



## wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 10:10 pm GMT

PDB ID : 6QZF  
EMDB ID : EMD-4685  
Title : The cryo-EM structure of the collar complex and tail axis in genome emptied bacteriophage phi29  
Authors : Xu, J.; Wang, D.; Gui, M.; Xiang, Y.  
Deposited on : 2019-03-11  
Resolution : 3.80 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](mailto: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>.

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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 3.80 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  $\geq 3$ , 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	0a	309	74% 91% 9%
1	0b	309	75% 91% 9%
1	0c	309	75% 91% 9%
1	0d	309	74% 91% 9%
1	0e	309	74% 91% 9%
1	0f	309	75% 91% 9%
1	0g	309	74% 91% 9%
1	0h	309	75% 91% 9%
1	0i	309	75% 91% 9%


























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Mol	Chain	Length	Quality of chain
1	0j	309	75% 91% 9%
1	0k	309	74% 91% 9%
1	0l	309	75% 91% 9%
2	0A	293	9% 98% ..
2	0B	293	9% 98% ..
2	0C	293	9% 98% ..
2	0D	293	9% 98% ..
2	0E	293	9% 98% ..
2	0F	293	9% 98% ..
2	0G	293	10% 98% ..
2	0H	293	10% 98% ..
2	0I	293	9% 98% ..
2	0J	293	9% 98% ..
2	0K	293	9% 98% ..
2	0L	293	9% 98% ..
3	A	854	5% 6% 94%
3	B	854	5% 7% 93%
3	C	854	6% 7% 93%
3	D	854	5% 6% 94%
3	E	854	5% 7% 93%
3	F	854	6% 7% 93%
3	G	854	5% 6% 94%
3	H	854	5% 7% 93%
3	I	854	6% 7% 93%
3	J	854	5% 6% 94%

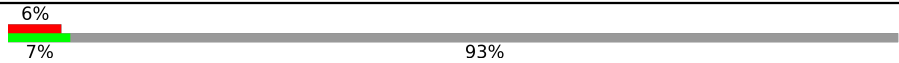
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Mol	Chain	Length	Quality of chain	
3	K	854		93%
3	L	854		93%
3	M	854		94%
3	N	854		93%
3	O	854		93%
3	P	854		94%
3	Q	854		93%
3	R	854		93%
3	S	854		94%
3	T	854		93%
3	U	854		93%
3	V	854		94%
3	W	854		93%
3	X	854		93%
3	Y	854		94%
3	Z	854		93%
3	a	854		93%
3	b	854		94%
3	c	854		93%
3	d	854		93%
3	e	854		94%
3	f	854		93%
3	g	854		93%
3	h	854		94%
3	i	854		93%

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Mol	Chain	Length	Quality of chain
3	j	854	 6% 7% 93%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 71628 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0a	280	2240	1429	376	428	7	0	0
1	0b	280	2240	1429	376	428	7	0	0
1	0c	280	2240	1429	376	428	7	0	0
1	0d	280	2240	1429	376	428	7	0	0
1	0e	280	2240	1429	376	428	7	0	0
1	0f	280	2240	1429	376	428	7	0	0
1	0g	280	2240	1429	376	428	7	0	0
1	0h	280	2240	1429	376	428	7	0	0
1	0i	280	2240	1429	376	428	7	0	0
1	0j	280	2240	1429	376	428	7	0	0
1	0k	280	2240	1429	376	428	7	0	0
1	0l	280	2240	1429	376	428	7	0	0

- Molecule 2 is a protein called Proximal tail tube connector protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	0A	291	2300	1416	397	479	8	0	0
2	0B	291	2300	1416	397	479	8	0	0
2	0C	291	2300	1416	397	479	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	0D	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0E	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0F	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0G	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0H	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0I	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0J	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0K	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0L	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		

- Molecule 3 is a protein called Pre-neck appendage protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	51	Total	C	N	O	S	0	0
			433	281	67	83	2		
3	B	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	C	61	Total	C	N	O	S	0	0
			514	334	78	98	4		
3	D	51	Total	C	N	O	S	0	0
			433	281	67	83	2		
3	E	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	F	61	Total	C	N	O	S	0	0
			514	334	78	98	4		
3	G	51	Total	C	N	O	S	0	0
			433	281	67	83	2		
3	H	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	I	61	Total	C	N	O	S	0	0
			514	334	78	98	4		
3	J	51	Total	C	N	O	S	0	0
			433	281	67	83	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	K	57	482	312	74	92	4	0	0
3	L	61	514	334	78	98	4	0	0
3	M	51	433	281	67	83	2	0	0
3	N	57	482	312	74	92	4	0	0
3	O	61	514	334	78	98	4	0	0
3	P	51	433	281	67	83	2	0	0
3	Q	57	482	312	74	92	4	0	0
3	R	61	514	334	78	98	4	0	0
3	S	51	433	281	67	83	2	0	0
3	T	57	482	312	74	92	4	0	0
3	U	61	514	334	78	98	4	0	0
3	V	51	433	281	67	83	2	0	0
3	W	57	482	312	74	92	4	0	0
3	X	61	514	334	78	98	4	0	0
3	Y	51	433	281	67	83	2	0	0
3	Z	57	482	312	74	92	4	0	0
3	a	61	514	334	78	98	4	0	0
3	b	51	433	281	67	83	2	0	0
3	c	57	482	312	74	92	4	0	0
3	d	61	514	334	78	98	4	0	0
3	e	51	433	281	67	83	2	0	0

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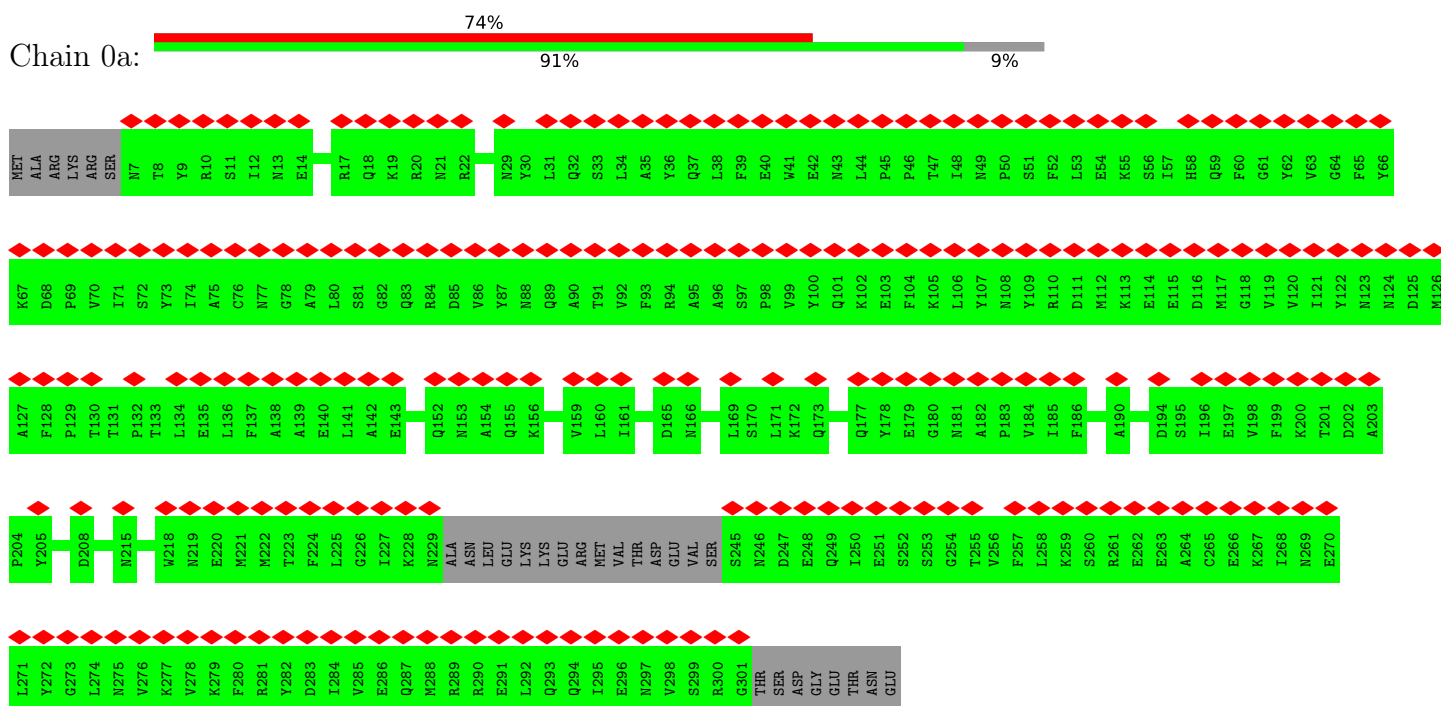
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	f	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	g	61	Total	C	N	O	S	0	0
			514	334	78	98	4		
3	h	51	Total	C	N	O	S	0	0
			433	281	67	83	2		
3	i	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	j	61	Total	C	N	O	S	0	0
			514	334	78	98	4		

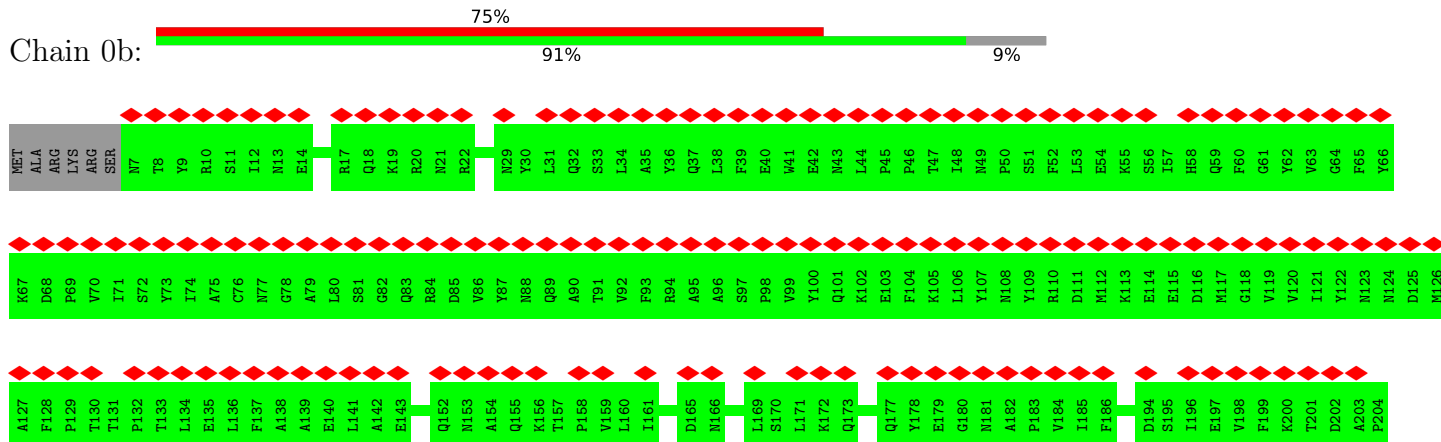
### 3 Residue-property plots [i](#)

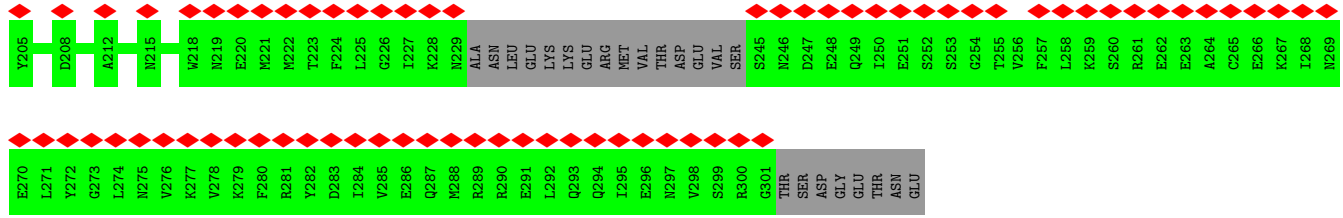
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Portal protein

