



Full wwPDB EM Validation Report ⓘ

Mar 25, 2025 – 03:35 PM JST

PDB ID : 9KI1
EMDB ID : EMD-62362
Title : Baseplate structure of Escherichia phage Mu
Authors : Zhou, J.Q.; Liu, H.R.
Deposited on : 2024-11-11
Resolution : 3.30 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
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) : 2.41.2

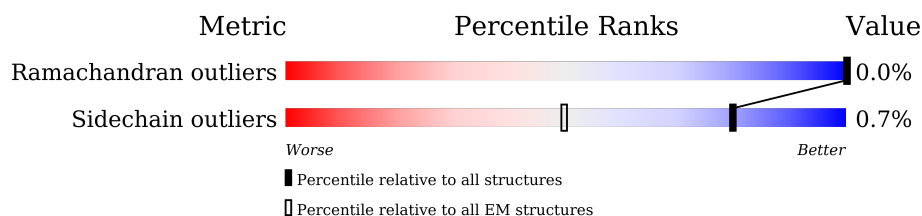
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY







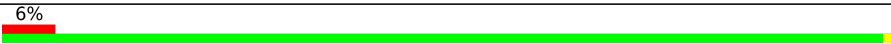


The reported resolution of this entry is 3.30 Å.

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 ≥ 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	495	 89% 10%
1	s	495	 88% 10%
1	t	495	 89% 10%
1	u	495	 84% 15%
1	v	495	 84% 15%
1	w	495	 84% 15%
2	1	495	 6% 99%
2	2	495	 7% 99%
2	3	495	 6% 99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	x	495	6% 99%
2	y	495	6% 99%
2	z	495	6% 99%
3	4	118	97% ..
3	5	118	95% ..
3	6	118	97% .
3	7	118	96% ..
3	8	118	97% ..
3	9	118	96% ..
4	A	145	98% ..
4	B	145	97% ..
4	C	145	98% ..
4	D	145	99% .
4	E	145	99% .
4	F	145	98% ..
5	G	379	96% .
5	N	379	96% .
5	U	379	96% ..
6	H	360	8% 98% ..
6	I	360	9% 98% ..
6	J	360	9% 98% ..
6	K	360	22% 98% ..
6	L	360	21% 98% ..
6	M	360	21% 98% ..
6	O	360	22% 99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	P	360	
6	Q	360	
6	R	360	
6	S	360	
6	T	360	
7	V	197	
7	W	197	
7	X	197	
8	a	180	
8	b	180	
8	c	180	
8	d	180	
8	e	180	
8	f	180	
9	g	690	
9	h	690	
9	i	690	
10	j	504	
10	k	504	
10	l	504	
10	m	504	
10	n	504	
10	o	504	
10	p	504	
10	q	504	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	r	504	<div><div></div><div>21%</div><div>79%</div></div>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 114473 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 DNA circularization protein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	446	Total	C	N	O	S	0	0
			3294	2035	579	666	14		
1	s	446	Total	C	N	O	S	0	0
			3294	2035	579	666	14		
1	t	446	Total	C	N	O	S	0	0
			3294	2035	579	666	14		
1	u	419	Total	C	N	O	S	0	0
			3119	1935	553	617	14		
1	v	419	Total	C	N	O	S	0	0
			3119	1935	553	617	14		
1	w	419	Total	C	N	O	S	0	0
			3119	1935	553	617	14		

- Molecule 2 is a protein called Tail sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	493	Total	C	N	O	S	0	0
			3719	2340	638	727	14		
2	2	493	Total	C	N	O	S	0	0
			3719	2340	638	727	14		
2	3	493	Total	C	N	O	S	0	0
			3719	2340	638	727	14		
2	x	493	Total	C	N	O	S	0	0
			3719	2340	638	727	14		
2	y	493	Total	C	N	O	S	0	0
			3719	2340	638	727	14		
2	z	493	Total	C	N	O	S	0	0
			3719	2340	638	727	14		

- Molecule 3 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	115	Total	C	N	O	S	0	0
			880	549	154	172	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	115	Total	C	N	O	S	0	0
			880	549	154	172	5		
3	6	115	Total	C	N	O	S	0	0
			880	549	154	172	5		
3	7	115	Total	C	N	O	S	0	0
			880	549	154	172	5		
3	8	115	Total	C	N	O	S	0	0
			880	549	154	172	5		
3	9	115	Total	C	N	O	S	0	0
			880	549	154	172	5		

- Molecule 4 is a protein called Baseplate protein gp46.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	143	Total	C	N	O	S	0	0
			1137	714	199	223	1		
4	B	143	Total	C	N	O	S	0	0
			1137	714	199	223	1		
4	C	143	Total	C	N	O	S	0	0
			1137	714	199	223	1		
4	D	143	Total	C	N	O	S	0	0
			1137	714	199	223	1		
4	E	143	Total	C	N	O	S	0	0
			1137	714	199	223	1		
4	F	143	Total	C	N	O	S	0	0
			1137	714	199	223	1		

- Molecule 5 is a protein called Baseplate hub protein gp44.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	366	Total	C	N	O	S	0	0
			2830	1769	499	554	8		
5	N	366	Total	C	N	O	S	0	0
			2830	1769	499	554	8		
5	U	366	Total	C	N	O	S	0	0
			2830	1769	499	554	8		

- Molecule 6 is a protein called Baseplate protein gp47.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	356	Total	C	N	O	S	0	0
			2694	1699	471	517	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	356	Total	C	N	O	S	0	0
			2694	1699	471	517	7		
6	J	356	Total	C	N	O	S	0	0
			2694	1699	471	517	7		
6	K	356	Total	C	N	O	S	0	0
			2694	1699	471	517	7		
6	L	356	Total	C	N	O	S	0	0
			2694	1699	471	517	7		
6	M	356	Total	C	N	O	S	0	0
			2694	1699	471	517	7		
6	O	359	Total	C	N	O	S	0	0
			2712	1711	474	520	7		
6	P	359	Total	C	N	O	S	0	0
			2712	1711	474	520	7		
6	Q	359	Total	C	N	O	S	0	0
			2712	1711	474	520	7		
6	R	343	Total	C	N	O	S	0	0
			2609	1652	455	495	7		
6	S	343	Total	C	N	O	S	0	0
			2609	1652	455	495	7		
6	T	343	Total	C	N	O	S	0	0
			2609	1652	455	495	7		

- Molecule 7 is a protein called Baseplate puncturing device gp45.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	194	Total	C	N	O	S	0	0
			1486	911	278	290	7		
7	W	194	Total	C	N	O	S	0	0
			1486	911	278	290	7		
7	X	194	Total	C	N	O	S	0	0
			1486	911	278	290	7		

- Molecule 8 is a protein called Baseplate protein gp48.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	174	Total	C	N	O	S	0	0
			1401	891	244	261	5		
8	b	150	Total	C	N	O	S	0	0
			1208	770	210	223	5		
8	c	174	Total	C	N	O	S	0	0
			1401	891	244	261	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	150	Total	C	N	O	S	0	0
			1208	770	210	223	5		
8	e	174	Total	C	N	O	S	0	0
			1401	891	244	261	5		
8	f	150	Total	C	N	O	S	0	0
			1208	770	210	223	5		

- Molecule 9 is a protein called Probable tape measure protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	17	Total	C	N	O	S	0	0
			130	83	20	26	1		
9	h	17	Total	C	N	O	S	0	0
			130	83	20	26	1		
9	i	17	Total	C	N	O	S	0	0
			130	83	20	26	1		

- Molecule 10 is a protein called Tail fiber protein S.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	k	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	l	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	m	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	n	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	o	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	p	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	q	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	r	108	Total	C	N	O	S	0	0
			836	529	142	162	3		

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	V	1	Total	Ca	0
			1	1	

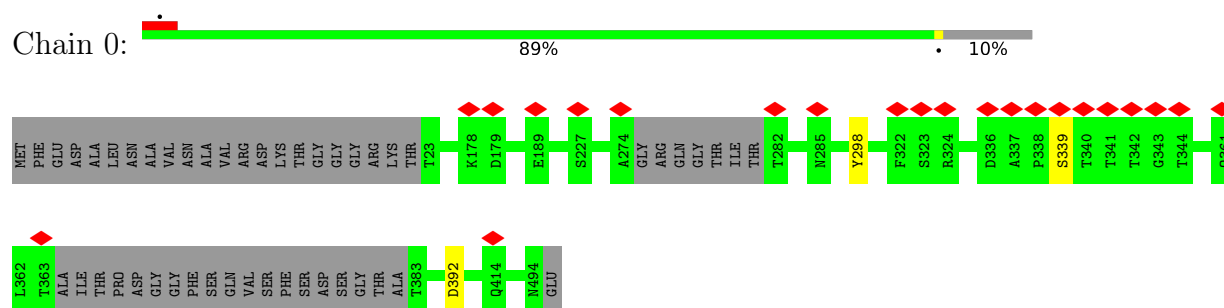
- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	V	1	Total	Fe	0
			1	1	

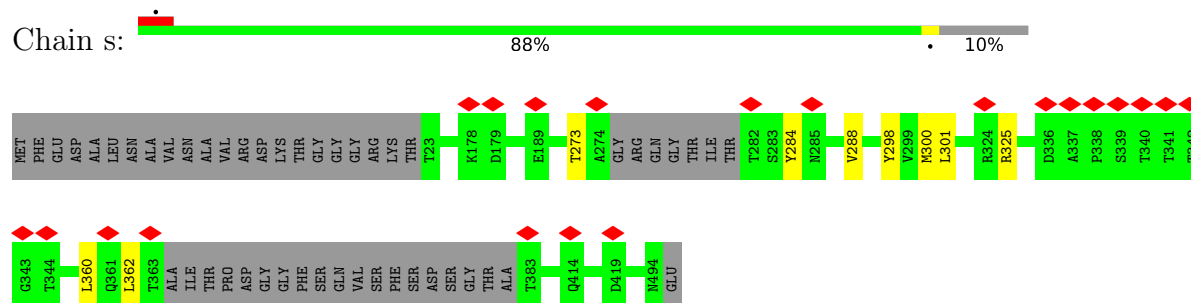
3 Residue-property plots [i](#)

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.

