP	SEE REMARK 999	UNP P13332
X	148	ALA	GLY	SEE REMARK 999	UNP P13332
X	150	ILE	ASN	SEE REMARK 999	UNP P13332
X	151	ILE	TYR	SEE REMARK 999	UNP P13332
X	301	GLY	GLU	SEE REMARK 999	UNP P13332
X	399	VAL	ALA	SEE REMARK 999	UNP P13332
X	454	TYR	HIS	SEE REMARK 999	UNP P13332
X	510	PRO	ARG	ENGINEERED MUTATION	UNP P13332
Y	100	GLU	ASP	SEE REMARK 999	UNP P13332
Y	148	ALA	GLY	SEE REMARK 999	UNP P13332
Y	150	ILE	ASN	SEE REMARK 999	UNP P13332
Y	151	ILE	TYR	SEE REMARK 999	UNP P13332
Y	301	GLY	GLU	SEE REMARK 999	UNP P13332
Y	399	VAL	ALA	SEE REMARK 999	UNP P13332
Y	454	TYR	HIS	SEE REMARK 999	UNP P13332
Y	510	PRO	ARG	ENGINEERED MUTATION	UNP P13332
Z	100	GLU	ASP	SEE REMARK 999	UNP P13332
Z	148	ALA	GLY	SEE REMARK 999	UNP P13332
Z	150	ILE	ASN	SEE REMARK 999	UNP P13332
Z	151	ILE	TYR	SEE REMARK 999	UNP P13332

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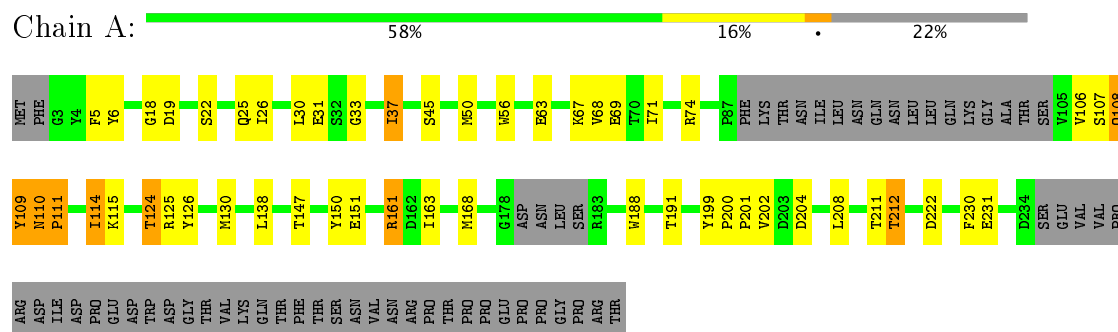
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Chain	Residue	Modelled	Actual	Comment	Reference
Z	301	GLY	GLU	SEE REMARK 999	UNP P13332
Z	399	VAL	ALA	SEE REMARK 999	UNP P13332
Z	454	TYR	HIS	SEE REMARK 999	UNP P13332
Z	510	PRO	ARG	ENGINEERED MUTATION	UNP P13332

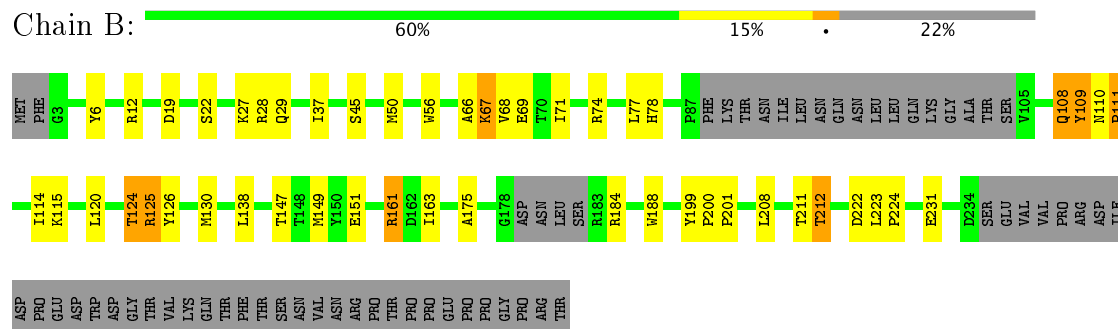
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