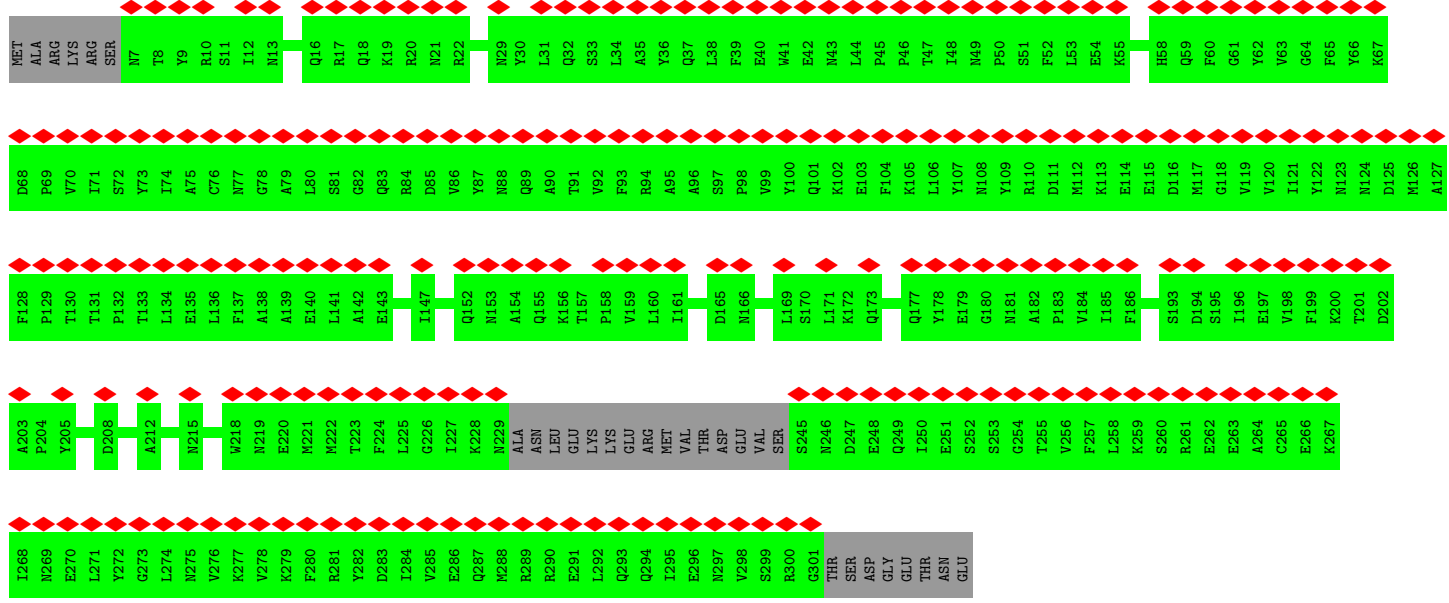
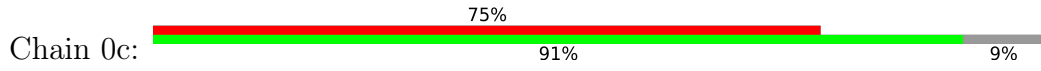


- Molecule 1: Portal protein

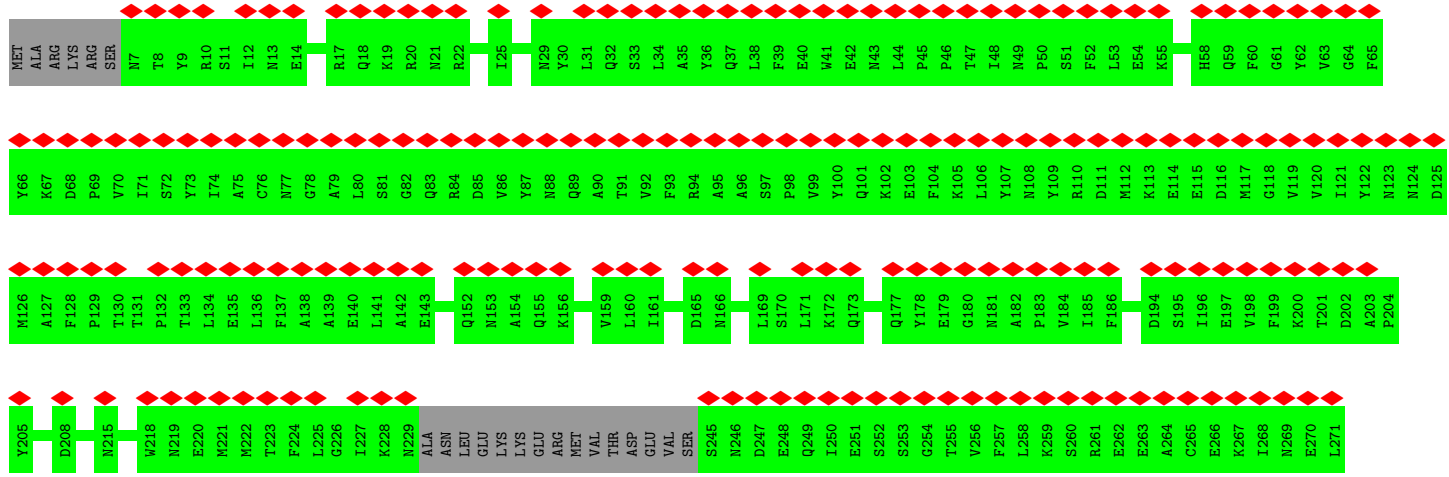
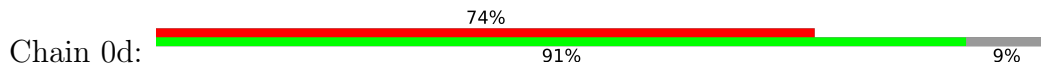


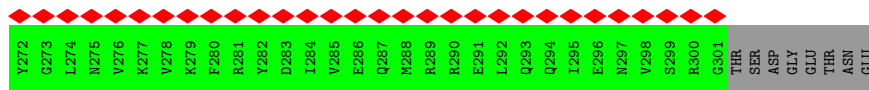


• Molecule 1: Portal protein

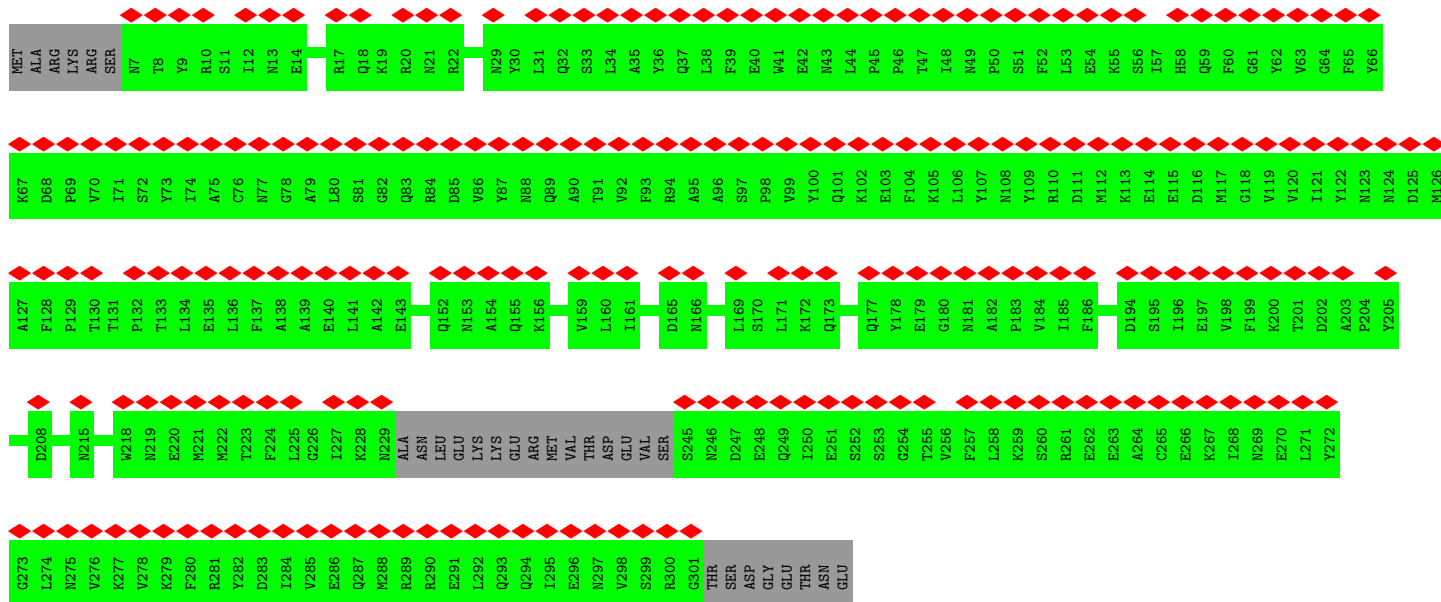
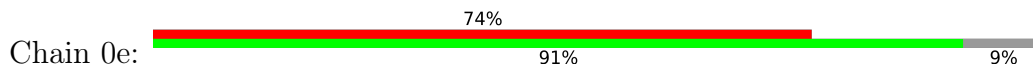


• Molecule 1: Portal protein

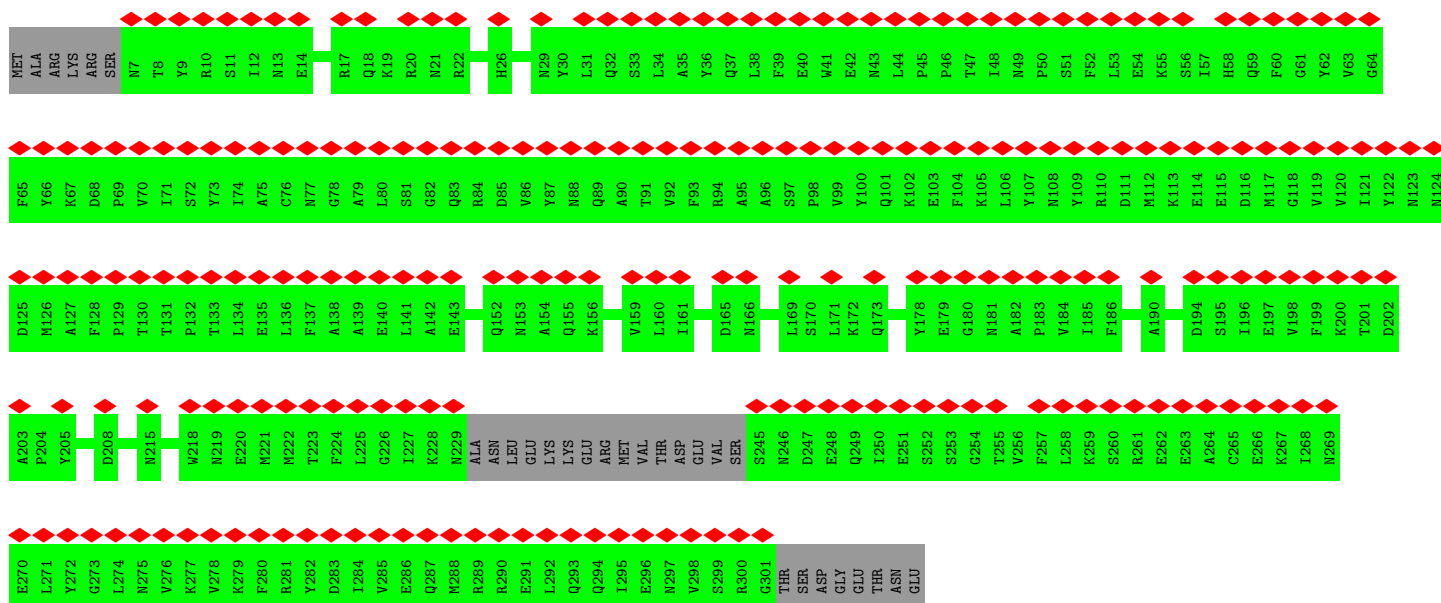
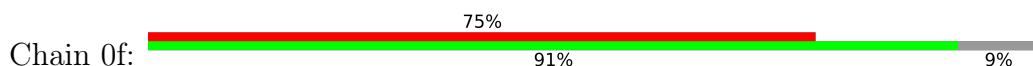




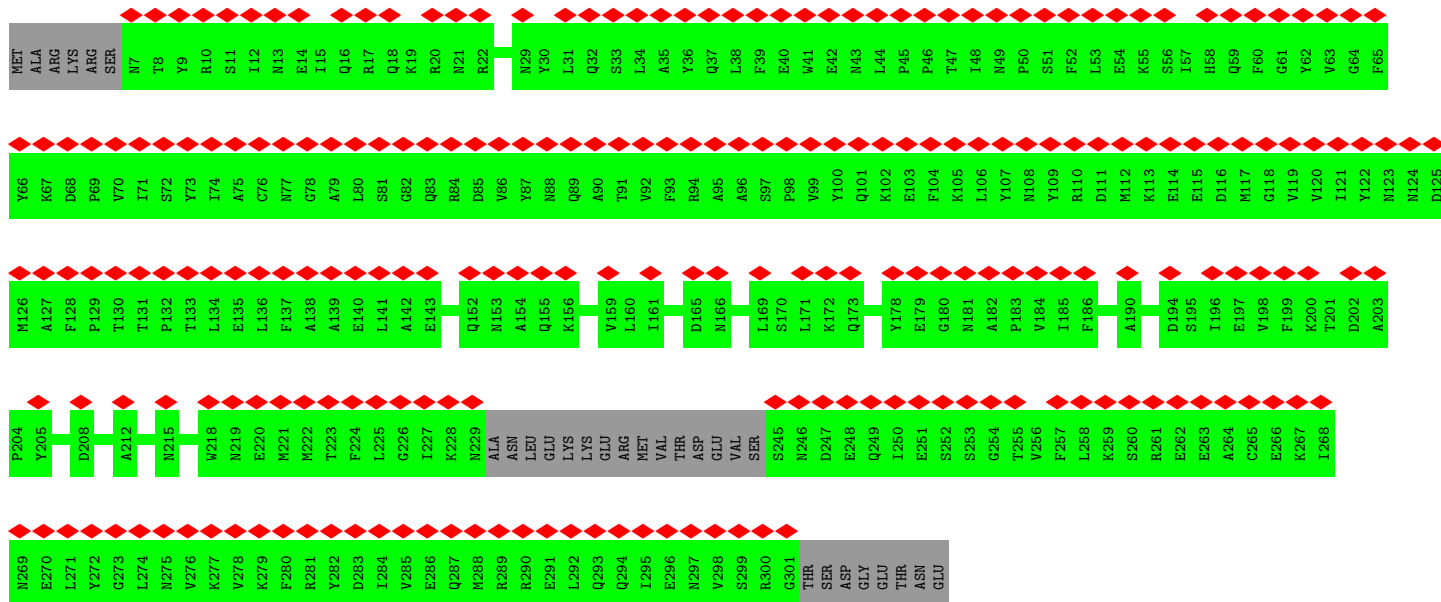
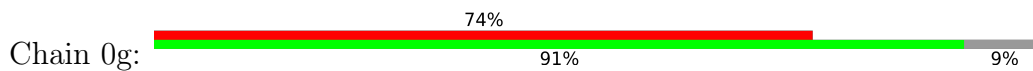
• Molecule 1: Portal protein



