



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 02:45 AM EDT

PDB ID : 8FWE  
EMDB ID : EMD-29503  
Title : Neck structure of Agrobacterium phage Milano, C3 symmetry  
Authors : Sonani, R.R.; Wang, F.; Esteves, N.C.; Kelly, R.J.; Sebastian, A.;  
Kreutzberger, M.A.B.; Leiman, P.G.; Scharf, B.E.; Egelman, E.H.  
Deposited on : 2023-01-21  
Resolution : 3.46 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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:

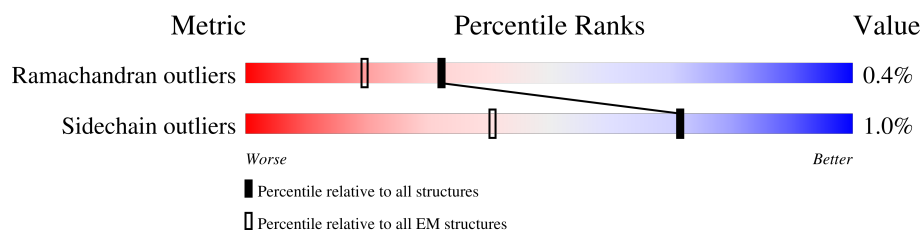
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 3.46 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	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	0	230	 5% 96%
1	1	230	 1% 96%
1	2	230	 5% 97%
1	3	230	 5% 97%
1	4	230	 5% 96%
1	5	230	 5% 97%
1	6	230	 7% 97%
1	7	230	 6% 96%
1	8	230	 5% 97%

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Mol	Chain	Length	Quality of chain
1	9	230	5% 96% ..
1	A	230	6% 97% .
1	B	230	5% 96% ..
1	C	230	5% 97% .
1	D	230	6% 96% ..
1	E	230	5% 97% .
1	F	230	7% 97% .
1	G	230	5% 96% ..
1	J	230	8% 97% .
1	K	230	7% 97% .
1	L	230	7% 97% .
1	M	230	7% 97% .
1	N	230	7% 97% .
1	O	230	7% 96% ..
1	P	230	7% 97% .
1	Q	230	7% 96% ..
1	R	230	7% 97% .
1	S	230	7% 97% .
1	T	230	7% 97% .
1	U	230	7% 97% .
1	V	230	6% 97% .
1	W	230	7% 97% .
1	X	230	8% 97% .
1	Y	230	. 97% .
1	Z	230	. 96% ..

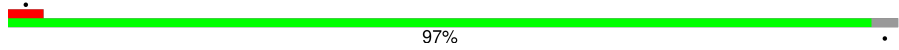

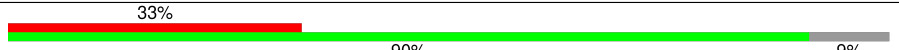
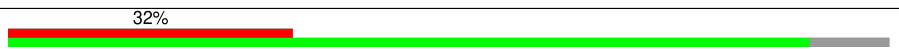
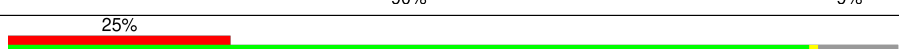
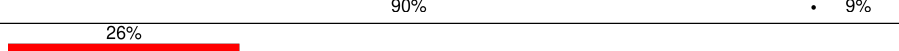
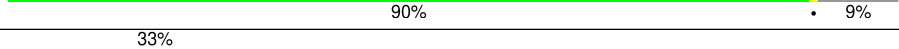

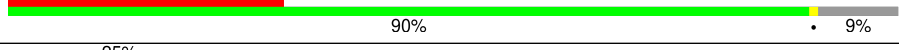



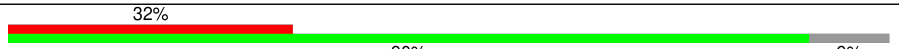


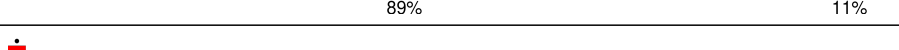








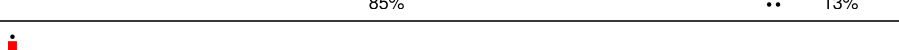
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Mol	Chain	Length	Quality of chain
1	a	230	5% 97% .
1	b	230	6% 97% .
1	c	230	5% 97% .
1	d	230	. 97% .
1	e	230	5% 96% ..
1	f	230	5% 97% .
1	g	230	6% 97% .
1	h	230	6% 97% .
1	i	230	. 97% .
1	j	230	6% 96% ..
1	k	230	5% 97% .
1	l	230	6% 97% .
1	m	230	5% 97% .
1	n	230	. 97% .
1	o	230	. 97% .
1	p	230	. 97% .
1	q	230	. 96% ..
1	r	230	5% 97% .
1	s	230	5% 97% .
1	t	230	. 97% .
1	u	230	. 97% .
1	v	230	. 97% .
1	w	230	. 97% .
1	x	230	5% 97% .
1	y	230	. 97% .

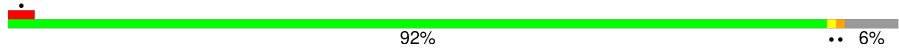
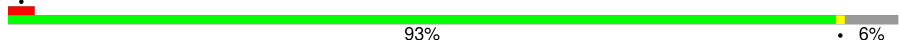
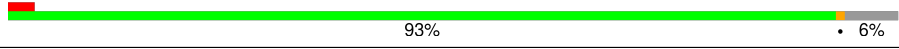
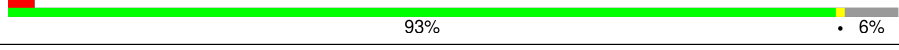
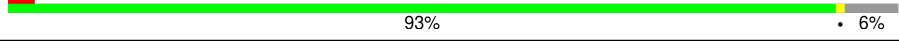
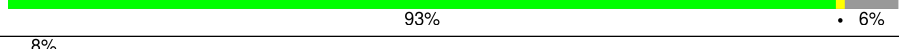
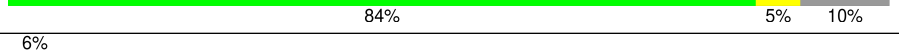
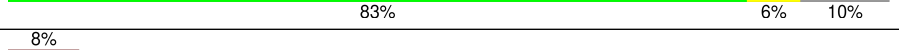
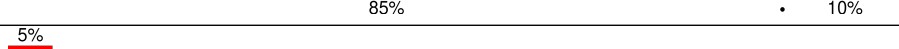
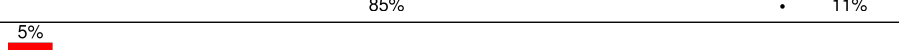




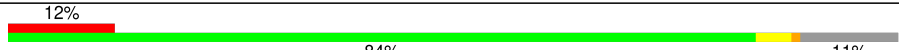



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Mol	Chain	Length	Quality of chain
1	z	230	
2	AA	420	
2	AB	420	
2	AC	420	
2	AD	420	
2	AE	420	
2	AF	420	
2	AG	420	
2	AH	420	
2	AI	420	
2	AJ	420	
2	AK	420	
2	AL	420	
3	AM	141	
3	AN	141	
3	AO	141	
3	AP	141	
3	H	141	
3	I	141	
4	AQ	178	
4	AR	178	
4	AS	178	
4	AT	178	
4	AW	178	
4	AX	178	

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Mol	Chain	Length	Quality of chain
5	AU	136	
5	AV	136	
5	AY	136	
5	AZ	136	
5	Aa	136	
5	Ab	136	
6	R3	202	
6	R4	202	
6	R5	202	
6	S3	202	
6	S4	202	
6	S5	202	
6	T3	202	
6	T4	202	
6	T5	202	
6	U3	202	
6	U4	202	
6	U5	202	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 171990 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 Collar sheath protein, gp13.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	K	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	L	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	M	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	N	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	O	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	P	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	Q	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	R	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	S	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	T	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	U	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	V	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	W	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	X	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	Y	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	Z	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	b	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	c	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	d	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	e	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	f	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	g	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	h	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	i	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	j	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	k	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	l	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	m	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	n	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	o	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	p	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	q	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	r	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	s	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	t	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	u	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	v	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	w	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	x	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	y	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	z	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	1	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	2	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	4	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	5	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	6	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	7	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	8	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	9	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	0	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	A	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	B	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	C	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	D	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	E	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
1	F	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		

- Molecule 2 is a protein called Portal protein, gp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AA	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AB	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AC	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AD	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AE	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AF	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AG	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AH	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AI	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AJ	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AK	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
2	AL	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		

- Molecule 3 is a protein called Neck 2 protein, gp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AM	125	Total	C	N	O	S	0	0
			997	621	183	185	8		
3	AP	125	Total	C	N	O	S	0	0
			997	621	183	185	8		
3	AN	125	Total	C	N	O	S	0	0
			997	621	183	185	8		
3	H	125	Total	C	N	O	S	0	0
			997	621	183	185	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	AO	125	Total	C	N	O	S	0	0
			997	621	183	185	8		
3	I	125	Total	C	N	O	S	0	0
			997	621	183	185	8		

- Molecule 4 is a protein called Tail-terminator protein, gp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AQ	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		
4	AR	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		
4	AS	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		
4	AT	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		
4	AW	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		
4	AX	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		

- Molecule 5 is a protein called Tail-tube, gp21.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AU	128	Total	C	N	O	S	0	0
			977	606	162	202	7		
5	AZ	128	Total	C	N	O	S	0	0
			977	606	162	202	7		
5	AV	128	Total	C	N	O	S	0	0
			977	606	162	202	7		
5	Aa	128	Total	C	N	O	S	0	0
			977	606	162	202	7		
5	AY	128	Total	C	N	O	S	0	0
			977	606	162	202	7		
5	Ab	128	Total	C	N	O	S	0	0
			977	606	162	202	7		

- Molecule 6 is a protein called Neck 1 protein, gp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R3	181	Total	C	N	O	S	0	0
			1395	887	249	255	4		

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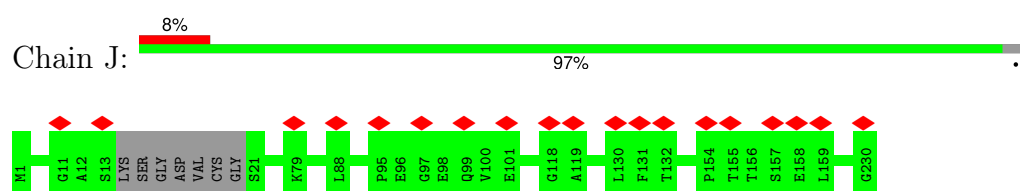
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Mol	Chain	Residues	Atoms					AltConf	Trace
6	S3	180	Total 1387	C 881	N 248	O 254	S 4	0	0
6	T3	179	Total 1379	C 875	N 247	O 253	S 4	0	0
6	U3	180	Total 1387	C 881	N 248	O 254	S 4	0	0
6	R4	181	Total 1395	C 887	N 249	O 255	S 4	0	0
6	S4	180	Total 1387	C 881	N 248	O 254	S 4	0	0
6	T4	179	Total 1379	C 875	N 247	O 253	S 4	0	0
6	U4	180	Total 1387	C 881	N 248	O 254	S 4	0	0
6	R5	181	Total 1395	C 887	N 249	O 255	S 4	0	0
6	S5	180	Total 1387	C 881	N 248	O 254	S 4	0	0
6	T5	179	Total 1379	C 875	N 247	O 253	S 4	0	0
6	U5	180	Total 1387	C 881	N 248	O 254	S 4	0	0

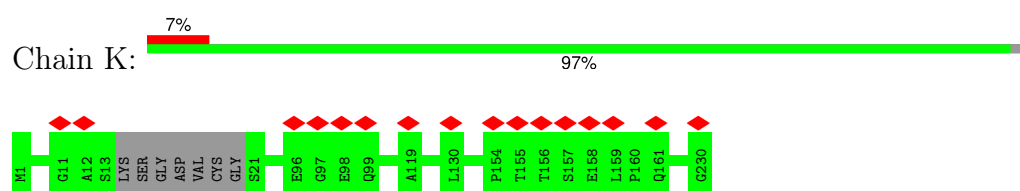
### 3 Residue-property plots [i](#)

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.

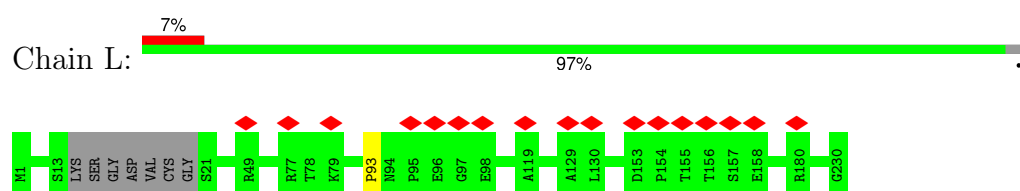
- Molecule 1: Collar sheath protein, gp13



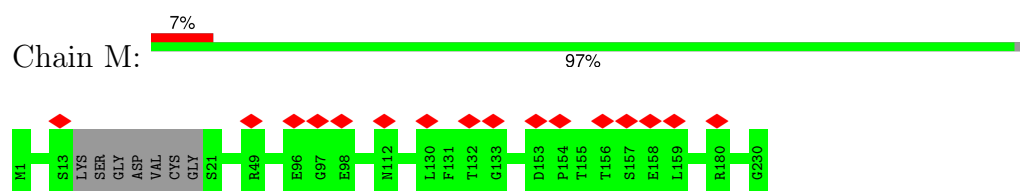
- Molecule 1: Collar sheath protein, gp13



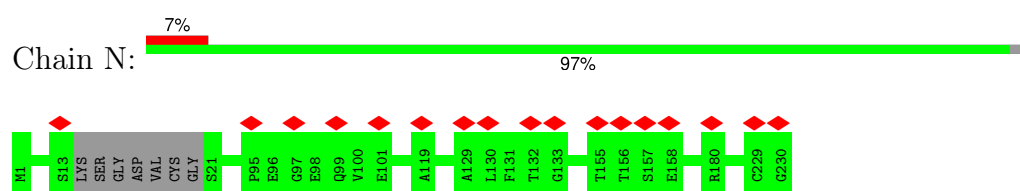
- Molecule 1: Collar sheath protein, gp13



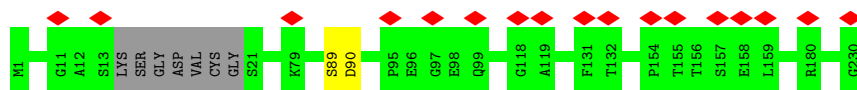
- Molecule 1: Collar sheath protein, gp13



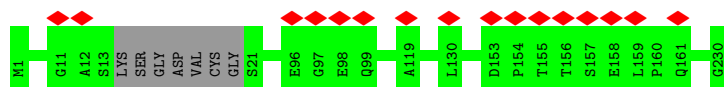
- Molecule 1: Collar sheath protein, gp13



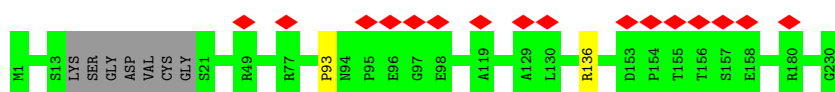
- Molecule 1: Collar sheath protein, gp13



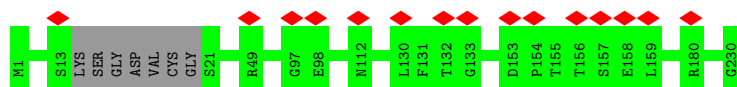
- Molecule 1: Collar sheath protein, gp13



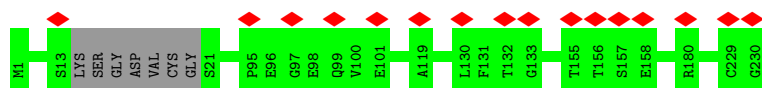
- Molecule 1: Collar sheath protein, gp13



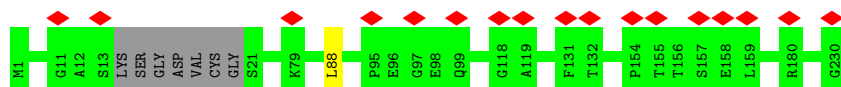
- Molecule 1: Collar sheath protein, gp13



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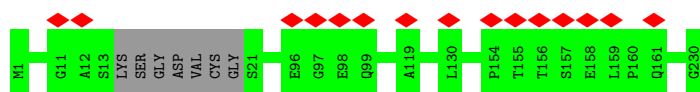


- Molecule 1: Collar sheath protein, gp13

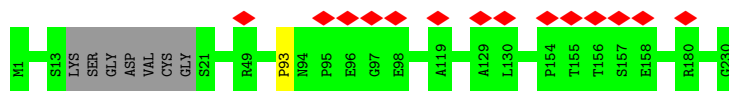


- Molecule 1: Collar sheath protein, gp13

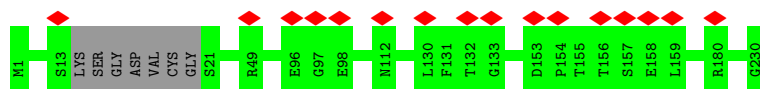




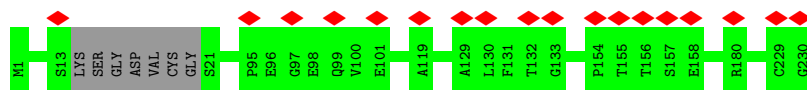
- Molecule 1: Collar sheath protein, gp13



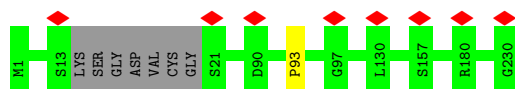
- Molecule 1: Collar sheath protein, gp13



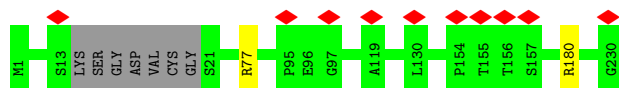
- Molecule 1: Collar sheath protein, gp13



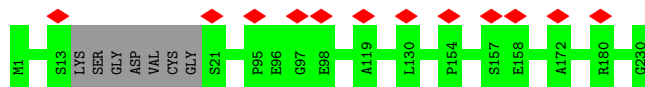
- Molecule 1: Collar sheath protein, gp13



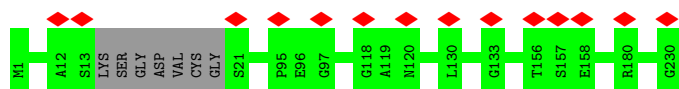
- Molecule 1: Collar sheath protein, gp13



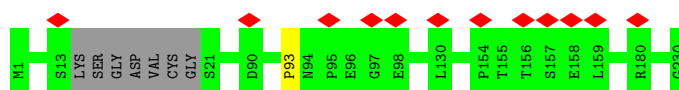
- Molecule 1: Collar sheath protein, gp13



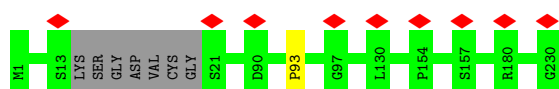
- Molecule 1: Collar sheath protein, gp13



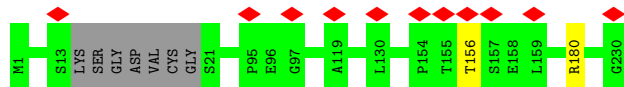
- Molecule 1: Collar sheath protein, gp13