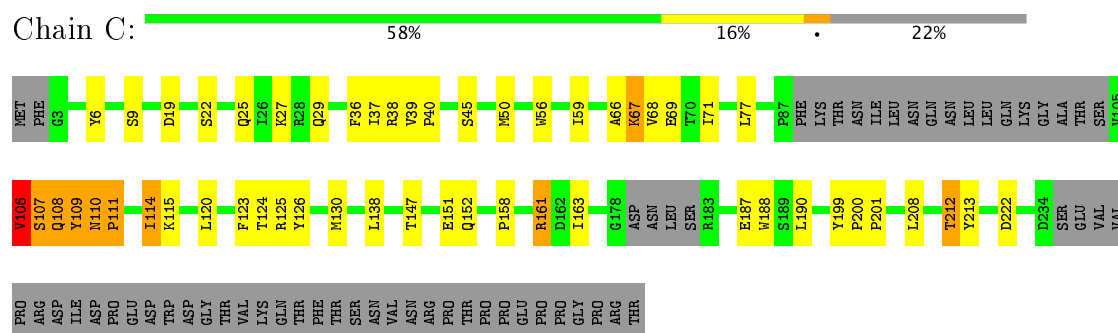
- Molecule 1: Tail connector protein Gp15



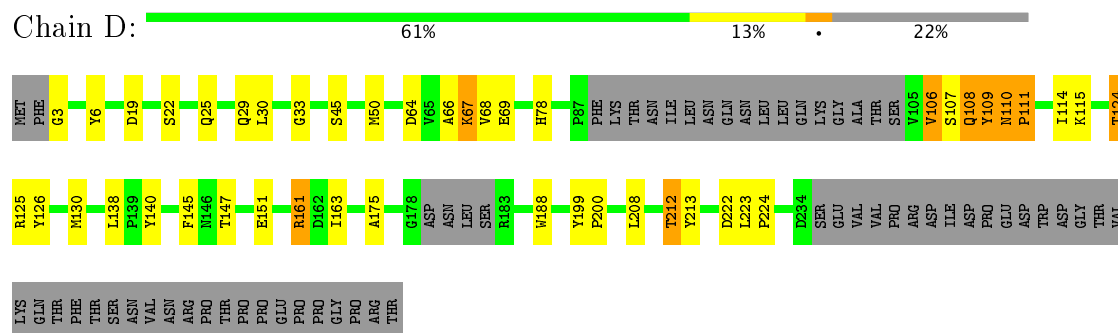
- Molecule 1: Tail connector protein Gp15



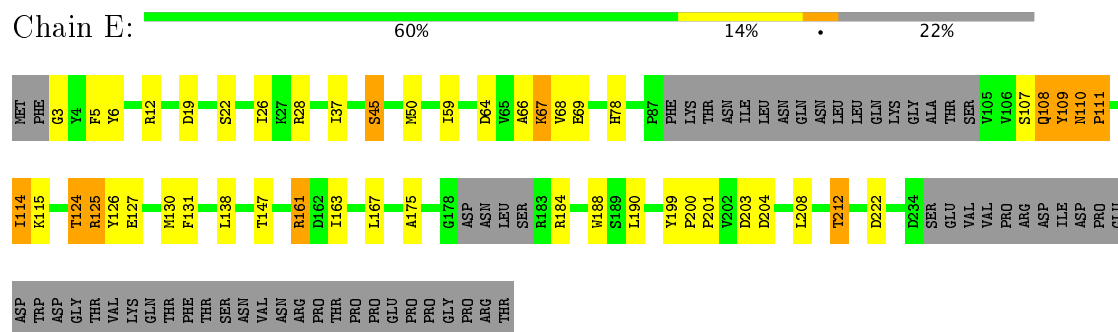
- Molecule 1: Tail connector protein Gp15



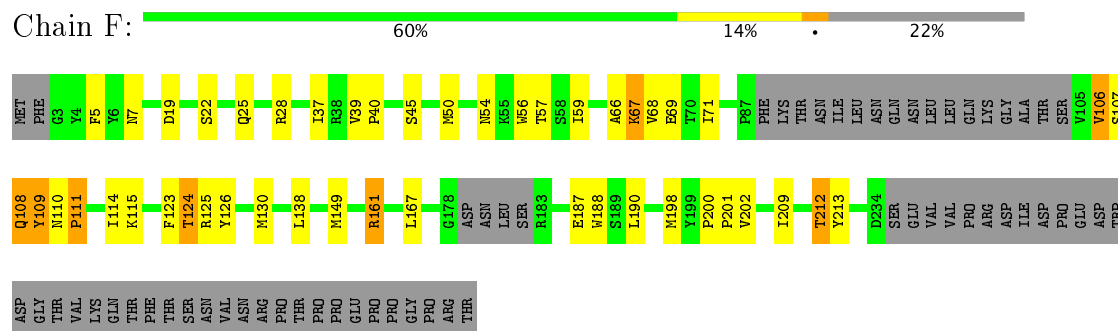
- Molecule 1: Tail connector protein Gp15