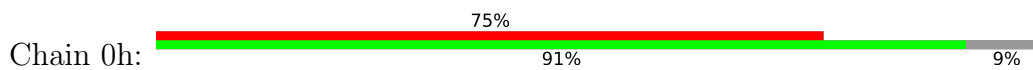
• Molecule 1: Portal protein



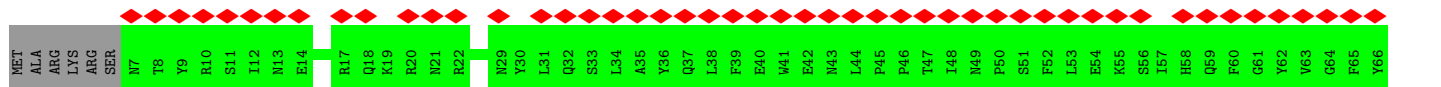
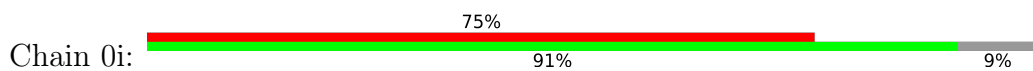
• Molecule 1: Portal protein

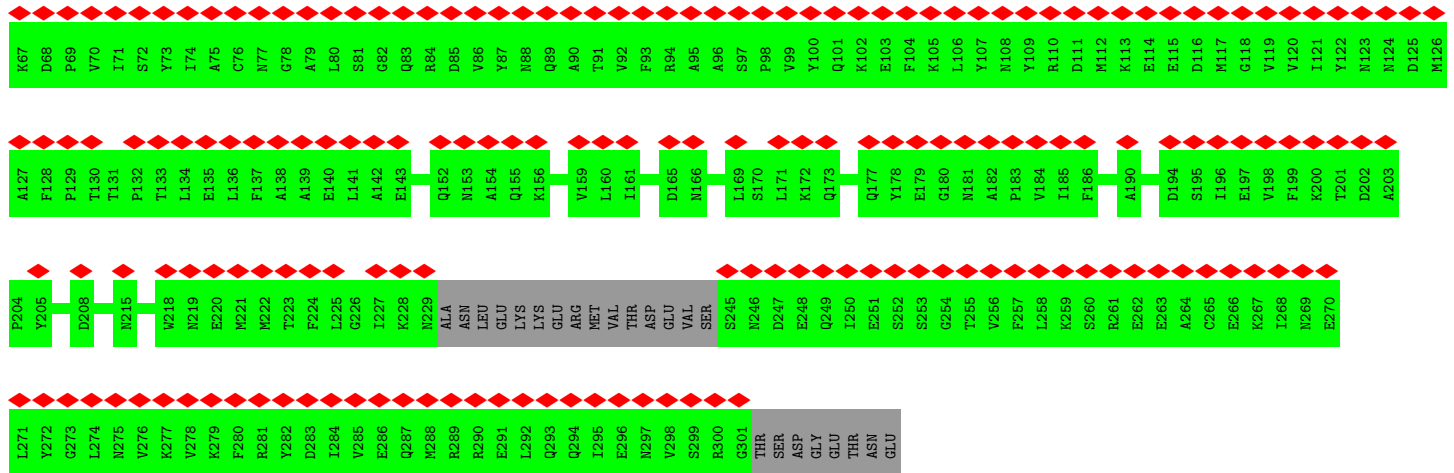


Molecule 1: Portal protein

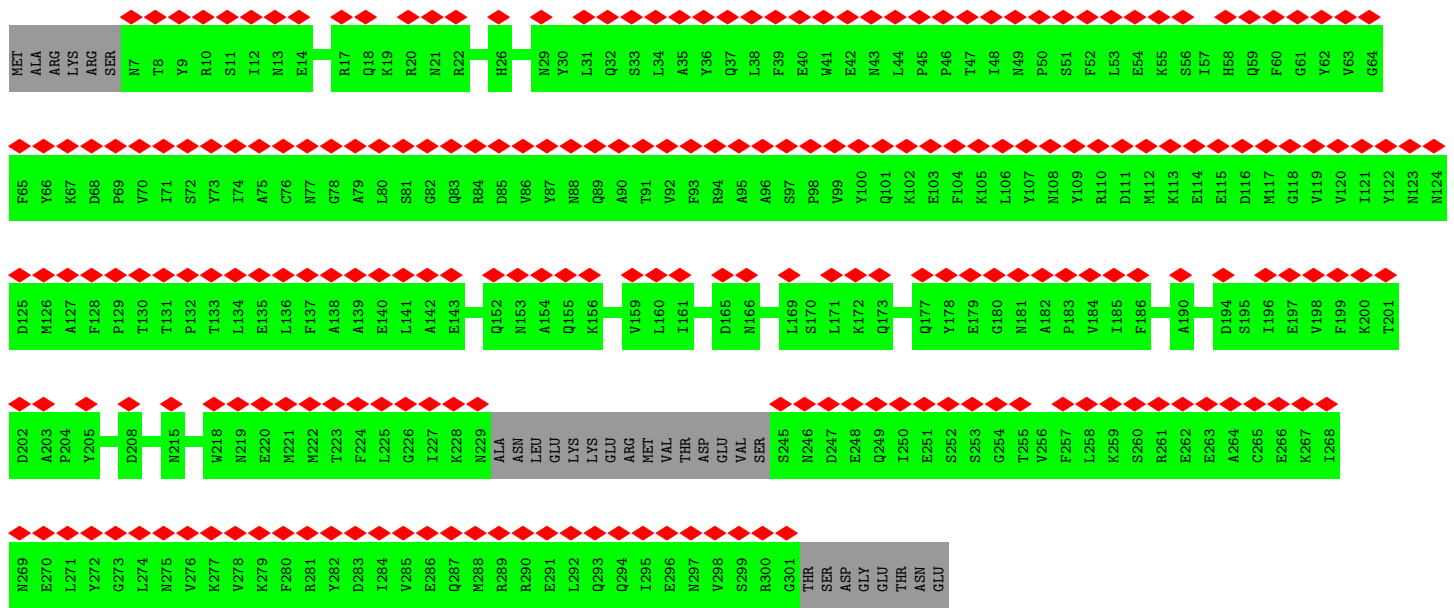
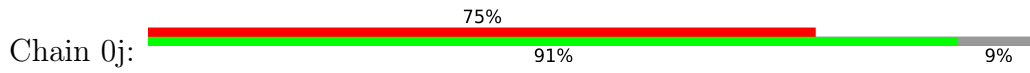


Molecule 1: Portal protein

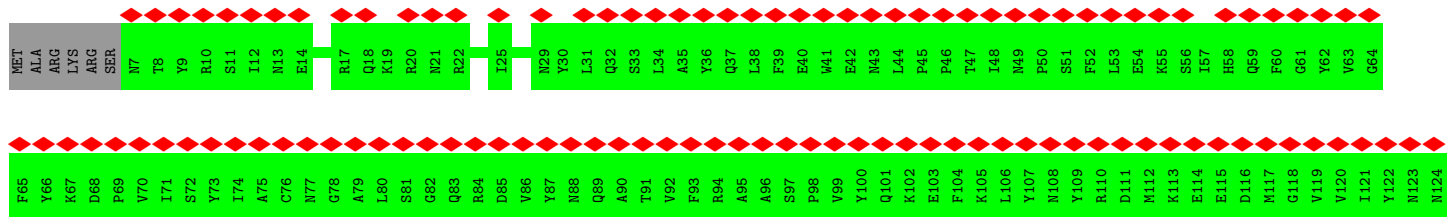
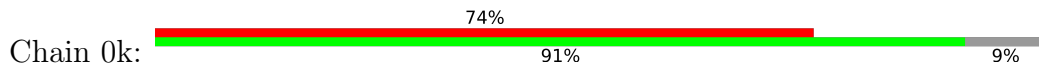


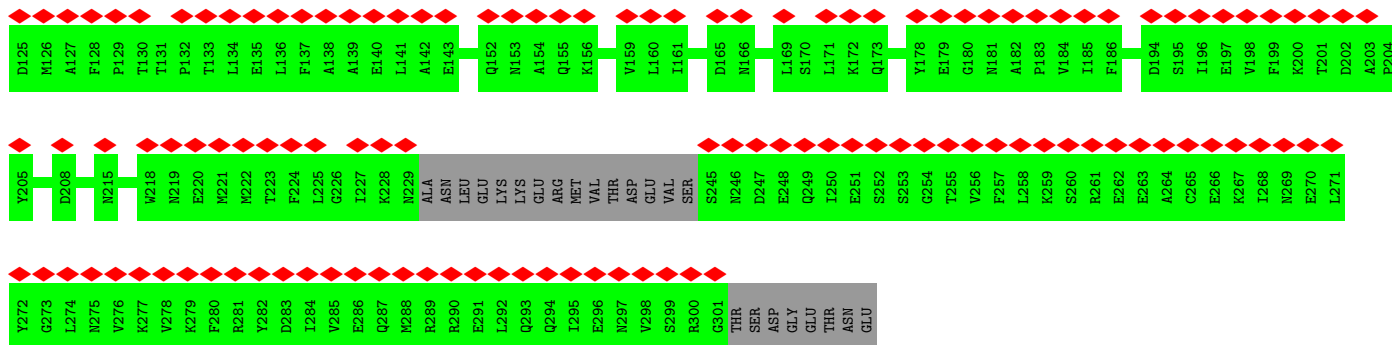


• Molecule 1: Portal protein

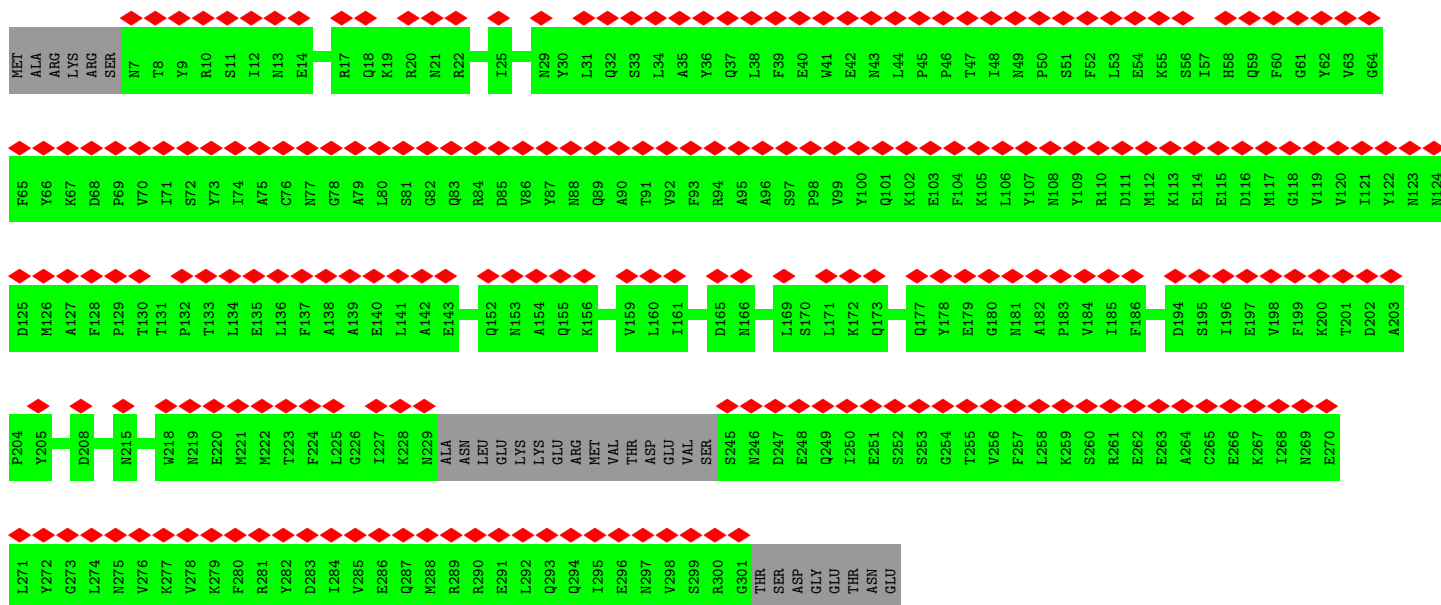
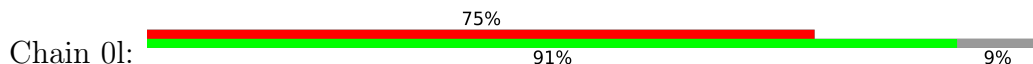