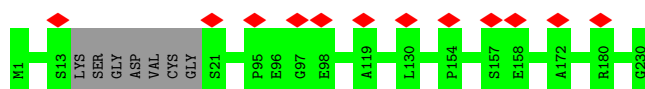
- Molecule 1: Collar sheath protein, gp13



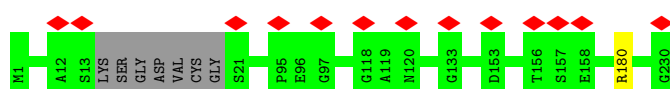
- Molecule 1: Collar sheath protein, gp13



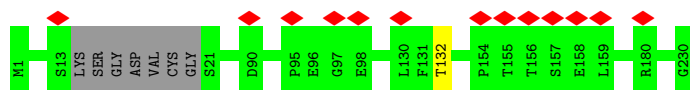
- Molecule 1: Collar sheath protein, gp13



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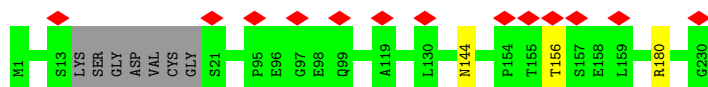
- Molecule 1: Collar sheath protein, gp13

Chain i:  97%



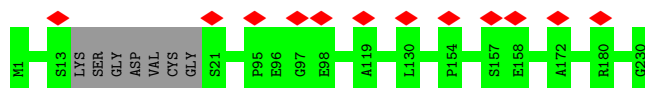
- Molecule 1: Collar sheath protein, gp13

Chain j:  96%



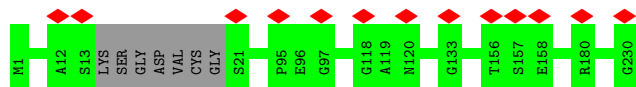
- Molecule 1: Collar sheath protein, gp13

Chain k:  97%



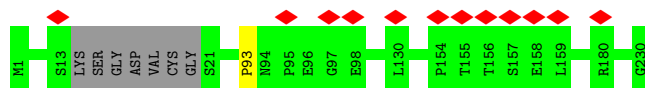
- Molecule 1: Collar sheath protein, gp13

Chain l:  97%



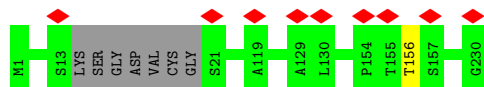
- Molecule 1: Collar sheath protein, gp13

Chain m:  97%



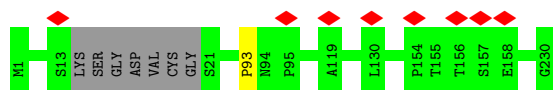
- Molecule 1: Collar sheath protein, gp13

Chain n:  97%

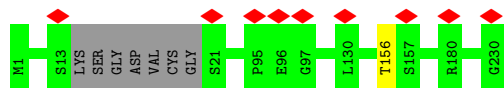


- Molecule 1: Collar sheath protein, gp13

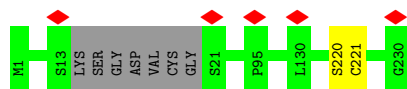
Chain o:  97%



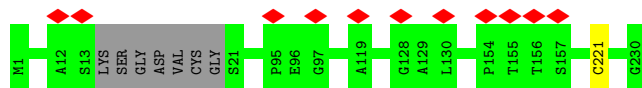
- Molecule 1: Collar sheath protein, gp13



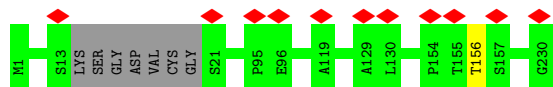
- Molecule 1: Collar sheath protein, gp13



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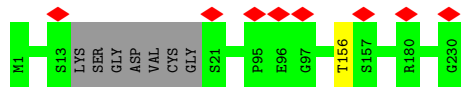
- Molecule 1: Collar sheath protein, gp13



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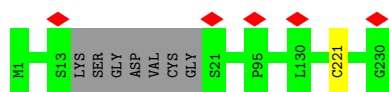


- Molecule 1: Collar sheath protein, gp13



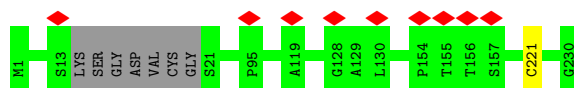
- Molecule 1: Collar sheath protein, gp13

Chain v:  97%



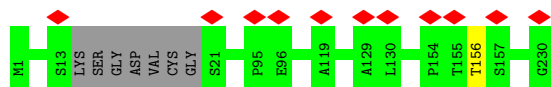
- Molecule 1: Collar sheath protein, gp13

Chain w:  97%



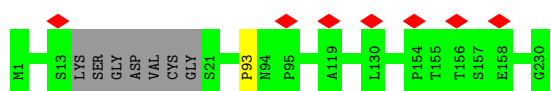
- Molecule 1: Collar sheath protein, gp13

Chain x:  5% 97%



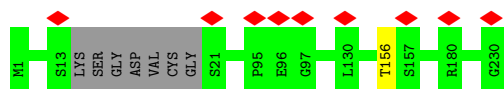
- Molecule 1: Collar sheath protein, gp13

Chain y:  97%



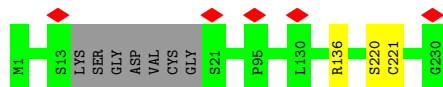
- Molecule 1: Collar sheath protein, gp13

Chain z:  97%



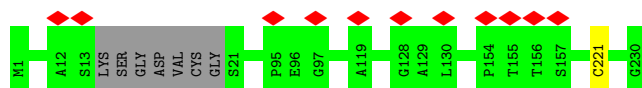
- Molecule 1: Collar sheath protein, gp13

Chain 1:  96%

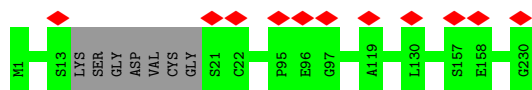


- Molecule 1: Collar sheath protein, gp13

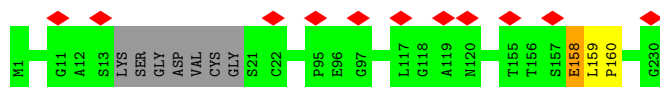
Chain 2:  5% 97%



- Molecule 1: Collar sheath protein, gp13



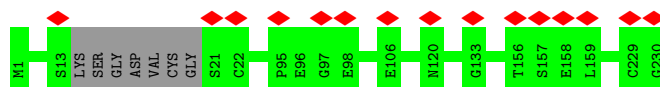
- Molecule 1: Collar sheath protein, gp13



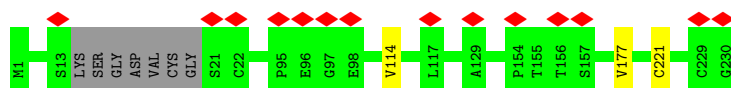
- Molecule 1: Collar sheath protein, gp13



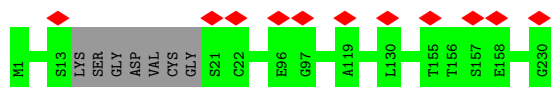
- Molecule 1: Collar sheath protein, gp13



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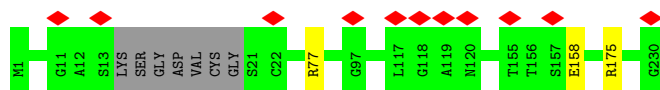


- Molecule 1: Collar sheath protein, gp13

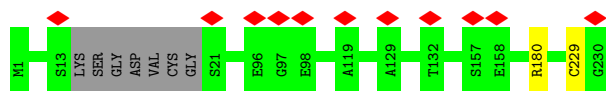


- Molecule 1: Collar sheath protein, gp13

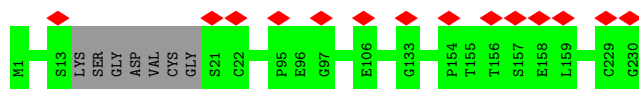




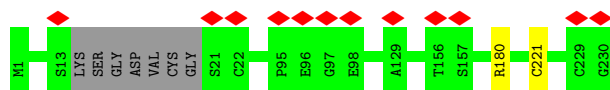
- Molecule 1: Collar sheath protein, gp13



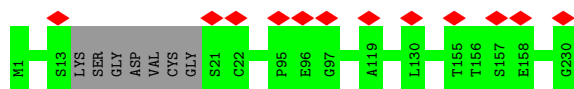
- Molecule 1: Collar sheath protein, gp13



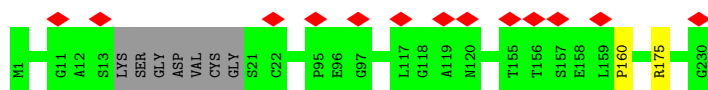
- Molecule 1: Collar sheath protein, gp13



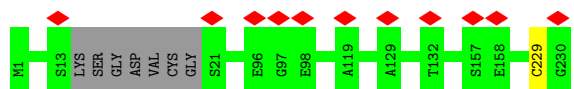
- Molecule 1: Collar sheath protein, gp13



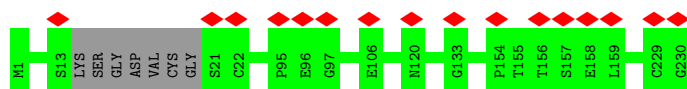
- Molecule 1: Collar sheath protein, gp13



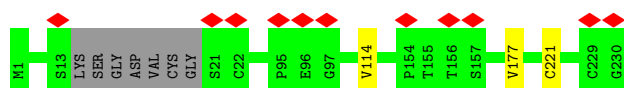
- Molecule 1: Collar sheath protein, gp13



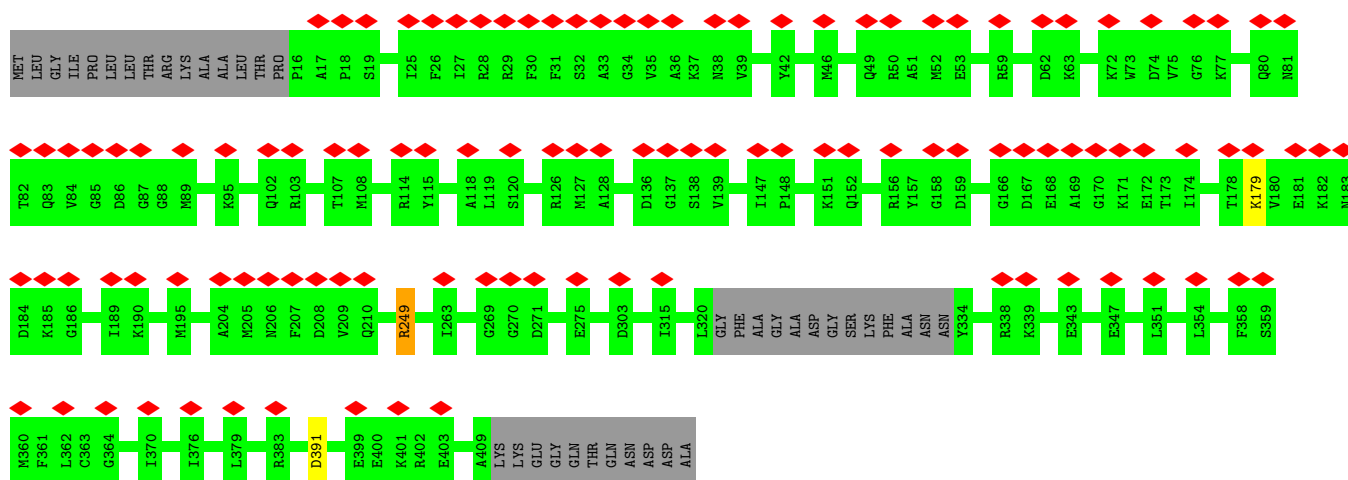
- Molecule 1: Collar sheath protein, gp13



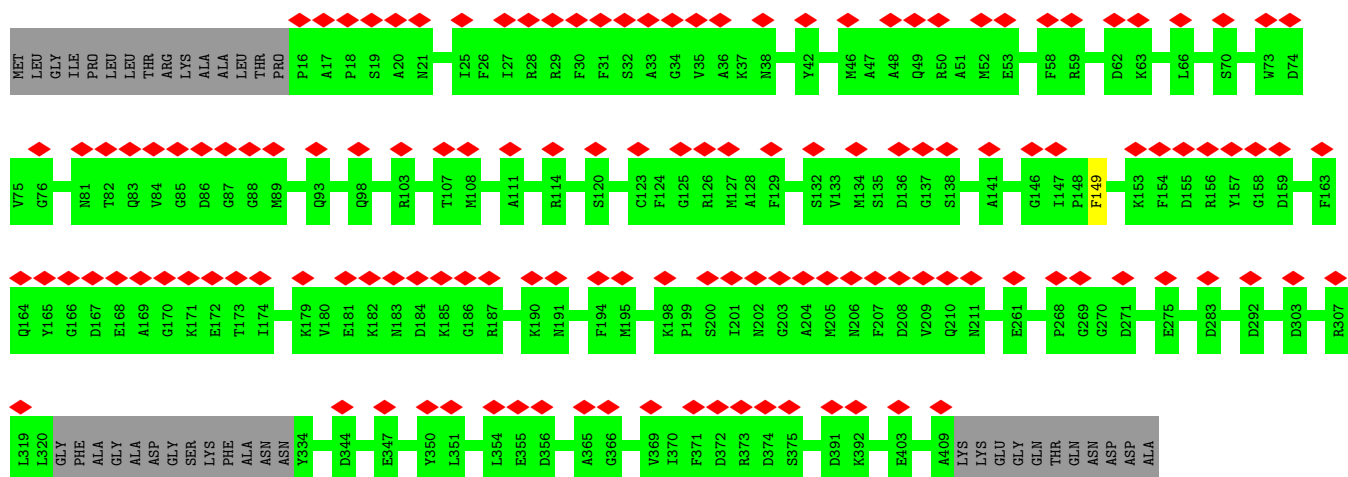
- Molecule 1: Collar sheath protein, gp13



- Molecule 2: Portal protein, gp7

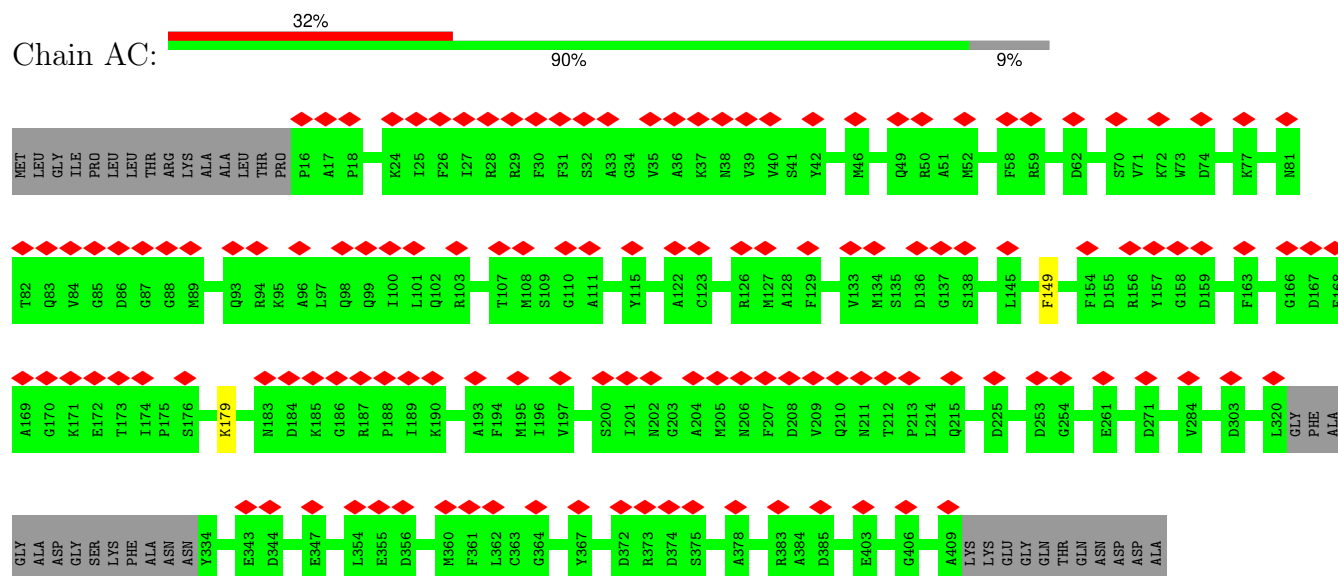


- Molecule 2: Portal protein, gp7



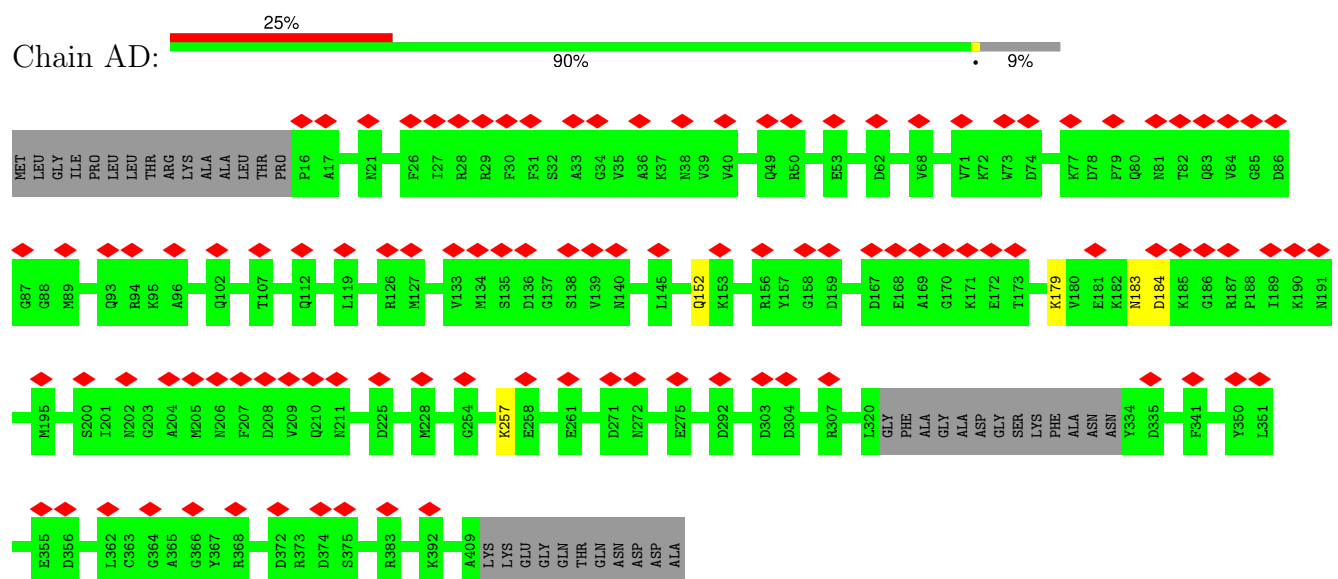
- Molecule 2: Portal protein, gp7

Chain AC:



