



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 07:24 AM EST

PDB ID : 3J2M
EMDB ID : EMD-1126
Title : The X-ray structure of the gp15 hexamer and the model of the gp18 protein fitted into the cryo-EM reconstruction of the extended T4 tail
Authors : Fokine, A.; Zhang, Z.; Kanamaru, S.; Bowman, V.D.; Aksyuk, A.; Arisaka, F.; Rao, V.B.; Rossmann, M.G.
Deposited on : 2012-11-09
Resolution : 15.00 Å(reported)

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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

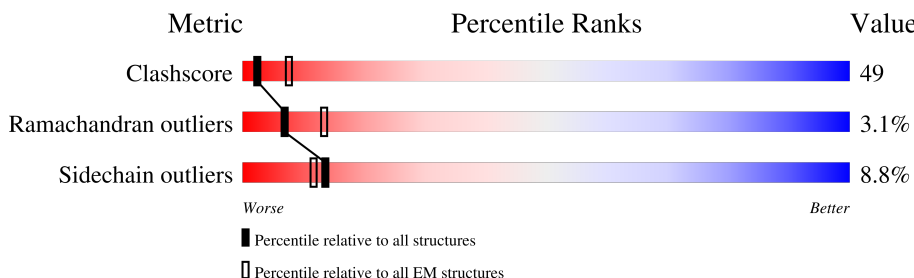
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 15.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	272	58% 17% • 22%
1	B	272	60% 15% • 22%
1	C	272	57% 17% • 22%
1	D	272	60% 14% • 22%
1	E	272	60% 14% • 22%
1	F	272	60% 15% • 22%
2	U	659	33% 50% 9% 8%
2	V	659	34% 49% 9% 8%

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Mol	Chain	Length	Quality of chain
2	W	659	<div><div></div><div></div><div></div><div></div></div> <div>34%49%9%8%</div>
2	X	659	<div><div></div><div></div><div></div><div></div></div> <div>34%49%9%8%</div>
2	Y	659	<div><div></div><div></div><div></div><div></div></div> <div>34%49%9%8%</div>
2	Z	659	<div><div></div><div></div><div></div><div></div></div> <div>33%50%9%8%</div>

2 Entry composition [i](#)

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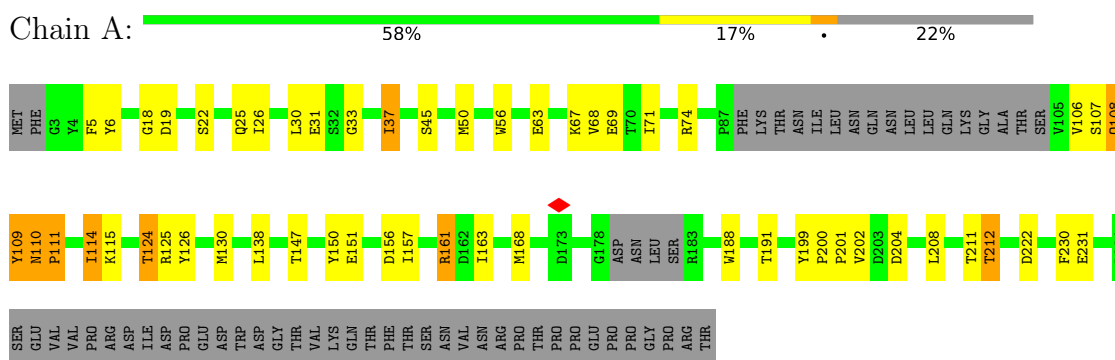
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Chain	Residue	Modelled	Actual	Comment	Reference
Z	301	GLY	GLU	SEE REMARK 999	UNP P13332
Z	399	VAL	ALA	SEE REMARK 999	UNP P13332
Z	454	TYR	HIS	SEE REMARK 999	UNP P13332
Z	510	PRO	ARG	ENGINEERED MUTATION	UNP P13332

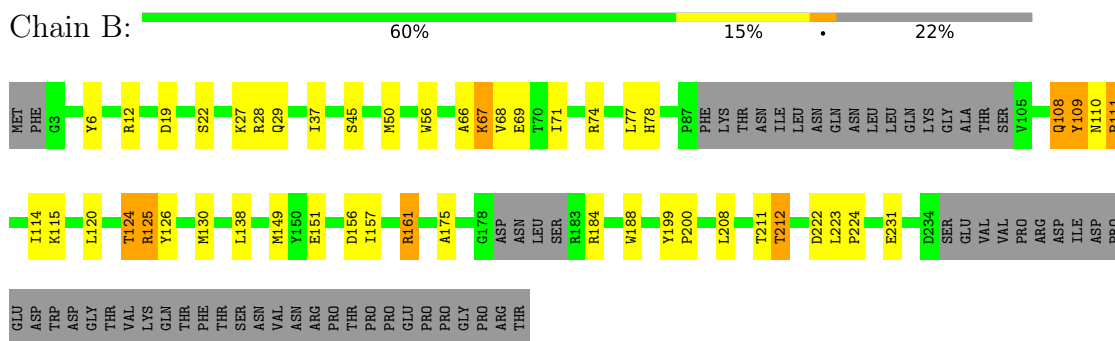
3 Residue-property plots

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.

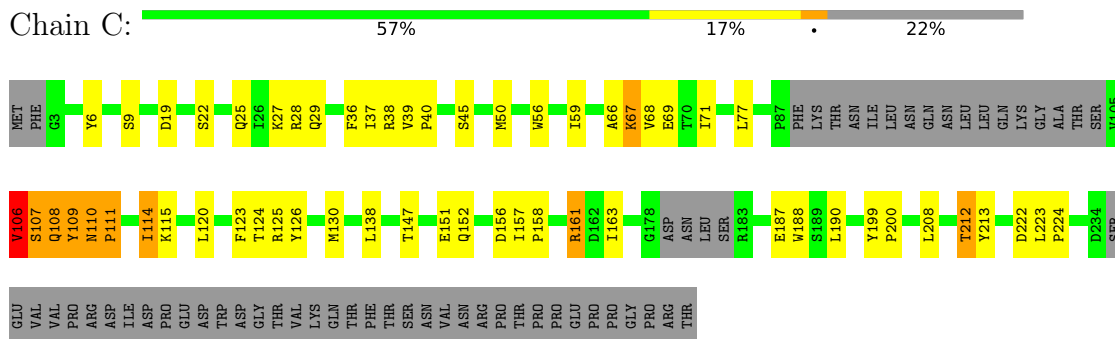
• Molecule 1: Tail connector protein Gp15