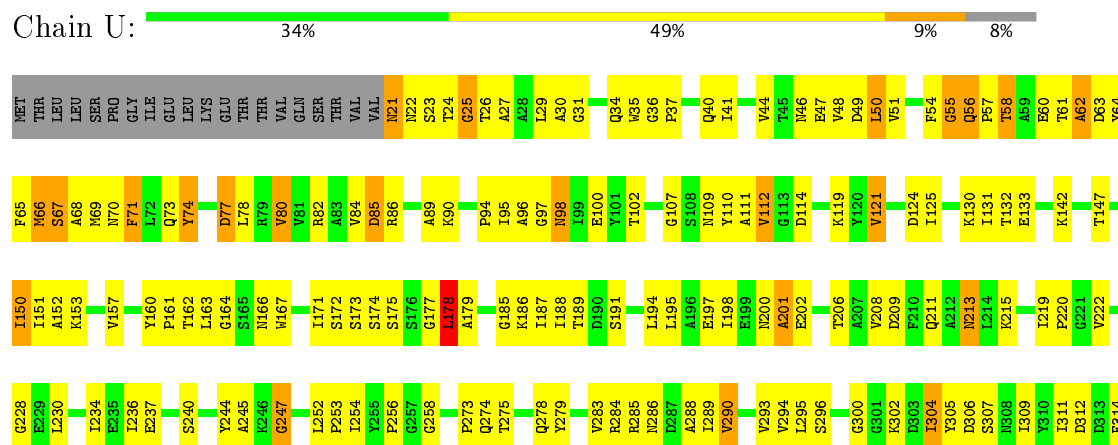
• Molecule 1: Tail connector protein Gp15