• Molecule 1: Portal protein

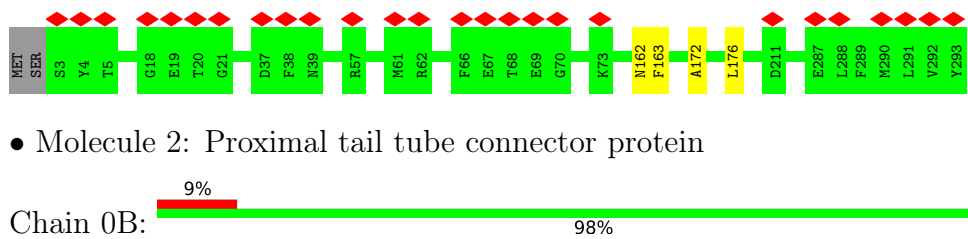




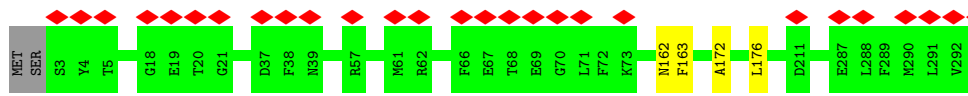
• Molecule 1: Portal protein



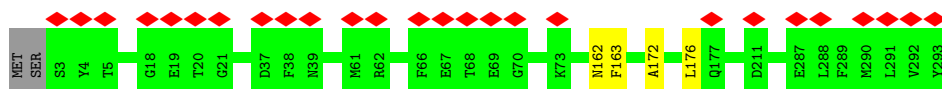
• Molecule 2: Proximal tail tube connector protein



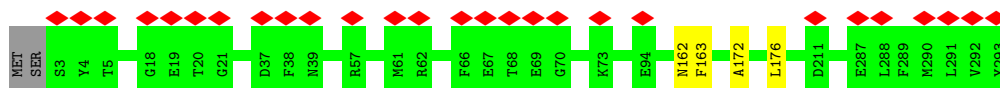
• Molecule 2: Proximal tail tube connector protein



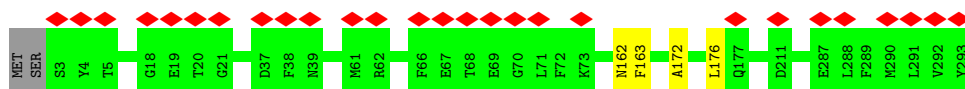
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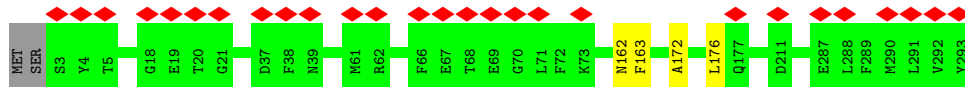
- Molecule 2: Proximal tail tube connector protein



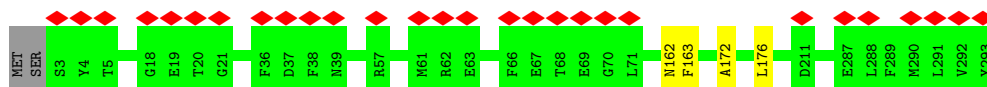
- Molecule 2: Proximal tail tube connector protein



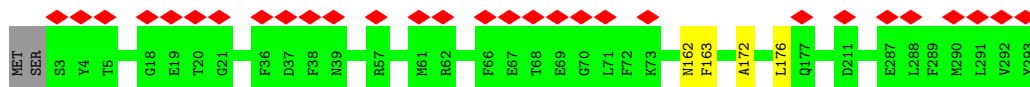
- Molecule 2: Proximal tail tube connector protein



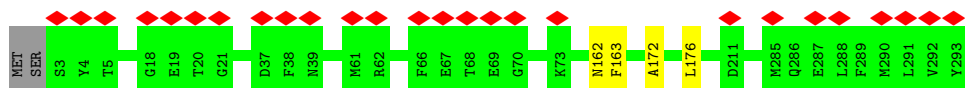
- Molecule 2: Proximal tail tube connector protein



- Molecule 2: Proximal tail tube connector protein



- Molecule 2: Proximal tail tube connector protein



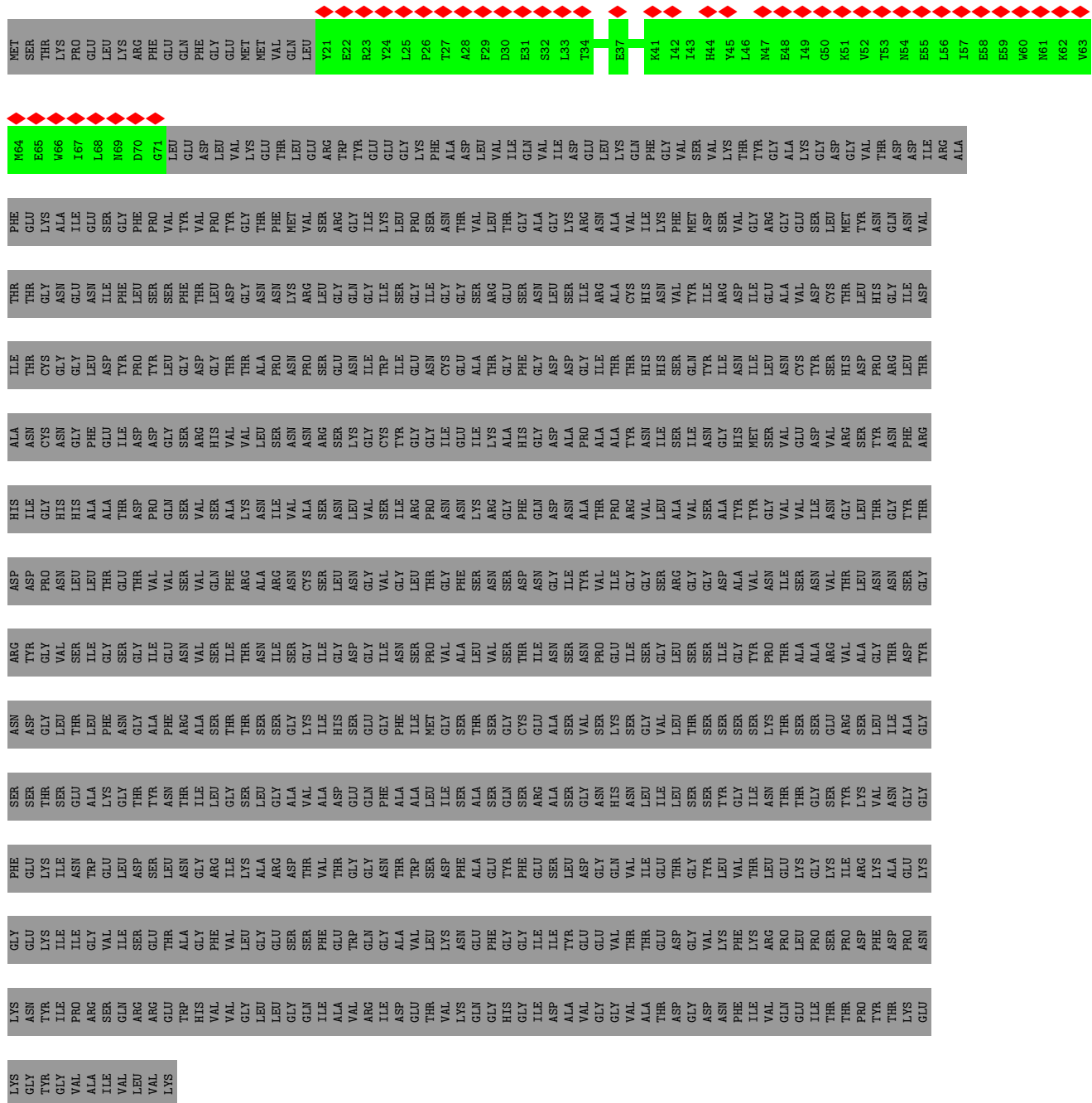




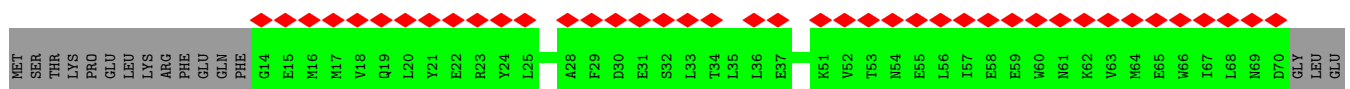




● Molecule 3: Pre-neck appendage protein



● Molecule 3: Pre-neck appendage protein

















MET	THR	PRO	LEU	LYS	PHE	GLU	GLN	PHE	G14	E15	M16	M17	V18	Q19	L20	Y21	E22	R23	Y24	L25	A28	F29	D30	E31	S32	L33	T34	L35	L36	E37	G50	K51	V52	T53	N54	E55	L56	I57	E58	E59	M60	M61	K62	V63	M64	E65	W66	I67	L68	N69	D70	GLY	LEU				
GLU	ASP	VAL	THR	LEU	ARG	TRP	TYR	GLU	GLY	LYS	PHE	ALA	ASP	LEU	VAL	ILE	GLN	VAL	ASP	GLY	GLY	PHE	GLY	VAL	LEU	GLN	GLY	ALA	GLY	ASP	GLY	VAL	THR	ASP	TYR	ILE	ASN	ARG	ALA	VAL	PHE	GLU	LYS	ALA	ILE	GLU	ASP	GLY	GLY	PHE	LEU						
PRO	VAL	TYR	VAL	PRO	GLY	THR	ASP	GLY	ASN	ARG	VAL	ARG	GLY	ASN	VAL	THR	GLY	ALA	ASP	GLY	GLY	ALA	VAL	GLY	ASN	ARG	ASP	VAL	GLY	GLY	ASP	GLY	VAL	THR	MET	TYR	ASN	GLN	ILE	ASN	VAL	THR	THR	GLY	ASN	ILE	ASN	PHE	LEU								
SER	SER	THR	PHE	LEU	ASP	THR	ASP	GLY	ASN	ARG	VAL	ARG	GLY	GLN	GLY	ILE	GLY	ASN	GLY	GLY	ASN	LEU	LEU	LYS	ILE	ARG	ASN	VAL	ALA	THR	CYS	HIS	THR	HIS	ASN	VAL	THR	THR	THR	THR	CYS	GLY	ASN	ILE	ASN	ASP	TYR	PRO									
TYR	LEU	GLY	ASP	GLY	THR	ALA	PRO	PRO	ASN	GLY	ASN	GLY	ASN	TYR	ILE	TRP	ILE	ASN	GLY	GLY	ASN	GLY	GLY	ALA	THR	THR	HIS	ASN	VAL	ILE	ILE	ASN	GLY	ASN	ALA	VAL	VAL	THR	HIS	ASN	PRO	CYS	GLY	ASN	ASN	PHE	GLU	ASP	ILE	ASP							
ASP	GLY	SER	ARG	HIS	VAL	VAL	LEU	ASN	SER	ARG	ASN	SER	LYS	ASN	TYR	CYS	TYR	GLY	GLY	ILE	GLY	GLU	GLU	ILE	ALA	PRO	ALA	ALA	TYR	ASN	ILE	ILE	SER	VAL	VAL	VAL	ASP	VAL	VAL	ARG	HIS	ASN	ILE	THR	ASP	THR	THR	THR	ASP	ASP							
PRO	GLN	VAL	VAL	VAL	GLN	ALA	LYS	ASN	ILE	ASN	VAL	ALA	SER	ASN	LEU	VAL	ILE	ASN	PRO	ASN	GLY	ASN	GLY	ASP	ALA	THR	ARG	VAL	VAL	TYR	VAL	ASN	GLY	ILE	ASN	THR	GLY	THR	ASP	THR	ASP	THR	ASP	THR	THR	THR	THR	THR	THR	THR	THR						
VAL	VAL	SER	VAL	VAL	SER	GLN	PHE	ARG	ALA	ARG	CYS	VAL	SER	ASN	LEU	GLY	VAL	THR	GLY	ASP	ASN	GLY	PHE	ASN	GLY	ILE	ASN	GLY	ALA	THR	ILE	VAL	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR					
ILE	GLU	ASN	VAL	VAL	THR	ASN	THR	THR	ASN	THR	ILE	ASN	ASP	ASP	GLY	VAL	ILE	ASN	PRO	VAL	THR	VAL	VAL	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR					
ALA	PHE	ARG	ALA	THR	THR	SER	SER	THR	LYS	GLY	ASN	HIS	SER	GLY	GLY	PHE	MET	GLY	ILE	ASN	SER	SER	ALA	ALA	VAL	VAL	LYS	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER				
TYR	ASN	THR	ILE	GLY	LEU	GLY	VAL	ALA	ALA	GLY	VAL	ASN	GLY	GLN	ALA	ALA	THR	GLY	GLY	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN		
SER	LEU	GLY	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE		
GLU	THR	ALA	GLY	PHE	VAL	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
ARG	GLU	TRP	HIS	VAL	VAL	GLY	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
VAL	LYS																																																								