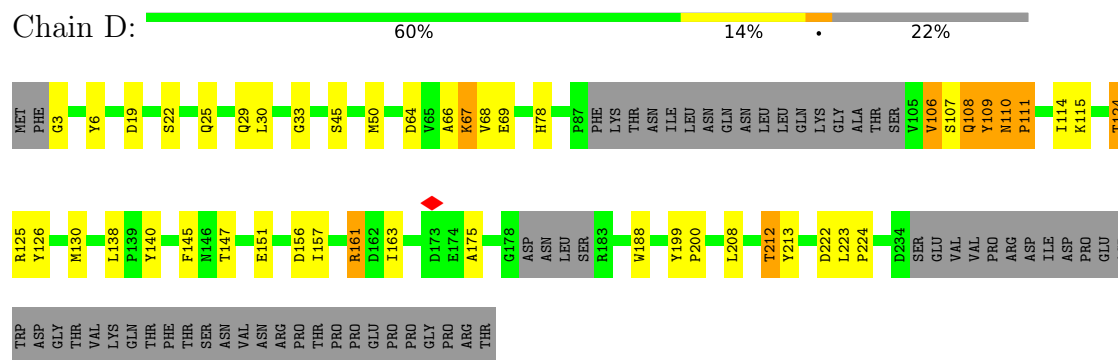
• Molecule 1: Tail connector protein Gp15



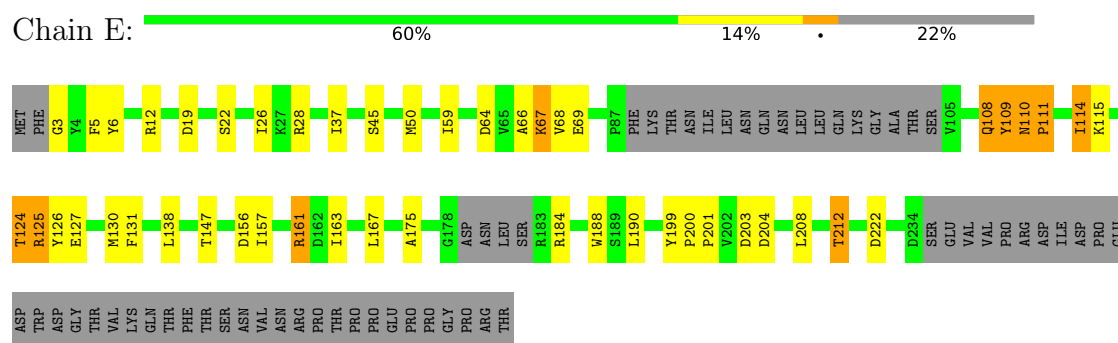
• Molecule 1: Tail connector protein Gp15



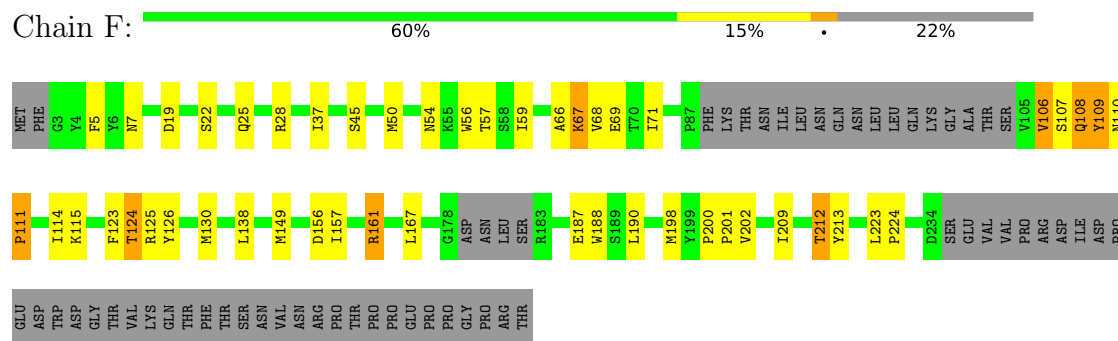
- Molecule 1: Tail connector protein Gp15



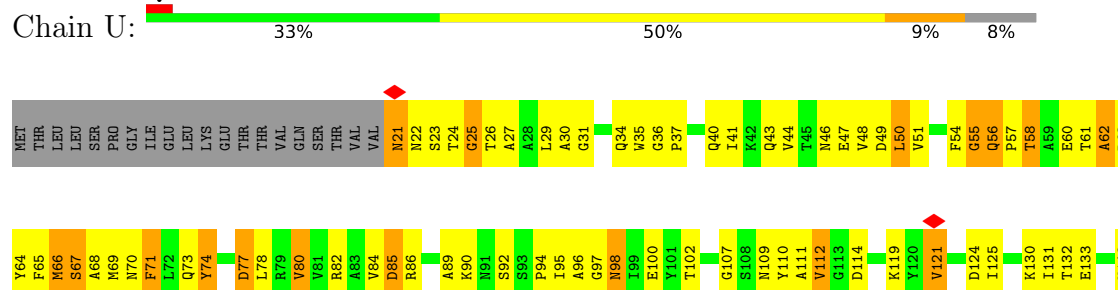
- Molecule 1: Tail connector protein Gp15