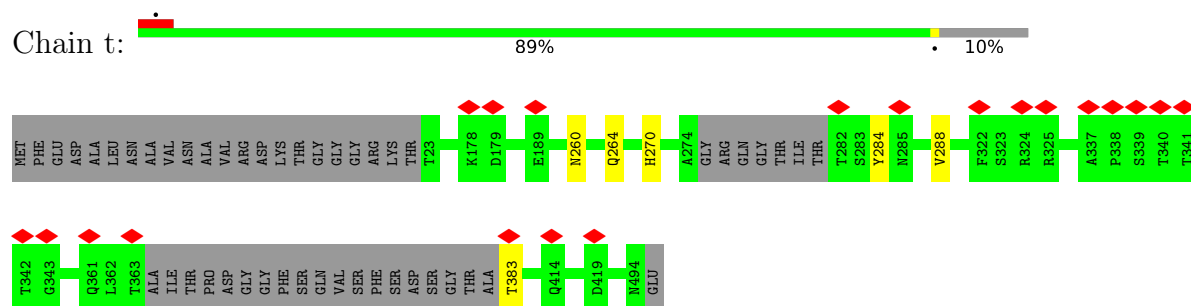
- Molecule 1: DNA circularization protein N



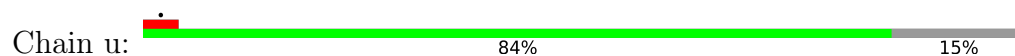
- Molecule 1: DNA circularization protein N

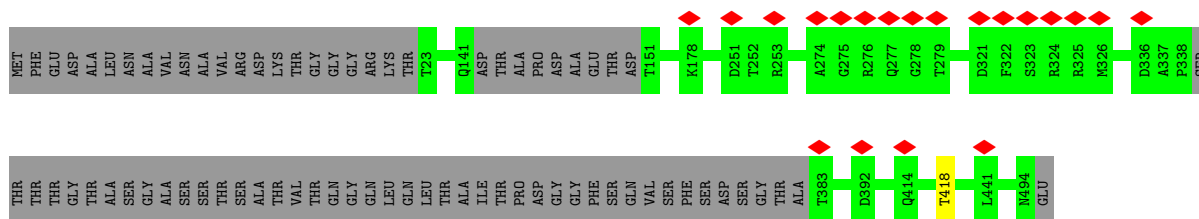


- Molecule 1: DNA circularization protein N

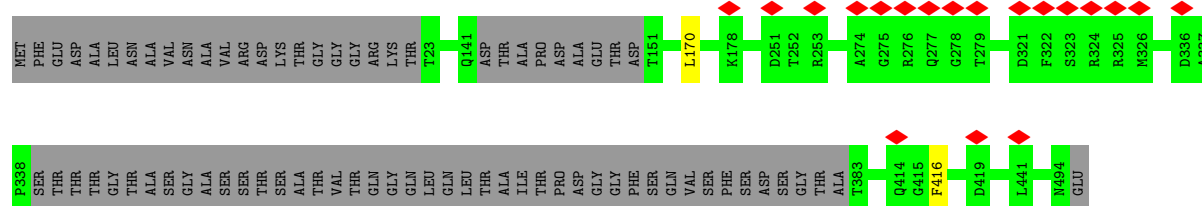
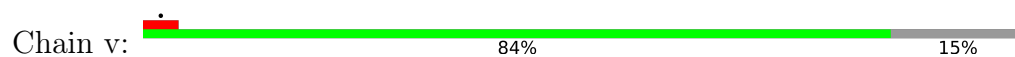


- Molecule 1: DNA circularization protein N

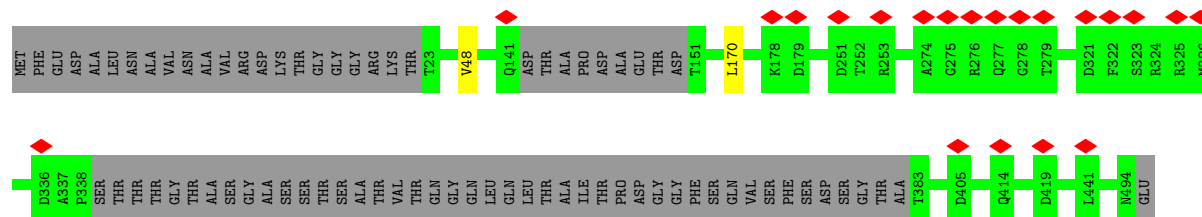
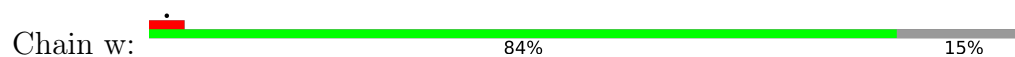




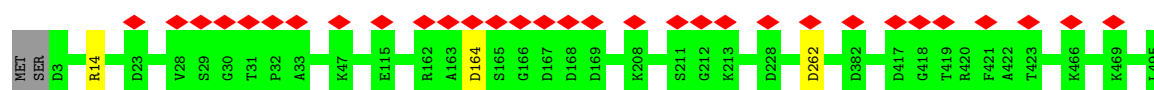
- Molecule 1: DNA circularization protein N



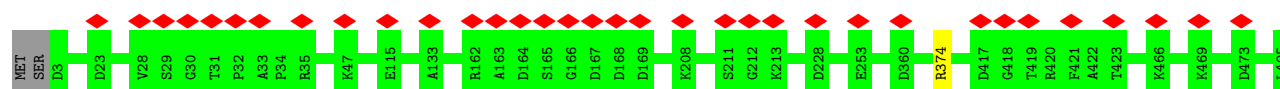
- Molecule 1: DNA circularization protein N



- Molecule 2: Tail sheath protein

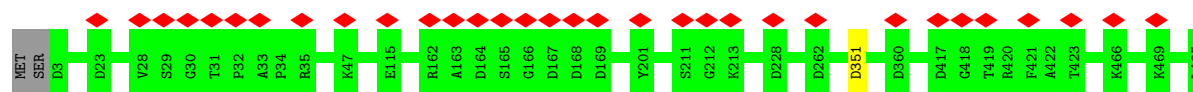


- Molecule 2: Tail sheath protein

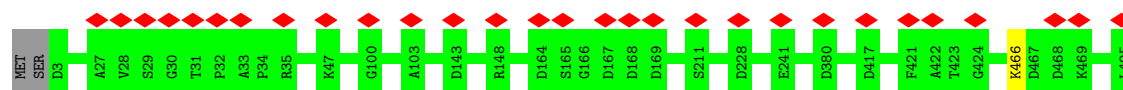


- Molecule 2: Tail sheath protein

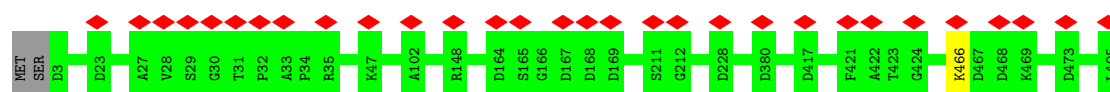




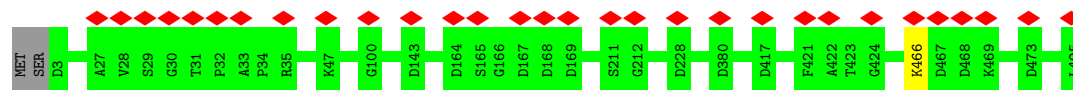
- Molecule 2: Tail sheath protein



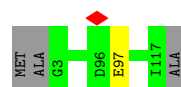
- Molecule 2: Tail sheath protein



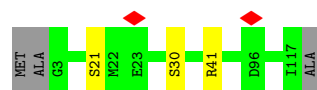
- Molecule 2: Tail sheath protein



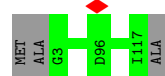
- Molecule 3: Tail tube protein



- Molecule 3: Tail tube protein

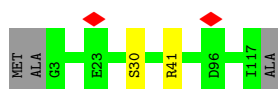


- Molecule 3: Tail tube protein



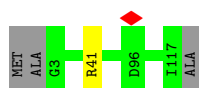
- Molecule 3: Tail tube protein

Chain 7:  96% ..



- Molecule 3: Tail tube protein

Chain 8:  97% ..



- Molecule 3: Tail tube protein

Chain 9:  96% ..



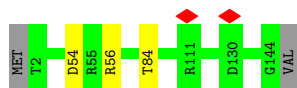
- Molecule 4: Baseplate protein gp46

Chain A:  98% ..



- Molecule 4: Baseplate protein gp46

Chain B:  97% ..



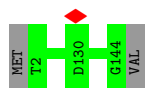
- Molecule 4: Baseplate protein gp46

Chain C:  98% ..



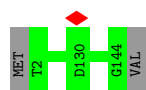
- Molecule 4: Baseplate protein gp46

Chain D:  99% .



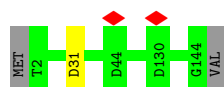
- Molecule 4: Baseplate protein gp46

Chain E:  99%



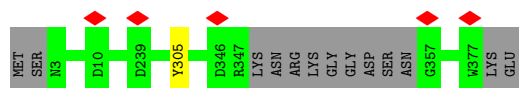
- Molecule 4: Baseplate protein gp46

Chain F:  98%



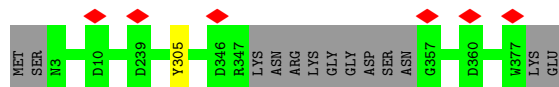
- Molecule 5: Baseplate hub protein gp44

Chain G:  96%



- Molecule 5: Baseplate hub protein gp44

Chain N:  96%



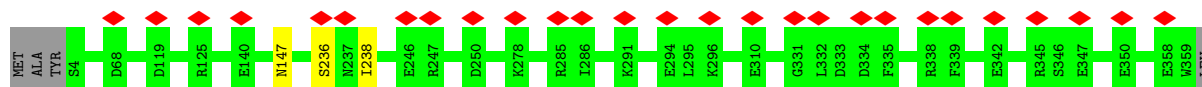
- Molecule 5: Baseplate hub protein gp44