Molecule 3: Pre-neck appendage protein



MET	THR	PRO	GLU	LEU	LYS	ARG	PHE	GLU	GLN	F13	G14	E15	M16	M17	V18	Q19	L20	Y21	E22	R23	Y24	L25	P26	T27	A28	F29	D30	E31	S32	L33	L36	N40	Y45	E48	I49	G50	K51	V52	T53	N54	E55	L56	I57	E58	E59	M60	M61	K62	V63	M64	E65	W66	I67					
L68	N69	D70	G71	L72	E73	ASP	LEU	VAL	LYS	GLU	THR	LEU	ARG	TRP	TYR	GLU	GLU	LYS	PHE	ALA	ASP	LEU	VAL	ILE	ASN	ASP	GLU	GLY	PHE	VAL	VAL	THR	TYR	GLY	ALA	LYS	ASP	ASP	ILE	ARG	ALA	PHE	GLU	LYS	ALA													









LYS  
GLY  
TYR  
GLY  
VAL  
ALA  
ILE  
VAL  
LEU  
VAL  
LYS

● Molecule 3: Pre-neck appendage protein



MET SER THR LYS PRO GLU LEU LYS ARG PHE GLU TRP VAL TYR PHE G14 E15 M16 H17 V18 Q19 L20 Y21 E22 R23 Y24 A28 F29 D30 E31 S32 L33 T34 L35 L36 E37 G50 K51 V52 T53 N54 E55 L56 I57 E58 E59 N60 H61 K62 V63 H64 E65 N66 I67 L68 H69 D70 LEU

GLU ASP LEU VAL LYS THR LEU ARG TRP VAL TYR PHE GLU G14 E15 M16 H17 V18 Q19 L20 Y21 E22 R23 Y24 A28 F29 D30 E31 S32 L33 T34 L35 L36 E37 G50 K51 V52 T53 N54 E55 L56 I57 E58 E59 N60 H61 K62 V63 H64 E65 N66 I67 L68 H69 D70 LEU

PRO VAL TYR ASP THR LYS PRO GLU LEU LYS ARG PHE GLU TRP VAL TYR PHE G14 E15 M16 H17 V18 Q19 L20 Y21 E22 R23 Y24 A28 F29 D30 E31 S32 L33 T34 L35 L36 E37 G50 K51 V52 T53 N54 E55 L56 I57 E58 E59 N60 H61 K62 V63 H64 E65 N66 I67 L68 H69 D70 LEU

SER SER THR LYS PRO GLU LEU LYS ARG PHE GLU TRP VAL TYR PHE G14 E15 M16 H17 V18 Q19 L20 Y21 E22 R23 Y24 A28 F29 D30 E31 S32 L33 T34 L35 L36 E37 G50 K51 V52 T53 N54 E55 L56 I57 E58 E59 N60 H61 K62 V63 H64 E65 N66 I67 L68 H69 D70 LEU

TYR LEU GLY ASP THR LYS PRO GLU LEU LYS ARG PHE GLU TRP VAL TYR PHE G14 E15 M16 H17 V18 Q19 L20 Y21 E22 R23 Y24 A28 F29 D30 E31 S32 L33 T34 L35 L36 E37 G50 K51 V52 T53 N54 E55 L56 I57 E58 E59 N60 H61 K62 V63 H64 E65 N66 I67 L68 H69 D70 LEU

ASP GLY SER ARG HIS GLY THR LYS PRO GLU LEU LYS ARG PHE GLU TRP VAL TYR PHE G14 E15 M16 H17 V18 Q19 L20 Y21 E22 R23 Y24 A28 F29 D30 E31 S32 L33 T34 L35 L36 E37 G50 K51 V52 T53 N54 E55 L56 I57 E58 E59 N60 H61 K62 V63 H64 E65 N66 I67 L68 H69 D70 LEU

PRO GLN SER VAL PHE ALA LYS ASN VAL LYS ARG PHE GLU TRP VAL TYR PHE G14 E15 M16 H17 V18 Q19 L20 Y21 E22 R23 Y24 A28 F29 D30 E31 S32 L33 T34 L35 L36 E37 G50 K51 V52 T53 N54 E55 L56 I57 E58 E59 N60 H61 K62 V63 H64 E65 N66 I67 L68 H69 D70 LEU

VAL VAL SER VAL PHE ARG ALA LYS ASN VAL LYS ARG PHE GLU TRP VAL TYR PHE G14 E15 M16 H17 V18 Q19 L20 Y21 E22 R23 Y24 A28 F29 D30 E31 S32 L33 T34 L35 L36 E37 G50 K51 V52 T53 N54 E55 L56 I57 E58 E59 N60 H61 K62 V63 H64 E65 N66 I67 L68 H69 D70 LEU

ILE GLU ASN VAL ILE ARG ALA LYS ASN VAL LYS ARG PHE GLU TRP VAL TYR PHE G14 E15 M16 H17 V18 Q19 L20 Y21 E22 R23 Y24 A28 F29 D30 E31 S32 L33 T34 L35 L36 E37 G50 K51 V52 T53 N54 E55 L56 I57 E58 E59 N60 H61 K62 V63 H64 E65 N66 I67 L68 H69 D70 LEU

ALA PHE ARG ALA THR SER ILE THR LYS ASN VAL LYS ARG PHE GLU TRP VAL TYR PHE G14 E15 M16 H17 V18 Q19 L20 Y21 E22 R23 Y24 A28 F29 D30 E31 S32 L33 T34 L35 L36 E37 G50 K51 V52 T53 N54 E55 L56 I57 E58 E59 N60 H61 K62 V63 H64 E65 N66 I67 L68 H69 D70 LEU

TYR ASN THR ILE LEU GLY VAL PHE ALA LYS ASN VAL LYS ARG PHE GLU TRP VAL TYR PHE G14 E15 M16 H17 V18 Q19 L20 Y21 E22 R23 Y24 A28 F29 D30 E31 S32 L33 T34 L35 L36 E37 G50 K51 V52 T53 N54 E55 L56 I57 E58 E59 N60 H61 K62 V63 H64 E65 N66 I67 L68 H69 D70 LEU

SER LEU ASN THR ILE LEU GLY VAL PHE ALA LYS ASN VAL LYS ARG PHE GLU TRP VAL TYR PHE G14 E15 M16 H17 V18 Q19 L20 Y21 E22 R23 Y24 A28 F29 D30 E31 S32 L33 T34 L35 L36 E37 G50 K51 V52 T53 N54 E55 L56 I57 E58 E59 N60 H61 K62 V63 H64 E65 N66 I67 L68 H69 D70 LEU

GLU THR ALA GLY PHE VAL LYS ASN VAL LYS ARG PHE GLU TRP VAL TYR PHE G14 E15 M16 H17 V18 Q19 L20 Y21 E22 R23 Y24 A28 F29 D30 E31 S32 L33 T34 L35 L36 E37 G50 K51 V52 T53 N54 E55 L56 I57 E58 E59 N60 H61 K62 V63 H64 E65 N66 I67 L68 H69 D70 LEU

ARG GLU TRP HIS VAL VAL GLY LEU ILE ILE ASP ALA LYS ASN VAL LYS ARG PHE GLU TRP VAL TYR PHE G14 E15 M16 H17 V18 Q19 L20 Y21 E22 R23 Y24 A28 F29 D30 E31 S32 L33 T34 L35 L36 E37 G50 K51 V52 T53 N54 E55 L56 I57 E58 E59 N60 H61 K62 V63 H64 E65 N66 I67 L68 H69 D70 LEU

VAL  
LYS

● Molecule 3: Pre-neck appendage protein







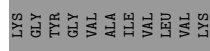
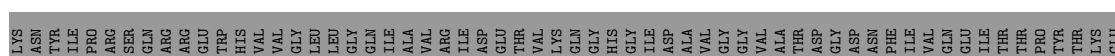
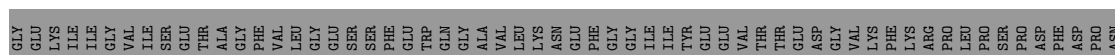
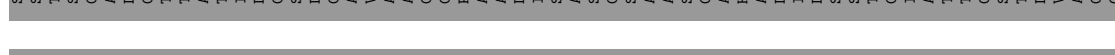
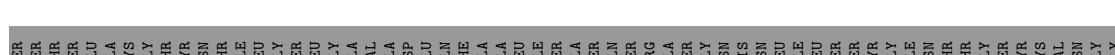
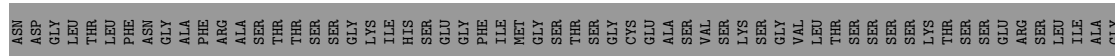
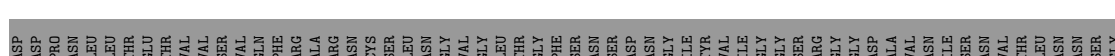
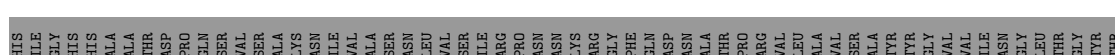
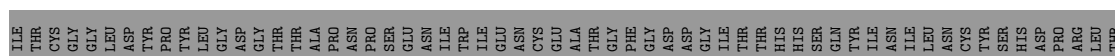
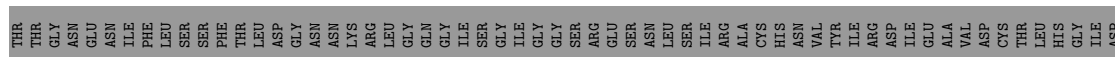
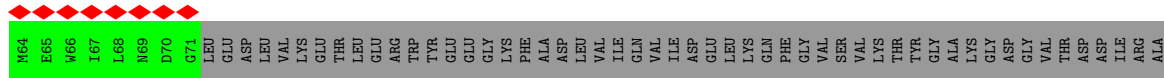
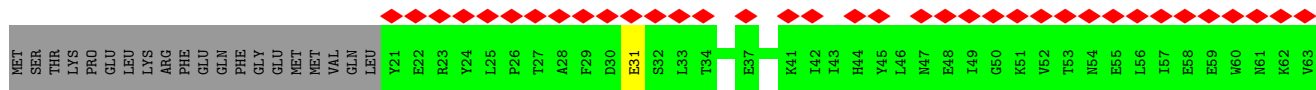




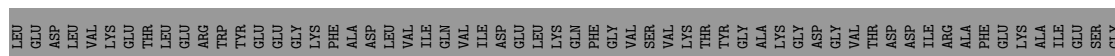
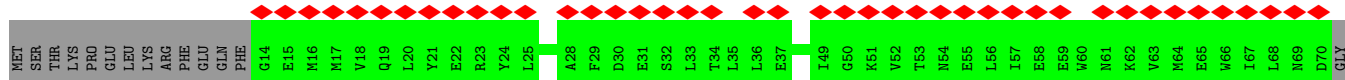








### • Molecule 3: Pre-neck appendage protein























GLY  
VAL  
ALA  
ILE  
VAL  
LEU  
VAL  
LYS



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31478	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	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	22.011	Depositor
Minimum map value	-4.860	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.233	Depositor
Recommended contour level	3.5	Depositor
Map size ( $\text{\AA}$ )	734.4, 734.4, 734.4	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.36, 1.36, 1.36	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	0a	0.43	0/2288	0.52	0/3103
1	0b	0.43	0/2288	0.52	0/3103
1	0c	0.43	0/2288	0.52	0/3103
1	0d	0.43	0/2288	0.52	0/3103
1	0e	0.43	0/2288	0.52	0/3103
1	0f	0.43	0/2288	0.52	0/3103
1	0g	0.43	0/2288	0.52	0/3103
1	0h	0.43	0/2288	0.52	0/3103
1	0i	0.43	0/2288	0.52	0/3103
1	0j	0.43	0/2288	0.52	0/3103
1	0k	0.43	0/2288	0.52	0/3103
1	0l	0.43	0/2288	0.52	0/3103
2	0A	0.62	0/2335	0.68	0/3149
2	0B	0.62	0/2335	0.68	0/3149
2	0C	0.62	0/2335	0.68	0/3149
2	0D	0.62	0/2335	0.68	0/3149
2	0E	0.62	0/2335	0.68	0/3149
2	0F	0.62	0/2335	0.68	0/3149
2	0G	0.62	0/2335	0.68	0/3149
2	0H	0.62	0/2335	0.68	0/3149
2	0I	0.62	0/2335	0.68	0/3149
2	0J	0.62	0/2335	0.68	0/3149
2	0K	0.62	0/2335	0.68	0/3149
2	0L	0.62	0/2335	0.68	0/3149
3	A	0.36	0/442	0.57	0/598
3	B	0.45	0/491	0.62	0/663
3	C	0.37	0/524	0.56	0/707
3	D	0.36	0/442	0.58	0/598
3	E	0.43	0/491	0.64	0/663
3	F	0.37	0/524	0.56	0/707
3	G	0.36	0/442	0.58	0/598
3	H	0.45	0/491	0.64	0/663
3	I	0.37	0/524	0.56	0/707
3	J	0.36	0/442	0.57	0/598