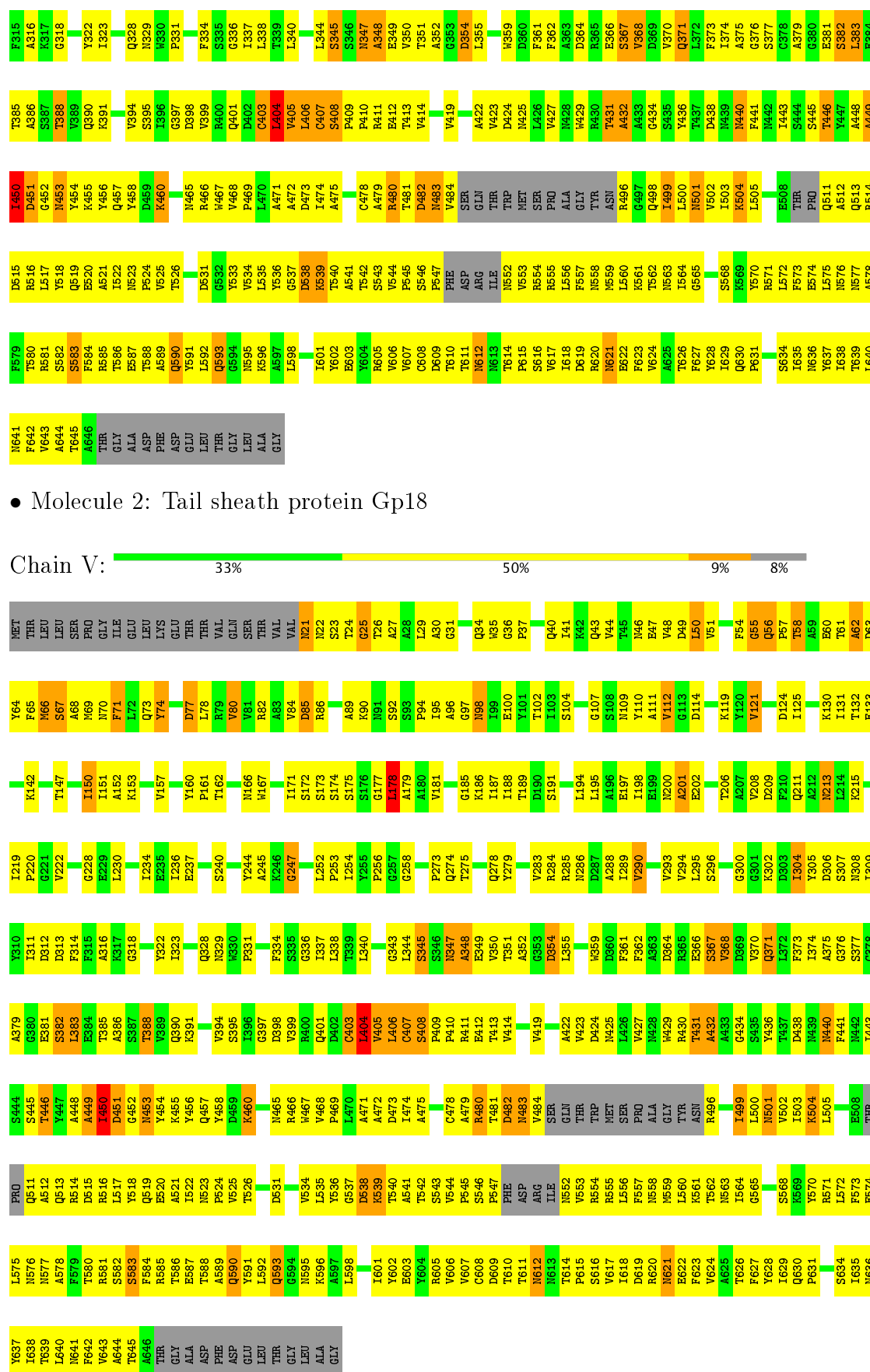


• Molecule 1: Tail connector protein Gp15

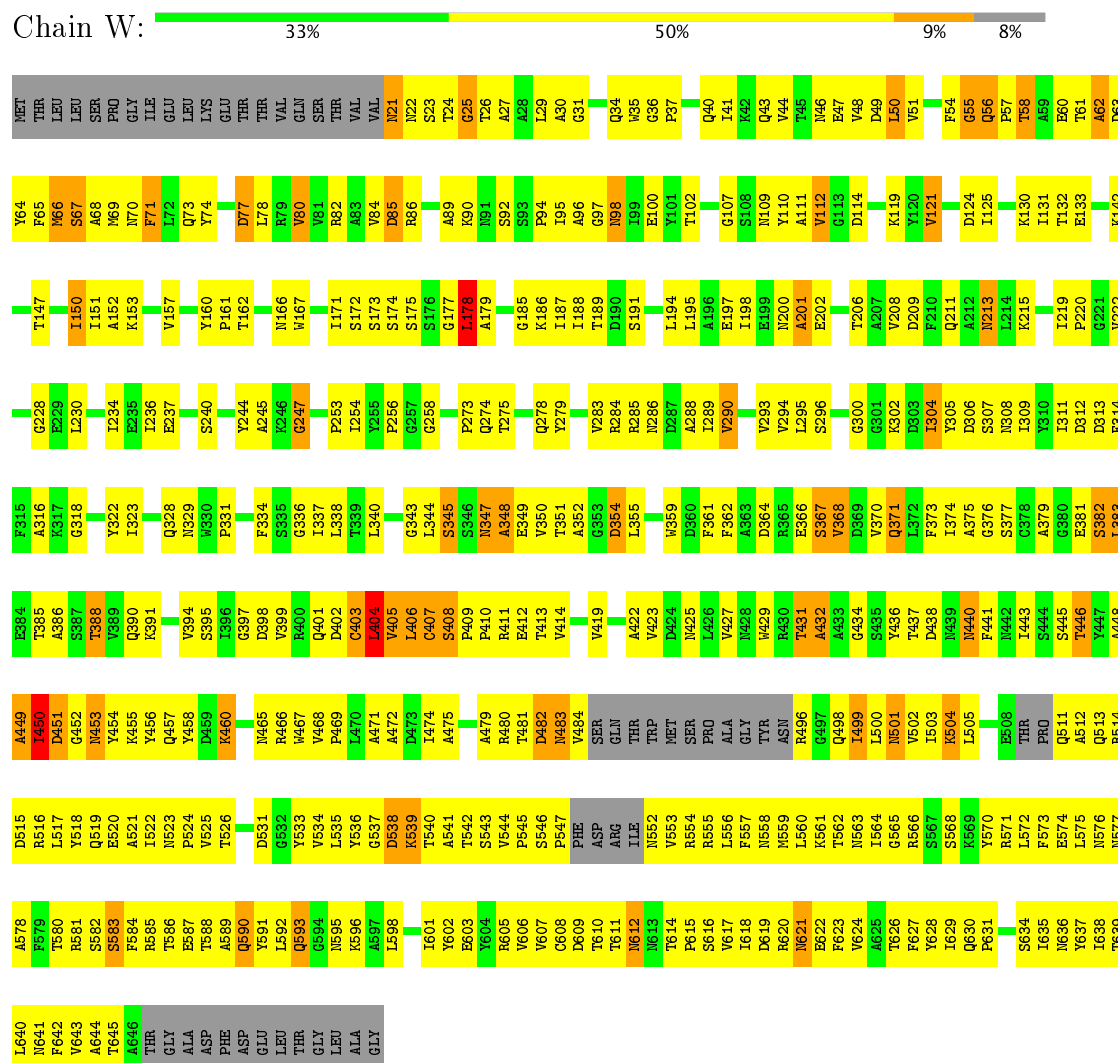


• Molecule 2: Tail sheath protein Gp18

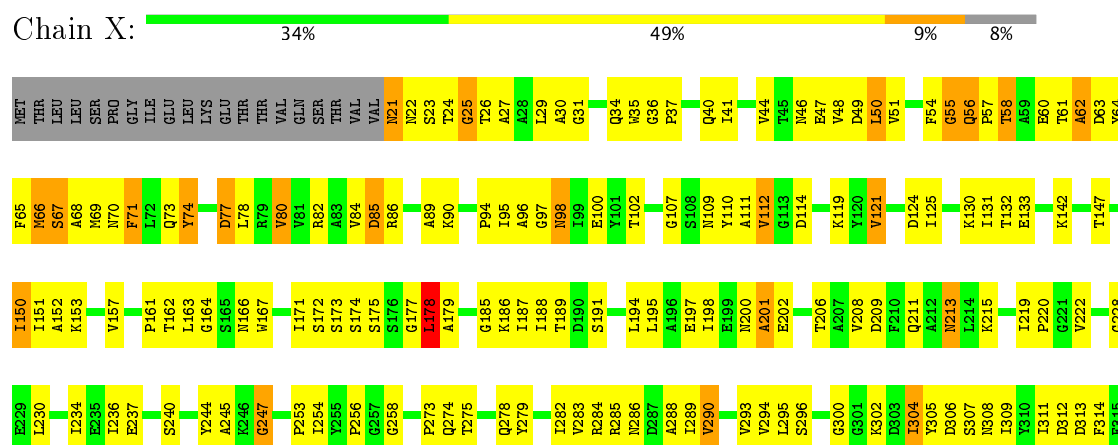




• Molecule 2: Tail sheath protein Gp18



• Molecule 2: Tail sheath protein Gp18



F642	T580	R516	D451	A386	A316
V643	R51	L517	G452	S387	K317
A644	S582	V518	H453	T388	G318
T645	S583	Q519	Y454	V369	
A646	R584	E520	K455	Q390	Y222
THR	A585	A521	Y456	K391	I233
GLY	T586	I522	Q457		
ALA	E587	N523	Y458	V394	Q328
ASP	A588	P524	D459	S395	N329
PHE	T589	V525	K460	I396	W330
ASP	Q590	T526		G397	P331
GLU	V591		H465	D398	
LEU	L592	D531	R466	V399	F334
THR	Q593	G532	W467	R400	S335
GLY	E594	G533	Y468	Q401	G336
LEU	V595	V534	P469	D402	I337
ALA	K596	L535	L470	C403	L338
A597	Y597	Y536	A471	L404	T339
	L598	G537	A472	V405	L340
		D538	D473	L406	
I601	V602	T540	I474	C407	L344
E603		K339	A475	S408	S345
T604		A541		P409	S346
R605	T542	T542	C478	P410	N347
V606	S543	S543	A479	R411	A348