Chain U:  96%



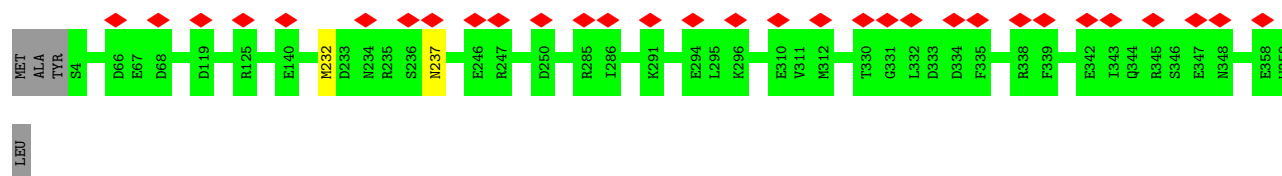
- Molecule 6: Baseplate protein gp47

Chain H:  8%  98%

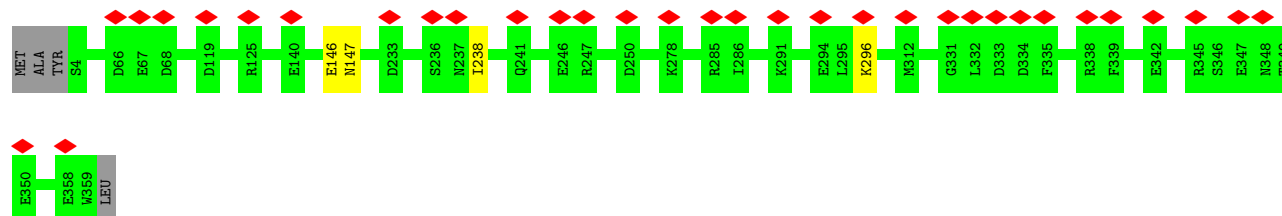


- Molecule 6: Baseplate protein gp47

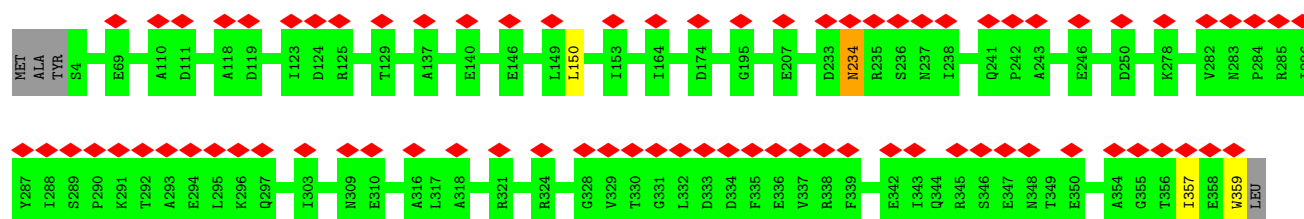
Chain I:  9%  98%



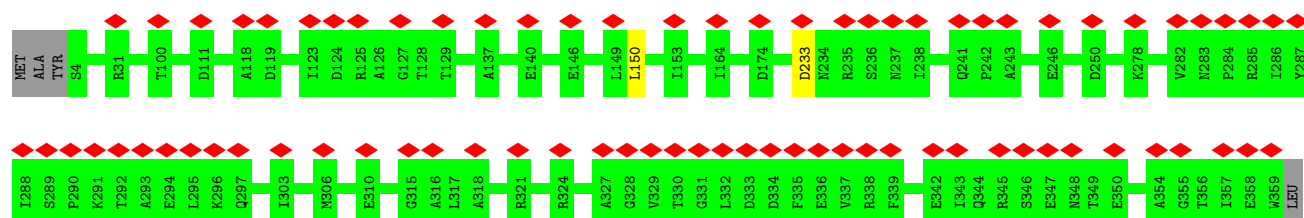
• Molecule 6: Baseplate protein gp47



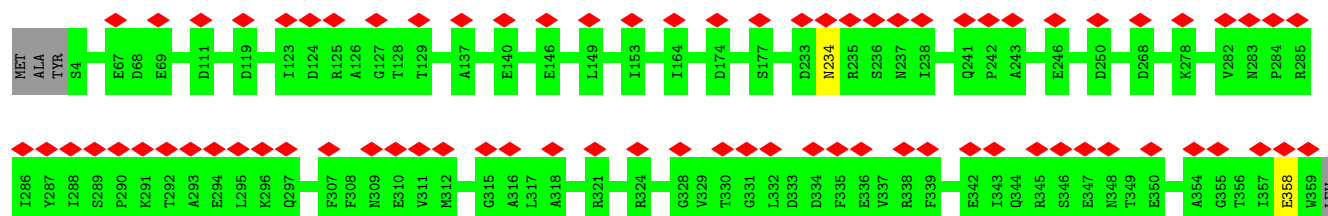
• Molecule 6: Baseplate protein gp47



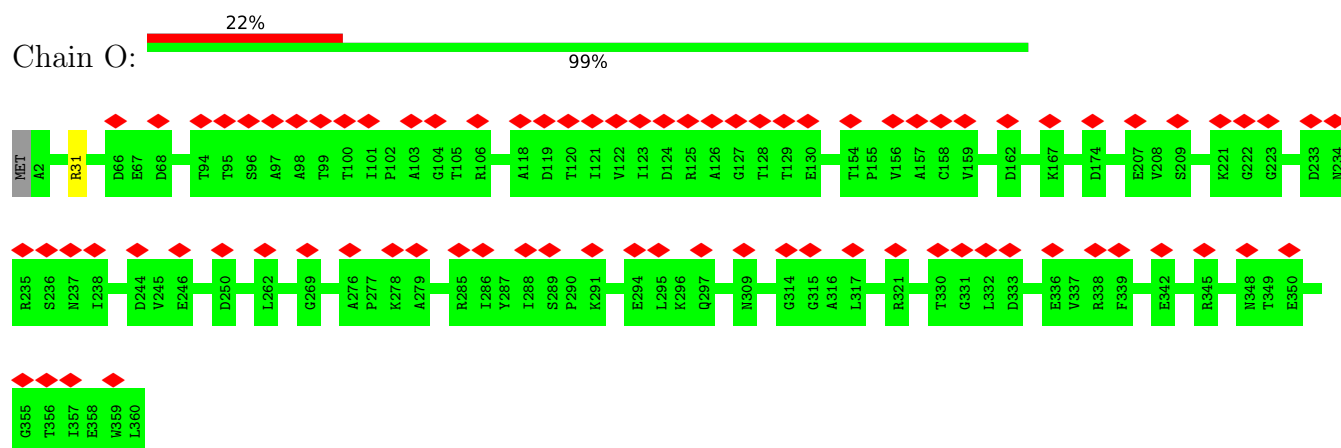
• Molecule 6: Baseplate protein gp47



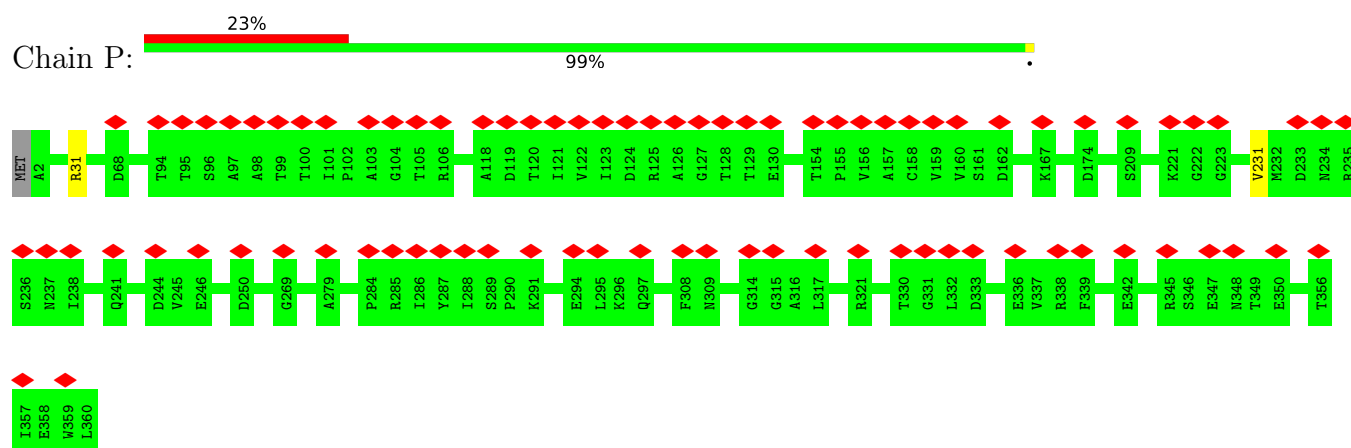
• Molecule 6: Baseplate protein gp47



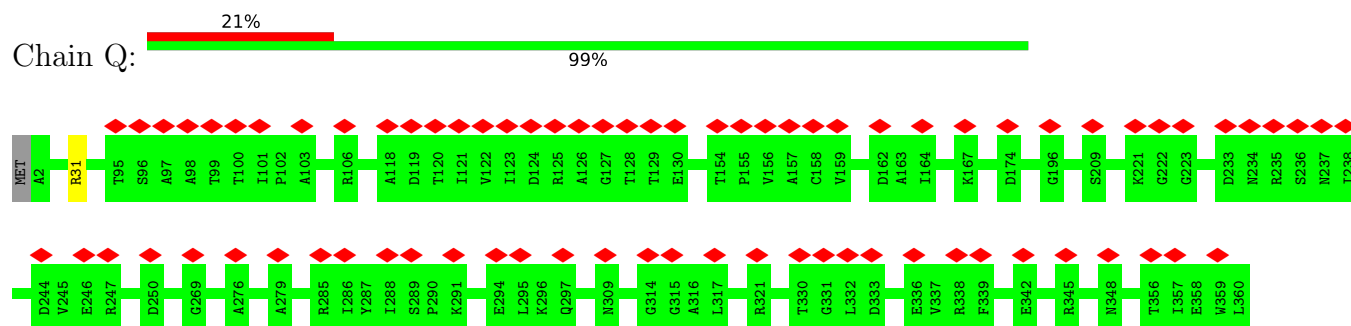
- Molecule 6: Baseplate protein gp47



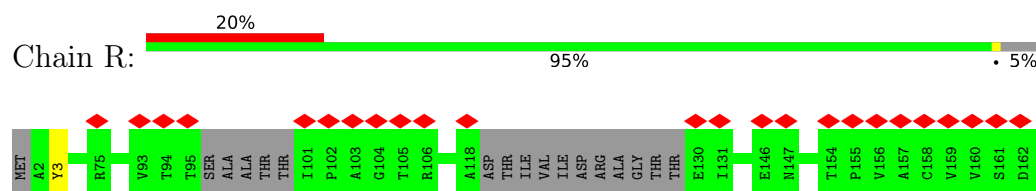
- Molecule 6: Baseplate protein gp47

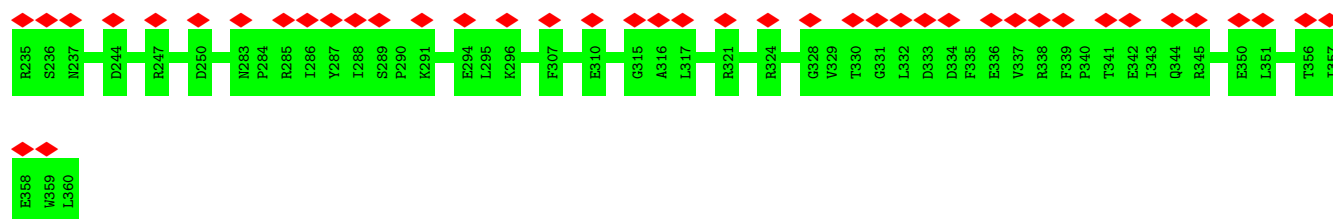


- Molecule 6: Baseplate protein gp47

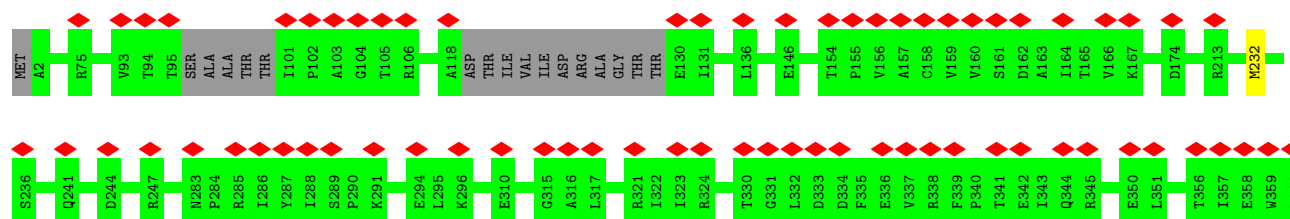


- Molecule 6: Baseplate protein gp47

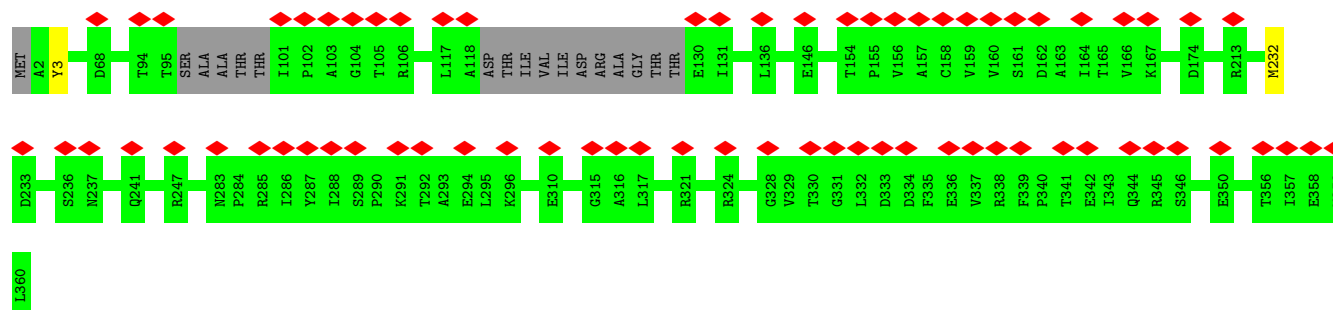
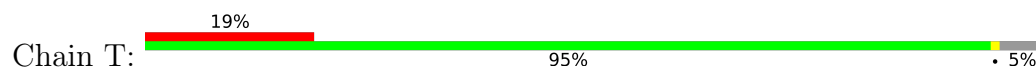




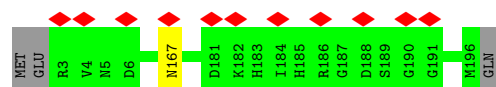