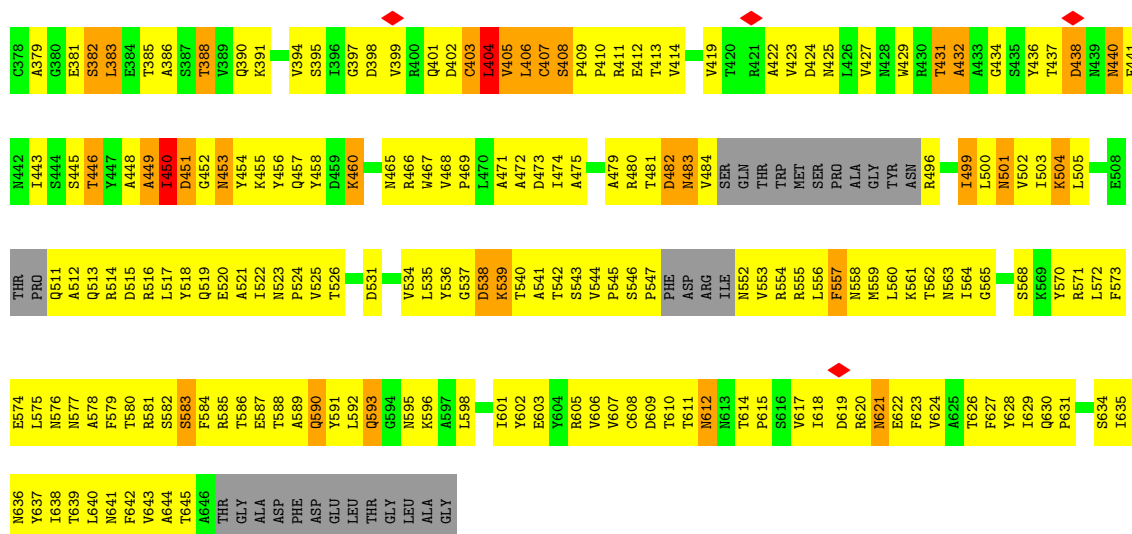


- Molecule 1: Tail connector protein Gp15

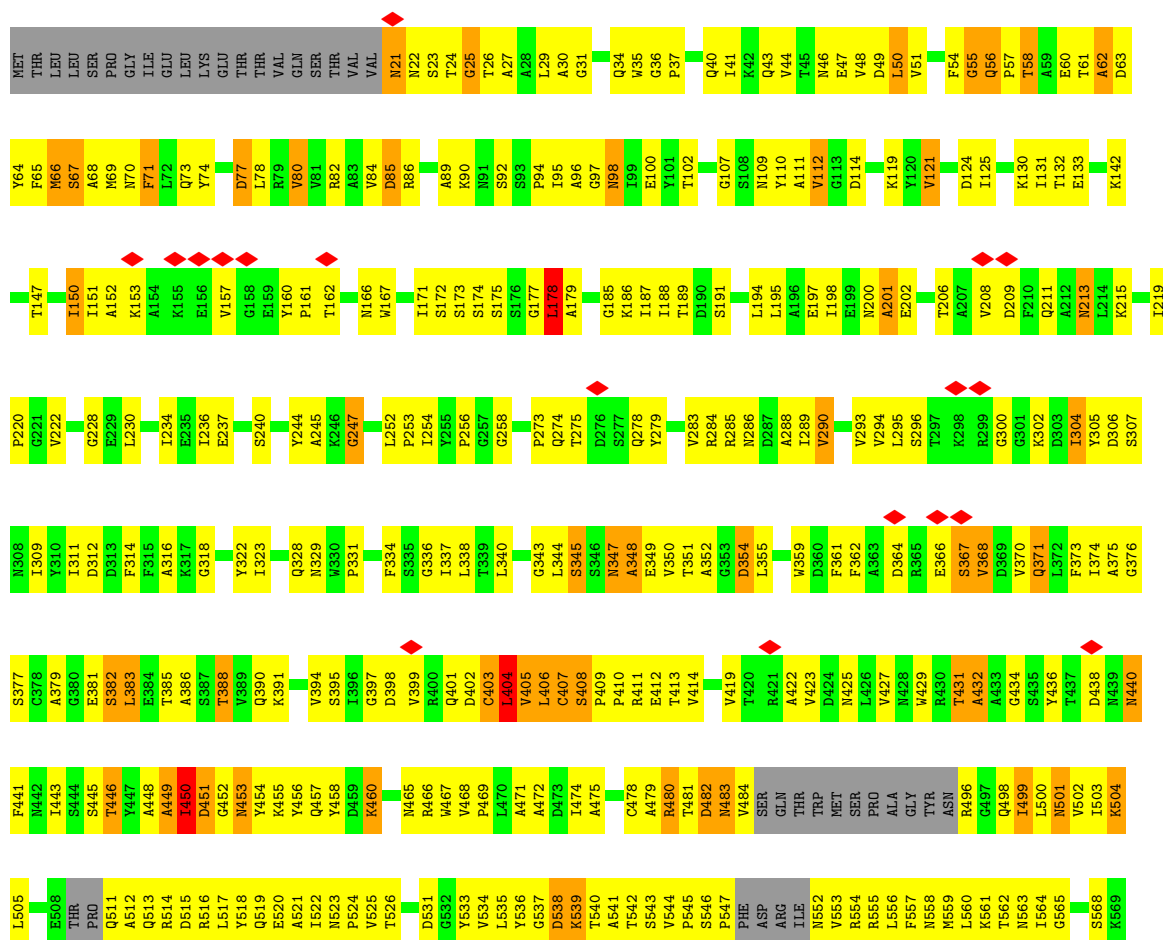


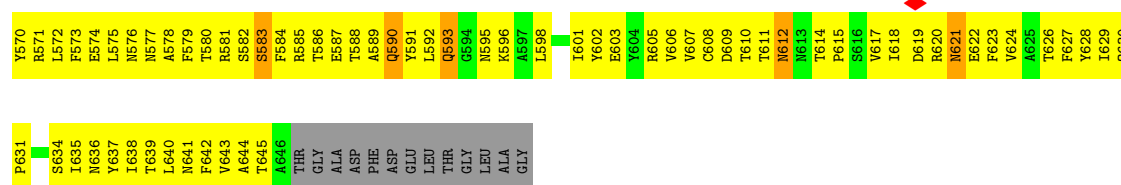
- Molecule 2: Tail sheath protein Gp18





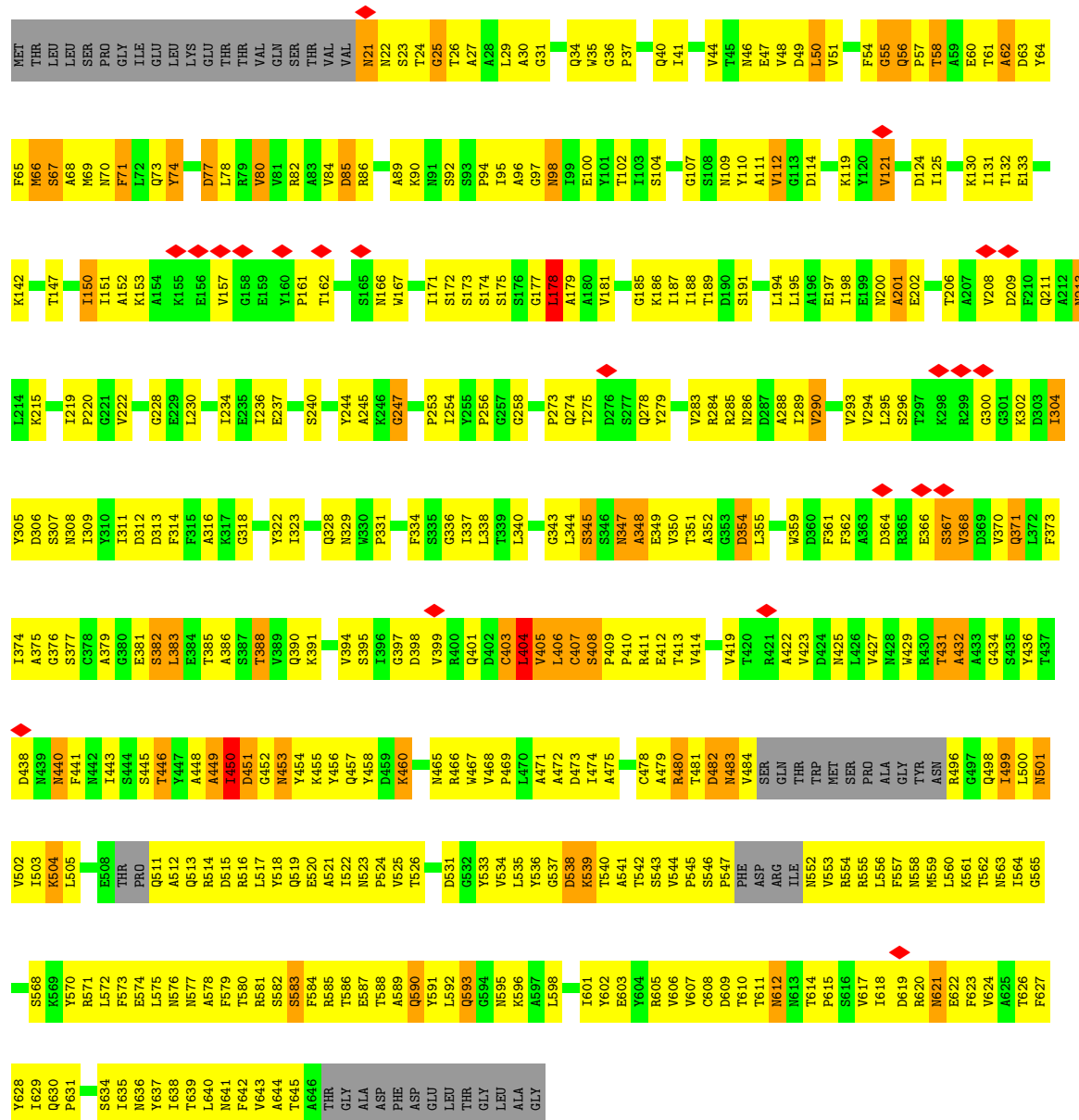
• Molecule 2: Tail sheath protein Gp18





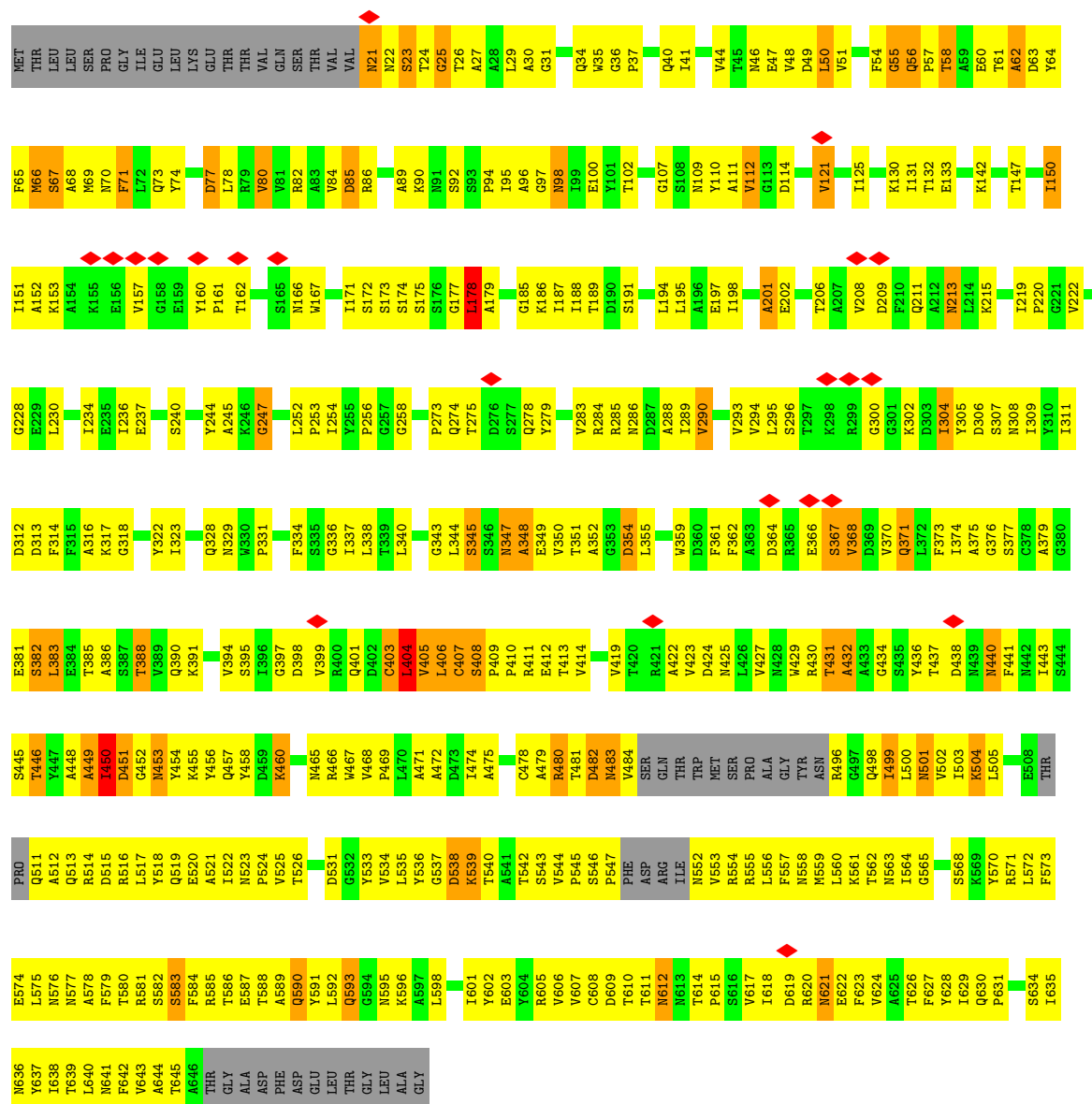
• Molecule 2: Tail sheath protein Gp18

Chain X: 34% 49% 9% 8%

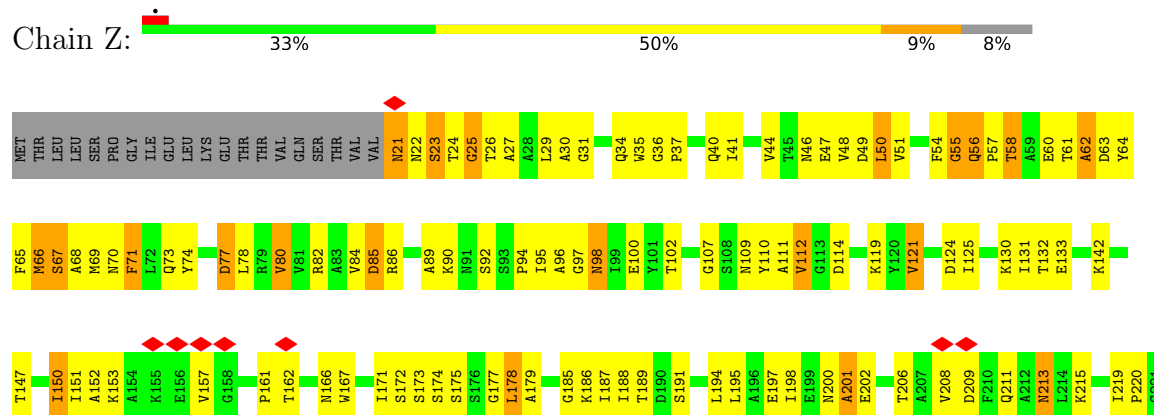


• Molecule 2: Tail sheath protein Gp18

Chain Y: 34% 49% 9% 8%



Chain Z: 33% 50% 9% 8%



S634	L572	E508	I443	A379	Y810	V222
I635	F573	THR	S444	G380	I311	G228
N636	E574	PRO	S445	E381	D312	G229
Y637	L575	Q511	T446	S382	D313	E229
I638	N576	A512	Y447	L383	F314	L230
T639	N577	Q513	Y448	E384	F315	L234
L640	A578	R514	A449	T385	A316	E235
M641	F579	D515	T450	A386	K317	I236
F642	T580	R516	D450	A387	G318	E237
V643	R581	L517	D451	T388	Y322	S240
A644	S582	Y518	N453	V389	I323	Y244
T645	S583	Q519	Y454	K390	Q328	A245
A646	F584	E520	K455	K391	N329	K246
THR	R585	A521	Y456	Q394	W330	G247
GLY	T586	I522	Q457	S395	Y334	L252
ALA	E587	N523	Y458	V396	G336	P253
ASP	T588	P524	D459	I396	I337	I254
PHE	A589	V525	K460	G397	L338	Y255
ASP	Q590	T526	N465	D398	T339	P256
GLU	Y591	D531	W466	V399	L340	G257
LEU	L592	G532	W467	R400	G343	G258
THR	Q593	Y533	V468	Q401	G344	P273
GLY	G594	V534	P469	D402	S345	Q274
LEU	N595	L535	L470	C403	S346	T275
ALA	K596	Y536	A471	L404	N347	D276
GLY	A597	G537	D472	V405	A348	S277
	L598	D538	A473	L406	E349	Q278
	I601	T540	I474	S408	V350	Y279
	Y602	A541	A475	P409	A352	V283
	E603	T542	C478	P410	G353	R284
	Y604	S543	A479	R411	D354	R285
	V606	V544	R480	E412	L355	N286
	V607	P545	T481	T413	W359	D287
	C608	S546	D482	V414	F361	I289
	D609	P547	N483	V419	F362	V290
	T610	PHE	V484	T420	A363	V293
	T611	ASP	SER	R421	D364	V294
	N612	ARG	GLN	A422	E365	L295
	N613	ILE	THR	A423	E366	S296
	P615	N552	TRP	D424	S367	T297
	S616	V553	MET	M425	R298	K299
	V617	R554	SER	N426	G300	G301
	I618	R555	PRO	L427	K302	K303
	D619	L556	ALA	W428	L372	I304
	R620	F557	GLY	M429	I374	Y305
	M621	N558	TYR	R430	A375	D306