V607	V544	V544	R490	E412	E349
C608	P545	P545	T481	T413	V350
D609	S546	S546	D482	V414	T351
T610	P547	P547	H483		A352
T611	PHE	PHE	V484	V419	G353
N612	ASP	ASP	SER		D354
N613	ARG	ARG	GLN	A422	L355
T614	ILE	N552	THR	V423	
P615	V553	V553	TRP	D424	W359
	R554	R554	MET	I425	D360
V617	R555	R555	SER	L426	F361
I618	L556	L556	PRO	V427	F362
D619	F557	F557	ALA	I428	A363
N620	N558	N558	GLY	W429	D364
	P559	P559	TYR	R430	R365
B622	L560	L560	ASN	T431	E366
F623	K561	K561	R496	A432	S367
V624	T562	T562	G497	A433	V368
A625	N563	N563	Q498	G434	D369
T626	L564	L564	I499	S435	V370
F627	G565	G565	L500	V436	Q371
V628			H501	T437	I372
I629			V502	D438	F373
	S568	S568	I503	I439	I374
	K569	K569	K504	I440	A375
	V570	V570	L505	F441	G376
P631					
				I442	S377
				I443	C378
S634	R571	R571	THR	S444	A379
I635	F573	F573	PRO	T446	G380
H636	E574	E574		S445	E381
	L575	L575	Q511	V447	S382
I638	N576	N576	A512	A448	L383
T639	N577	N577	Q513		
	F578	F578	R514	A449	F384
L640	A578	A578	D515	T460	T385
	E579	E579			