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	K	0.47	0/491	0.64	0/663
3	L	0.37	0/524	0.56	0/707
3	M	0.35	0/442	0.57	0/598
3	N	0.42	0/491	0.60	0/663
3	O	0.37	0/524	0.56	0/707
3	P	0.34	0/442	0.57	0/598
3	Q	0.41	0/491	0.60	0/663
3	R	0.37	0/524	0.56	0/707
3	S	0.34	0/442	0.57	0/598
3	T	0.41	0/491	0.60	0/663
3	U	0.37	0/524	0.56	0/707
3	V	0.34	0/442	0.57	0/598
3	W	0.43	0/491	0.60	0/663
3	X	0.37	0/524	0.56	0/707
3	Y	0.35	0/442	0.58	0/598
3	Z	0.42	0/491	0.59	0/663
3	a	0.37	0/524	0.56	0/707
3	b	0.34	0/442	0.57	0/598
3	c	0.41	0/491	0.60	0/663
3	d	0.37	0/524	0.56	0/707
3	e	0.36	0/442	0.58	0/598
3	f	0.43	0/491	0.62	0/663
3	g	0.37	0/524	0.56	0/707
3	h	0.38	0/442	0.59	0/598
3	i	0.43	0/491	0.62	0/663
3	j	0.37	0/524	0.56	0/707
All	All	0.50	0/72960	0.60	0/98640

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	0A	0	3
2	0B	0	3
2	0C	0	3
2	0D	0	3
2	0E	0	3
2	0F	0	3
2	0G	0	3
2	0H	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	0I	0	3
2	0J	0	3
2	0K	0	3
2	0L	0	3
All	All	0	36

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	0A	163	PHE	Peptide
2	0A	172	ALA	Peptide
2	0A	176	LEU	Peptide
2	0B	163	PHE	Peptide
2	0B	172	ALA	Peptide

## 5.2 Too-close contacts [i](#)

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

## 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	0a	276/309 (89%)	258 (94%)	18 (6%)	0	100   100
1	0b	276/309 (89%)	258 (94%)	18 (6%)	0	100   100
1	0c	276/309 (89%)	258 (94%)	18 (6%)	0	100   100
1	0d	276/309 (89%)	258 (94%)	18 (6%)	0	100   100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0e	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0f	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0g	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0h	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0i	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0j	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0k	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0l	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
2	0A	289/293 (99%)	248 (86%)	41 (14%)	0	100	100
2	0B	289/293 (99%)	249 (86%)	40 (14%)	0	100	100
2	0C	289/293 (99%)	249 (86%)	40 (14%)	0	100	100
2	0D	289/293 (99%)	248 (86%)	41 (14%)	0	100	100
2	0E	289/293 (99%)	249 (86%)	40 (14%)	0	100	100
2	0F	289/293 (99%)	248 (86%)	41 (14%)	0	100	100
2	0G	289/293 (99%)	248 (86%)	41 (14%)	0	100	100
2	0H	289/293 (99%)	249 (86%)	40 (14%)	0	100	100
2	0I	289/293 (99%)	249 (86%)	40 (14%)	0	100	100
2	0J	289/293 (99%)	249 (86%)	40 (14%)	0	100	100
2	0K	289/293 (99%)	248 (86%)	41 (14%)	0	100	100
2	0L	289/293 (99%)	249 (86%)	40 (14%)	0	100	100
3	A	49/854 (6%)	44 (90%)	5 (10%)	0	100	100
3	B	55/854 (6%)	52 (94%)	3 (6%)	0	100	100
3	C	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	D	49/854 (6%)	44 (90%)	5 (10%)	0	100	100
3	E	55/854 (6%)	52 (94%)	3 (6%)	0	100	100
3	F	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	G	49/854 (6%)	43 (88%)	6 (12%)	0	100	100
3	H	55/854 (6%)	52 (94%)	3 (6%)	0	100	100
3	I	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	J	49/854 (6%)	43 (88%)	5 (10%)	1 (2%)	7	41
3	K	55/854 (6%)	52 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	M	49/854 (6%)	44 (90%)	5 (10%)	0	100	100
3	N	55/854 (6%)	52 (94%)	3 (6%)	0	100	100
3	O	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	P	49/854 (6%)	43 (88%)	6 (12%)	0	100	100
3	Q	55/854 (6%)	52 (94%)	3 (6%)	0	100	100
3	R	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	S	49/854 (6%)	43 (88%)	6 (12%)	0	100	100
3	T	55/854 (6%)	53 (96%)	2 (4%)	0	100	100
3	U	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	V	49/854 (6%)	44 (90%)	5 (10%)	0	100	100
3	W	55/854 (6%)	52 (94%)	3 (6%)	0	100	100
3	X	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	Y	49/854 (6%)	43 (88%)	5 (10%)	1 (2%)	7	41
3	Z	55/854 (6%)	51 (93%)	4 (7%)	0	100	100
3	a	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	b	49/854 (6%)	44 (90%)	4 (8%)	1 (2%)	7	41
3	c	55/854 (6%)	53 (96%)	2 (4%)	0	100	100
3	d	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	e	49/854 (6%)	44 (90%)	5 (10%)	0	100	100
3	f	55/854 (6%)	51 (93%)	4 (7%)	0	100	100
3	g	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	h	49/854 (6%)	44 (90%)	5 (10%)	0	100	100
3	i	55/854 (6%)	52 (94%)	3 (6%)	0	100	100
3	j	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
All	All	8736/37968 (23%)	7874 (90%)	859 (10%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	31	GLU
3	Y	31	GLU
3	b	31	GLU

### 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	0a	235/277 (85%)	235 (100%)	0	100	100
1	0b	235/277 (85%)	235 (100%)	0	100	100
1	0c	235/277 (85%)	235 (100%)	0	100	100
1	0d	235/277 (85%)	235 (100%)	0	100	100
1	0e	235/277 (85%)	235 (100%)	0	100	100
1	0f	235/277 (85%)	235 (100%)	0	100	100
1	0g	235/277 (85%)	235 (100%)	0	100	100
1	0h	235/277 (85%)	235 (100%)	0	100	100
1	0i	235/277 (85%)	235 (100%)	0	100	100
1	0j	235/277 (85%)	235 (100%)	0	100	100
1	0k	235/277 (85%)	235 (100%)	0	100	100
1	0l	235/277 (85%)	235 (100%)	0	100	100
2	0A	250/270 (93%)	249 (100%)	1 (0%)	91	95
2	0B	250/270 (93%)	249 (100%)	1 (0%)	91	95
2	0C	250/270 (93%)	249 (100%)	1 (0%)	91	95
2	0D	250/270 (93%)	249 (100%)	1 (0%)	91	95
2	0E	250/270 (93%)	249 (100%)	1 (0%)	91	95
2	0F	250/270 (93%)	249 (100%)	1 (0%)	91	95
2	0G	250/270 (93%)	249 (100%)	1 (0%)	91	95
2	0H	250/270 (93%)	249 (100%)	1 (0%)	91	95
2	0I	250/270 (93%)	249 (100%)	1 (0%)	91	95
2	0J	250/270 (93%)	249 (100%)	1 (0%)	91	95
2	0K	250/270 (93%)	249 (100%)	1 (0%)	91	95
2	0L	250/270 (93%)	249 (100%)	1 (0%)	91	95
3	A	48/706 (7%)	48 (100%)	0	100	100
3	B	54/706 (8%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	57/706 (8%)	57 (100%)	0	100	100
3	D	48/706 (7%)	48 (100%)	0	100	100
3	E	54/706 (8%)	54 (100%)	0	100	100
3	F	57/706 (8%)	57 (100%)	0	100	100
3	G	48/706 (7%)	48 (100%)	0	100	100
3	H	54/706 (8%)	54 (100%)	0	100	100
3	I	57/706 (8%)	57 (100%)	0	100	100
3	J	48/706 (7%)	48 (100%)	0	100	100
3	K	54/706 (8%)	54 (100%)	0	100	100
3	L	57/706 (8%)	57 (100%)	0	100	100
3	M	48/706 (7%)	48 (100%)	0	100	100
3	N	54/706 (8%)	54 (100%)	0	100	100
3	O	57/706 (8%)	57 (100%)	0	100	100
3	P	48/706 (7%)	48 (100%)	0	100	100
3	Q	54/706 (8%)	54 (100%)	0	100	100
3	R	57/706 (8%)	57 (100%)	0	100	100
3	S	48/706 (7%)	48 (100%)	0	100	100
3	T	54/706 (8%)	54 (100%)	0	100	100
3	U	57/706 (8%)	57 (100%)	0	100	100
3	V	48/706 (7%)	48 (100%)	0	100	100
3	W	54/706 (8%)	54 (100%)	0	100	100
3	X	57/706 (8%)	57 (100%)	0	100	100
3	Y	48/706 (7%)	48 (100%)	0	100	100
3	Z	54/706 (8%)	54 (100%)	0	100	100
3	a	57/706 (8%)	57 (100%)	0	100	100
3	b	48/706 (7%)	48 (100%)	0	100	100
3	c	54/706 (8%)	54 (100%)	0	100	100
3	d	57/706 (8%)	57 (100%)	0	100	100
3	e	48/706 (7%)	48 (100%)	0	100	100
3	f	54/706 (8%)	54 (100%)	0	100	100
3	g	57/706 (8%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	h	48/706 (7%)	48 (100%)	0	100	100
3	i	54/706 (8%)	54 (100%)	0	100	100
3	j	57/706 (8%)	57 (100%)	0	100	100
All	All	7728/31980 (24%)	7716 (100%)	12 (0%)	93	97

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	0H	162	ASN
2	0I	162	ASN
2	0L	162	ASN
2	0J	162	ASN
2	0D	162	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	54	ASN
3	i	61	ASN
3	H	61	ASN
3	T	61	ASN
1	0l	168	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.

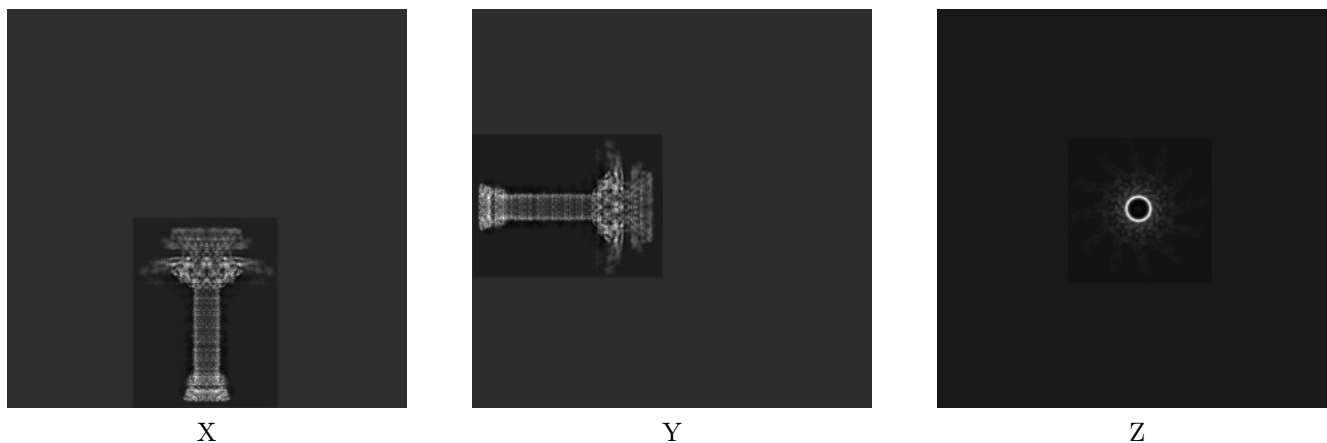
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4685. 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](#)

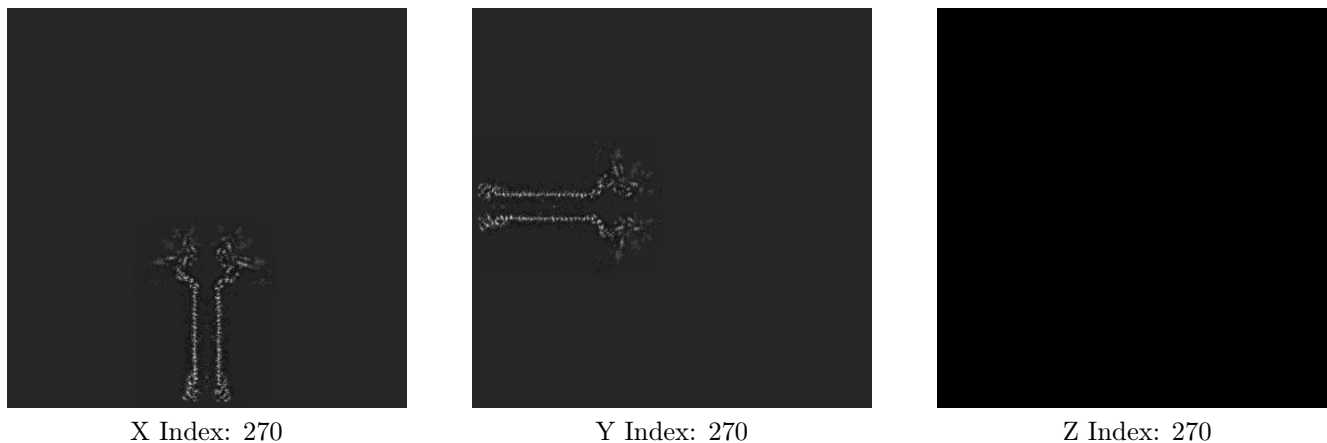
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