- Molecule 6: Baseplate protein gp47



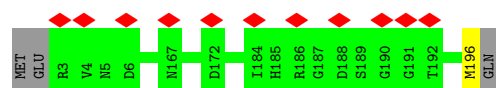
- Molecule 6: Baseplate protein gp47



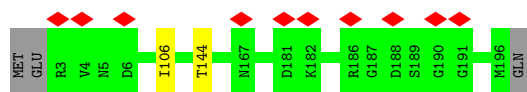
- Molecule 7: Baseplate puncturing device gp45



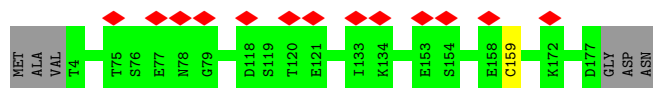
- Molecule 7: Baseplate puncturing device gp45



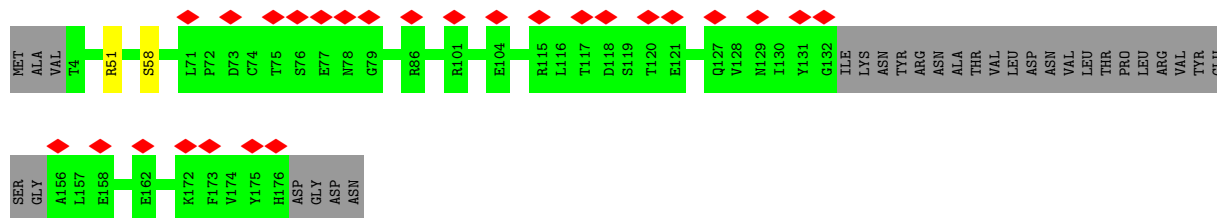
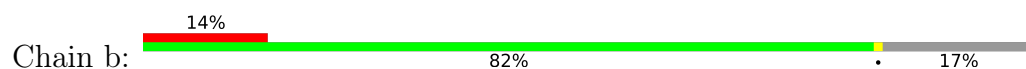
- Molecule 7: Baseplate puncturing device gp45



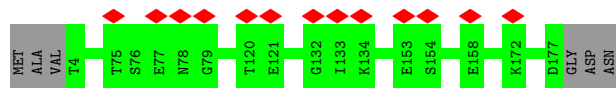
- Molecule 8: Baseplate protein gp48



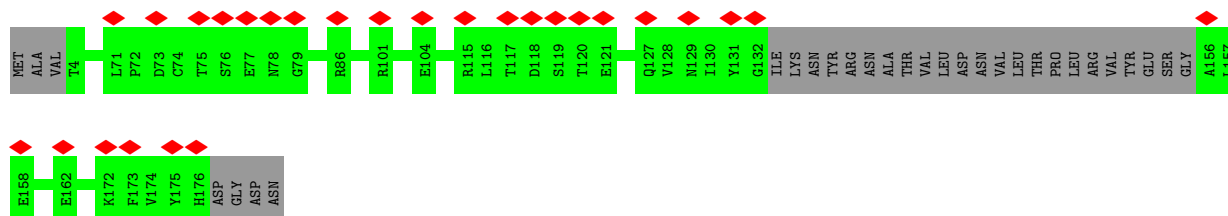
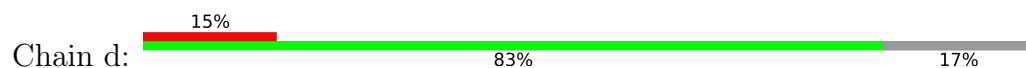
- Molecule 8: Baseplate protein gp48



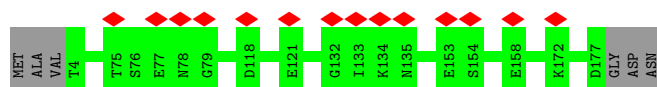
- Molecule 8: Baseplate protein gp48

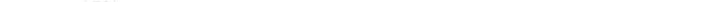


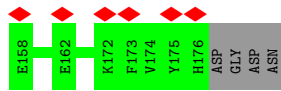
- Molecule 8: Baseplate protein gp48

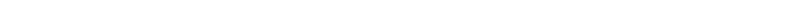


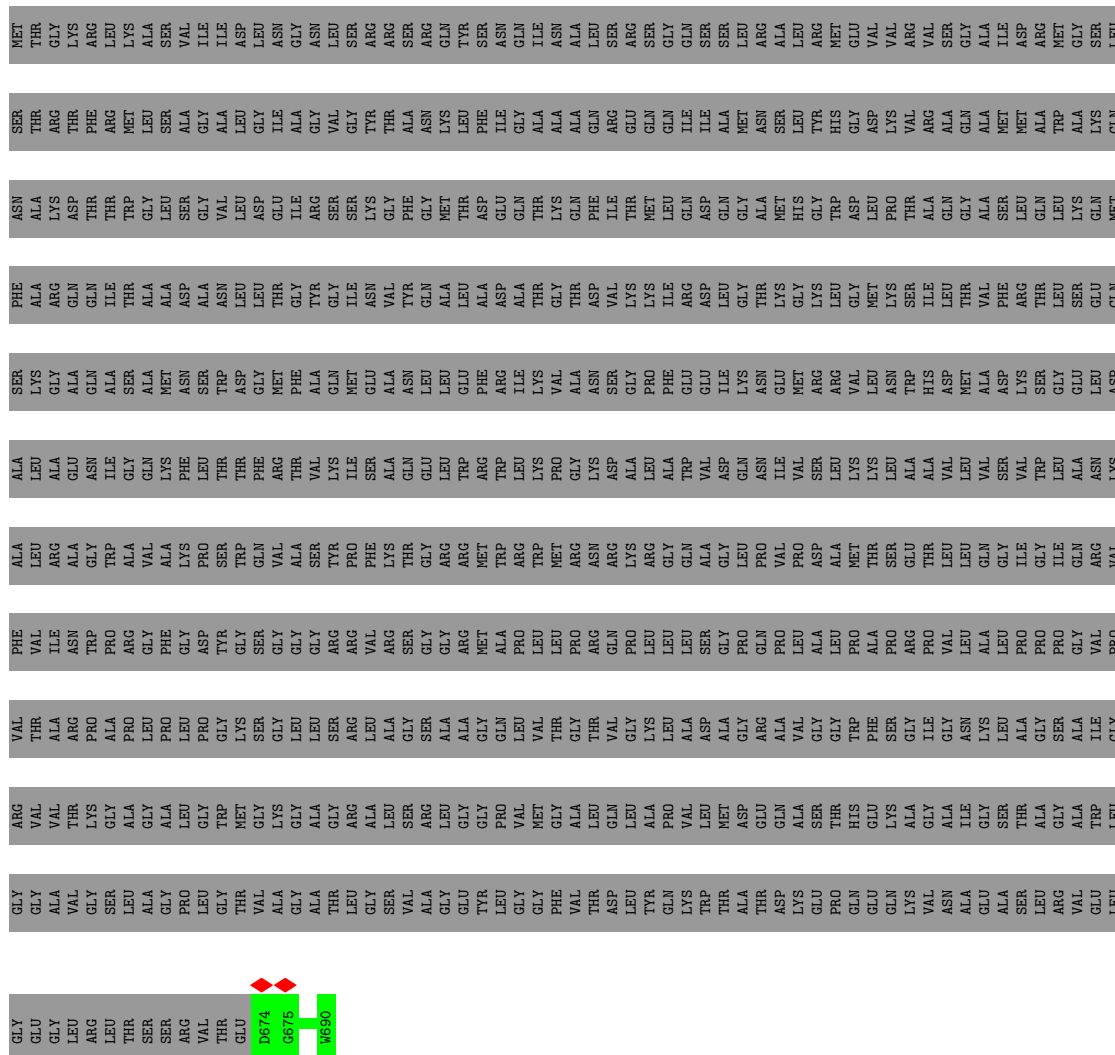
- Molecule 8: Baseplate protein gp48

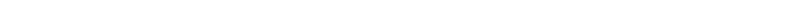


Chain f: 