	E622	M559	ASN	T431	G376	S307
	F623	L560	R496	A432	S377	N308
	V624	T562	Q498	A433	D369	I309
	A625	I564	I499	G434	V370	
	T626	F564	L500	S435	L372	
	F627	G565	N501	Y436	I304	
	Y628	S568	V502	T437	I374	
	I629	K569	I503	D438	A375	
	Q630	Y570	K504	M439	G376	
	P631	R571	L505	M440	S377	
				N442	C378	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	3029	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	each particle image	Depositor
Microscope	FEI/PHILIPS CM300FEG/ST	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	47000	Depositor
Image detector	Not provided	
Maximum map value	7.953	Depositor
Minimum map value	-2.953	Depositor
Average map value	0.059	Depositor
Map value standard deviation	0.533	Depositor
Recommended contour level	1.01	Depositor
Map size (\AA)	714.6, 714.6, 1508.6	wwPDB
Map dimensions	180, 180, 380	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\AA)	3.97, 3.97, 3.97	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	0.49	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	0.89	21/6427 (0.3%)
2	V	0.60	0/4729	0.90	21/6427 (0.3%)
2	W	0.60	0/4729	0.89	21/6427 (0.3%)
2	X	0.60	0/4729	0.90	21/6427 (0.3%)
2	Y	0.60	1/4729 (0.0%)	0.89	20/6427 (0.3%)
2	Z	0.60	1/4729 (0.0%)	0.89	19/6427 (0.3%)
All	All	0.57	2/39096 (0.0%)	0.83	124/53088 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	23	SER	C-O	5.16	1.33	1.23
2	Y	23	SER	C-O	5.03	1.32	1.23

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	55	GLY	N-CA-C	18.09	158.33	113.10
2	U	55	GLY	N-CA-C	18.03	158.18	113.10
2	Y	55	GLY	N-CA-C	18.01	158.12	113.10
2	W	55	GLY	N-CA-C	17.99	158.08	113.10
2	X	55	GLY	N-CA-C	17.93	157.92	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	54	0
1	B	1742	0	1673	59	0
1	C	1742	0	1673	49	0
1	D	1742	0	1673	44	0
1	E	1742	0	1673	46	0
1	F	1742	0	1673	36	0
2	U	4647	0	4564	595	0
2	V	4647	0	4564	592	0
2	W	4647	0	4564	588	0
2	X	4647	0	4564	587	0
2	Y	4647	0	4562	576	0
2	Z	4647	0	4564	577	0
All	All	38334	0	37420	3690	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 49.