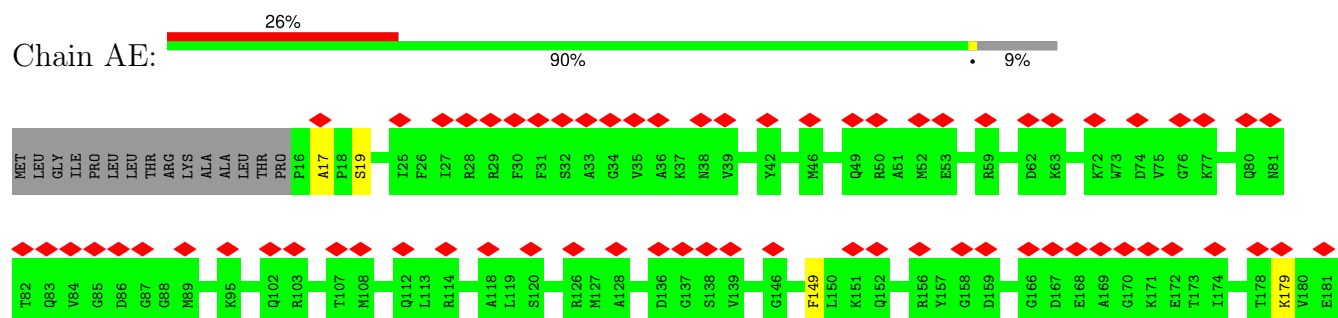
- Molecule 2: Portal protein, gp7

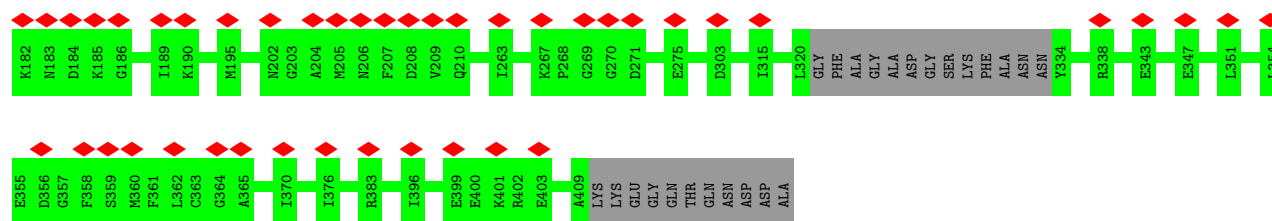
Chain AD:



- Molecule 2: Portal protein, gp7

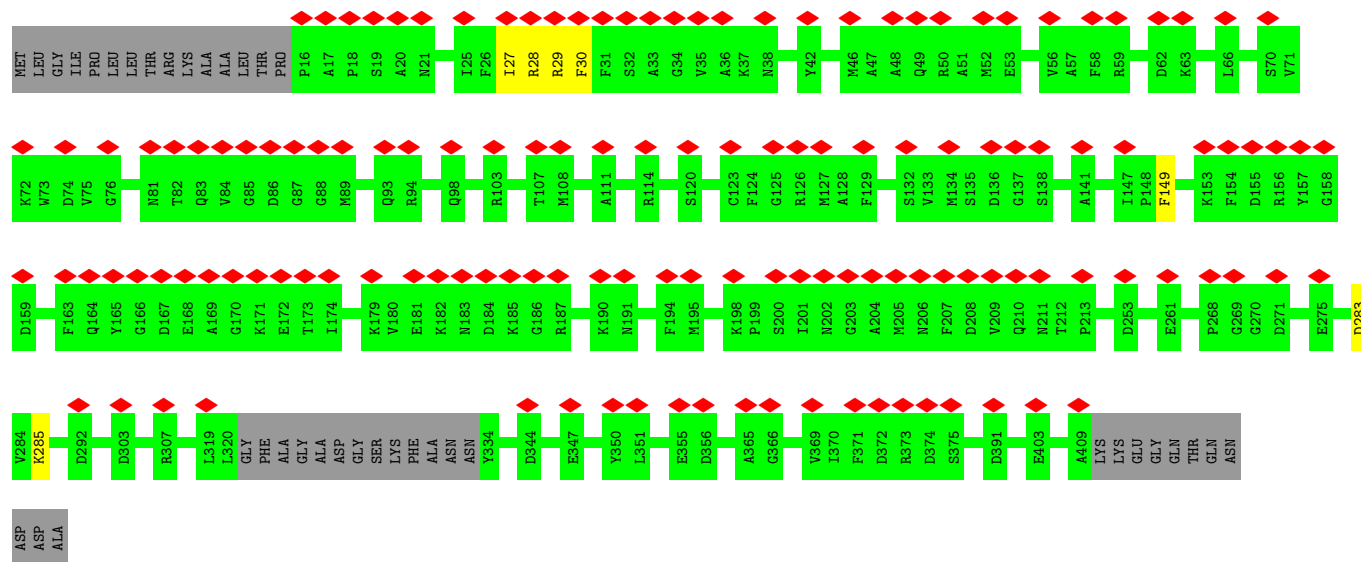
Chain AE:





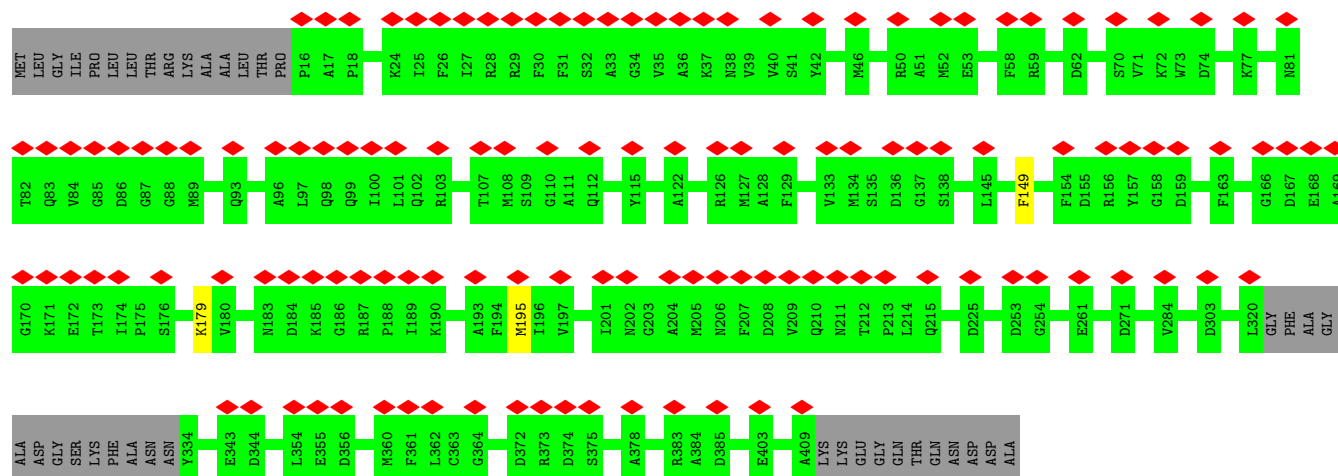
• Molecule 2: Portal protein, gp7

Chain AF: 33% 89% 9%



• Molecule 2: Portal protein, gp7

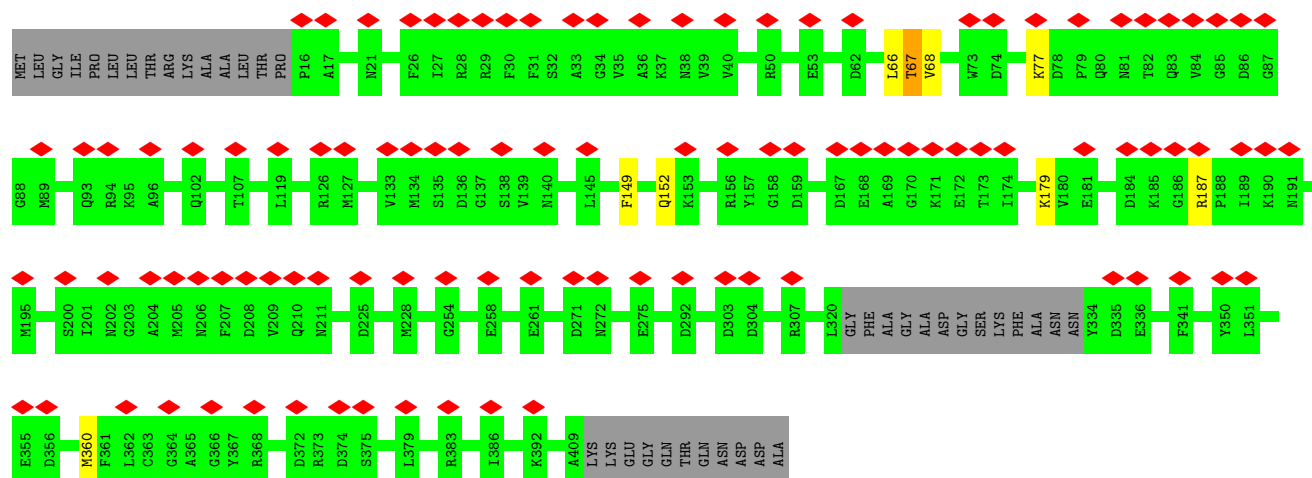
Chain AG: 31% 90% 9%



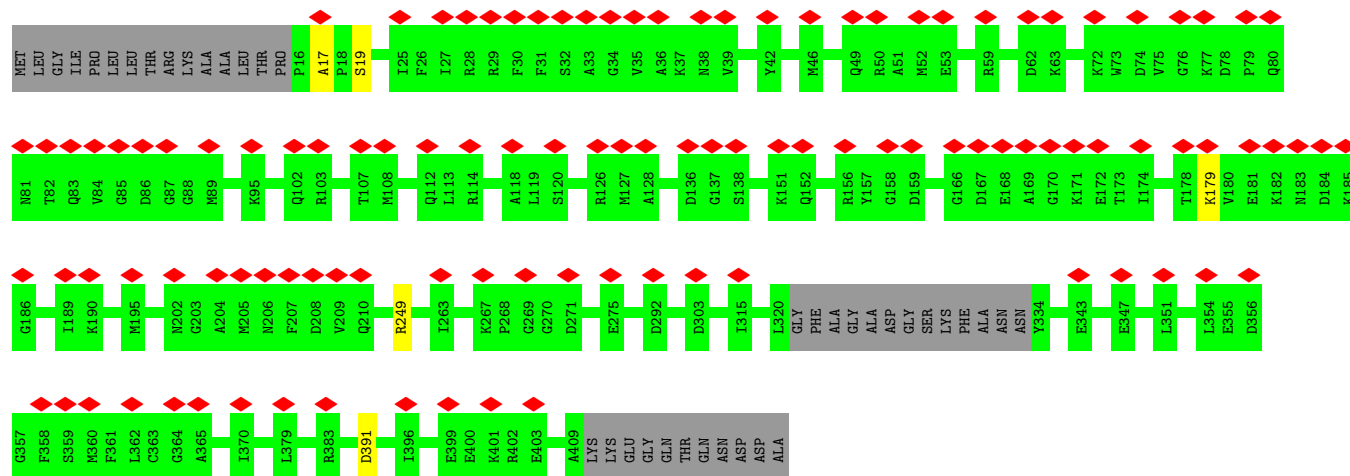
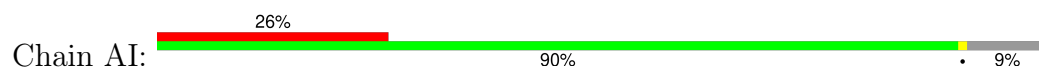
• Molecule 2: Portal protein, gp7

Chain AH: 25% 89% 9%

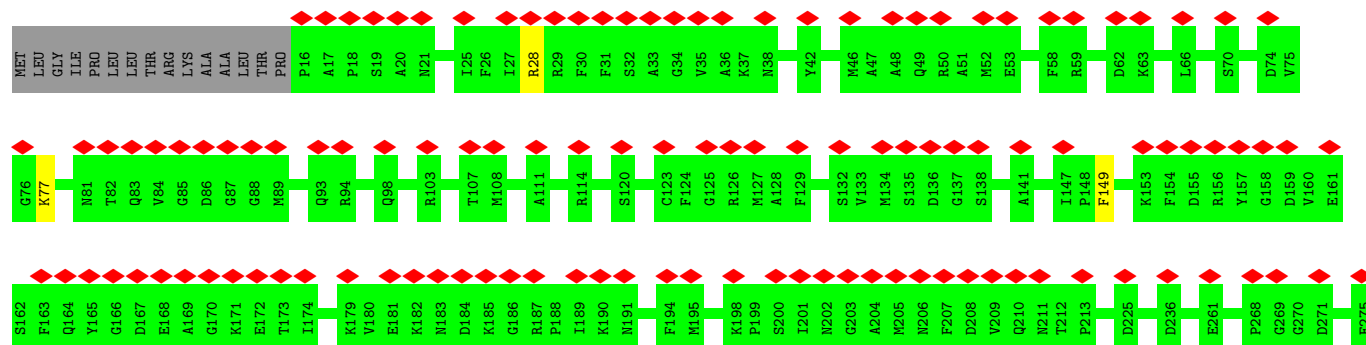
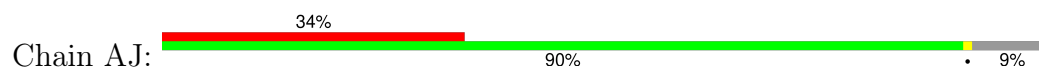


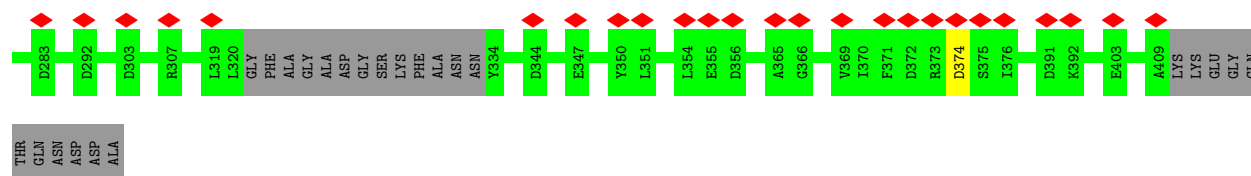


• Molecule 2: Portal protein, gp7

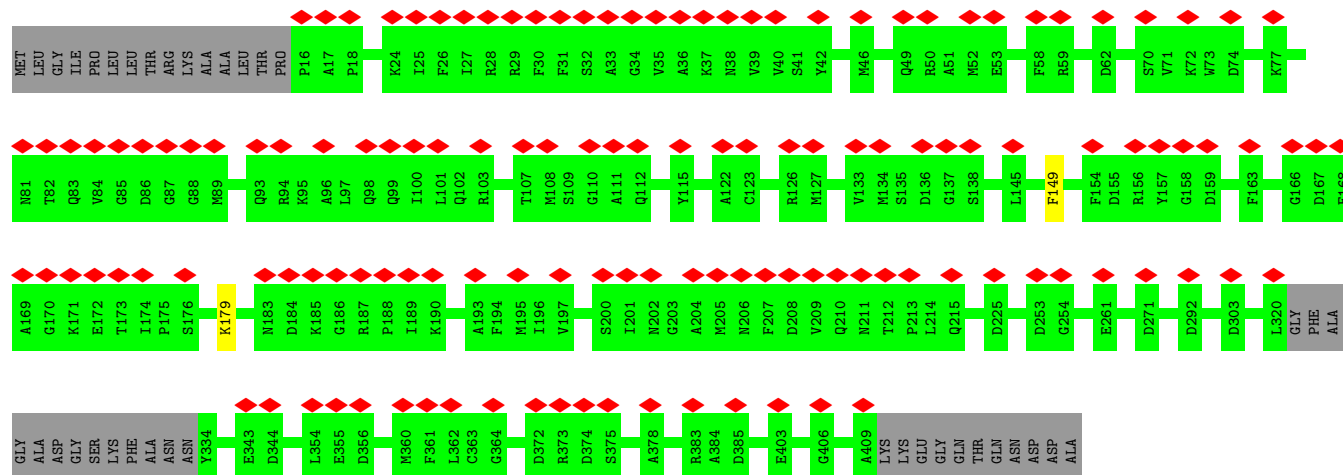


• Molecule 2: Portal protein, gp7

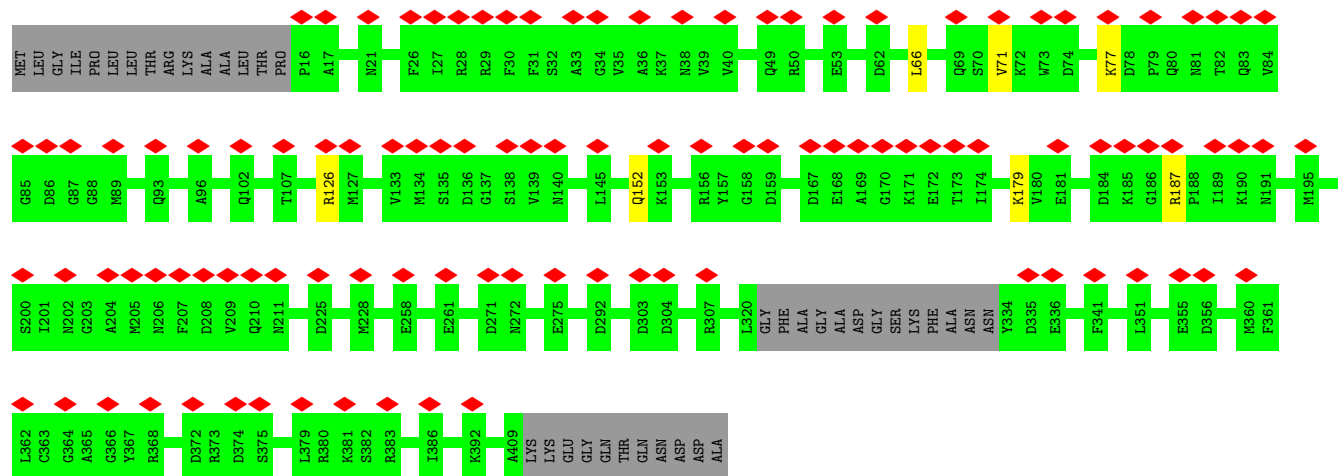
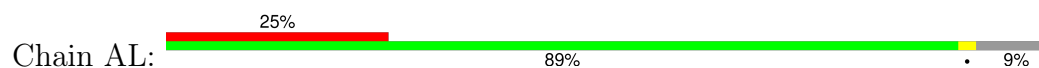




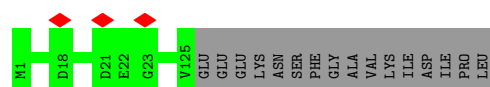
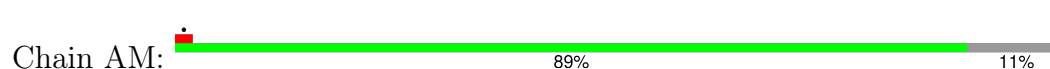
• Molecule 2: Portal protein, gp7




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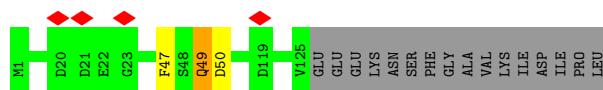