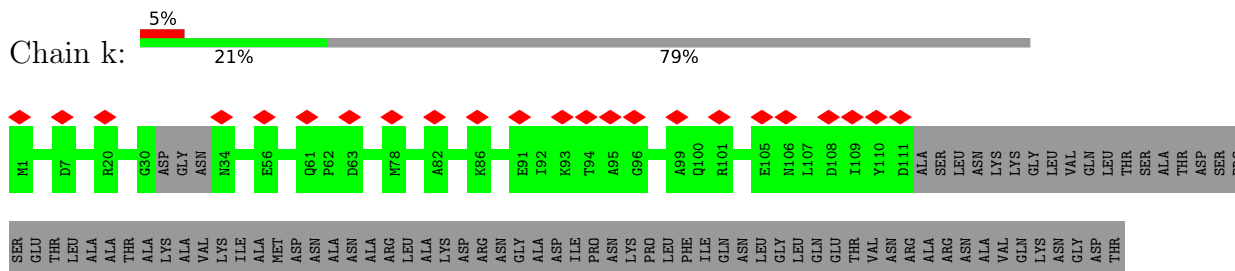


Chain g:  98%



Chain h:  98%

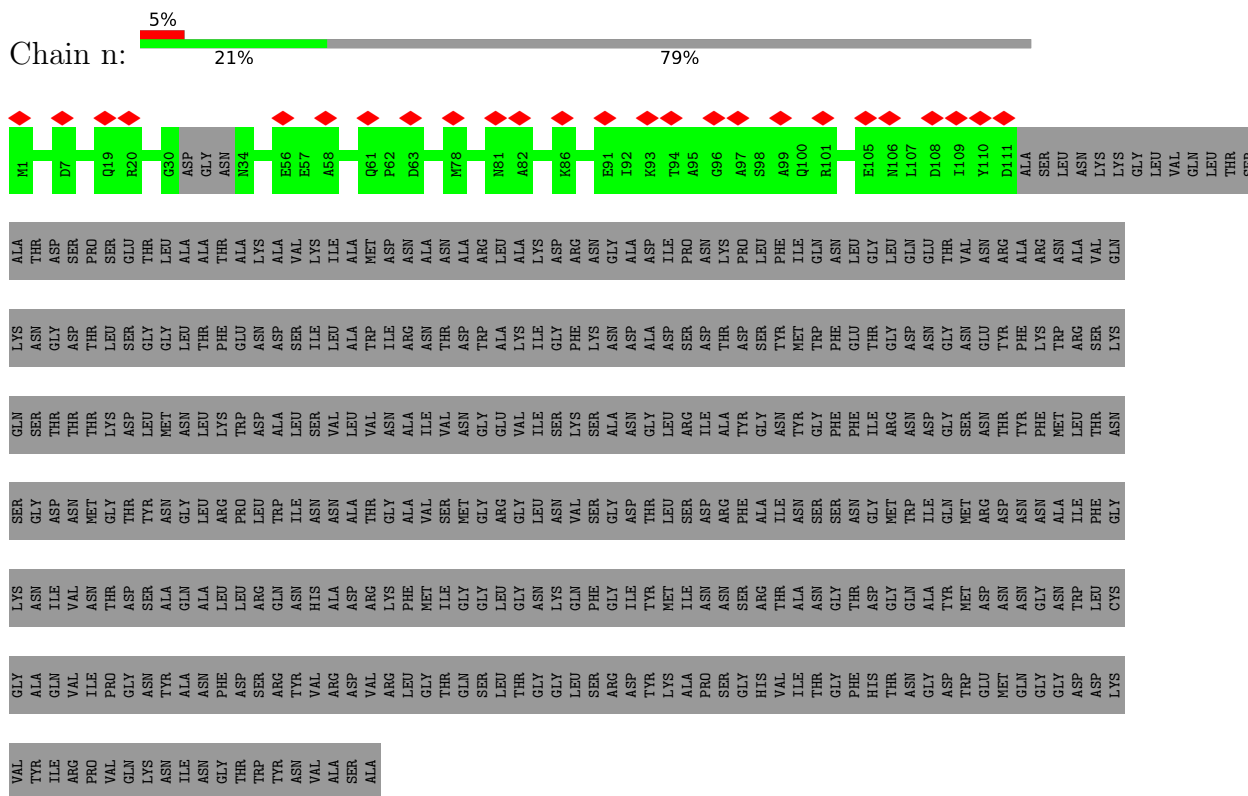




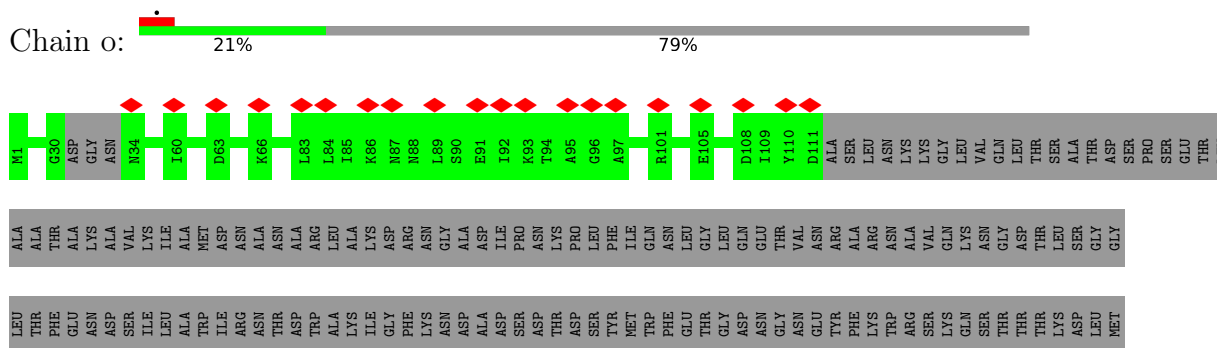


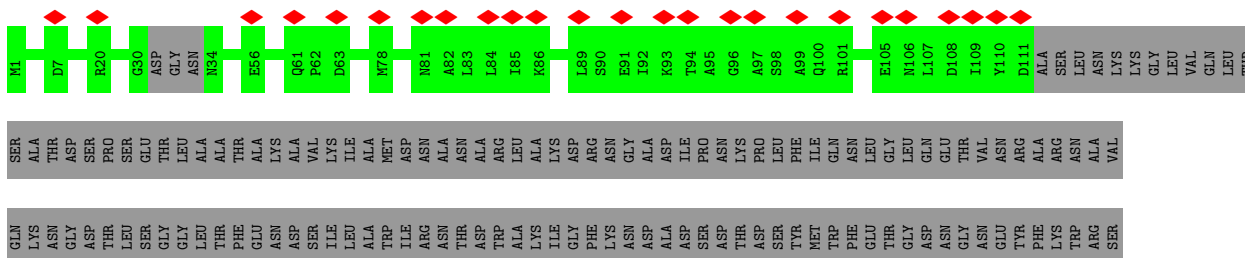
[illegible]

- Molecule 10: Tail fiber protein S



- Molecule 10: Tail fiber protein S





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	408.0, 408.0, 408.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FE

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	0.32	0/3340	0.53	0/4545
1	s	0.37	0/3340	0.55	0/4545
1	t	0.36	0/3340	0.57	0/4545
1	u	0.30	0/3164	0.49	0/4300
1	v	0.29	0/3164	0.50	0/4300
1	w	0.28	0/3164	0.50	0/4300
2	1	0.26	0/3793	0.49	0/5166
2	2	0.26	0/3793	0.49	0/5166
2	3	0.27	0/3793	0.49	0/5166
2	x	0.26	0/3793	0.49	0/5166
2	y	0.27	0/3793	0.50	0/5166
2	z	0.27	0/3793	0.50	0/5166
3	4	0.25	0/896	0.51	0/1208
3	5	0.25	0/896	0.51	0/1208
3	6	0.25	0/896	0.50	0/1208
3	7	0.25	0/896	0.52	0/1208
3	8	0.25	0/896	0.51	0/1208
3	9	0.25	0/896	0.51	0/1208
4	A	0.31	0/1162	0.53	0/1582
4	B	0.34	0/1162	0.56	0/1582
4	C	0.27	0/1162	0.53	0/1582
4	D	0.25	0/1162	0.54	0/1582
4	E	0.30	0/1162	0.55	0/1582
4	F	0.28	0/1162	0.54	0/1582
5	G	0.28	0/2876	0.53	0/3895
5	N	0.28	0/2876	0.55	0/3895
5	U	0.29	0/2876	0.55	0/3895
6	H	0.33	0/2754	0.53	0/3766
6	I	0.31	0/2754	0.53	0/3766
6	J	0.31	0/2754	0.54	0/3766
6	K	0.29	0/2754	0.53	0/3766
6	L	0.30	0/2754	0.53	0/3766

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	M	0.28	0/2754	0.52	0/3766
6	O	0.28	0/2772	0.50	0/3791
6	P	0.28	0/2772	0.51	0/3791
6	Q	0.27	0/2772	0.50	0/3791
6	R	0.28	0/2668	0.51	0/3644
6	S	0.29	0/2668	0.49	0/3644
6	T	0.30	0/2668	0.51	0/3644
7	V	0.31	0/1506	0.59	0/2037
7	W	0.33	0/1506	0.58	0/2037
7	X	0.31	0/1506	0.57	0/2037
8	a	0.28	0/1436	0.51	0/1952
8	b	0.25	0/1239	0.50	0/1681
8	c	0.27	0/1436	0.50	0/1952
8	d	0.34	0/1239	0.49	0/1681
8	e	0.30	0/1436	0.52	0/1952
8	f	0.29	0/1239	0.51	0/1681
9	g	0.27	0/133	0.44	0/180
9	h	0.28	0/133	0.43	0/180
9	i	0.28	0/133	0.45	0/180
10	j	0.29	0/849	0.48	0/1153
10	k	0.26	0/849	0.47	0/1153
10	l	0.32	0/849	0.45	0/1153
10	m	0.37	0/849	0.49	0/1153
10	n	0.26	0/849	0.46	0/1153
10	o	0.28	0/849	0.46	0/1153
10	p	0.28	0/849	0.48	0/1153
10	q	0.28	0/849	0.46	0/1153
10	r	0.28	0/849	0.45	0/1153
All	All	0.29	0/116673	0.52	0/158784