The worst 5 of 3690 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ASP:HB3	2:U:579:PHE:CE1	1.23	1.68
1:B:157:ILE:CD1	2:V:579:PHE:HB3	1.20	1.63
1:B:157:ILE:HG13	2:V:579:PHE:CB	1.21	1.57
1:B:156:ASP:HB3	2:V:579:PHE:CE1	1.39	1.54
1:A:157:ILE:HG13	2:U:579:PHE:CB	1.22	1.54

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%)	10	46
1	B	205/272 (75%)	184 (90%)	17 (8%)	4 (2%)	7	38
1	C	205/272 (75%)	184 (90%)	17 (8%)	4 (2%)	7	38
1	D	205/272 (75%)	184 (90%)	17 (8%)	4 (2%)	7	38
1	E	205/272 (75%)	183 (89%)	18 (9%)	4 (2%)	7	38
1	F	205/272 (75%)	184 (90%)	18 (9%)	3 (2%)	10	46
2	U	601/659 (91%)	479 (80%)	101 (17%)	21 (4%)	3	25
2	V	601/659 (91%)	480 (80%)	100 (17%)	21 (4%)	3	25
2	W	601/659 (91%)	479 (80%)	101 (17%)	21 (4%)	3	25
2	X	601/659 (91%)	479 (80%)	101 (17%)	21 (4%)	3	25
2	Y	601/659 (91%)	479 (80%)	101 (17%)	21 (4%)	3	25
2	Z	601/659 (91%)	480 (80%)	100 (17%)	21 (4%)	3	25
All	All	4836/5586 (87%)	3979 (82%)	709 (15%)	148 (3%)	7	27

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
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%)	11	34
1	B	192/250 (77%)	181 (94%)	11 (6%)	20	45
1	C	192/250 (77%)	176 (92%)	16 (8%)	11	34
1	D	192/250 (77%)	180 (94%)	12 (6%)	18	43
1	E	192/250 (77%)	180 (94%)	12 (6%)	18	43
1	F	192/250 (77%)	179 (93%)	13 (7%)	16	41
2	U	494/536 (92%)	446 (90%)	48 (10%)	8	27
2	V	494/536 (92%)	447 (90%)	47 (10%)	8	27
2	W	494/536 (92%)	448 (91%)	46 (9%)	9	28
2	X	494/536 (92%)	448 (91%)	46 (9%)	9	28
2	Y	494/536 (92%)	446 (90%)	48 (10%)	8	27
2	Z	494/536 (92%)	446 (90%)	48 (10%)	8	27
All	All	4116/4716 (87%)	3753 (91%)	363 (9%)	13	31

5 of 363 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	X	102	THR
2	Y	345	SER
2	X	213	ASN
2	X	483	ASN
2	Y	436	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
2	X	453	ASN
2	Y	390	GLN
2	Z	641	ASN
2	X	511	GLN
2	X	630	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

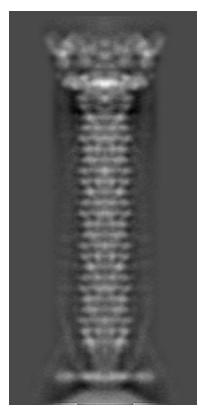
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1126. These allow visual inspection of the internal detail of the map and identification of artifacts.