• Molecule 3: Neck 2 protein, gp15




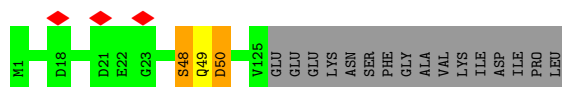
- Molecule 3: Neck 2 protein, gp15

Chain AP:  87% 11%




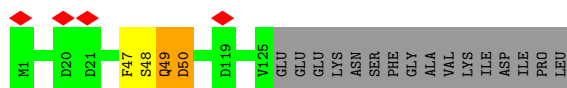
- Molecule 3: Neck 2 protein, gp15

Chain AN:  87% 11%



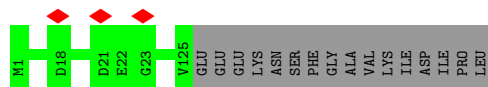
- Molecule 3: Neck 2 protein, gp15

Chain H:  86% 11%




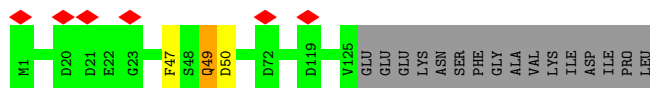
- Molecule 3: Neck 2 protein, gp15

Chain AO:  89% 11%




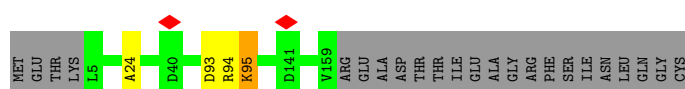
- Molecule 3: Neck 2 protein, gp15

Chain I:  87% 11%




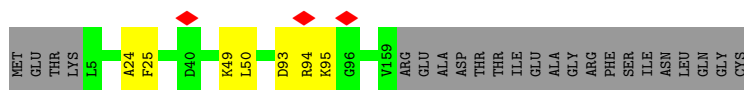
- Molecule 4: Tail-terminator protein, gp18

Chain AQ:  85% 13%

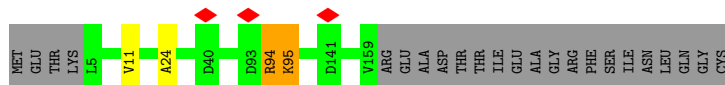
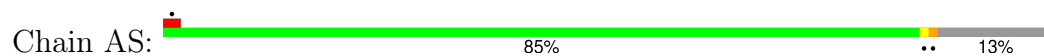


- Molecule 4: Tail-terminator protein, gp18

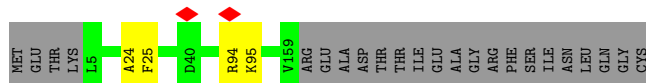
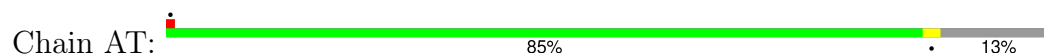
Chain AR:  83% 13%



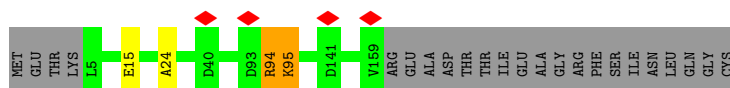
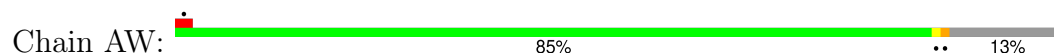
- Molecule 4: Tail-terminator protein, gp18



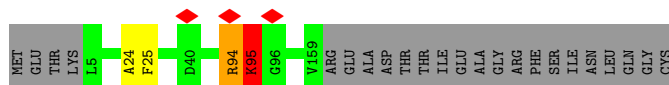
- Molecule 4: Tail-terminator protein, gp18



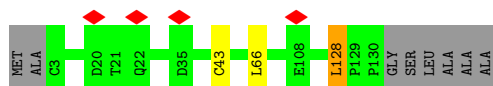
- Molecule 4: Tail-terminator protein, gp18



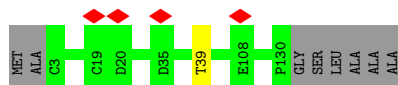
- Molecule 4: Tail-terminator protein, gp18



- Molecule 5: Tail-tube, gp21

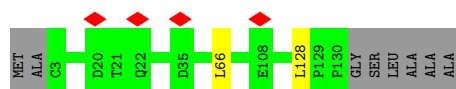


- Molecule 5: Tail-tube, gp21



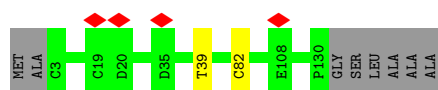
- Molecule 5: Tail-tube, gp21

Chain AV:  93% 6%



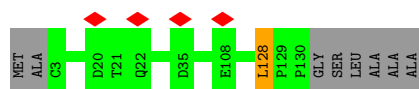
- Molecule 5: Tail-tube, gp21

Chain Aa:  93% 6%



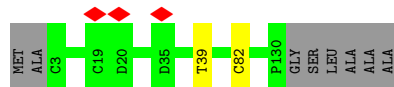
- Molecule 5: Tail-tube, gp21

Chain AY:  93% 6%




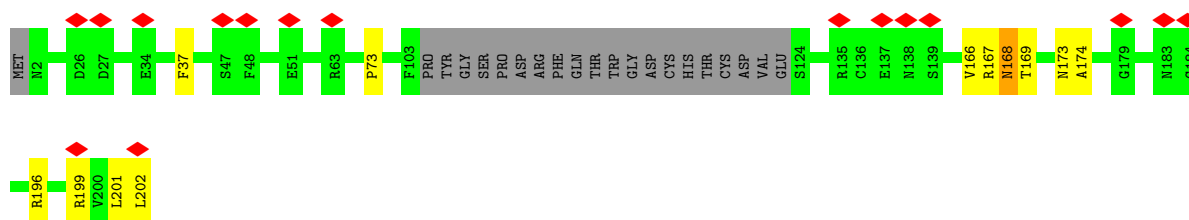
- Molecule 5: Tail-tube, gp21

Chain Ab:  93% 6%




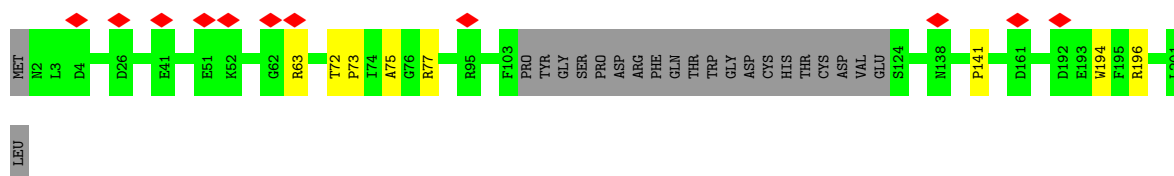
- Molecule 6: Neck 1 protein, gp14

Chain R3:  8% 84% 5% 10%

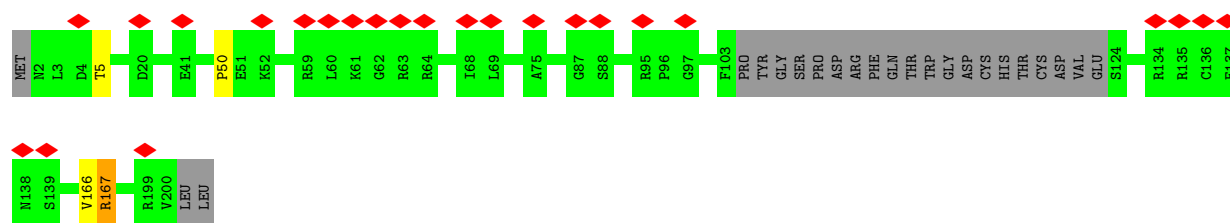
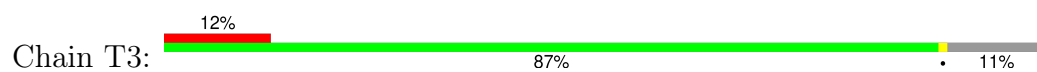


- Molecule 6: Neck 1 protein, gp14

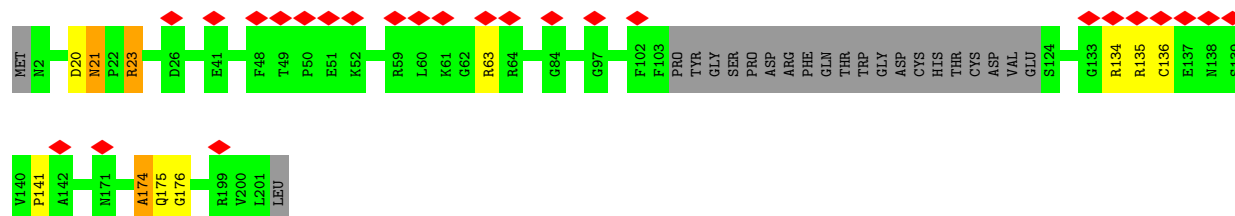
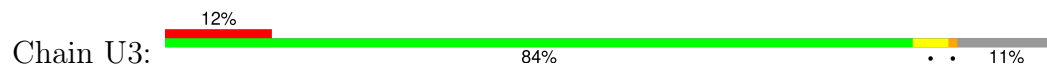
Chain S3:  5% 85% 11%



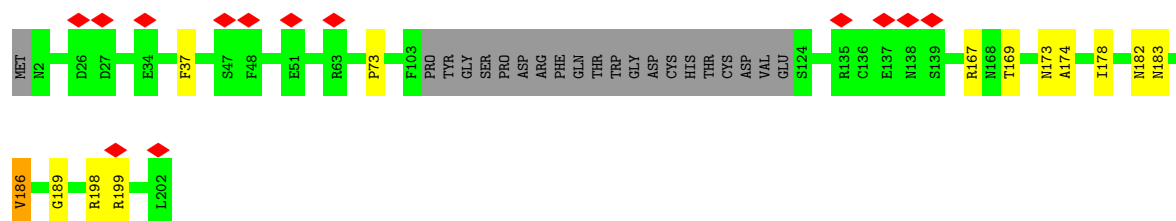
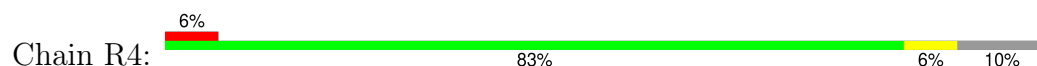
- Molecule 6: Neck 1 protein, gp14



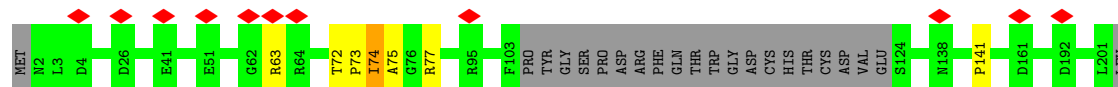
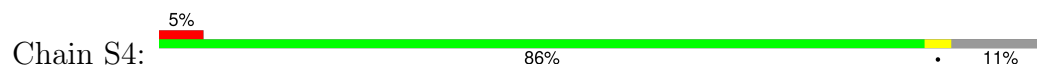
- Molecule 6: Neck 1 protein, gp14



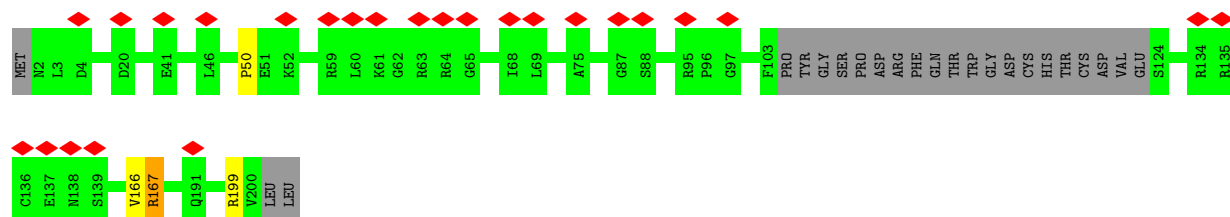
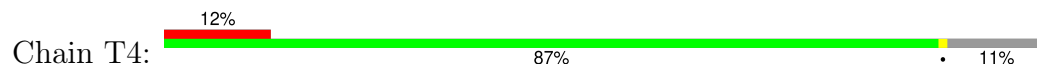
- Molecule 6: Neck 1 protein, gp14



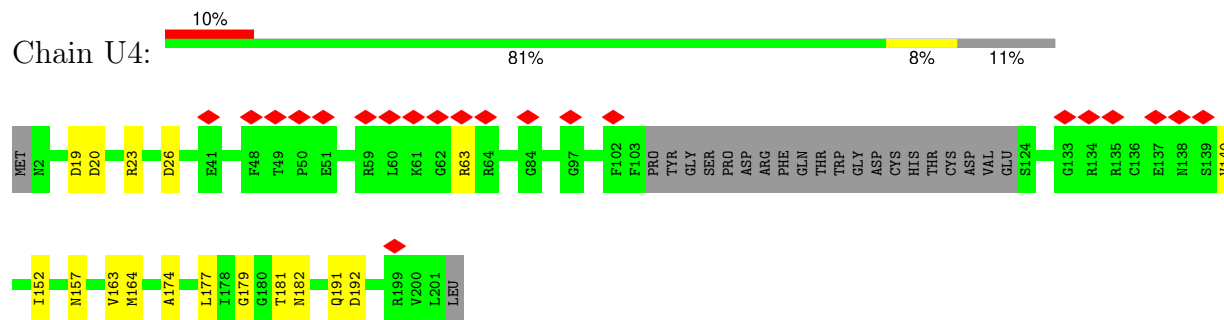
- Molecule 6: Neck 1 protein, gp14



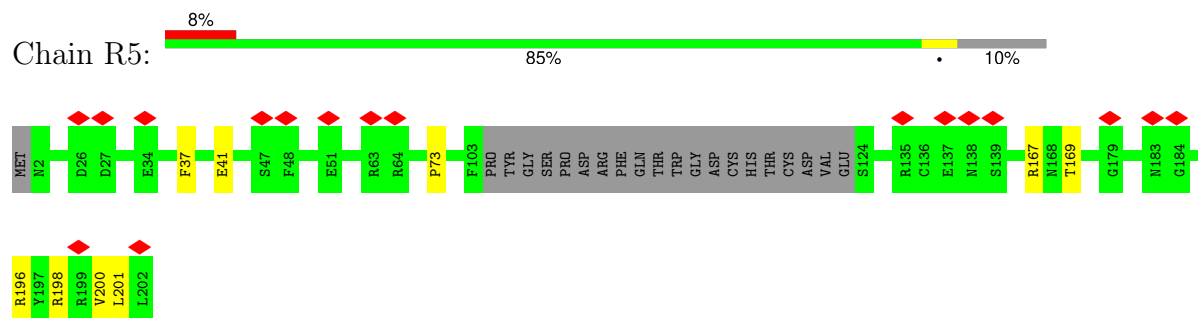
- Molecule 6: Neck 1 protein, gp14



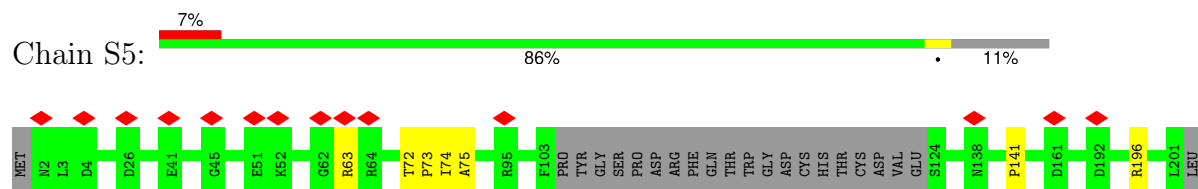
- Molecule 6: Neck 1 protein, gp14



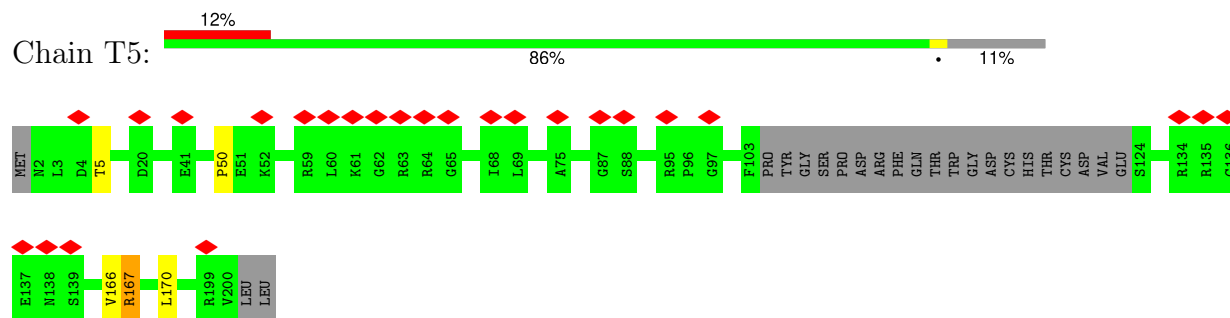
- Molecule 6: Neck 1 protein, gp14



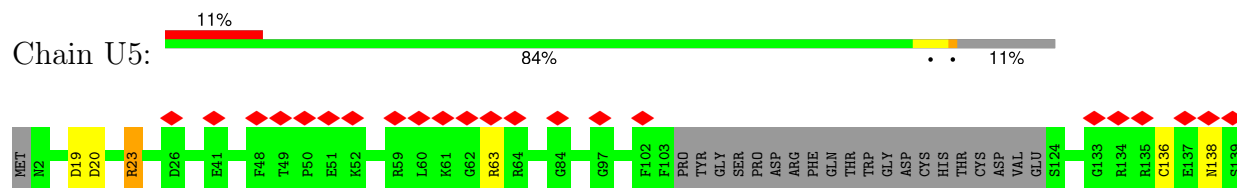
- Molecule 6: Neck 1 protein, gp14



- Molecule 6: Neck 1 protein, gp14



- Molecule 6: Neck 1 protein, gp14







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10216	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.780	Depositor
Minimum map value	-0.421	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	483.84003, 483.84003, 483.84003	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	0	0.45	0/1723	0.52	0/2353
1	1	0.47	0/1723	0.53	0/2353
1	2	0.49	0/1723	0.55	0/2353
1	3	0.44	0/1723	0.52	0/2353
1	4	0.44	0/1723	0.51	0/2353
1	5	0.45	0/1723	0.52	0/2353
1	6	0.43	0/1723	0.52	0/2353
1	7	0.43	0/1723	0.54	0/2353
1	8	0.44	0/1723	0.52	0/2353
1	9	0.44	0/1723	0.51	0/2353
1	A	0.43	0/1723	0.52	0/2353
1	B	0.44	0/1723	0.54	0/2353
1	C	0.44	0/1723	0.52	0/2353
1	D	0.44	0/1723	0.51	0/2353
1	E	0.45	0/1723	0.52	0/2353
1	F	0.43	0/1723	0.52	0/2353
1	G	0.44	0/1723	0.53	0/2353
1	J	0.48	0/1723	0.53	0/2353
1	K	0.47	0/1723	0.54	0/2353
1	L	0.46	0/1723	0.52	1/2353 (0.0%)
1	M	0.44	0/1723	0.52	0/2353
1	N	0.46	0/1723	0.52	0/2353
1	O	0.48	0/1723	0.53	0/2353
1	P	0.48	0/1723	0.54	0/2353
1	Q	0.46	0/1723	0.52	1/2353 (0.0%)
1	R	0.43	0/1723	0.52	0/2353
1	S	0.46	0/1723	0.52	0/2353
1	T	0.48	0/1723	0.53	0/2353
1	U	0.47	0/1723	0.54	0/2353
1	V	0.46	0/1723	0.53	1/2353 (0.0%)
1	W	0.44	0/1723	0.52	0/2353
1	X	0.46	0/1723	0.52	0/2353
1	Y	0.48	0/1723	0.53	1/2353 (0.0%)
1	Z	0.49	0/1723	0.53	0/2353