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

5.3.1 Protein backbone ⓘ

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	440/495 (89%)	417 (95%)	23 (5%)	0	100	100
1	s	440/495 (89%)	414 (94%)	26 (6%)	0	100	100
1	t	440/495 (89%)	406 (92%)	33 (8%)	1 (0%)	44	71
1	u	413/495 (83%)	397 (96%)	16 (4%)	0	100	100
1	v	413/495 (83%)	395 (96%)	18 (4%)	0	100	100
1	w	413/495 (83%)	395 (96%)	18 (4%)	0	100	100
2	1	491/495 (99%)	469 (96%)	22 (4%)	0	100	100
2	2	491/495 (99%)	470 (96%)	21 (4%)	0	100	100
2	3	491/495 (99%)	469 (96%)	22 (4%)	0	100	100
2	x	491/495 (99%)	459 (94%)	32 (6%)	0	100	100
2	y	491/495 (99%)	455 (93%)	36 (7%)	0	100	100
2	z	491/495 (99%)	458 (93%)	33 (7%)	0	100	100
3	4	113/118 (96%)	104 (92%)	9 (8%)	0	100	100
3	5	113/118 (96%)	106 (94%)	7 (6%)	0	100	100
3	6	113/118 (96%)	105 (93%)	8 (7%)	0	100	100
3	7	113/118 (96%)	106 (94%)	7 (6%)	0	100	100
3	8	113/118 (96%)	102 (90%)	11 (10%)	0	100	100
3	9	113/118 (96%)	107 (95%)	6 (5%)	0	100	100
4	A	141/145 (97%)	133 (94%)	8 (6%)	0	100	100
4	B	141/145 (97%)	136 (96%)	5 (4%)	0	100	100
4	C	141/145 (97%)	136 (96%)	5 (4%)	0	100	100
4	D	141/145 (97%)	136 (96%)	5 (4%)	0	100	100
4	E	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
4	F	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
5	G	362/379 (96%)	349 (96%)	13 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	N	362/379 (96%)	350 (97%)	12 (3%)	0	100	100
5	U	362/379 (96%)	350 (97%)	12 (3%)	0	100	100
6	H	354/360 (98%)	343 (97%)	10 (3%)	1 (0%)	37	66
6	I	354/360 (98%)	341 (96%)	13 (4%)	0	100	100
6	J	354/360 (98%)	344 (97%)	9 (2%)	1 (0%)	37	66
6	K	354/360 (98%)	340 (96%)	13 (4%)	1 (0%)	37	66
6	L	354/360 (98%)	341 (96%)	13 (4%)	0	100	100
6	M	354/360 (98%)	341 (96%)	13 (4%)	0	100	100
6	O	357/360 (99%)	339 (95%)	18 (5%)	0	100	100
6	P	357/360 (99%)	342 (96%)	15 (4%)	0	100	100
6	Q	357/360 (99%)	342 (96%)	15 (4%)	0	100	100
6	R	337/360 (94%)	323 (96%)	14 (4%)	0	100	100
6	S	337/360 (94%)	327 (97%)	10 (3%)	0	100	100
6	T	337/360 (94%)	327 (97%)	10 (3%)	0	100	100
7	V	192/197 (98%)	170 (88%)	22 (12%)	0	100	100
7	W	192/197 (98%)	172 (90%)	20 (10%)	0	100	100
7	X	192/197 (98%)	174 (91%)	18 (9%)	0	100	100
8	a	172/180 (96%)	161 (94%)	11 (6%)	0	100	100
8	b	146/180 (81%)	140 (96%)	6 (4%)	0	100	100
8	c	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
8	d	146/180 (81%)	138 (94%)	8 (6%)	0	100	100
8	e	172/180 (96%)	165 (96%)	7 (4%)	0	100	100
8	f	146/180 (81%)	139 (95%)	7 (5%)	0	100	100
9	g	15/690 (2%)	15 (100%)	0	0	100	100
9	h	15/690 (2%)	15 (100%)	0	0	100	100
9	i	15/690 (2%)	14 (93%)	1 (7%)	0	100	100
10	j	104/504 (21%)	102 (98%)	2 (2%)	0	100	100
10	k	104/504 (21%)	100 (96%)	4 (4%)	0	100	100
10	l	104/504 (21%)	102 (98%)	2 (2%)	0	100	100
10	m	104/504 (21%)	102 (98%)	2 (2%)	0	100	100
10	n	104/504 (21%)	99 (95%)	5 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	o	104/504 (21%)	102 (98%)	2 (2%)	0	100	100
10	p	104/504 (21%)	101 (97%)	3 (3%)	0	100	100
10	q	104/504 (21%)	99 (95%)	5 (5%)	0	100	100
10	r	104/504 (21%)	102 (98%)	2 (2%)	0	100	100
All	All	14832/21252 (70%)	14120 (95%)	708 (5%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	t	270	HIS
6	K	234	ASN
6	J	238	ILE
6	H	238	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	353/391 (90%)	350 (99%)	3 (1%)	79	87
1	s	353/391 (90%)	344 (98%)	9 (2%)	42	67
1	t	353/391 (90%)	348 (99%)	5 (1%)	62	78
1	u	333/391 (85%)	332 (100%)	1 (0%)	91	94
1	v	333/391 (85%)	331 (99%)	2 (1%)	84	90
1	w	333/391 (85%)	331 (99%)	2 (1%)	84	90
2	1	391/394 (99%)	388 (99%)	3 (1%)	79	87
2	2	391/394 (99%)	390 (100%)	1 (0%)	91	94
2	3	391/394 (99%)	390 (100%)	1 (0%)	91	94
2	x	391/394 (99%)	390 (100%)	1 (0%)	91	94
2	y	391/394 (99%)	390 (100%)	1 (0%)	91	94
2	z	391/394 (99%)	390 (100%)	1 (0%)	91	94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	4	91/92 (99%)	90 (99%)	1 (1%)	70	82
3	5	91/92 (99%)	88 (97%)	3 (3%)	33	60
3	6	91/92 (99%)	91 (100%)	0	100	100
3	7	91/92 (99%)	89 (98%)	2 (2%)	47	69
3	8	91/92 (99%)	90 (99%)	1 (1%)	70	82
3	9	91/92 (99%)	89 (98%)	2 (2%)	47	69
4	A	118/120 (98%)	117 (99%)	1 (1%)	79	87
4	B	118/120 (98%)	115 (98%)	3 (2%)	42	67
4	C	118/120 (98%)	117 (99%)	1 (1%)	79	87
4	D	118/120 (98%)	118 (100%)	0	100	100
4	E	118/120 (98%)	118 (100%)	0	100	100
4	F	118/120 (98%)	117 (99%)	1 (1%)	79	87
5	G	300/313 (96%)	299 (100%)	1 (0%)	91	94
5	N	300/313 (96%)	299 (100%)	1 (0%)	91	94
5	U	300/313 (96%)	298 (99%)	2 (1%)	81	88
6	H	283/286 (99%)	281 (99%)	2 (1%)	81	88
6	I	283/286 (99%)	281 (99%)	2 (1%)	81	88
6	J	283/286 (99%)	280 (99%)	3 (1%)	70	82
6	K	283/286 (99%)	279 (99%)	4 (1%)	62	78
6	L	283/286 (99%)	281 (99%)	2 (1%)	81	88
6	M	283/286 (99%)	281 (99%)	2 (1%)	81	88
6	O	284/286 (99%)	283 (100%)	1 (0%)	89	93
6	P	284/286 (99%)	282 (99%)	2 (1%)	81	88
6	Q	284/286 (99%)	283 (100%)	1 (0%)	89	93
6	R	273/286 (96%)	271 (99%)	2 (1%)	81	88
6	S	273/286 (96%)	272 (100%)	1 (0%)	89	93
6	T	273/286 (96%)	271 (99%)	2 (1%)	81	88
7	V	162/166 (98%)	161 (99%)	1 (1%)	84	90
7	W	162/166 (98%)	161 (99%)	1 (1%)	84	90
7	X	162/166 (98%)	160 (99%)	2 (1%)	67	80
8	a	147/152 (97%)	146 (99%)	1 (1%)	81	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	b	125/152 (82%)	123 (98%)	2 (2%)	58	76
8	c	147/152 (97%)	147 (100%)	0	100	100
8	d	125/152 (82%)	125 (100%)	0	100	100
8	e	147/152 (97%)	147 (100%)	0	100	100
8	f	125/152 (82%)	125 (100%)	0	100	100
9	g	12/520 (2%)	12 (100%)	0	100	100
9	h	12/520 (2%)	12 (100%)	0	100	100
9	i	12/520 (2%)	12 (100%)	0	100	100
10	j	90/412 (22%)	89 (99%)	1 (1%)	70	82
10	k	90/412 (22%)	90 (100%)	0	100	100
10	l	90/412 (22%)	90 (100%)	0	100	100
10	m	90/412 (22%)	89 (99%)	1 (1%)	70	82
10	n	90/412 (22%)	90 (100%)	0	100	100
10	o	90/412 (22%)	90 (100%)	0	100	100
10	p	90/412 (22%)	90 (100%)	0	100	100
10	q	90/412 (22%)	90 (100%)	0	100	100
10	r	90/412 (22%)	90 (100%)	0	100	100
All	All	12075/17031 (71%)	11993 (99%)	82 (1%)	80	88

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	298	TYR
1	0	339	SER
1	0	392	ASP
2	1	14	ARG
2	1	164	ASP
2	1	262	ASP
2	2	374	ARG
2	3	351	ASP
3	4	97	GLU
3	5	21	SER
3	5	30	SER
3	5	41	ARG
3	7	30	SER
3	7	41	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	8	41	ARG
3	9	30	SER
3	9	41	ARG
4	A	28	LEU
4	B	54	ASP
4	B	56	ARG
4	B	84	THR
4	C	53	ASP
4	F	31	ASP
5	G	305	TYR
6	H	147	ASN
6	H	236	SER
6	I	232	MET
6	I	237	ASN
6	J	146	GLU
6	J	147	ASN
6	J	296	LYS
6	K	150	LEU
6	K	234	ASN
6	K	357	ILE
6	K	359	TRP
6	L	150	LEU
6	L	233	ASP
6	M	234	ASN
6	M	358	GLU
5	N	305	TYR
6	O	31	ARG
6	P	31	ARG
6	P	231	VAL
6	Q	31	ARG
6	R	3	TYR
6	R	232	MET
6	S	232	MET
6	T	3	TYR
6	T	232	MET
5	U	264	LEU
5	U	305	TYR
7	V	167	ASN
7	W	196	MET
7	X	106	ILE
7	X	144	THR
8	a	159	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	b	51	ARG
8	b	58	SER
10	j	78	MET
10	m	86	LYS
1	s	273	THR
1	s	284	TYR
1	s	288	VAL
1	s	298	TYR
1	s	300	MET
1	s	301	LEU
1	s	325	ARG
1	s	360	LEU
1	s	362	LEU
1	t	260	ASN
1	t	264	GLN
1	t	284	TYR
1	t	288	VAL
1	t	383	THR
1	u	418	THR
1	v	170	LEU
1	v	416	PHE
1	w	48	VAL
1	w	170	LEU
2	x	466	LYS
2	y	466	LYS
2	z	466	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	231	GLN
1	0	297	ASN
2	3	346	ASN
4	A	17	GLN
6	I	237	ASN
6	J	108	GLN
6	J	147	ASN
6	M	283	ASN
5	N	260	GLN
6	Q	348	ASN
6	R	309	ASN
6	S	309	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	T	309	ASN
8	b	127	GLN
8	b	129	ASN
8	d	127	GLN
8	d	129	ASN
8	d	176	HIS
8	f	127	GLN
8	f	129	ASN
10	m	53	ASN
10	m	80	ASN
10	m	88	ASN
10	r	6	ASN
1	s	297	ASN
1	t	297	ASN
1	u	61	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

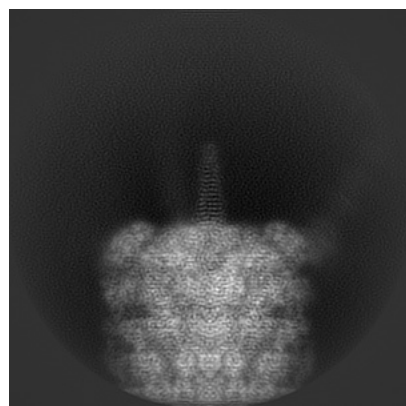
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62362. These allow visual inspection of the internal detail of the map and identification of artifacts.