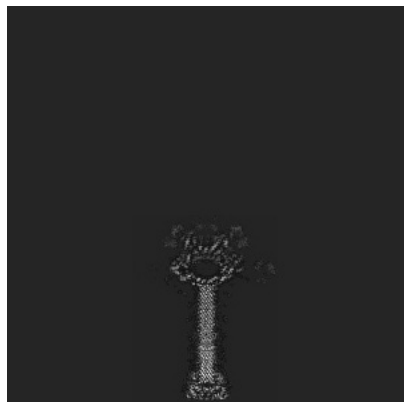
#### 6.2.1 Primary map



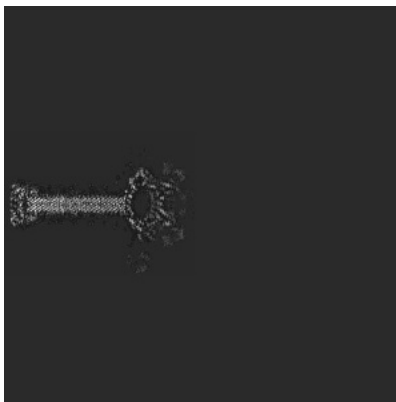
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

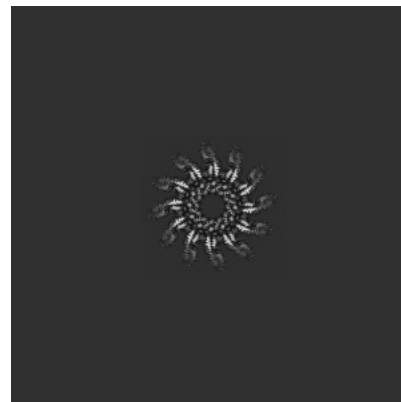
### 6.3.1 Primary map



X Index: 256



Y Index: 254

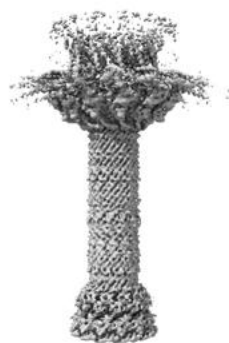


Z Index: 194

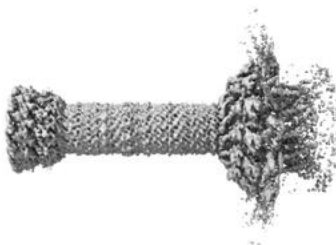
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

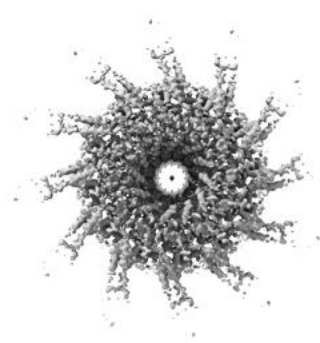
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

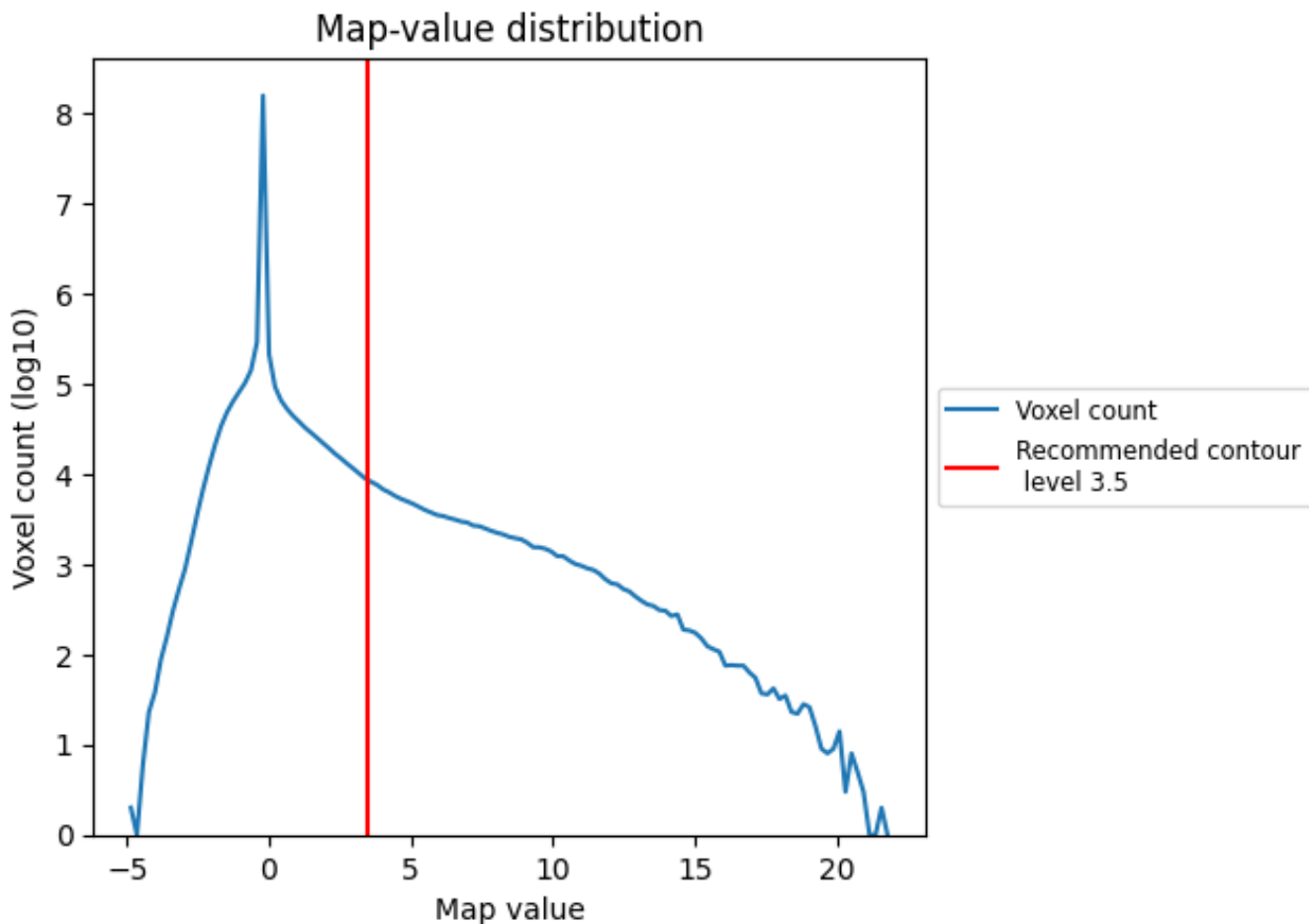
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

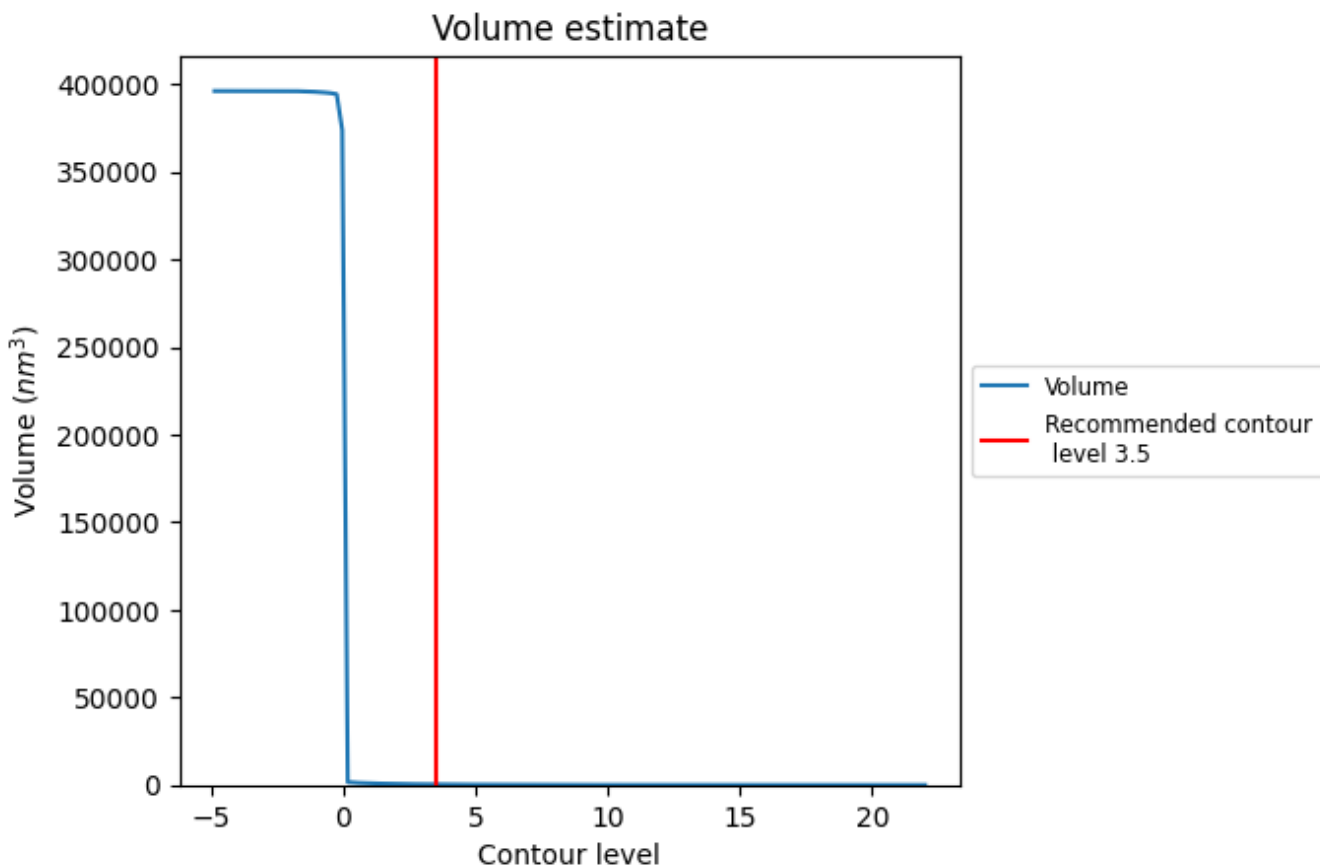
This section contains the results of statistical analysis of the map.

### 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.

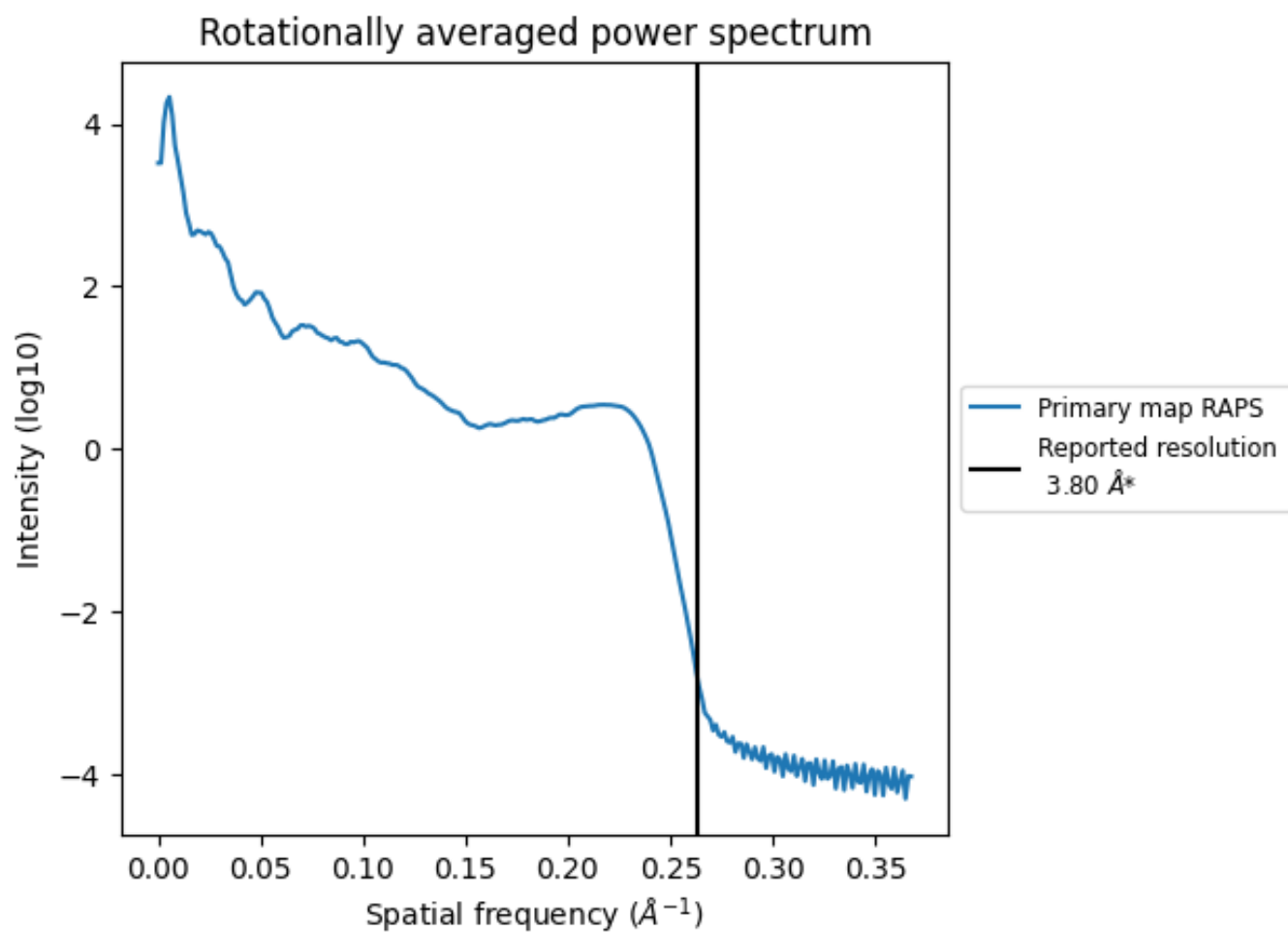
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 323  $\text{nm}^3$ ; this corresponds to an approximate mass of 291 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  $0.263 \text{\AA}^{-1}$