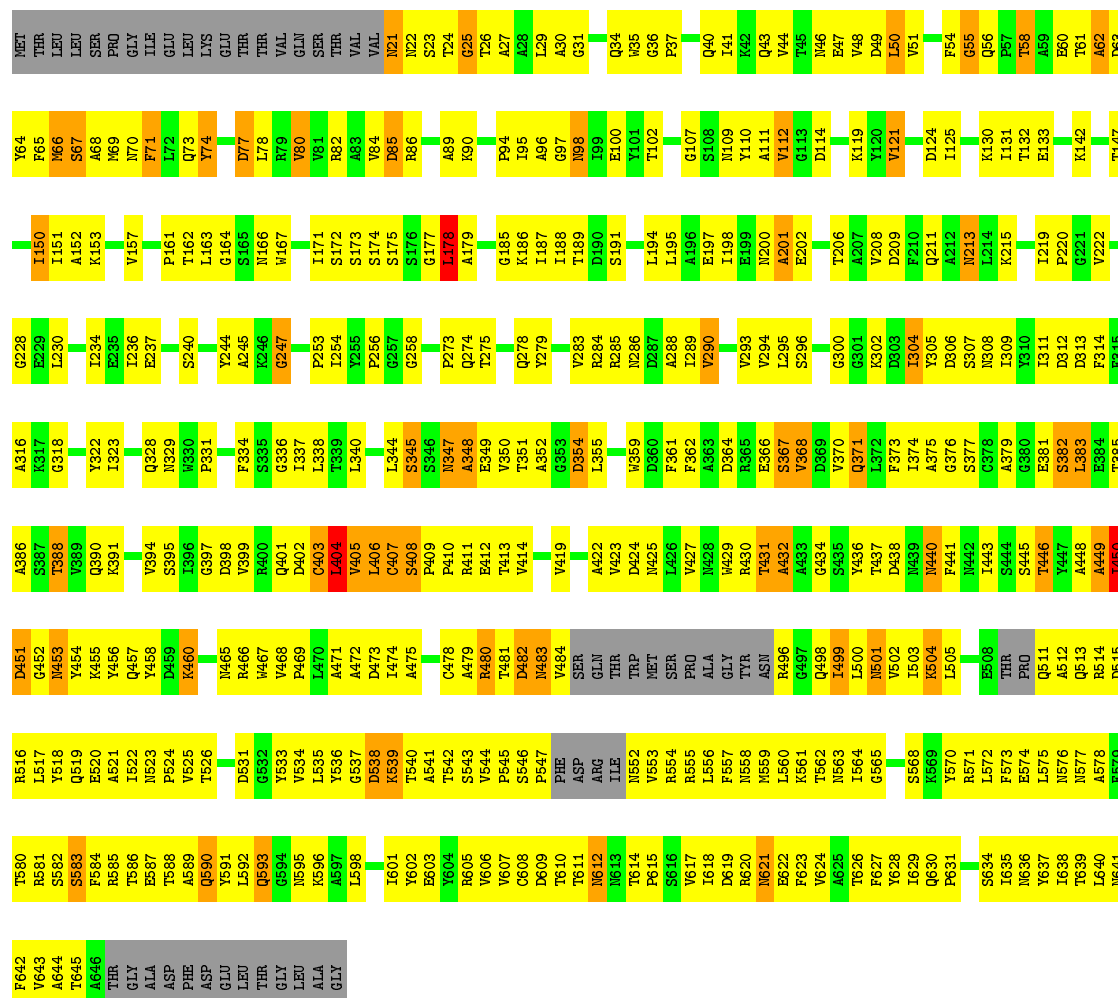
• Molecule 2: Tail sheath protein Gp18

Chain Y: 34% 50% 9% 8%

F642	T580	D515	A449	E384	F315	G228	T147	Y64
V643	R581	R516	D450	T385	A316	E229		F65
A644	S582	L517	D451	A386	F317	L230		LEU
A646	S583	Y518	G452	S387	G318		I150	S67
	F584	Q519	D453	T388		I234		A68
THR	R585	E520	Y454	T389	Y322	E235		SR
GLY	T586	A521	K455	Q390	I323		A152	PRD
ALA	E587	T522	Y456	K391		E237		GLY
ASP	T588	N523	Q457		Q328		V157	ILE
PHE	A589	F524	Y458		K329	S240		GLU
ASP	Q590	V525	D459	S395	K330		P161	LEU
GLU	Y591	T526	K460	L396	P331		T162	LVS
LEU	L592			G397		Y244		GLU
THR	Q593	D531		D398	F334	A245		THR
GLY	G594		R466	T399	S335	G246		THR
LEU	N595	V534	V467	R400	G336	E247		GLN
ALA	K596	L536	V468	Q401	I337		I171	SER
GLY	A597	Y536	P469	D402	L338	P253	S172	R81
		G537	L470	C403	T339	I254	S173	R82
		D538	A471	L404	L340	Y255	S174	A83
	I601	K539	A472	V405		G257	S175	R85
	Y602	T540	D473	L406	G343	G257	S176	N21
	E603	A541	I474	C407	L344	G258	G177	N22
	Y604	T542	A475	S408	S345		L178	S23
	R605	S543		P409	S346	P273	A179	R86
	V606	V544	C478	P410	N347	Q274		A89
	V607	F545	A479	R411	A348	T275	G185	G90
	C608	S546	R480	E412	S349	K186	S93	N91
	D609	P547	T481	T413	V350	Q278	I187	S92
T610	PHE	ASP	D482	V414	T351	Y279	I188	P94
T611	ARG	ASP	N483		A352		T189	I95
N612	ILE	ARG	V484	V419	G353	V283	D190	A96
N613	N552	ILE	SER		L355	R284	S191	G97
T614	P615	P553	THR	V423	D354	R285		N98
S616	S616	R554	TRP	D424		N286	L194	K35
V617	R555	R555	MET	N425	K359	D287	L195	N35
L618	L556	L556	SER	L426	D360	A288	A196	G36
D619	F557	F557	PRQ	V427	F361	I289	E197	P37
R620	N558	N558	ALA	N428	F362	V290	I198	S97
N621	N559	N559	GLY	V429	A363		A199	
E622	L560	L560	THR	R430	D364	V293	K200	K42