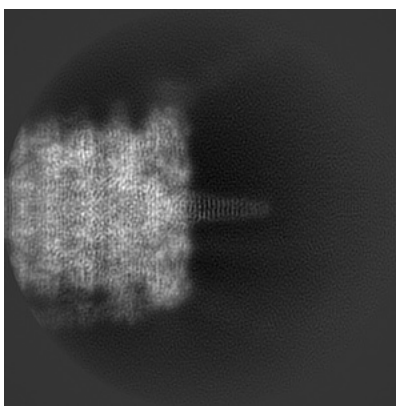
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

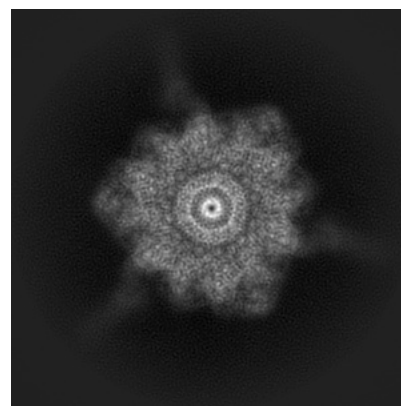
6.1.1 Primary map



X

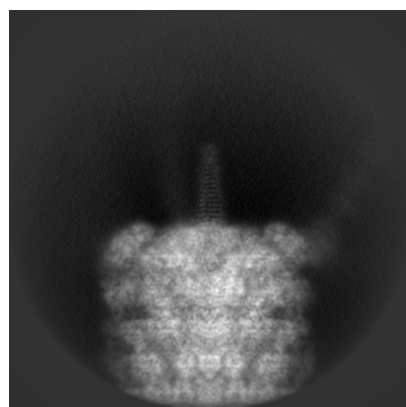


Y

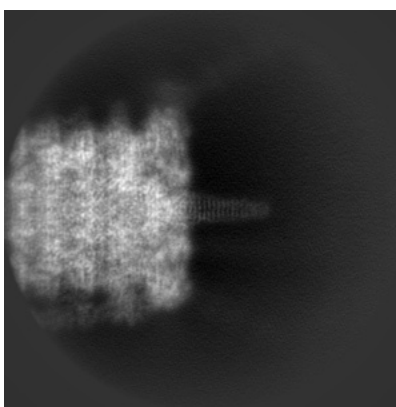


Z

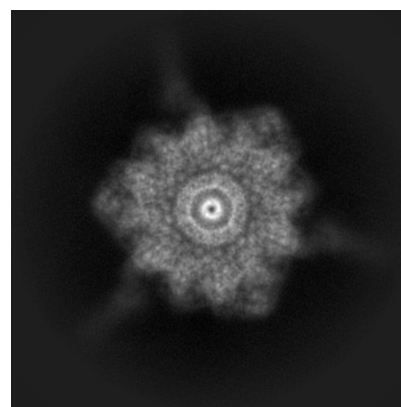
6.1.2 Raw map



X



Y

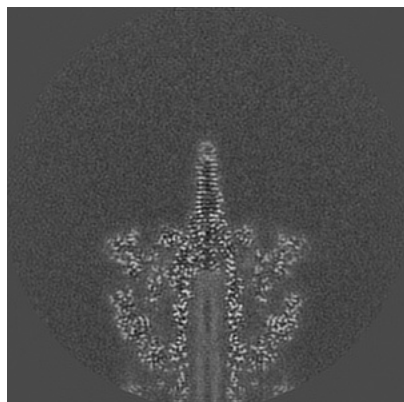


Z

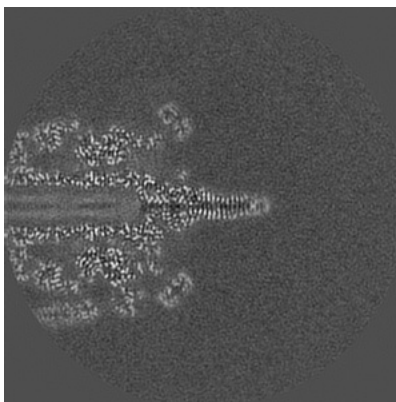
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

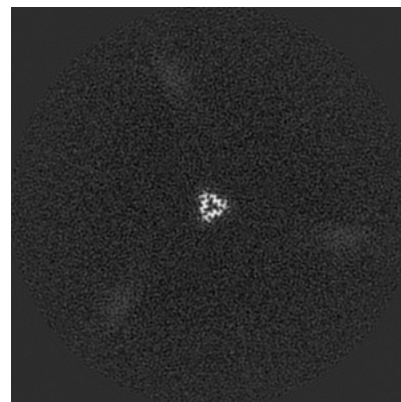
6.2.1 Primary map



X Index: 150

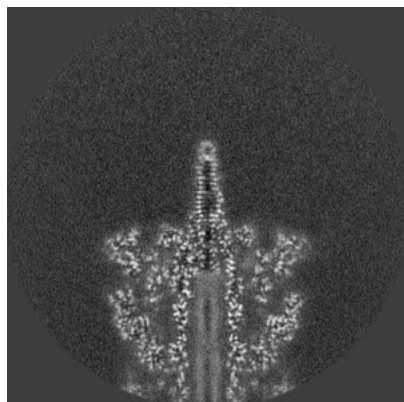


Y Index: 150

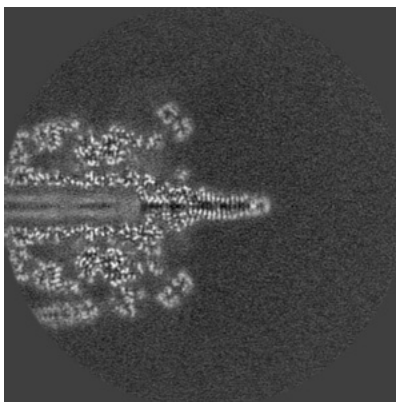


Z Index: 150

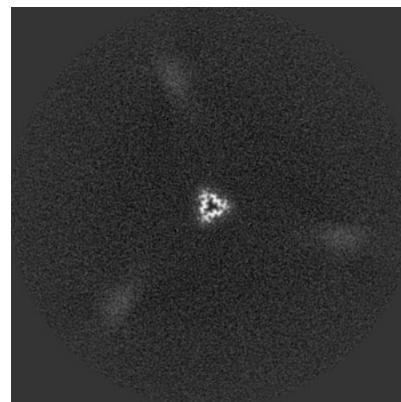
6.2.2 Raw map



X Index: 150



Y Index: 150

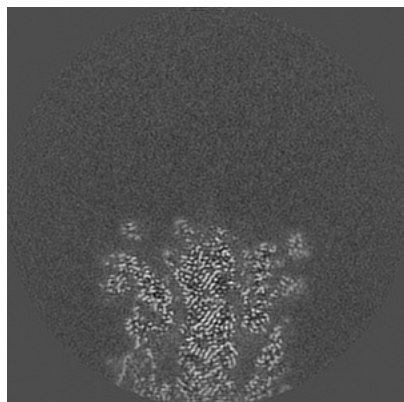


Z Index: 150

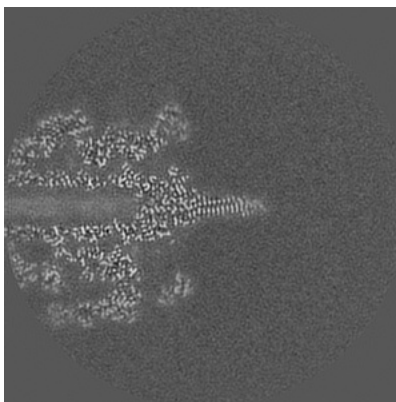
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

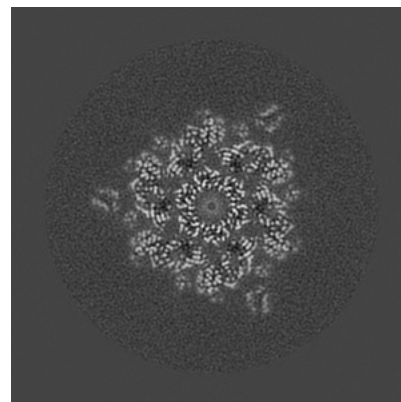
6.3.1 Primary map



X Index: 167

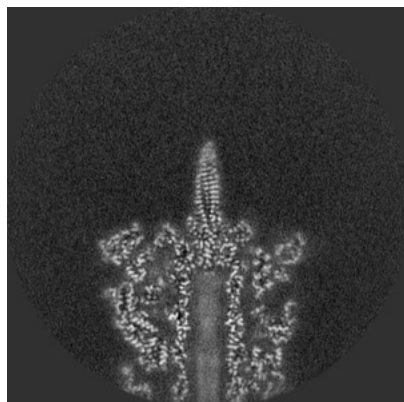


Y Index: 155

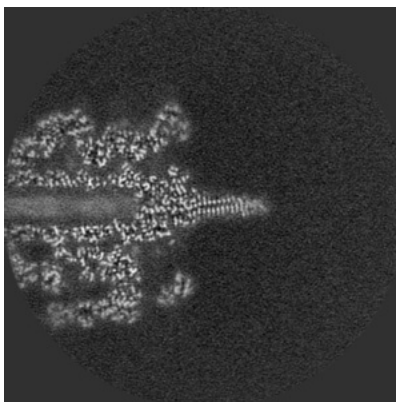


Z Index: 65

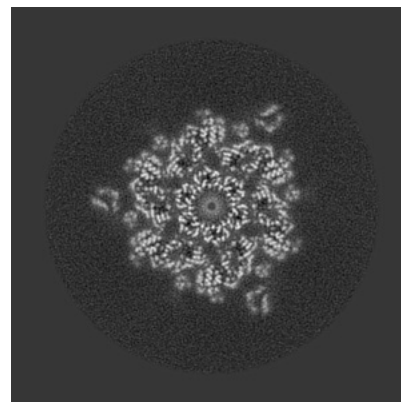
6.3.2 Raw map



X Index: 154



Y Index: 155

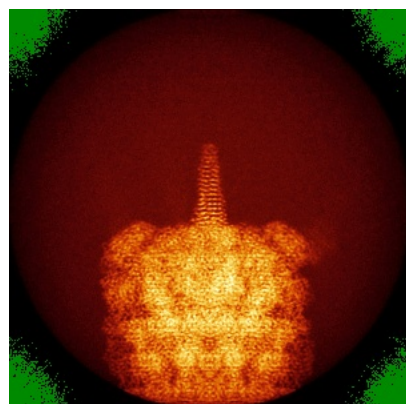


Z Index: 65

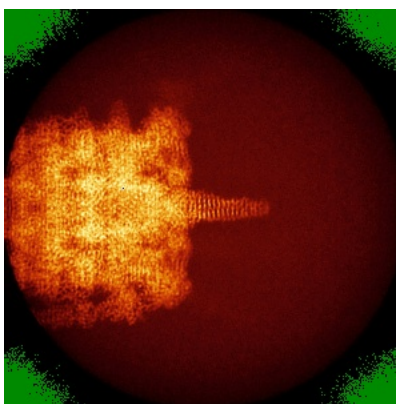
The images above show the largest variance slices of the map in three orthogonal directions.