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	a	0.48	0/1723	0.53	0/2353
1	b	0.48	0/1723	0.53	0/2353
1	c	0.48	0/1723	0.54	1/2353 (0.0%)
1	d	0.48	0/1723	0.53	1/2353 (0.0%)
1	e	0.49	0/1723	0.53	0/2353
1	f	0.48	0/1723	0.53	0/2353
1	g	0.48	0/1723	0.53	0/2353
1	h	0.48	0/1723	0.53	0/2353
1	i	0.48	0/1723	0.53	1/2353 (0.0%)
1	j	0.49	0/1723	0.53	0/2353
1	k	0.48	0/1723	0.52	0/2353
1	l	0.48	0/1723	0.52	0/2353
1	m	0.48	0/1723	0.53	1/2353 (0.0%)
1	n	0.49	0/1723	0.52	0/2353
1	o	0.48	0/1723	0.53	1/2353 (0.0%)
1	p	0.47	0/1723	0.53	0/2353
1	q	0.48	0/1723	0.53	0/2353
1	r	0.49	0/1723	0.56	0/2353
1	s	0.49	0/1723	0.53	0/2353
1	t	0.48	0/1723	0.53	1/2353 (0.0%)
1	u	0.47	0/1723	0.52	0/2353
1	v	0.49	0/1723	0.54	0/2353
1	w	0.48	0/1723	0.55	0/2353
1	x	0.49	0/1723	0.53	0/2353
1	y	0.48	0/1723	0.52	1/2353 (0.0%)
1	z	0.48	0/1723	0.53	0/2353
2	AA	0.37	0/3000	0.52	2/4056 (0.0%)
2	AB	0.37	0/3000	0.53	0/4056
2	AC	0.35	0/3000	0.51	0/4056
2	AD	0.36	0/3000	0.53	0/4056
2	AE	0.36	0/3000	0.52	0/4056
2	AF	0.36	0/3000	0.52	0/4056
2	AG	0.35	0/3000	0.51	0/4056
2	AH	0.36	0/3000	0.53	1/4056 (0.0%)
2	AI	0.37	0/3000	0.51	0/4056
2	AJ	0.36	0/3000	0.53	2/4056 (0.0%)
2	AK	0.35	0/3000	0.51	0/4056
2	AL	0.36	0/3000	0.53	1/4056 (0.0%)
3	AM	0.43	0/1017	0.50	0/1381
3	AN	0.44	0/1017	0.50	0/1381
3	AO	0.43	0/1017	0.50	0/1381
3	AP	0.43	0/1017	0.53	0/1381
3	H	0.43	0/1017	0.51	0/1381

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	I	0.43	0/1017	0.52	0/1381
4	AQ	0.46	0/1281	0.49	0/1734
4	AR	0.47	0/1281	0.49	0/1734
4	AS	0.47	0/1281	0.52	0/1734
4	AT	0.47	0/1281	0.49	0/1734
4	AW	0.47	0/1281	0.52	0/1734
4	AX	0.48	0/1281	0.51	1/1734 (0.1%)
5	AU	0.45	0/993	0.55	0/1358
5	AV	0.45	0/993	0.55	0/1358
5	AY	0.46	0/993	0.55	0/1358
5	AZ	0.45	0/993	0.53	0/1358
5	Aa	0.44	0/993	0.53	0/1358
5	Ab	0.44	0/993	0.54	0/1358
6	R3	0.47	0/1420	0.56	0/1927
6	R4	0.47	0/1420	0.57	0/1927
6	R5	0.47	0/1420	0.58	1/1927 (0.1%)
6	S3	0.46	0/1412	0.56	0/1916
6	S4	0.46	0/1412	0.56	0/1916
6	S5	0.46	0/1412	0.57	0/1916
6	T3	0.39	0/1404	0.54	0/1905
6	T4	0.40	0/1404	0.55	0/1905
6	T5	0.39	0/1404	0.55	0/1905
6	U3	0.48	0/1412	0.61	1/1916 (0.1%)
6	U4	0.50	0/1412	0.59	0/1916
6	U5	0.46	0/1412	0.57	1/1916 (0.1%)
All	All	0.44	0/176070	0.53	21/239682 (0.0%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AA	249	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	t	93	PRO	C-N-CA	-5.58	107.75	121.70
1	Q	93	PRO	C-N-CA	-5.47	108.02	121.70
4	AX	95	LYS	N-CA-C	-5.36	96.52	111.00
1	o	93	PRO	C-N-CA	-5.27	108.53	121.70
1	c	93	PRO	C-N-CA	-5.27	108.53	121.70
2	AA	249	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	L	93	PRO	C-N-CA	-5.25	108.57	121.70
1	V	93	PRO	C-N-CA	-5.21	108.67	121.70
1	i	93	PRO	C-N-CA	-5.19	108.73	121.70
2	AL	77	LYS	C-N-CA	-5.16	108.80	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	93	PRO	C-N-CA	-5.11	108.93	121.70
1	m	93	PRO	C-N-CA	-5.07	109.02	121.70
6	R5	41	GLU	N-CA-C	-5.06	97.34	111.00
2	AH	77	LYS	C-N-CA	-5.05	109.08	121.70
1	y	93	PRO	C-N-CA	-5.04	109.10	121.70
6	U3	174	ALA	N-CA-C	-5.02	97.44	111.00
1	Y	93	PRO	C-N-CA	-5.01	109.18	121.70
2	AJ	77	LYS	C-N-CA	-5.01	109.18	121.70
2	AJ	28	ARG	NE-CZ-NH1	-5.00	117.80	120.30
6	U5	174	ALA	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	0	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
1	1	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
1	2	219/230 (95%)	195 (89%)	24 (11%)	0	100	100
1	3	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
1	4	219/230 (95%)	196 (90%)	21 (10%)	2 (1%)	14	48
1	5	219/230 (95%)	200 (91%)	19 (9%)	0	100	100
1	6	219/230 (95%)	197 (90%)	22 (10%)	0	100	100
1	7	219/230 (95%)	202 (92%)	17 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8	219/230 (95%)	202 (92%)	17 (8%)	0	100	100
1	9	219/230 (95%)	195 (89%)	23 (10%)	1 (0%)	25	59
1	A	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
1	B	219/230 (95%)	204 (93%)	15 (7%)	0	100	100
1	C	219/230 (95%)	202 (92%)	17 (8%)	0	100	100
1	D	219/230 (95%)	198 (90%)	20 (9%)	1 (0%)	25	59
1	E	219/230 (95%)	200 (91%)	19 (9%)	0	100	100
1	F	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
1	G	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
1	J	219/230 (95%)	194 (89%)	25 (11%)	0	100	100
1	K	219/230 (95%)	193 (88%)	26 (12%)	0	100	100
1	L	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	M	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
1	N	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	O	219/230 (95%)	193 (88%)	25 (11%)	1 (0%)	25	59
1	P	219/230 (95%)	192 (88%)	27 (12%)	0	100	100
1	Q	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	R	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	S	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	T	219/230 (95%)	191 (87%)	28 (13%)	0	100	100
1	U	219/230 (95%)	195 (89%)	24 (11%)	0	100	100
1	V	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
1	W	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	X	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	Y	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	Z	219/230 (95%)	197 (90%)	22 (10%)	0	100	100
1	a	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
1	b	219/230 (95%)	200 (91%)	19 (9%)	0	100	100
1	c	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
1	d	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
1	e	219/230 (95%)	199 (91%)	20 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	f	219/230 (95%)	197 (90%)	22 (10%)	0	100	100
1	g	219/230 (95%)	200 (91%)	19 (9%)	0	100	100
1	h	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
1	i	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	j	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	k	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	l	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
1	m	219/230 (95%)	197 (90%)	22 (10%)	0	100	100
1	n	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	o	219/230 (95%)	197 (90%)	22 (10%)	0	100	100
1	p	219/230 (95%)	194 (89%)	25 (11%)	0	100	100
1	q	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
1	r	219/230 (95%)	194 (89%)	25 (11%)	0	100	100
1	s	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	t	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	u	219/230 (95%)	195 (89%)	24 (11%)	0	100	100
1	v	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
1	w	219/230 (95%)	195 (89%)	24 (11%)	0	100	100
1	x	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	y	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
1	z	219/230 (95%)	194 (89%)	25 (11%)	0	100	100
2	AA	377/420 (90%)	323 (86%)	54 (14%)	0	100	100
2	AB	377/420 (90%)	324 (86%)	53 (14%)	0	100	100
2	AC	377/420 (90%)	324 (86%)	53 (14%)	0	100	100
2	AD	377/420 (90%)	323 (86%)	54 (14%)	0	100	100
2	AE	377/420 (90%)	322 (85%)	53 (14%)	2 (0%)	25	59
2	AF	377/420 (90%)	324 (86%)	52 (14%)	1 (0%)	37	69
2	AG	377/420 (90%)	323 (86%)	54 (14%)	0	100	100
2	AH	377/420 (90%)	321 (85%)	55 (15%)	1 (0%)	37	69
2	AI	377/420 (90%)	323 (86%)	52 (14%)	2 (0%)	25	59
2	AJ	377/420 (90%)	323 (86%)	54 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AK	377/420 (90%)	323 (86%)	54 (14%)	0	100	100
2	AL	377/420 (90%)	315 (84%)	62 (16%)	0	100	100
3	AM	123/141 (87%)	107 (87%)	16 (13%)	0	100	100
3	AN	123/141 (87%)	107 (87%)	14 (11%)	2 (2%)	8	37
3	AO	123/141 (87%)	108 (88%)	15 (12%)	0	100	100
3	AP	123/141 (87%)	110 (89%)	11 (9%)	2 (2%)	8	37
3	H	123/141 (87%)	109 (89%)	11 (9%)	3 (2%)	5	30
3	I	123/141 (87%)	108 (88%)	13 (11%)	2 (2%)	8	37
4	AQ	153/178 (86%)	136 (89%)	15 (10%)	2 (1%)	10	41
4	AR	153/178 (86%)	137 (90%)	15 (10%)	1 (1%)	19	53
4	AS	153/178 (86%)	132 (86%)	18 (12%)	3 (2%)	6	33
4	AT	153/178 (86%)	137 (90%)	15 (10%)	1 (1%)	19	53
4	AW	153/178 (86%)	134 (88%)	16 (10%)	3 (2%)	6	33
4	AX	153/178 (86%)	135 (88%)	15 (10%)	3 (2%)	6	33
5	AU	126/136 (93%)	112 (89%)	13 (10%)	1 (1%)	16	50
5	AV	126/136 (93%)	114 (90%)	11 (9%)	1 (1%)	16	50
5	AY	126/136 (93%)	113 (90%)	12 (10%)	1 (1%)	16	50
5	AZ	126/136 (93%)	115 (91%)	11 (9%)	0	100	100
5	Aa	126/136 (93%)	115 (91%)	11 (9%)	0	100	100
5	Ab	126/136 (93%)	115 (91%)	11 (9%)	0	100	100
6	R3	177/202 (88%)	142 (80%)	30 (17%)	5 (3%)	4	27
6	R4	177/202 (88%)	142 (80%)	29 (16%)	6 (3%)	3	24
6	R5	177/202 (88%)	141 (80%)	31 (18%)	5 (3%)	4	27
6	S3	176/202 (87%)	142 (81%)	30 (17%)	4 (2%)	5	31
6	S4	176/202 (87%)	143 (81%)	28 (16%)	5 (3%)	4	27
6	S5	176/202 (87%)	142 (81%)	30 (17%)	4 (2%)	5	31
6	T3	175/202 (87%)	143 (82%)	30 (17%)	2 (1%)	12	44
6	T4	175/202 (87%)	146 (83%)	27 (15%)	2 (1%)	12	44
6	T5	175/202 (87%)	143 (82%)	30 (17%)	2 (1%)	12	44
6	U3	176/202 (87%)	143 (81%)	27 (15%)	6 (3%)	3	24
6	U4	176/202 (87%)	139 (79%)	32 (18%)	5 (3%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	U5	176/202 (87%)	142 (81%)	29 (16%)	5 (3%)	4	27
All	All	22188/23994 (92%)	19565 (88%)	2536 (11%)	87 (0%)	32	64

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AP	50	ASP
6	R3	168	ASN
6	S3	73	PRO
6	U3	141	PRO
6	U3	174	ALA
3	AN	50	ASP
4	AS	95	LYS
3	H	50	ASP
6	R4	174	ALA
6	S4	73	PRO
6	U4	174	ALA
6	U4	181	THR
4	AW	95	LYS
4	AX	95	LYS
3	I	50	ASP
6	S5	73	PRO
6	S5	75	ALA
6	U5	171	ASN
6	U5	174	ALA
1	4	158	GLU
1	9	158	GLU
2	AE	19	SER
2	AI	19	SER
6	S3	63	ARG
6	S3	75	ALA
6	U3	176	GLY
3	H	48	SER
3	H	49	GLN
6	S4	63	ARG
6	S4	75	ALA
4	AX	94	ARG
6	R5	167	ARG
6	R5	196	ARG
6	S5	63	ARG
6	U5	176	GLY
1	O	90	ASP

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Mol	Chain	Res	Type
1	4	160	PRO
2	AI	17	ALA
4	AQ	95	LYS
3	AP	49	GLN
6	S3	141	PRO
6	T3	50	PRO
6	T3	167	ARG
4	AS	94	ARG
5	AV	128	LEU
6	R4	167	ARG
6	R4	186	VAL
6	R4	189	GLY
6	T4	50	PRO
6	U4	179	GLY
4	AW	94	ARG
3	I	49	GLN
6	R5	201	LEU
6	T5	50	PRO
2	AE	17	ALA
2	AF	30	PHE
4	AQ	24	ALA
5	AU	128	LEU
6	U3	21	ASN
6	U3	23	ARG
3	AN	48	SER
4	AS	24	ALA
4	AT	24	ALA
6	S4	141	PRO
6	U4	191	GLN
4	AW	24	ALA
5	AY	128	LEU
6	R5	200	VAL
6	S5	141	PRO
6	T5	167	ARG
2	AH	67	THR
4	AR	24	ALA
6	R3	73	PRO
6	R3	167	ARG
6	R4	73	PRO
6	R4	199	ARG
6	T4	167	ARG
6	U4	63	ARG

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Mol	Chain	Res	Type
4	AX	24	ALA
6	R5	73	PRO
6	U5	23	ARG
6	R3	166	VAL
6	R3	174	ALA
6	U3	63	ARG
6	U5	63	ARG
1	D	160	PRO
6	S4	74	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	186/191 (97%)	184 (99%)	2 (1%)	70	83
1	1	186/191 (97%)	183 (98%)	3 (2%)	58	76
1	2	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	3	186/191 (97%)	186 (100%)	0	100	100
1	4	186/191 (97%)	184 (99%)	2 (1%)	70	83
1	5	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	6	186/191 (97%)	186 (100%)	0	100	100
1	7	186/191 (97%)	183 (98%)	3 (2%)	58	76
1	8	186/191 (97%)	186 (100%)	0	100	100
1	9	186/191 (97%)	184 (99%)	2 (1%)	70	83
1	A	186/191 (97%)	186 (100%)	0	100	100
1	B	186/191 (97%)	184 (99%)	2 (1%)	70	83
1	C	186/191 (97%)	186 (100%)	0	100	100
1	D	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	E	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	F	186/191 (97%)	186 (100%)	0	100	100
1	G	186/191 (97%)	183 (98%)	3 (2%)	58	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	186/191 (97%)	186 (100%)	0	100	100
1	K	186/191 (97%)	186 (100%)	0	100	100
1	L	186/191 (97%)	186 (100%)	0	100	100
1	M	186/191 (97%)	186 (100%)	0	100	100
1	N	186/191 (97%)	186 (100%)	0	100	100
1	O	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	P	186/191 (97%)	186 (100%)	0	100	100
1	Q	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	R	186/191 (97%)	186 (100%)	0	100	100
1	S	186/191 (97%)	186 (100%)	0	100	100
1	T	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	U	186/191 (97%)	186 (100%)	0	100	100
1	V	186/191 (97%)	186 (100%)	0	100	100
1	W	186/191 (97%)	186 (100%)	0	100	100
1	X	186/191 (97%)	186 (100%)	0	100	100
1	Y	186/191 (97%)	186 (100%)	0	100	100
1	Z	186/191 (97%)	184 (99%)	2 (1%)	70	83
1	a	186/191 (97%)	186 (100%)	0	100	100
1	b	186/191 (97%)	186 (100%)	0	100	100
1	c	186/191 (97%)	186 (100%)	0	100	100
1	d	186/191 (97%)	186 (100%)	0	100	100
1	e	186/191 (97%)	184 (99%)	2 (1%)	70	83
1	f	186/191 (97%)	186 (100%)	0	100	100
1	g	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	h	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	i	186/191 (97%)	186 (100%)	0	100	100
1	j	186/191 (97%)	183 (98%)	3 (2%)	58	76
1	k	186/191 (97%)	186 (100%)	0	100	100
1	l	186/191 (97%)	186 (100%)	0	100	100
1	m	186/191 (97%)	186 (100%)	0	100	100
1	n	186/191 (97%)	185 (100%)	1 (0%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	186/191 (97%)	186 (100%)	0	100	100
1	p	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	q	186/191 (97%)	184 (99%)	2 (1%)	70	83
1	r	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	s	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	t	186/191 (97%)	186 (100%)	0	100	100
1	u	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	v	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	w	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	x	186/191 (97%)	185 (100%)	1 (0%)	86	92
1	y	186/191 (97%)	186 (100%)	0	100	100
1	z	186/191 (97%)	185 (100%)	1 (0%)	86	92
2	AA	311/339 (92%)	308 (99%)	3 (1%)	73	84
2	AB	311/339 (92%)	310 (100%)	1 (0%)	91	96
2	AC	311/339 (92%)	309 (99%)	2 (1%)	84	91
2	AD	311/339 (92%)	306 (98%)	5 (2%)	58	76
2	AE	311/339 (92%)	309 (99%)	2 (1%)	84	91
2	AF	311/339 (92%)	305 (98%)	6 (2%)	52	74
2	AG	311/339 (92%)	308 (99%)	3 (1%)	73	84
2	AH	311/339 (92%)	303 (97%)	8 (3%)	41	68
2	AI	311/339 (92%)	308 (99%)	3 (1%)	73	84
2	AJ	311/339 (92%)	309 (99%)	2 (1%)	84	91
2	AK	311/339 (92%)	309 (99%)	2 (1%)	84	91
2	AL	311/339 (92%)	305 (98%)	6 (2%)	52	74
3	AM	114/128 (89%)	114 (100%)	0	100	100
3	AN	114/128 (89%)	111 (97%)	3 (3%)	41	68
3	AO	114/128 (89%)	114 (100%)	0	100	100
3	AP	114/128 (89%)	112 (98%)	2 (2%)	54	75
3	H	114/128 (89%)	111 (97%)	3 (3%)	41	68
3	I	114/128 (89%)	112 (98%)	2 (2%)	54	75
4	AQ	134/153 (88%)	131 (98%)	3 (2%)	47	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AR	134/153 (88%)	128 (96%)	6 (4%)	23	54
4	AS	134/153 (88%)	131 (98%)	3 (2%)	47	71
4	AT	134/153 (88%)	131 (98%)	3 (2%)	47	71
4	AW	134/153 (88%)	131 (98%)	3 (2%)	47	71
4	AX	134/153 (88%)	131 (98%)	3 (2%)	47	71
5	AU	113/116 (97%)	110 (97%)	3 (3%)	40	67
5	AV	113/116 (97%)	112 (99%)	1 (1%)	75	86
5	AY	113/116 (97%)	112 (99%)	1 (1%)	75	86
5	AZ	113/116 (97%)	112 (99%)	1 (1%)	75	86
5	Aa	113/116 (97%)	111 (98%)	2 (2%)	54	75
5	Ab	113/116 (97%)	111 (98%)	2 (2%)	54	75
6	R3	149/168 (89%)	141 (95%)	8 (5%)	18	47
6	R4	149/168 (89%)	141 (95%)	8 (5%)	18	47
6	R5	149/168 (89%)	146 (98%)	3 (2%)	50	73
6	S3	148/168 (88%)	144 (97%)	4 (3%)	40	67
6	S4	148/168 (88%)	145 (98%)	3 (2%)	50	73
6	S5	148/168 (88%)	145 (98%)	3 (2%)	50	73
6	T3	147/168 (88%)	144 (98%)	3 (2%)	50	73
6	T4	147/168 (88%)	144 (98%)	3 (2%)	50	73
6	T5	147/168 (88%)	143 (97%)	4 (3%)	40	67
6	U3	148/168 (88%)	141 (95%)	7 (5%)	22	52
6	U4	148/168 (88%)	136 (92%)	12 (8%)	9	34
6	U5	148/168 (88%)	141 (95%)	7 (5%)	22	52
All	All	18834/19926 (94%)	18641 (99%)	193 (1%)	71	84