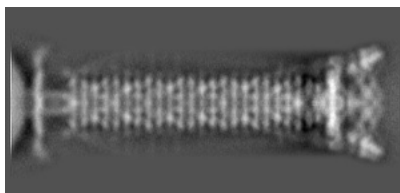
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

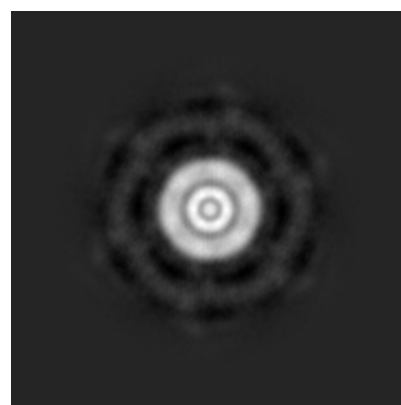
6.1.1 Primary map



X



Y

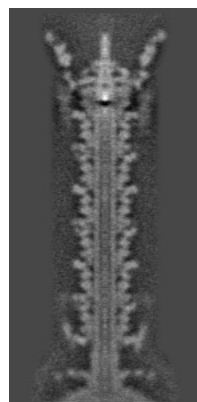


Z

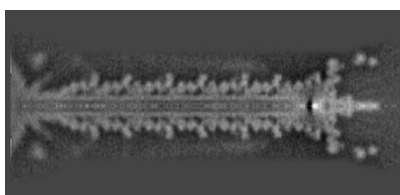
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

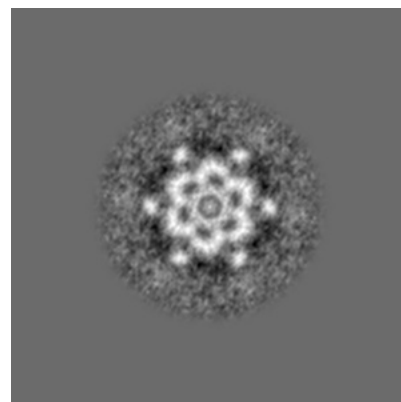
6.2.1 Primary map



X Index: 90



Y Index: 90

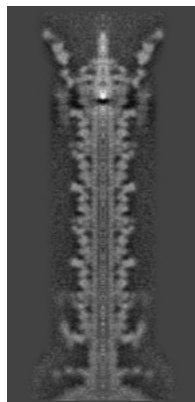


Z Index: 190

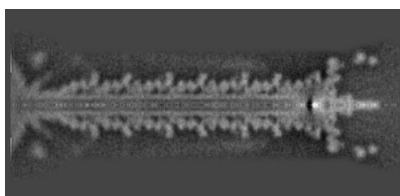
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

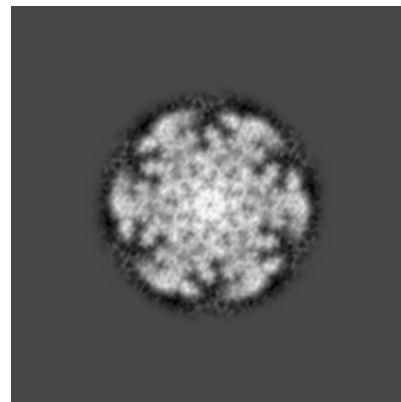
6.3.1 Primary map



X Index: 89



Y Index: 90



Z Index: 310

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

6.4 Orthogonal surface views [i](#)

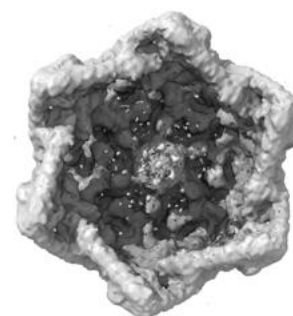
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