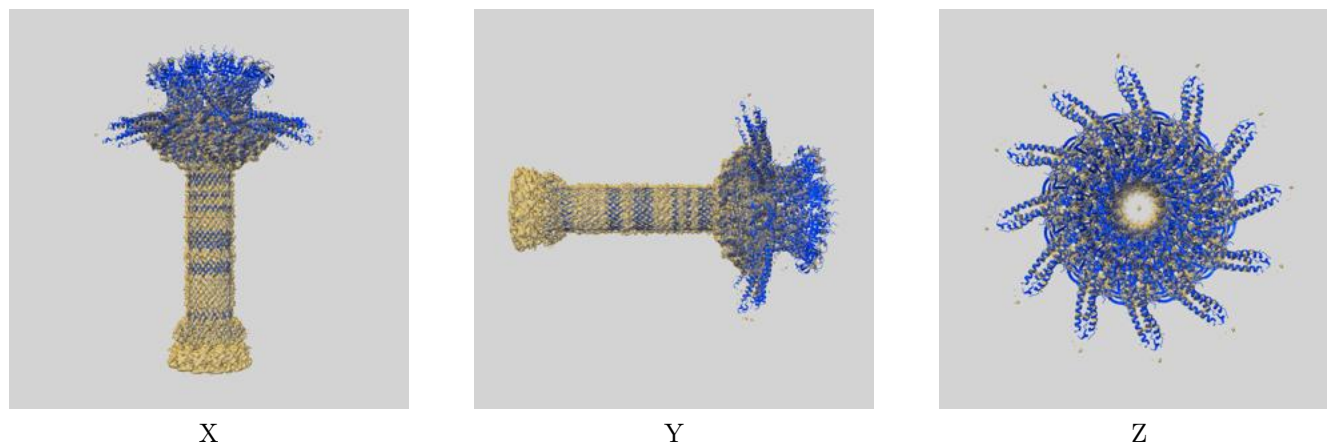
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

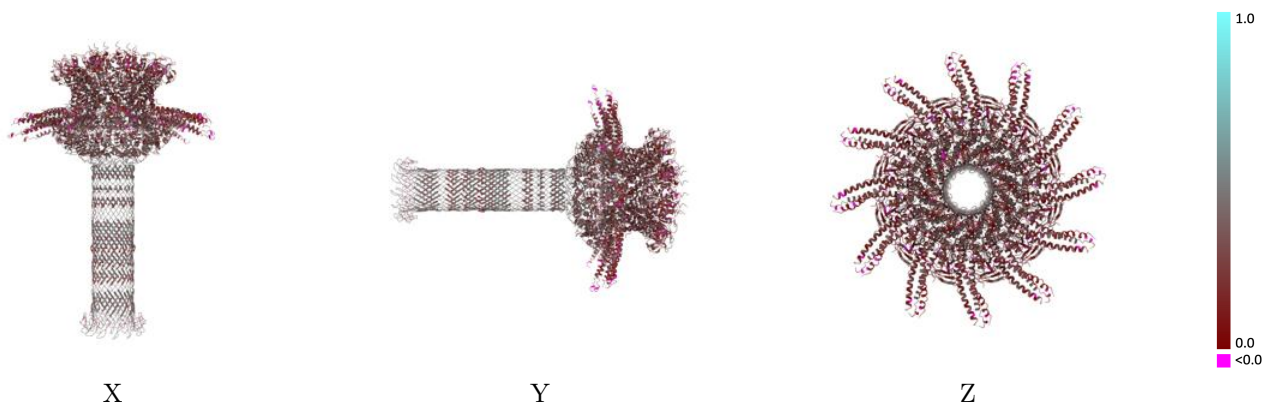
This section contains information regarding the fit between EMDB map EMD-4685 and PDB model 6QZF. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlay [i](#)



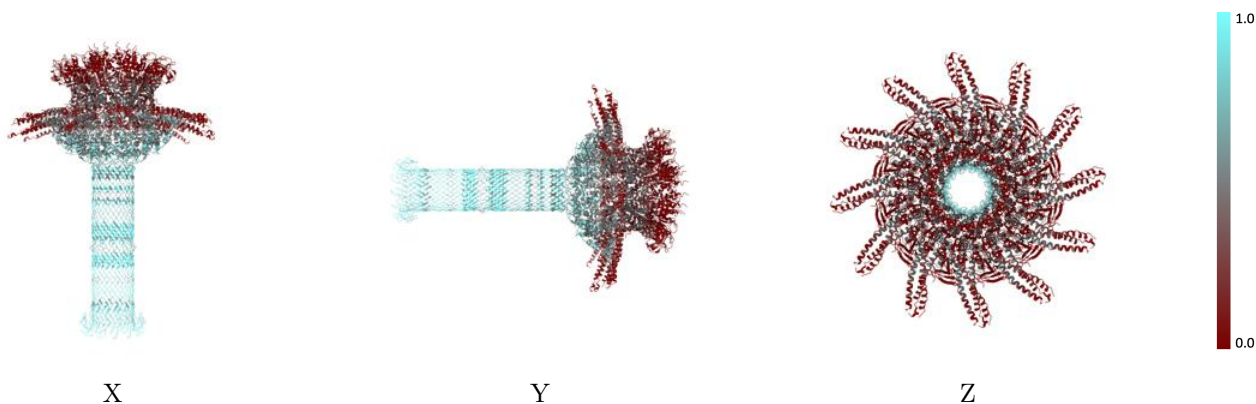
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



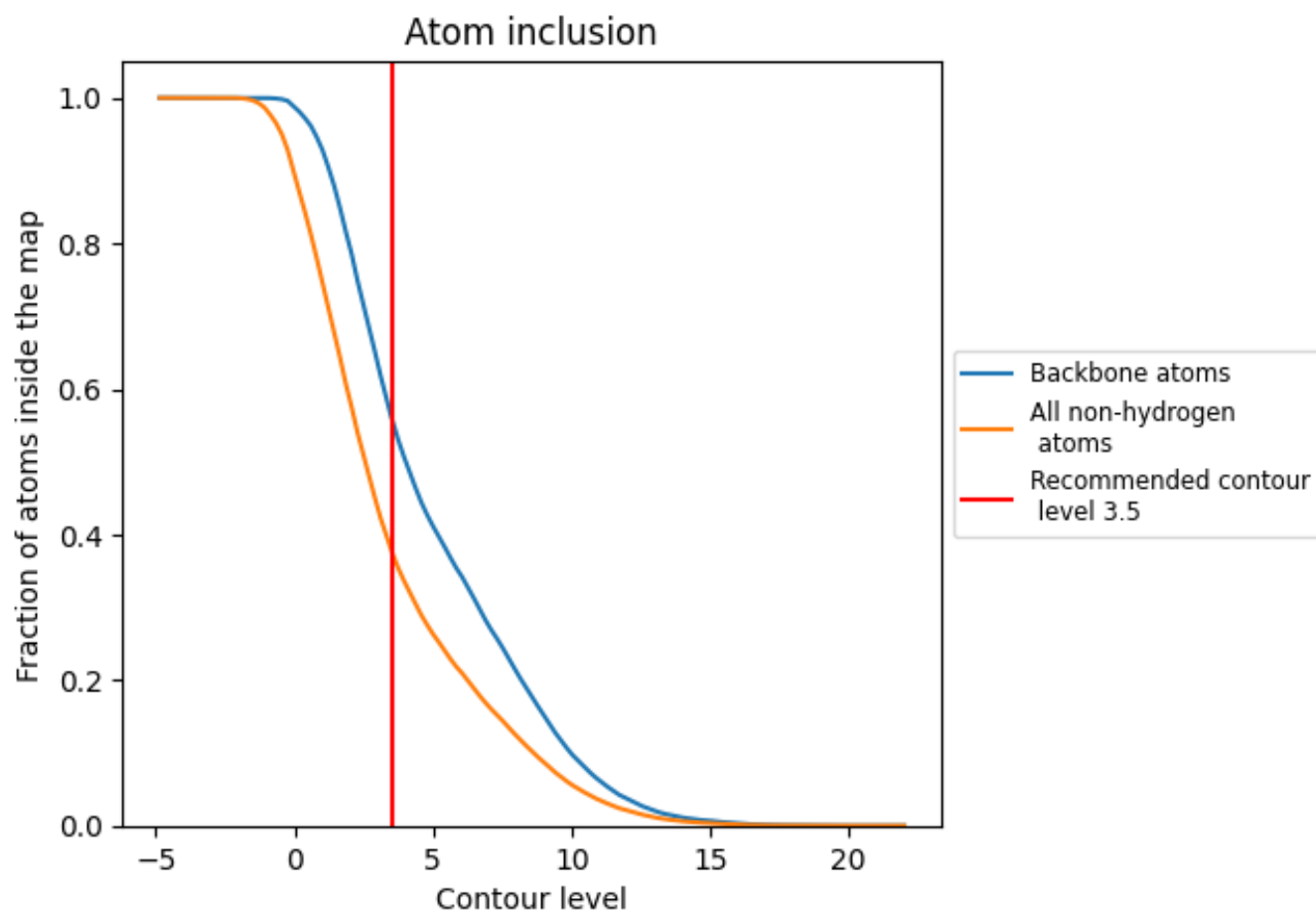
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 38% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3777	 0.3050
0A	 0.6739	 0.3690
0B	 0.6743	 0.3690
0C	 0.6757	 0.3730
0D	 0.6761	 0.3720
0E	 0.6783	 0.3720
0F	 0.6774	 0.3740
0G	 0.6743	 0.3720
0H	 0.6779	 0.3730
0I	 0.6752	 0.3730
0J	 0.6761	 0.3720
0K	 0.6774	 0.3700
0L	 0.6717	 0.3710
0a	 0.1891	 0.2840
0b	 0.1909	 0.2840
0c	 0.1914	 0.2840
0d	 0.1923	 0.2820
0e	 0.1927	 0.2860
0f	 0.1873	 0.2830
0g	 0.1882	 0.2820
0h	 0.1909	 0.2850
0i	 0.1900	 0.2850
0j	 0.1882	 0.2830
0k	 0.1873	 0.2830
0l	 0.1882	 0.2850
A	 0.1737	 0.2080
B	 0.2274	 0.2470
C	 0.1874	 0.2480
D	 0.1667	 0.2090
E	 0.2316	 0.2420
F	 0.1933	 0.2530
G	 0.1620	 0.2100
H	 0.2295	 0.2390
I	 0.1874	 0.2500
J	 0.1667	 0.2020



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Chain	Atom inclusion	Q-score
K	0.2232	0.2330
L	0.1913	0.2470
M	0.1690	0.2010
N	0.2189	0.2330
O	0.1933	0.2490
P	0.1690	0.2010
Q	0.2189	0.2310
R	0.1913	0.2420
S	0.1714	0.2040
T	0.2211	0.2340
U	0.1874	0.2500
V	0.1737	0.2080
W	0.2189	0.2260
X	0.1815	0.2400
Y	0.1690	0.2010
Z	0.2211	0.2290
a	0.1815	0.2430
b	0.1667	0.2000
c	0.2168	0.2290
d	0.1933	0.2480
e	0.1690	0.1960
f	0.2211	0.2390
g	0.1775	0.2390
h	0.1714	0.1950
i	0.2232	0.2390
j	0.1893	0.2500