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	89	SER
1	Q	136	ARG
1	T	88	LEU
1	Z	77	ARG
1	Z	180	ARG
1	e	156	THR

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Mol	Chain	Res	Type
1	e	180	ARG
1	g	180	ARG
1	h	132	THR
1	j	144	ASN
1	j	156	THR
1	j	180	ARG
1	n	156	THR
1	p	156	THR
1	q	220	SER
1	q	221	CYS
1	r	221	CYS
1	s	156	THR
1	u	156	THR
1	v	221	CYS
1	w	221	CYS
1	x	156	THR
1	z	156	THR
1	1	136	ARG
1	1	220	SER
1	1	221	CYS
1	2	221	CYS
1	4	158	GLU
1	4	159	LEU
1	5	229	CYS
1	7	114	VAL
1	7	177	VAL
1	7	221	CYS
1	9	77	ARG
1	9	175	ARG
1	0	180	ARG
1	0	229	CYS
1	B	180	ARG
1	B	221	CYS
1	D	175	ARG
1	E	229	CYS
1	G	114	VAL
1	G	177	VAL
1	G	221	CYS
2	AA	179	LYS
2	AA	249	ARG
2	AA	391	ASP
2	AB	149	PHE

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Mol	Chain	Res	Type
2	AC	149	PHE
2	AC	179	LYS
2	AD	152	GLN
2	AD	179	LYS
2	AD	183	ASN
2	AD	184	ASP
2	AD	257	LYS
2	AE	149	PHE
2	AE	179	LYS
2	AF	27	ILE
2	AF	28	ARG
2	AF	29	ARG
2	AF	149	PHE
2	AF	283	ASP
2	AF	285	LYS
2	AG	149	PHE
2	AG	179	LYS
2	AG	195	MET
2	AH	66	LEU
2	AH	67	THR
2	AH	68	VAL
2	AH	149	PHE
2	AH	152	GLN
2	AH	179	LYS
2	AH	187	ARG
2	AH	360	MET
2	AI	179	LYS
2	AI	249	ARG
2	AI	391	ASP
2	AJ	149	PHE
2	AJ	374	ASP
2	AK	149	PHE
2	AK	179	LYS
2	AL	66	LEU
2	AL	71	VAL
2	AL	126	ARG
2	AL	152	GLN
2	AL	179	LYS
2	AL	187	ARG
4	AQ	93	ASP
4	AQ	94	ARG
4	AQ	95	LYS

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Mol	Chain	Res	Type
5	AU	43	CYS
5	AU	66	LEU
5	AU	128	LEU
4	AR	25	PHE
4	AR	49	LYS
4	AR	50	LEU
4	AR	93	ASP
4	AR	94	ARG
4	AR	95	LYS
3	AP	47	PHE
3	AP	49	GLN
5	AZ	39	THR
6	R3	37	PHE
6	R3	168	ASN
6	R3	169	THR
6	R3	173	ASN
6	R3	196	ARG
6	R3	199	ARG
6	R3	201	LEU
6	R3	202	LEU
6	S3	72	THR
6	S3	77	ARG
6	S3	194	TRP
6	S3	196	ARG
6	T3	5	THR
6	T3	166	VAL
6	T3	167	ARG
6	U3	20	ASP
6	U3	21	ASN
6	U3	23	ARG
6	U3	134	ARG
6	U3	135	ARG
6	U3	136	CYS
6	U3	175	GLN
3	AN	48	SER
3	AN	49	GLN
3	AN	50	ASP
4	AS	11	VAL
4	AS	94	ARG
4	AS	95	LYS
5	AV	66	LEU
4	AT	25	PHE

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Mol	Chain	Res	Type
4	AT	94	ARG
4	AT	95	LYS
3	H	47	PHE
3	H	49	GLN
3	H	50	ASP
5	Aa	39	THR
5	Aa	82	CYS
6	R4	37	PHE
6	R4	169	THR
6	R4	173	ASN
6	R4	178	ILE
6	R4	182	ASN
6	R4	183	ASN
6	R4	186	VAL
6	R4	198	ARG
6	S4	72	THR
6	S4	74	ILE
6	S4	77	ARG
6	T4	166	VAL
6	T4	167	ARG
6	T4	199	ARG
6	U4	19	ASP
6	U4	20	ASP
6	U4	23	ARG
6	U4	26	ASP
6	U4	140	VAL
6	U4	152	ILE
6	U4	157	ASN
6	U4	163	VAL
6	U4	164	MET
6	U4	177	LEU
6	U4	182	ASN
6	U4	192	ASP
4	AW	15	GLU
4	AW	94	ARG
4	AW	95	LYS
5	AY	128	LEU
4	AX	25	PHE
4	AX	94	ARG
4	AX	95	LYS
3	I	47	PHE
3	I	49	GLN

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Mol	Chain	Res	Type
5	Ab	39	THR
5	Ab	82	CYS
6	R5	37	PHE
6	R5	169	THR
6	R5	198	ARG
6	S5	72	THR
6	S5	74	ILE
6	S5	196	ARG
6	T5	5	THR
6	T5	166	VAL
6	T5	167	ARG
6	T5	170	LEU
6	U5	19	ASP
6	U5	20	ASP
6	U5	23	ARG
6	U5	136	CYS
6	U5	138	ASN
6	U5	140	VAL
6	U5	144	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (203) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	112	ASN
1	K	112	ASN
1	M	55	ASN
1	N	142	ASN
1	O	112	ASN
1	P	112	ASN
1	R	55	ASN
1	S	142	ASN
1	T	112	ASN
1	U	112	ASN
1	W	55	ASN
1	X	142	ASN
1	Z	182	HIS
1	a	112	ASN
1	a	120	ASN
1	e	182	HIS
1	f	112	ASN
1	f	120	ASN
1	k	112	ASN

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Mol	Chain	Res	Type
1	k	120	ASN
1	o	112	ASN
1	p	112	ASN
1	q	112	ASN
1	r	112	ASN
1	t	112	ASN
1	u	112	ASN
1	v	51	HIS
1	w	112	ASN
1	y	112	ASN
1	z	112	ASN
1	1	112	ASN
1	2	112	ASN
1	5	112	ASN
1	6	112	ASN
1	6	218	HIS
1	7	55	ASN
1	7	112	ASN
1	7	120	ASN
1	0	112	ASN
1	A	112	ASN
1	B	112	ASN
1	B	120	ASN
1	D	99	GLN
1	E	112	ASN
1	F	112	ASN
1	F	218	HIS
1	G	112	ASN
1	G	120	ASN
2	AA	38	ASN
2	AA	69	GLN
2	AA	191	ASN
2	AA	202	ASN
2	AA	240	ASN
2	AA	291	ASN
2	AA	312	ASN
2	AB	69	GLN
2	AB	81	ASN
2	AB	112	GLN
2	AB	191	ASN
2	AB	202	ASN
2	AB	255	GLN

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Mol	Chain	Res	Type
2	AB	291	ASN
2	AC	44	ASN
2	AC	69	GLN
2	AC	99	GLN
2	AC	112	GLN
2	AC	164	GLN
2	AC	191	ASN
2	AC	211	ASN
2	AC	240	ASN
2	AC	291	ASN
2	AD	44	ASN
2	AD	81	ASN
2	AD	112	GLN
2	AD	140	ASN
2	AD	164	GLN
2	AD	183	ASN
2	AD	191	ASN
2	AD	202	ASN
2	AD	272	ASN
2	AD	291	ASN
2	AD	297	HIS
2	AD	312	ASN
2	AE	191	ASN
2	AE	202	ASN
2	AE	240	ASN
2	AE	291	ASN
2	AF	44	ASN
2	AF	69	GLN
2	AF	81	ASN
2	AF	112	GLN
2	AF	191	ASN
2	AF	202	ASN
2	AF	206	ASN
2	AF	291	ASN
2	AG	69	GLN
2	AG	99	GLN
2	AG	112	GLN
2	AG	164	GLN
2	AG	191	ASN
2	AG	202	ASN
2	AG	206	ASN
2	AG	240	ASN

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Mol	Chain	Res	Type
2	AG	291	ASN
2	AH	44	ASN
2	AH	81	ASN
2	AH	112	GLN
2	AH	140	ASN
2	AH	164	GLN
2	AH	191	ASN
2	AH	202	ASN
2	AH	272	ASN
2	AH	297	HIS
2	AI	69	GLN
2	AI	81	ASN
2	AI	191	ASN
2	AI	202	ASN
2	AI	240	ASN
2	AJ	69	GLN
2	AJ	81	ASN
2	AJ	112	GLN
2	AJ	191	ASN
2	AJ	202	ASN
2	AJ	206	ASN
2	AJ	255	GLN
2	AJ	291	ASN
2	AK	69	GLN
2	AK	99	GLN
2	AK	112	GLN
2	AK	152	GLN
2	AK	164	GLN
2	AK	183	ASN
2	AK	191	ASN
2	AK	202	ASN
2	AK	206	ASN
2	AK	240	ASN
2	AK	291	ASN
2	AL	44	ASN
2	AL	81	ASN
2	AL	112	GLN
2	AL	164	GLN
2	AL	191	ASN
2	AL	202	ASN
2	AL	291	ASN
2	AL	297	HIS

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Mol	Chain	Res	Type
3	AM	68	ASN
5	AU	4	ASN
5	AU	6	GLN
5	AU	42	ASN
4	AR	75	ASN
4	AR	125	HIS
4	AR	151	GLN
3	AP	8	HIS
5	AZ	6	GLN
6	R3	125	GLN
6	R3	168	ASN
6	R3	191	GLN
6	S3	125	GLN
6	S3	138	ASN
6	S3	155	ASN
6	S3	158	ASN
6	T3	125	GLN
6	U3	2	ASN
6	U3	155	ASN
3	AN	49	GLN
3	AN	68	ASN
5	AV	4	ASN
5	AV	6	GLN
5	AV	42	ASN
5	AV	84	GLN
4	AT	75	ASN
4	AT	125	HIS
4	AT	151	GLN
3	H	8	HIS
5	Aa	6	GLN
6	R4	125	GLN
6	R4	173	ASN
6	R4	183	ASN
6	S4	125	GLN
6	S4	155	ASN
6	S4	158	ASN
6	T4	125	GLN
6	U4	2	ASN
6	U4	168	ASN
4	AW	151	GLN
5	AY	4	ASN
5	AY	6	GLN

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Mol	Chain	Res	Type
5	AY	42	ASN
4	AX	75	ASN
4	AX	125	HIS
4	AX	151	GLN
3	I	8	HIS
3	I	49	GLN
5	Ab	6	GLN
6	R5	125	GLN
6	R5	191	GLN
6	S5	125	GLN
6	S5	155	ASN
6	S5	158	ASN
6	T5	125	GLN
6	U5	2	ASN
6	U5	138	ASN
6	U5	155	ASN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

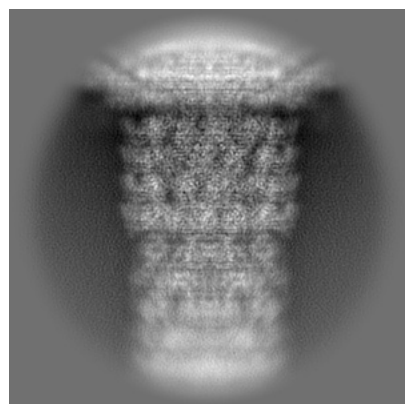
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29503. These allow visual inspection of the internal detail of the map and identification of artifacts.

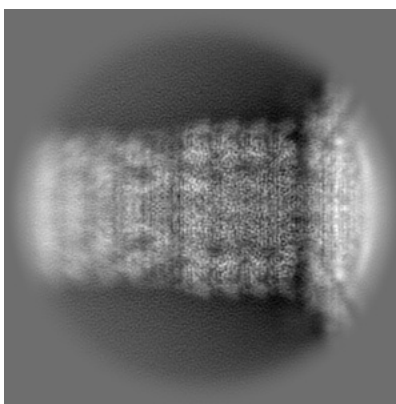
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

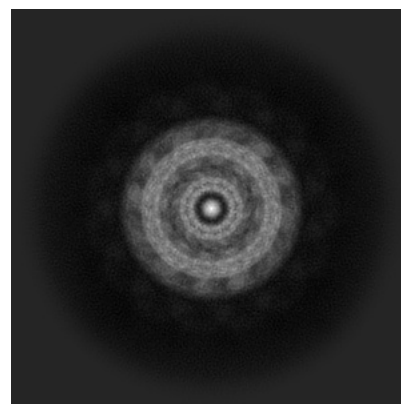
#### 6.1.1 Primary map



X

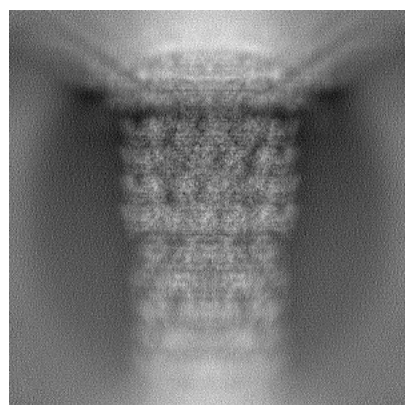


Y

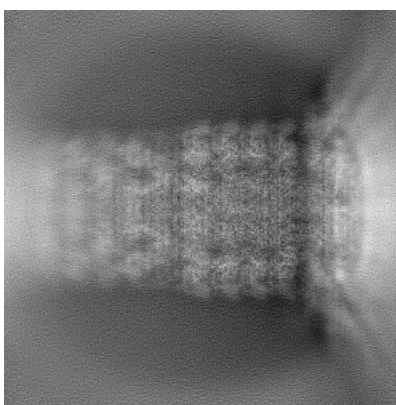


Z

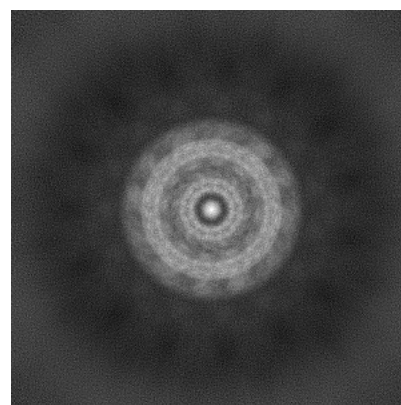
#### 6.1.2 Raw map



X



Y

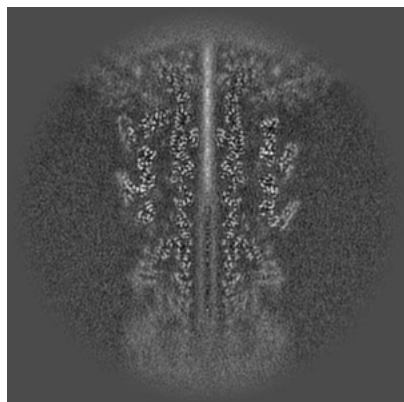


Z

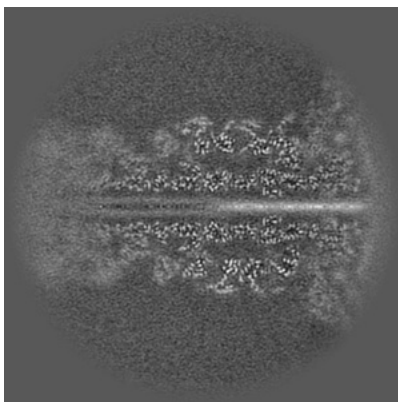
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

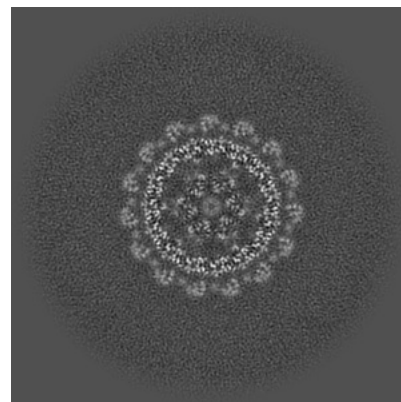
### 6.2.1 Primary map



X Index: 224

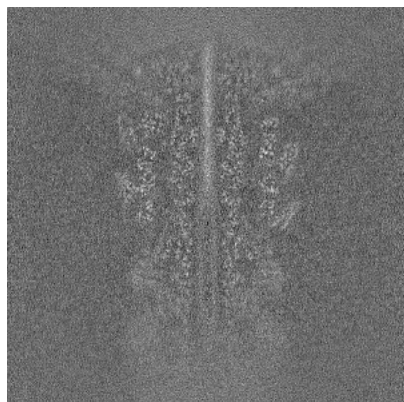


Y Index: 224

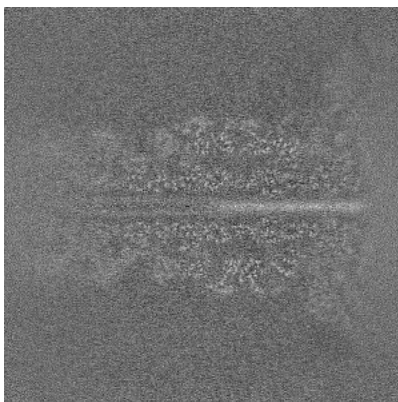


Z Index: 224

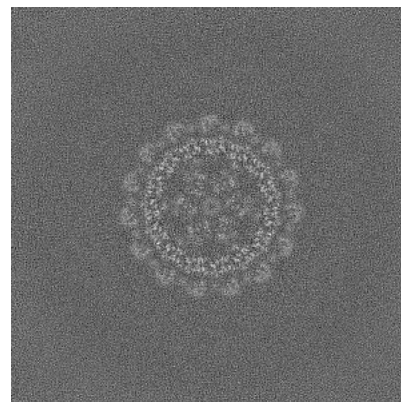
### 6.2.2 Raw map



X Index: 224



Y Index: 224

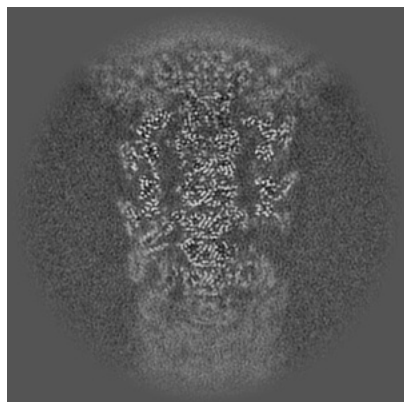


Z Index: 224

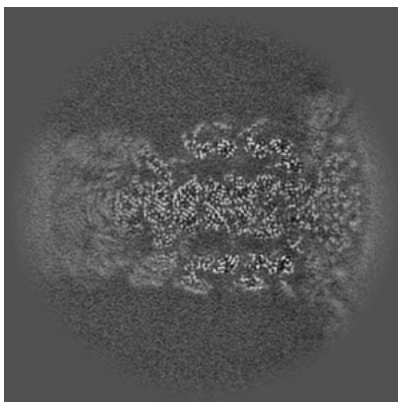
The images above show central slices of the map in three orthogonal directions.