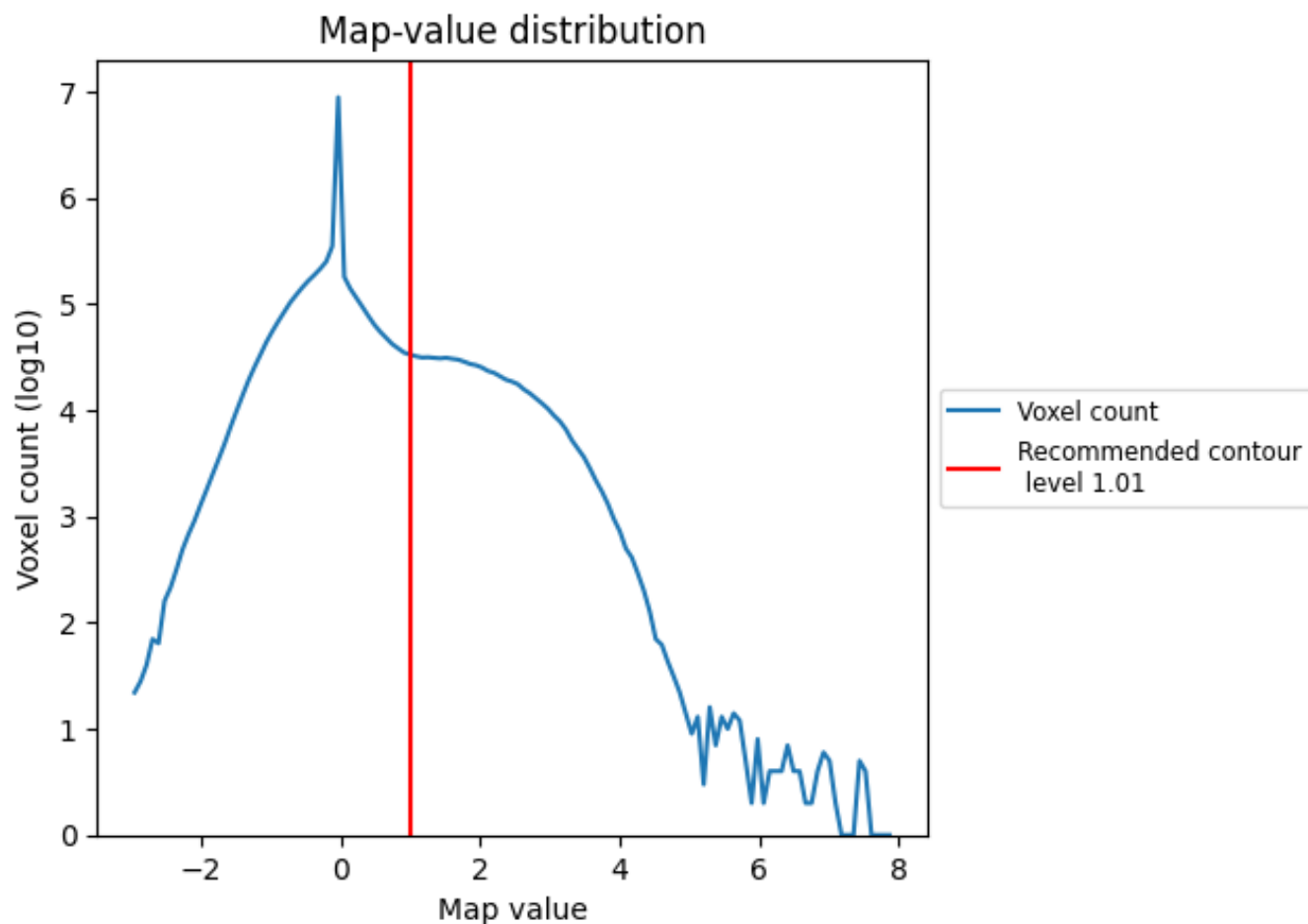
6.5 Mask visualisation

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

7 Map analysis [i](#)

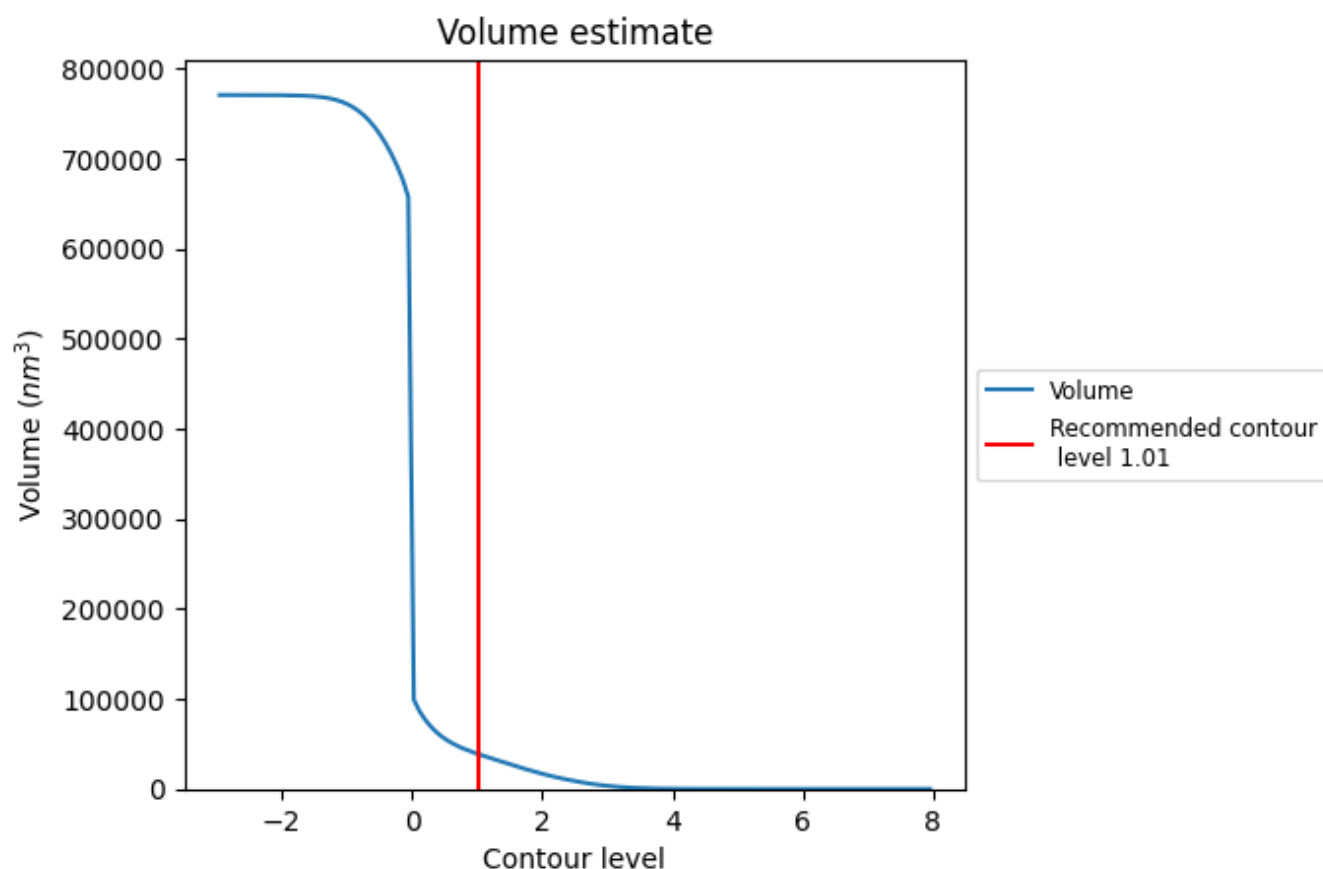
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 38892 nm³; this corresponds to an approximate mass of 35132 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

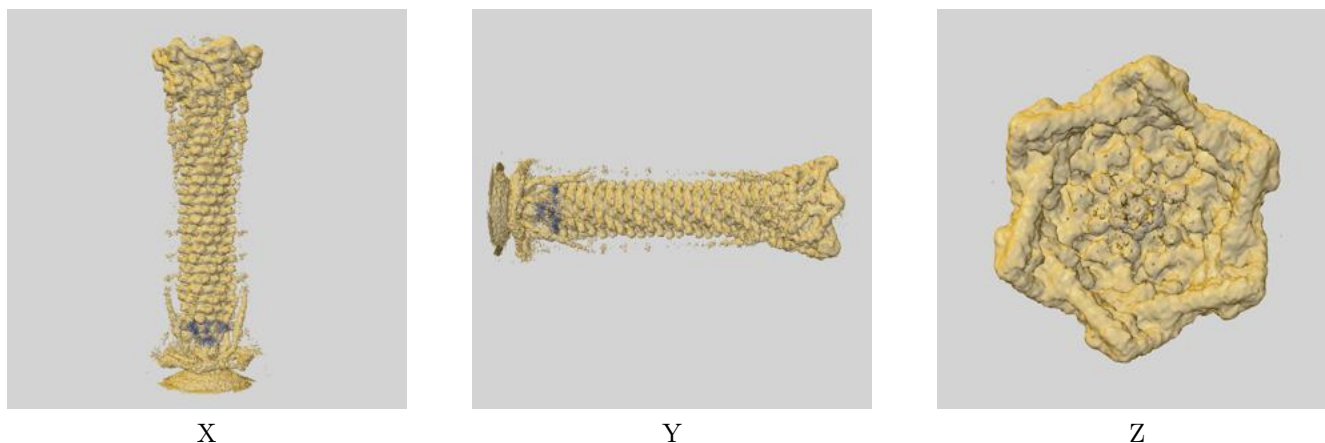
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