F623	T561	T561	ASN	T431	R365	V294	A201	Q43
V624	T562	T562	A496	A432	E366	L295	E202	N109
A625	N563	N563		A433	S367	S296		Y110
T626	I564	I564	I499	G434	V368		T206	I46
F627	G565	G565	L500	S435	D369	G300	A207	G107
Y628			N501	T436	V370	G301	V208	K42
	S568	S568	N502	Y437	Q371	K302	D209	V44
	K569	K569	F503	D438	L372	D303	F210	Y111
P631	Y570	Y570	K504	N439	F373	Q211	A212	
	R571	R571	L505	N440	I374	Y305	K213	D124
	L572	L572		F441	A375	S307	L214	I125
S634	F573	F573	E508	N442	G376	S307	K215	
I635	E574	E574	THR	L443	S377	N308		K430
K636	L575	L575	PRQ	S444	G378	I309		I131
	N576	N576		S445	A379	Y310	T219	A59
T639	N577	N577	Q511	T446	G380	I311	P220	B60
	N578	N578	A512		E381	G312	G221	T61
	N579	N579	Q513	Y447	S382	G313	Y222	
N641	E580	E580	R514	L448	L392	D314		A62
								D62

- Molecule 2: Tail sheath protein Gp18

Chain Z:  33% 50% 9% 8%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	1965	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	47000	Depositor
Image detector	KODAK SO-163 FILM	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 >2	RMSZ	# Z >2
1	A	0.49	0/1787	0.64	0/2421
1	B	0.47	0/1787	0.63	0/2421
1	C	0.48	0/1787	0.64	1/2421 (0.0%)
1	D	0.49	0/1787	0.63	0/2421
1	E	0.49	0/1787	0.63	0/2421
1	F	0.50	0/1787	0.65	0/2421
2	U	0.60	0/4729	0.90	21/6427 (0.3%)
2	V	0.60	0/4729	0.89	21/6427 (0.3%)
2	W	0.60	0/4729	0.90	21/6427 (0.3%)
2	X	0.59	0/4729	0.90	21/6427 (0.3%)
2	Y	0.60	0/4729	0.90	21/6427 (0.3%)
2	Z	0.60	0/4729	0.90	21/6427 (0.3%)
All	All	0.57	0/39096	0.83	127/53088 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	U	0	4
2	V	0	4
2	W	0	4
2	X	0	4
2	Y	0	4
2	Z	0	4
All	All	0	24

There are no bond length outliers.