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

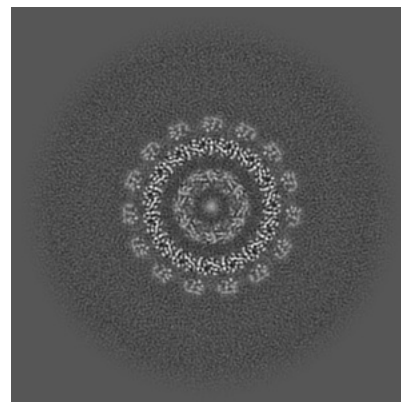
### 6.3.1 Primary map



X Index: 246

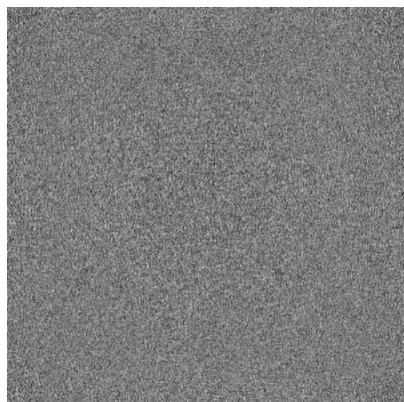


Y Index: 246

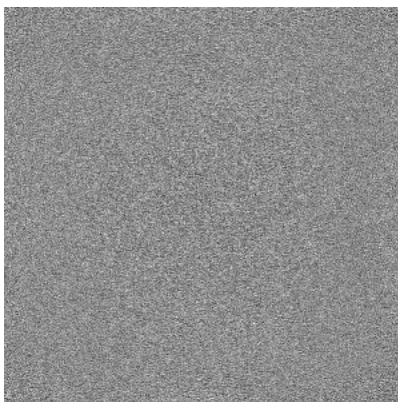


Z Index: 284

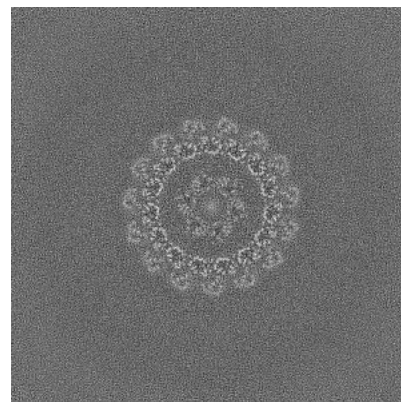
### 6.3.2 Raw map



X Index: 0



Y Index: 0



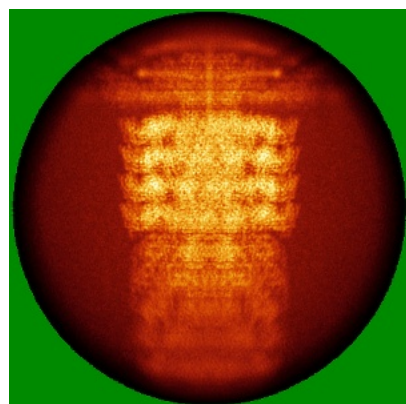
Z Index: 249

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

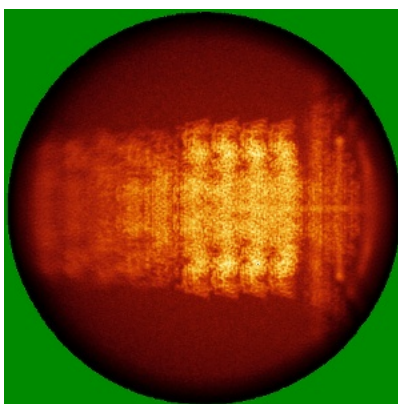


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

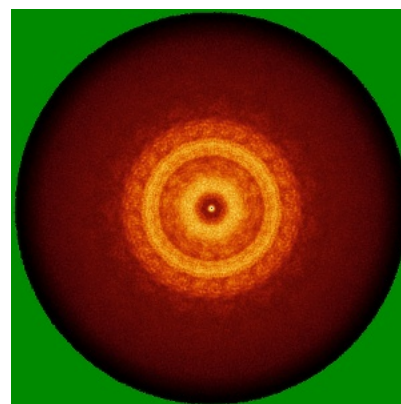
### 6.4.1 Primary map



X

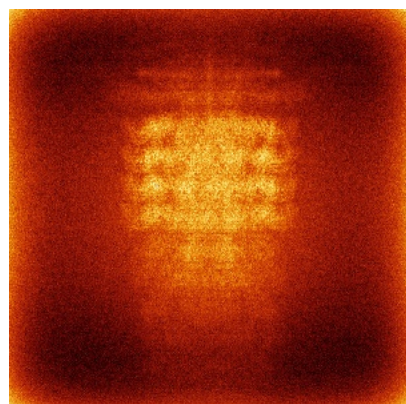


Y

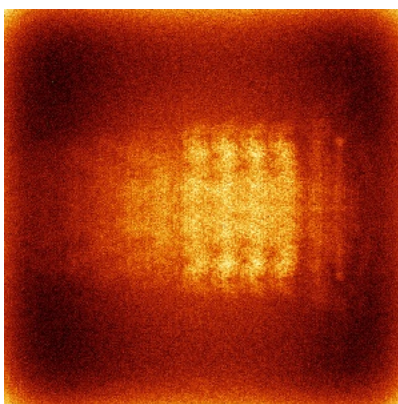


Z

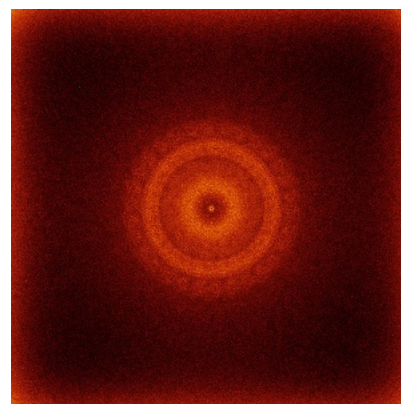
### 6.4.2 Raw map



X



Y

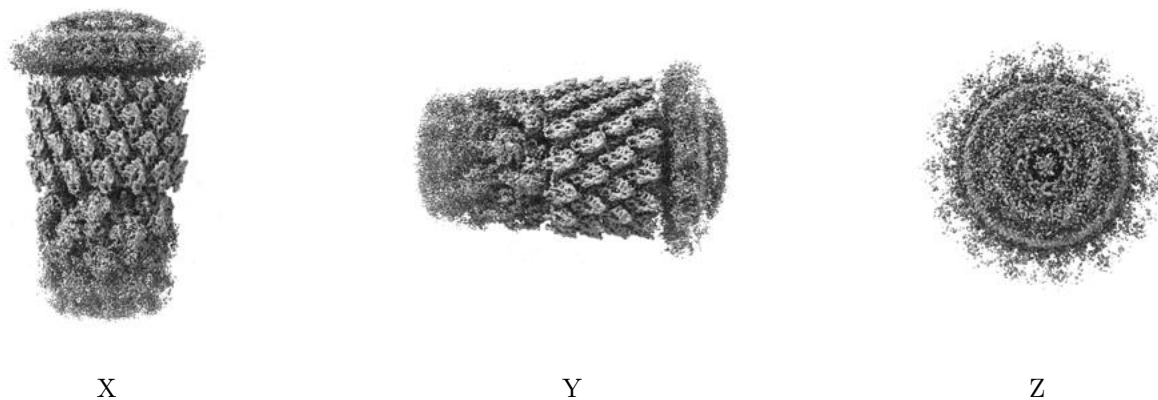


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

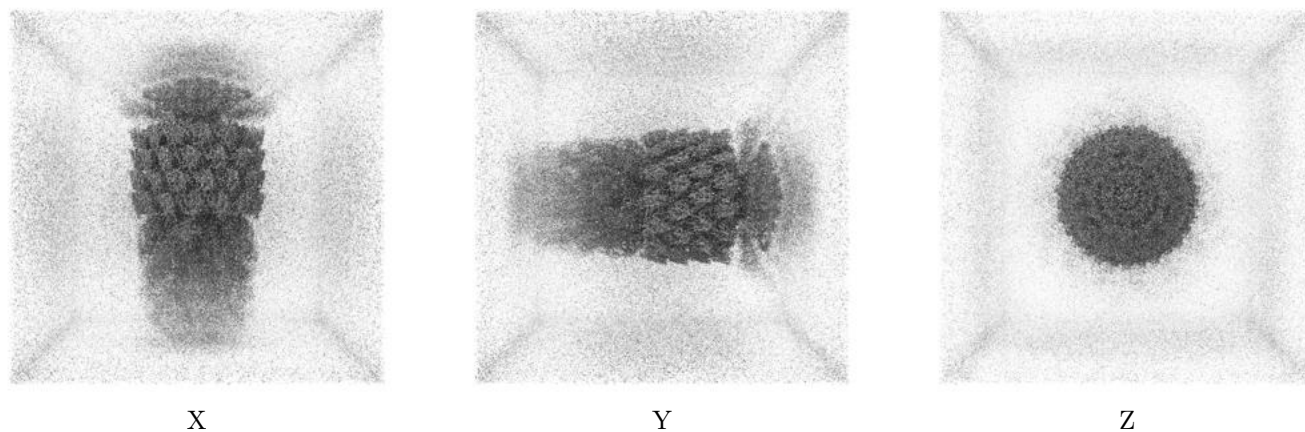
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

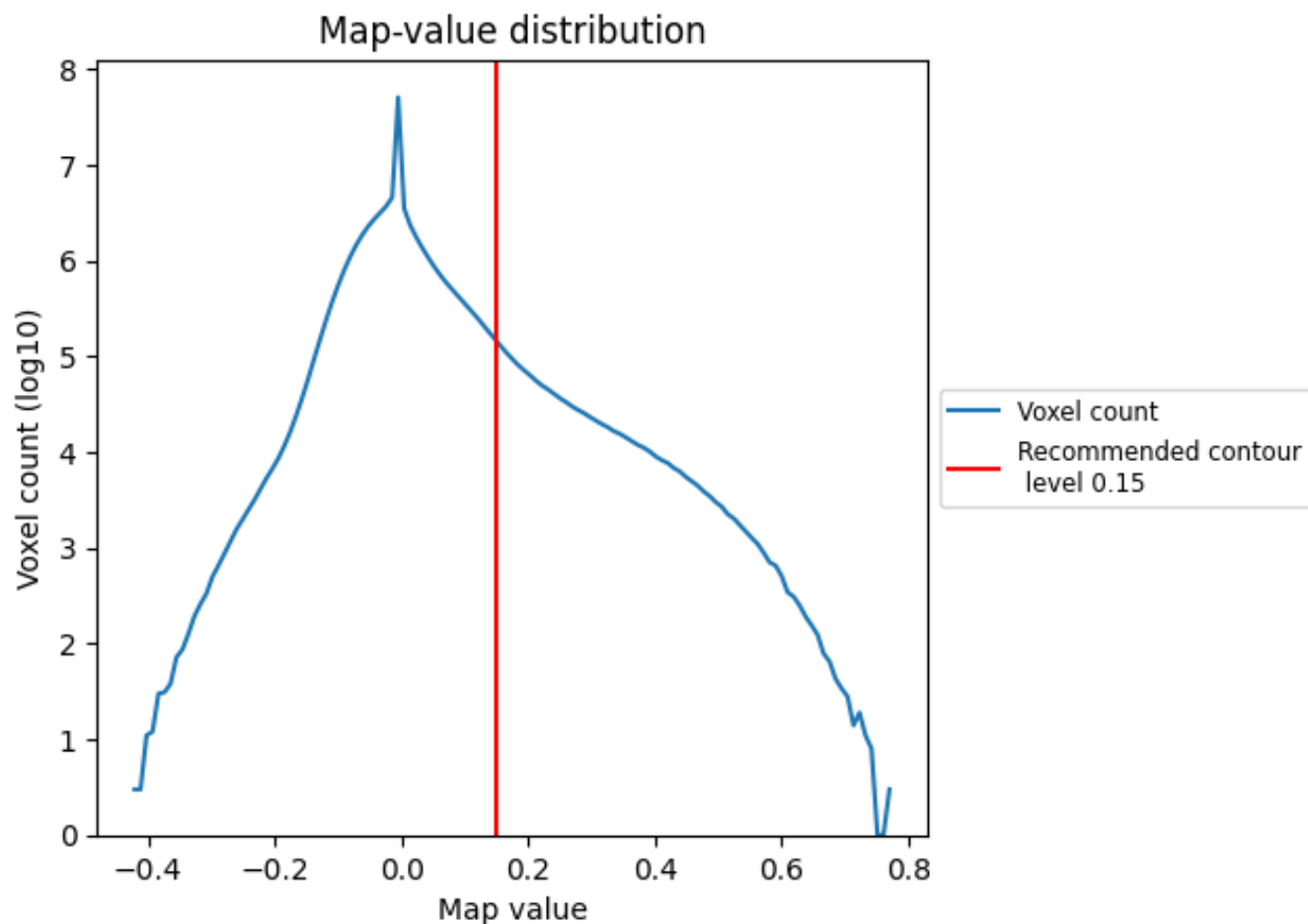
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

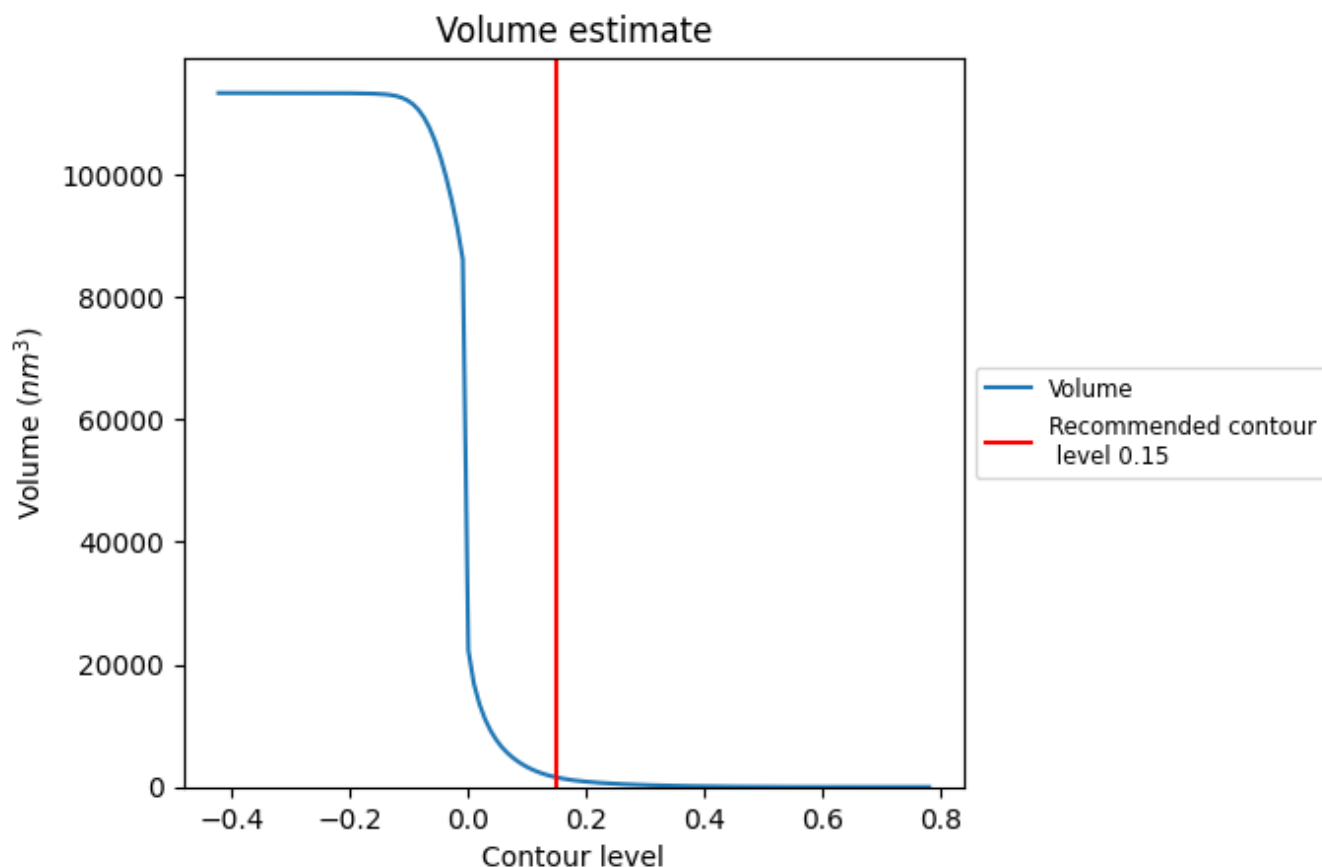
This section contains the results of statistical analysis of the map.