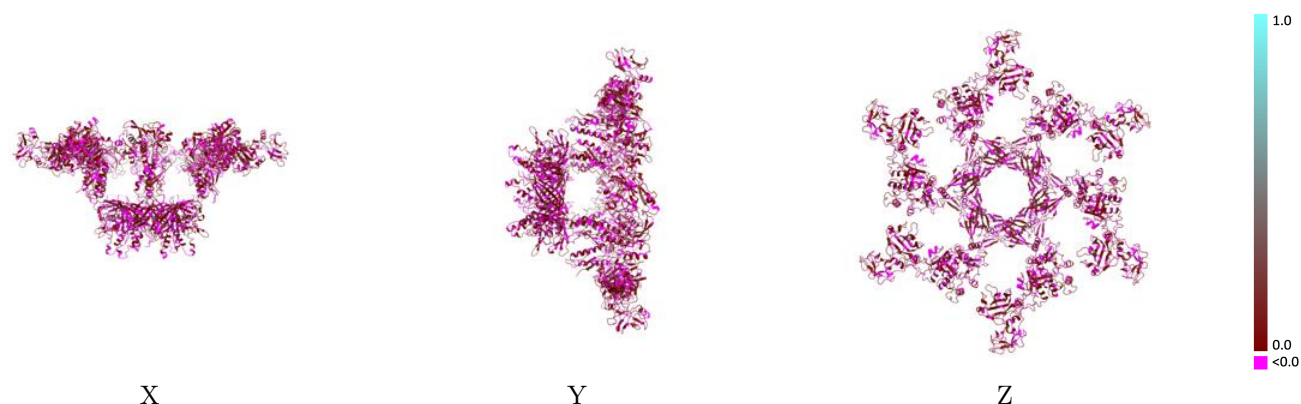
This section contains information regarding the fit between EMDB map EMD-1126 and PDB model 3J2M. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



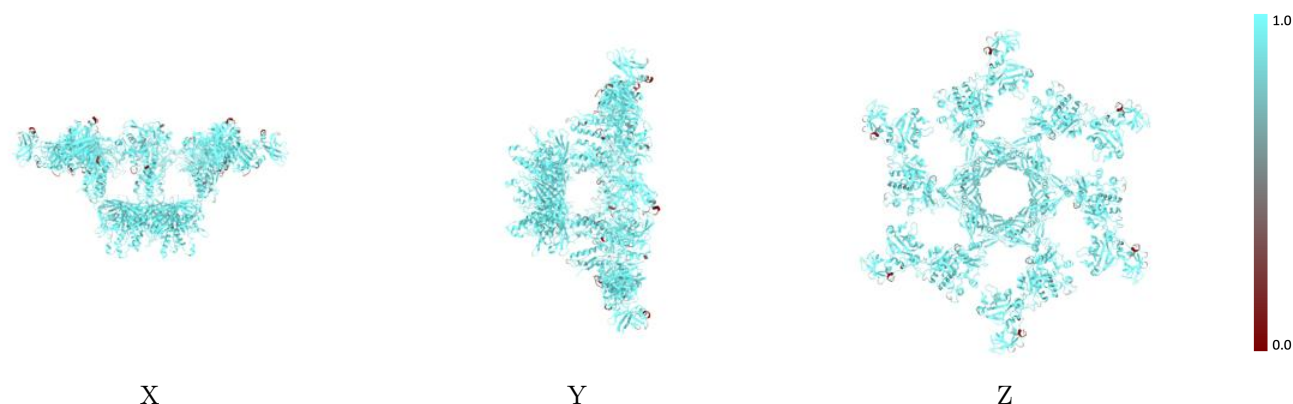
The images above show the 3D surface view of the map at the recommended contour level 1.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



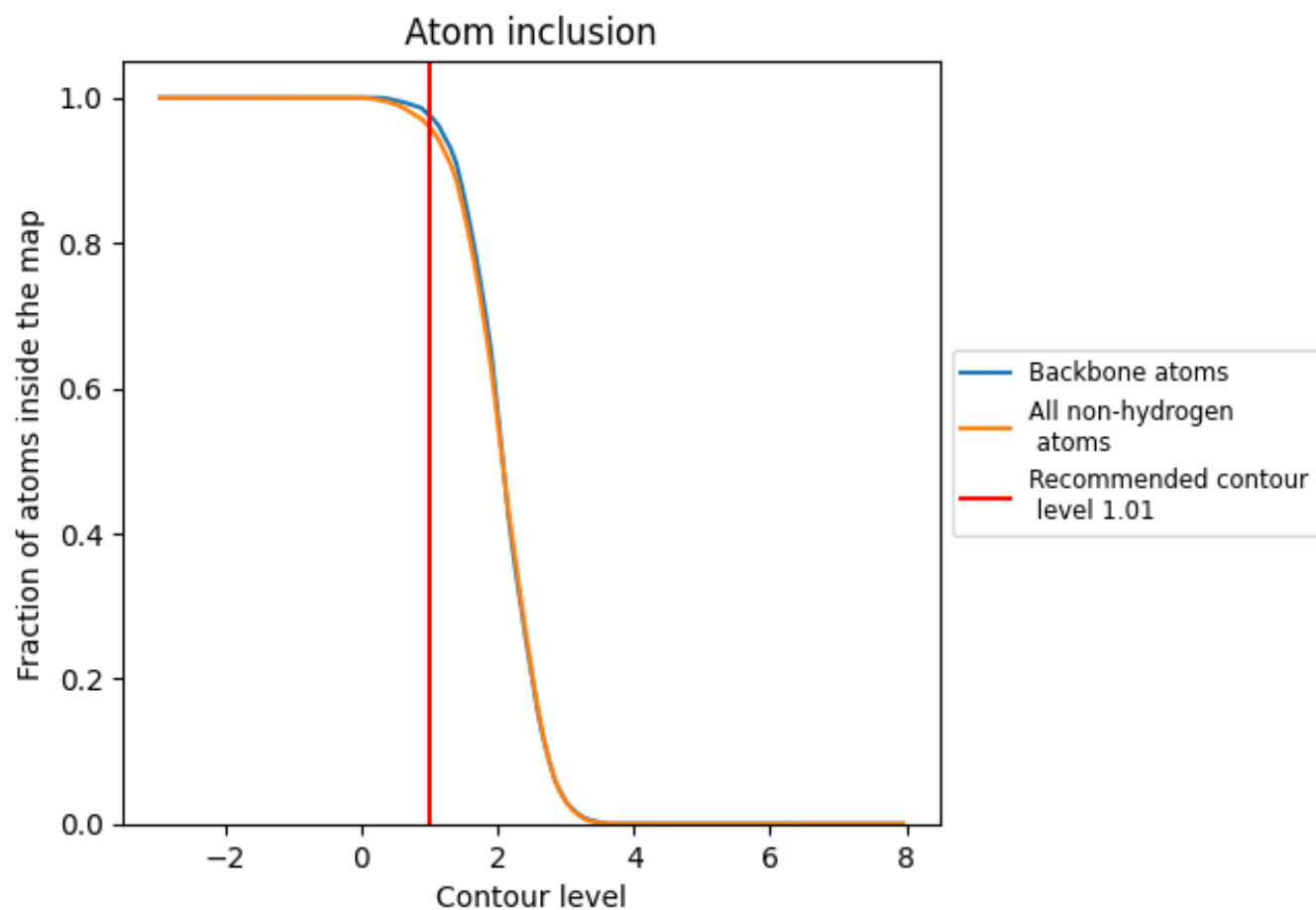
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.01).



























9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 96% 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 (1.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9584	 0.0430
A	 0.9930	 0.0230
B	 0.9924	 0.0260
C	 0.9924	 0.0260
D	 0.9924	 0.0220
E	 0.9924	 0.0260
F	 0.9935	 0.0250
U	 0.9445	 0.0540
V	 0.9456	 0.0500
W	 0.9467	 0.0480
X	 0.9443	 0.0510
Y	 0.9456	 0.0500
Z	 0.9471	 0.0490