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	55	GLY	N-CA-C	18.05	158.21	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	55	GLY	N-CA-C	18.03	158.18	113.10
2	X	55	GLY	N-CA-C	18.03	158.16	113.10
2	W	55	GLY	N-CA-C	18.01	158.13	113.10
2	Z	55	GLY	N-CA-C	18.01	158.12	113.10

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	U	21	ASN	Peptide
2	U	450	ILE	Peptide
2	U	451	ASP	Peptide
2	U	452	GLY	Peptide
2	V	21	ASN	Peptide

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	A	1742	0	1673	29	0
1	B	1742	0	1673	33	0
1	C	1742	0	1673	30	0
1	D	1742	0	1673	29	0
1	E	1742	0	1673	32	0
1	F	1742	0	1673	28	0
2	U	4647	0	4563	565	0
2	V	4647	0	4564	571	0
2	W	4647	0	4564	568	0
2	X	4647	0	4564	565	0
2	Y	4647	0	4564	557	0
2	Z	4647	0	4564	561	0
All	All	38334	0	37421	3566	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 47.

The worst 5 of 3566 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)
2:U:404:LEU:CG	2:U:554:ARG:HH12	1.22	1.52
2:V:404:LEU:CG	2:V:554:ARG:HH12	1.22	1.51
2:Z:404:LEU:CG	2:Z:554:ARG:HH12	1.23	1.51
2:Y:404:LEU:CG	2:Y:554:ARG:HH12	1.22	1.50
2:X:496:ARG:N	2:X:534:VAL:CB	1.73	1.50

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	A	205/272 (75%)	184 (90%)	18 (9%)	3 (2%)	12	53
1	B	205/272 (75%)	184 (90%)	17 (8%)	4 (2%)	9	46
1	C	205/272 (75%)	184 (90%)	17 (8%)	4 (2%)	9	46
1	D	205/272 (75%)	184 (90%)	17 (8%)	4 (2%)	9	46
1	E	205/272 (75%)	183 (89%)	18 (9%)	4 (2%)	9	46
1	F	205/272 (75%)	184 (90%)	18 (9%)	3 (2%)	12	53
2	U	601/659 (91%)	479 (80%)	101 (17%)	21 (4%)	4	34
2	V	601/659 (91%)	479 (80%)	101 (17%)	21 (4%)	4	34
2	W	601/659 (91%)	479 (80%)	101 (17%)	21 (4%)	4	34
2	X	601/659 (91%)	479 (80%)	101 (17%)	21 (4%)	4	34
2	Y	601/659 (91%)	481 (80%)	99 (16%)	21 (4%)	4	34
2	Z	601/659 (91%)	479 (80%)	101 (17%)	21 (4%)	4	34
All	All	4836/5586 (87%)	3979 (82%)	709 (15%)	148 (3%)	8	37

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	GLN

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Mol	Chain	Res	Type
1	B	67	LYS
1	B	108	GLN
1	C	67	LYS
1	C	108	GLN

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	A	192/250 (77%)	176 (92%)	16 (8%)	13	43
1	B	192/250 (77%)	181 (94%)	11 (6%)	24	56
1	C	192/250 (77%)	176 (92%)	16 (8%)	13	43
1	D	192/250 (77%)	180 (94%)	12 (6%)	21	53
1	E	192/250 (77%)	180 (94%)	12 (6%)	21	53
1	F	192/250 (77%)	179 (93%)	13 (7%)	18	51
2	U	494/536 (92%)	448 (91%)	46 (9%)	10	37
2	V	494/536 (92%)	447 (90%)	47 (10%)	10	36
2	W	494/536 (92%)	447 (90%)	47 (10%)	10	36
2	X	494/536 (92%)	448 (91%)	46 (9%)	10	37
2	Y	494/536 (92%)	446 (90%)	48 (10%)	9	35
2	Z	494/536 (92%)	446 (90%)	48 (10%)	9	35
All	All	4116/4716 (87%)	3754 (91%)	362 (9%)	16	39

5 of 362 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	V	450	ILE
2	W	395	SER
2	Z	347	ASN
2	V	501	ASN
2	W	102	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
2	W	513	GLN
2	X	440	ASN
2	Z	511	GLN
2	W	612	ASN
2	X	43	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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.