### 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](#)

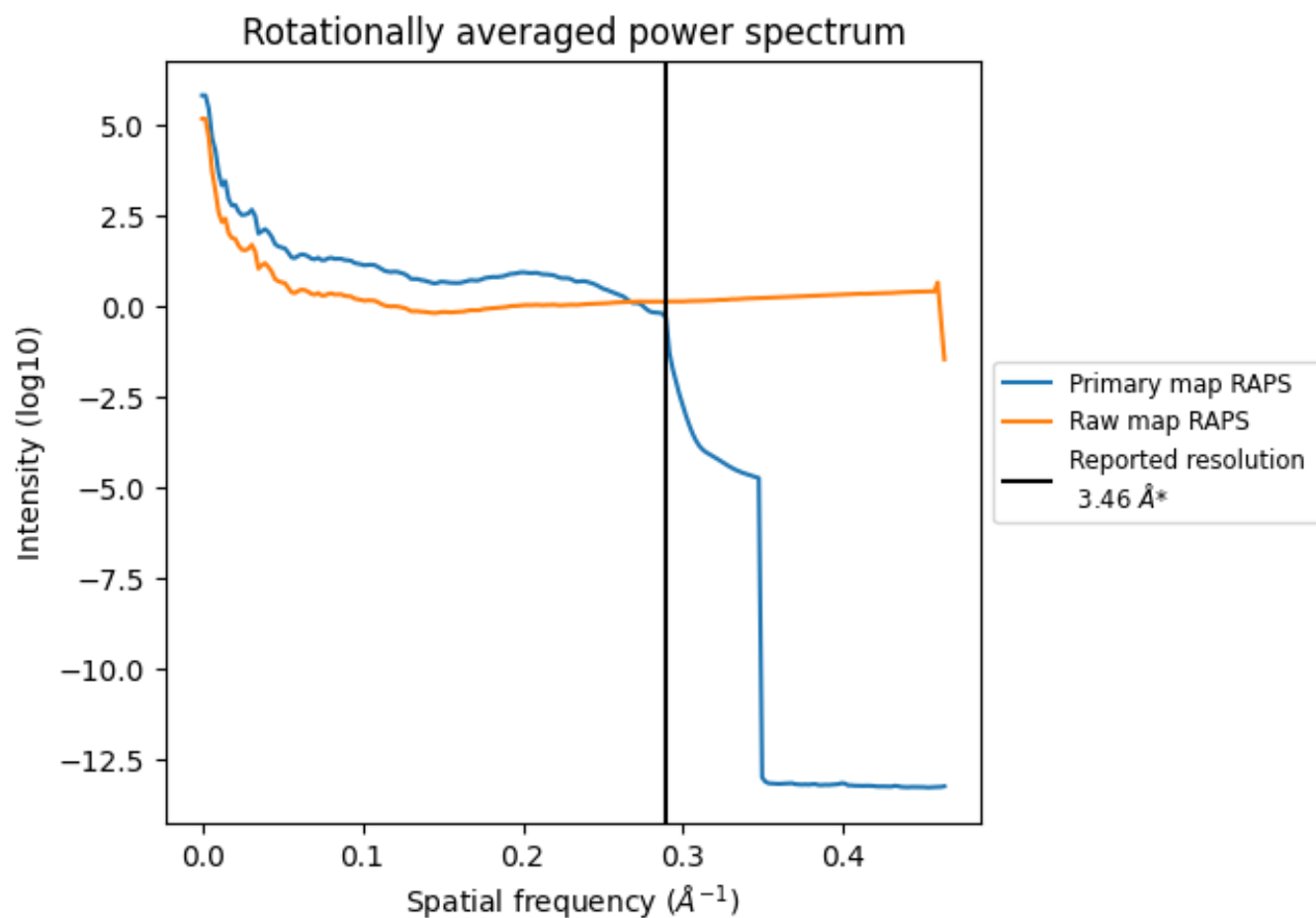


The volume at the recommended contour level is 1570  $\text{nm}^3$ ; this corresponds to an approximate mass of 1418 kDa.

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 ⓘ

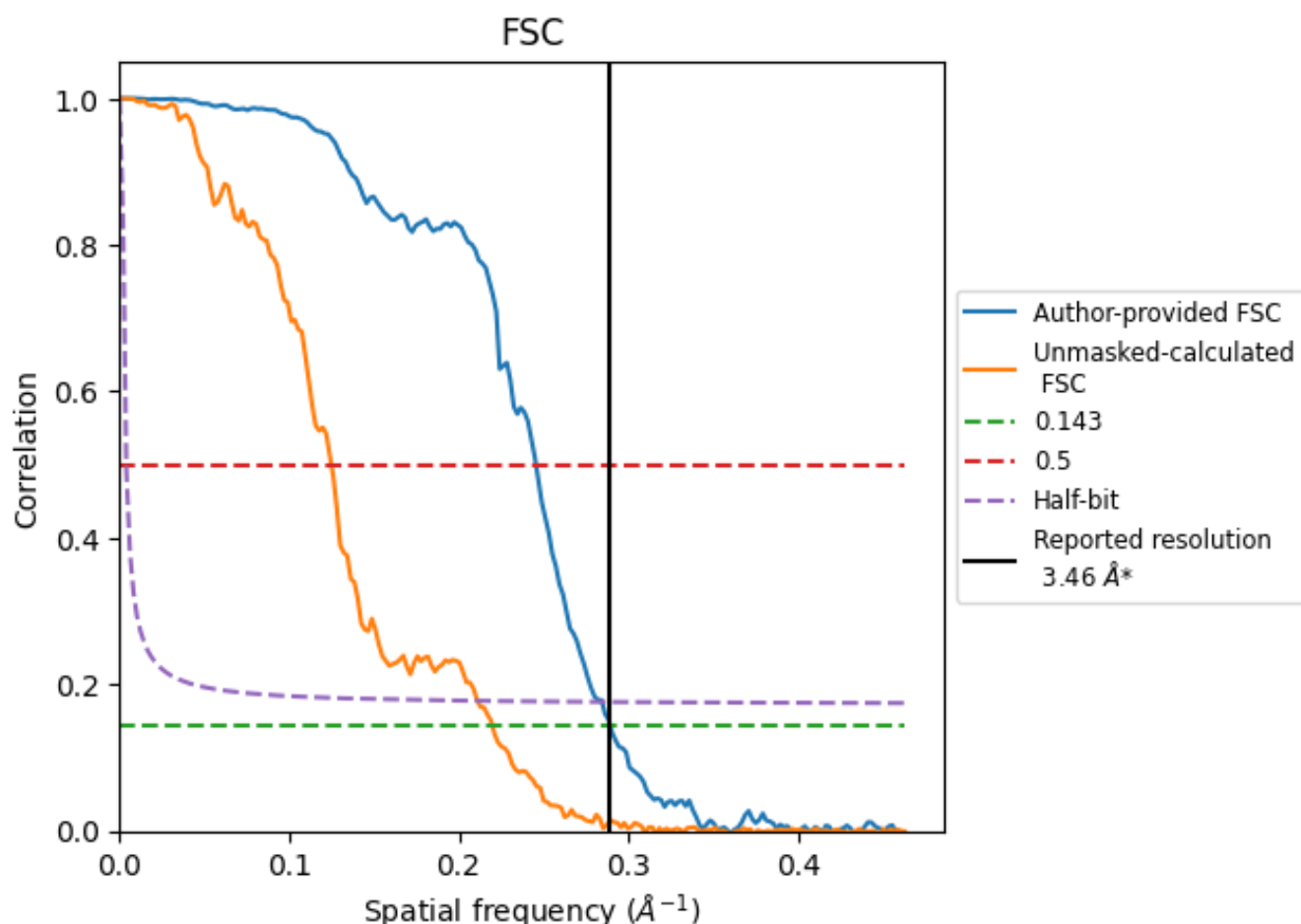


\*Reported resolution corresponds to spatial frequency of 0.289 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.289  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

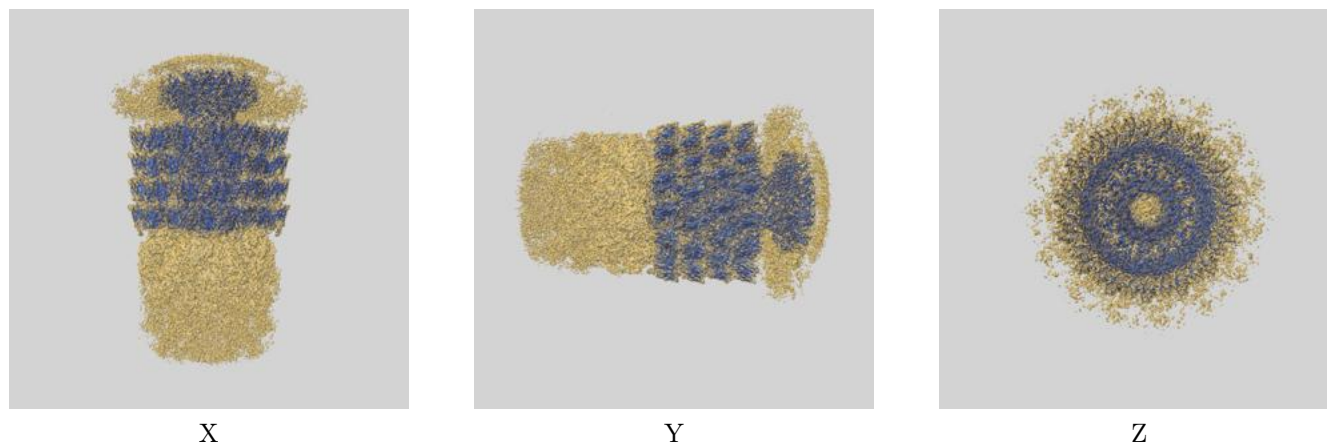
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	3.46	4.07	3.51
Unmasked-calculated*	4.55	8.01	4.74

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.55 differs from the reported value 3.46 by more than 10 %

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

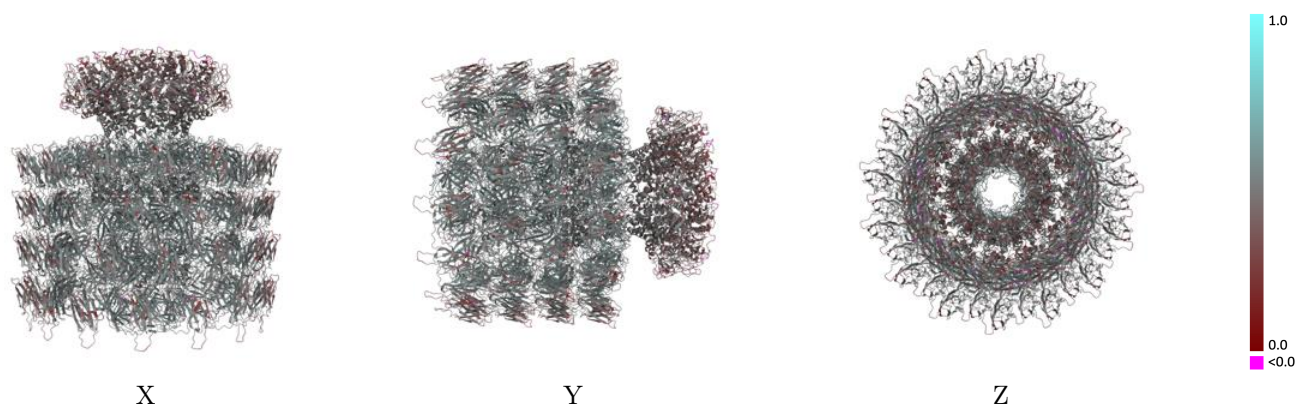
This section contains information regarding the fit between EMDB map EMD-29503 and PDB model 8FWE. Per-residue inclusion information can be found in section [3](#) on page [13](#).

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



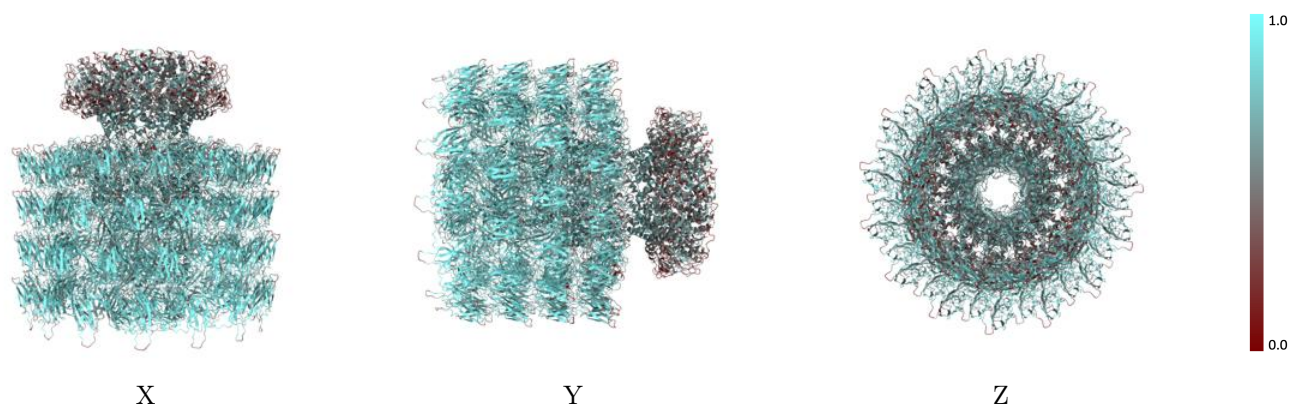
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



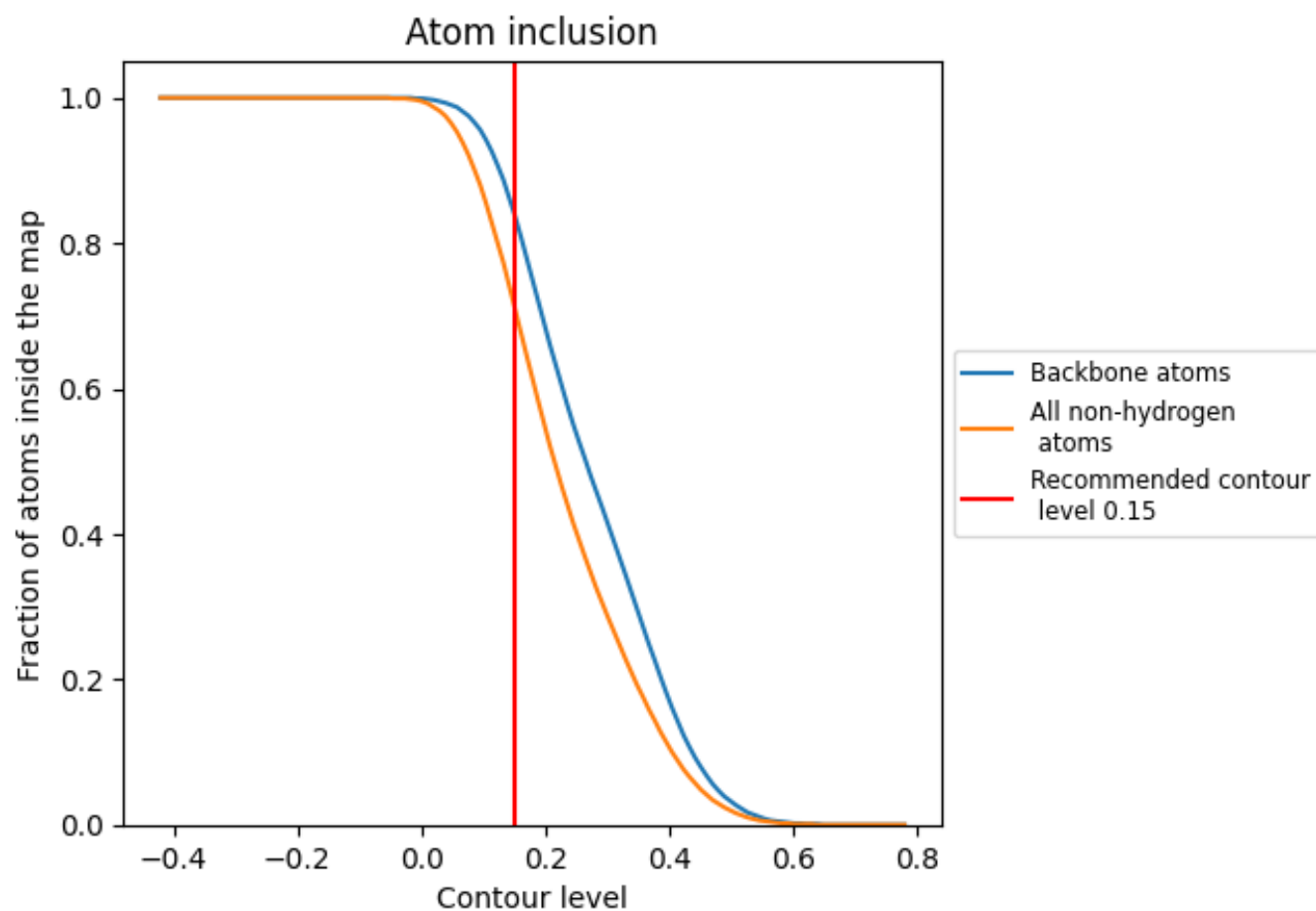
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 71% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7140	 0.4750
0	 0.7990	 0.4700
1	 0.8180	 0.4950
2	 0.8130	 0.4880
3	 0.7890	 0.4700
4	 0.7910	 0.4670
5	 0.7960	 0.4710
6	 0.7940	 0.4650
7	 0.7830	 0.4660
8	 0.7880	 0.4720
9	 0.7860	 0.4660
A	 0.8000	 0.4650
AA	 0.5160	 0.4230
AB	 0.4750	 0.3970
AC	 0.4810	 0.4030
AD	 0.5070	 0.4190
AE	 0.5210	 0.4250
AF	 0.4770	 0.4000
AG	 0.4870	 0.4030
AH	 0.5080	 0.4200
AI	 0.5170	 0.4240
AJ	 0.4730	 0.3980
AK	 0.4860	 0.4020
AL	 0.5120	 0.4200
AM	 0.7670	 0.5320
AN	 0.7700	 0.5300
AO	 0.7740	 0.5260
AP	 0.7530	 0.5310
AQ	 0.7740	 0.5200
AR	 0.7680	 0.5160
AS	 0.7750	 0.5200
AT	 0.7660	 0.5180
AU	 0.7650	 0.5150
AV	 0.7680	 0.5180
AW	 0.7660	 0.5220



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Chain	Atom inclusion	Q-score
AX	 0.7620	 0.5180
AY	 0.7630	 0.5180
AZ	 0.7570	 0.5220
Aa	 0.7570	 0.5220
Ab	 0.7580	 0.5210
B	 0.7850	 0.4660
C	 0.7910	 0.4700
D	 0.7800	 0.4620
E	 0.7980	 0.4720
F	 0.7940	 0.4650
G	 0.7800	 0.4670
H	 0.7550	 0.5280
I	 0.7530	 0.5280
J	 0.7510	 0.4910
K	 0.7490	 0.4920
L	 0.7520	 0.4840
M	 0.7250	 0.4830
N	 0.7210	 0.4810
O	 0.7580	 0.4920
P	 0.7450	 0.4900
Q	 0.7510	 0.4830
R	 0.7240	 0.4830
R3	 0.7010	 0.5040
R4	 0.6930	 0.5070
R5	 0.6940	 0.5030
S	 0.7250	 0.4810
S3	 0.6950	 0.5080
S4	 0.6940	 0.5100
S5	 0.6880	 0.5100
T	 0.7570	 0.4890
T3	 0.6420	 0.5120
T4	 0.6410	 0.5090
T5	 0.6440	 0.5110
U	 0.7530	 0.4920
U3	 0.6420	 0.4980
U4	 0.6400	 0.5010
U5	 0.6430	 0.5000
V	 0.7550	 0.4880
W	 0.7260	 0.4840
X	 0.7240	 0.4820
Y	 0.8100	 0.4960
Z	 0.7940	 0.4910

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Chain	Atom inclusion	Q-score
a	 0.8080	 0.4890
b	 0.7970	 0.4830
c	 0.7940	 0.4890
d	 0.8080	 0.4920
e	 0.7930	 0.4910
f	 0.8060	 0.4890
g	 0.7990	 0.4830
h	 0.7930	 0.4900
i	 0.8090	 0.4930
j	 0.7910	 0.4900
k	 0.8110	 0.4910
l	 0.7950	 0.4850
m	 0.7920	 0.4910
n	 0.8290	 0.4920
o	 0.8260	 0.4980
p	 0.8170	 0.4910
q	 0.8240	 0.4930
r	 0.8110	 0.4880
s	 0.8260	 0.4900
t	 0.8280	 0.4980
u	 0.8180	 0.4930
v	 0.8190	 0.4930
w	 0.8180	 0.4880
x	 0.8250	 0.4910
y	 0.8210	 0.4980
z	 0.8210	 0.4930