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

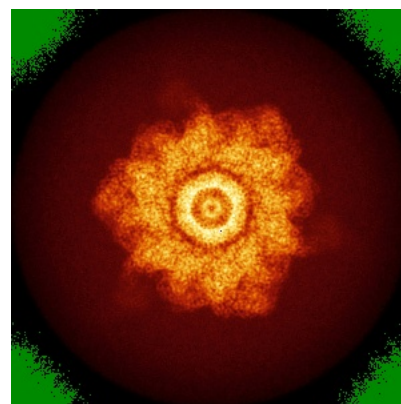
6.4.1 Primary map



X

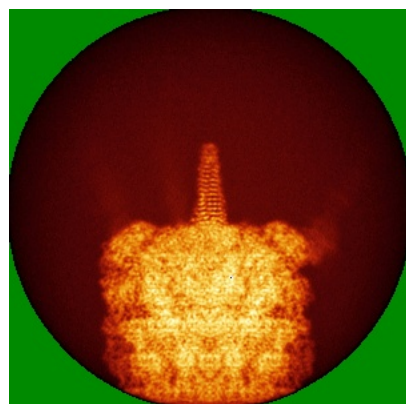


Y

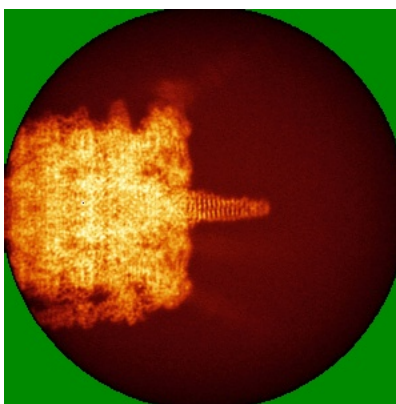


Z

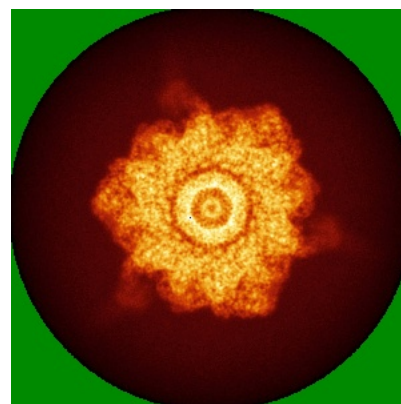
6.4.2 Raw map



X



Y

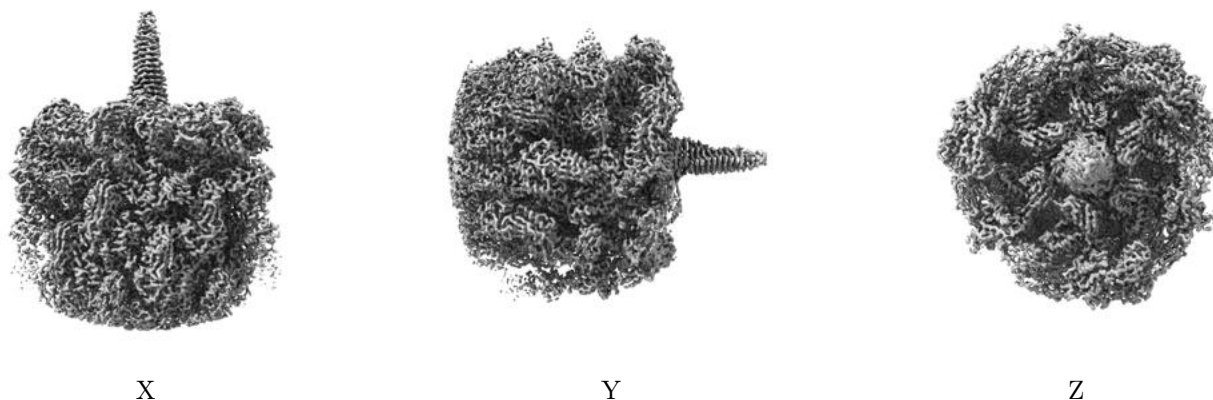


Z

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.

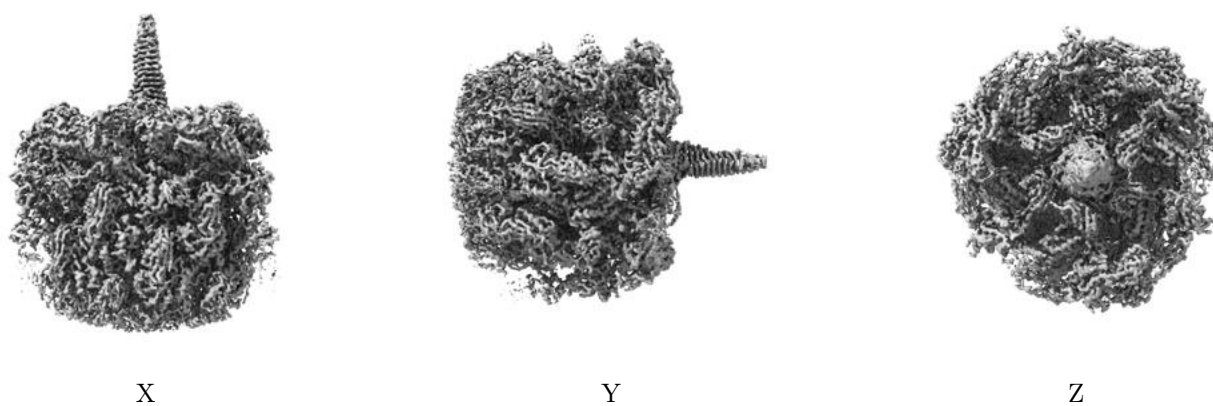
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

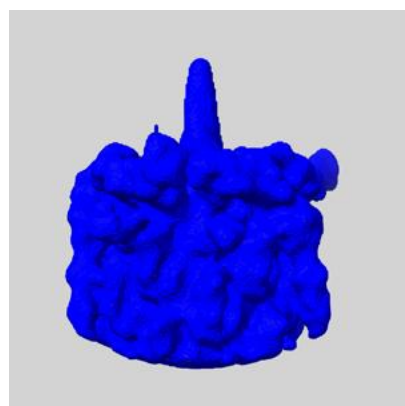
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

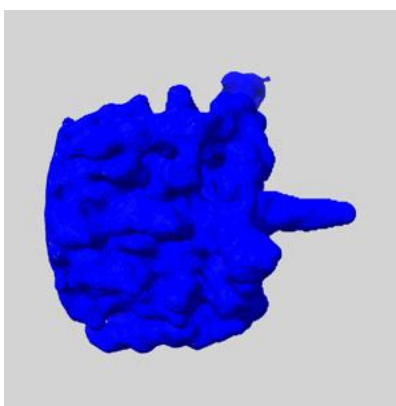
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

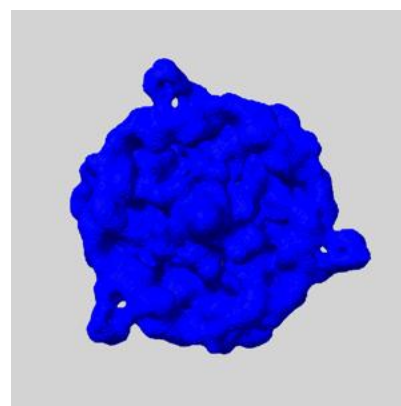
6.6.1 emd_62362_msk_1.map [i](#)



X



Y

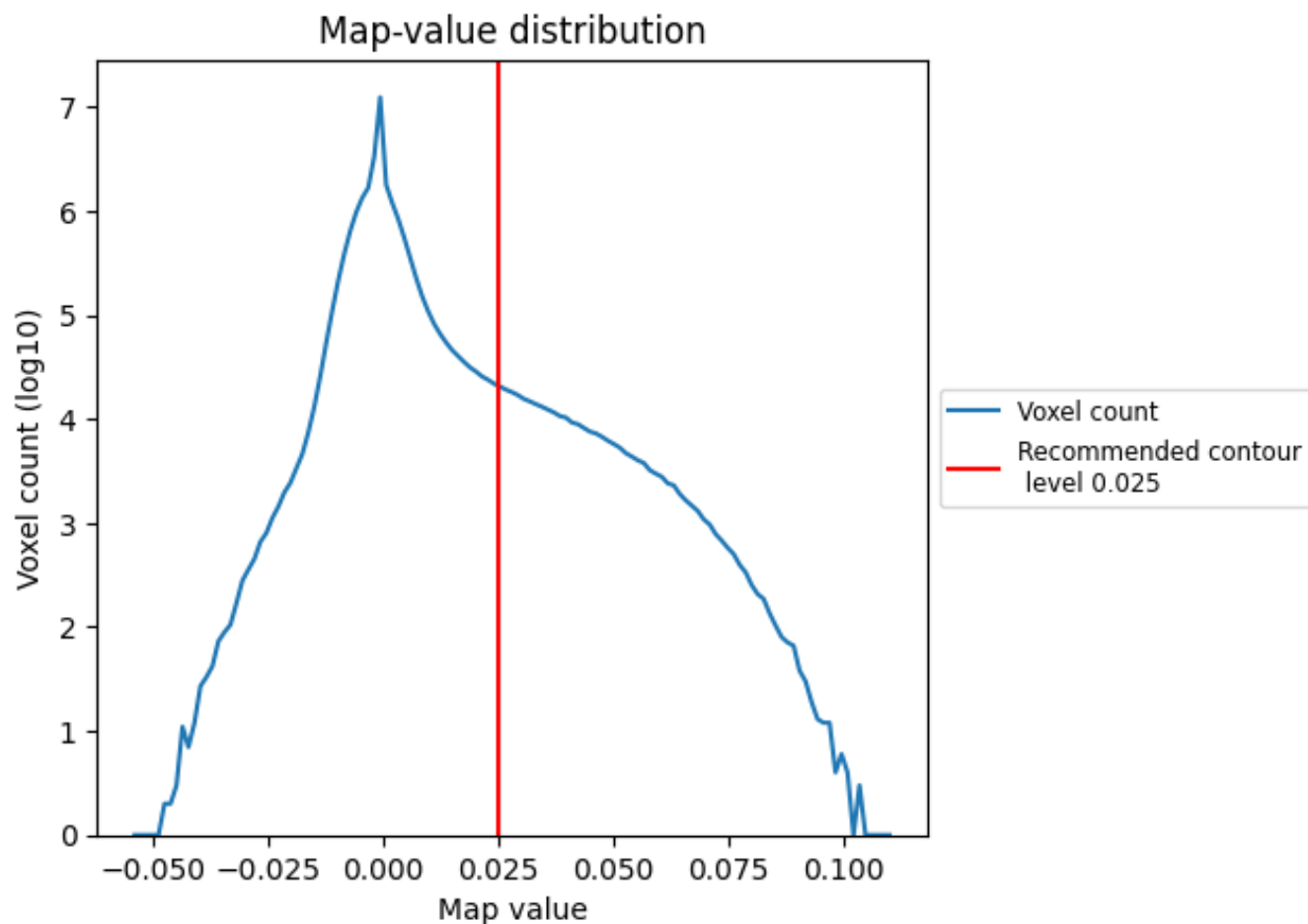


Z

7 Map analysis [i](#)

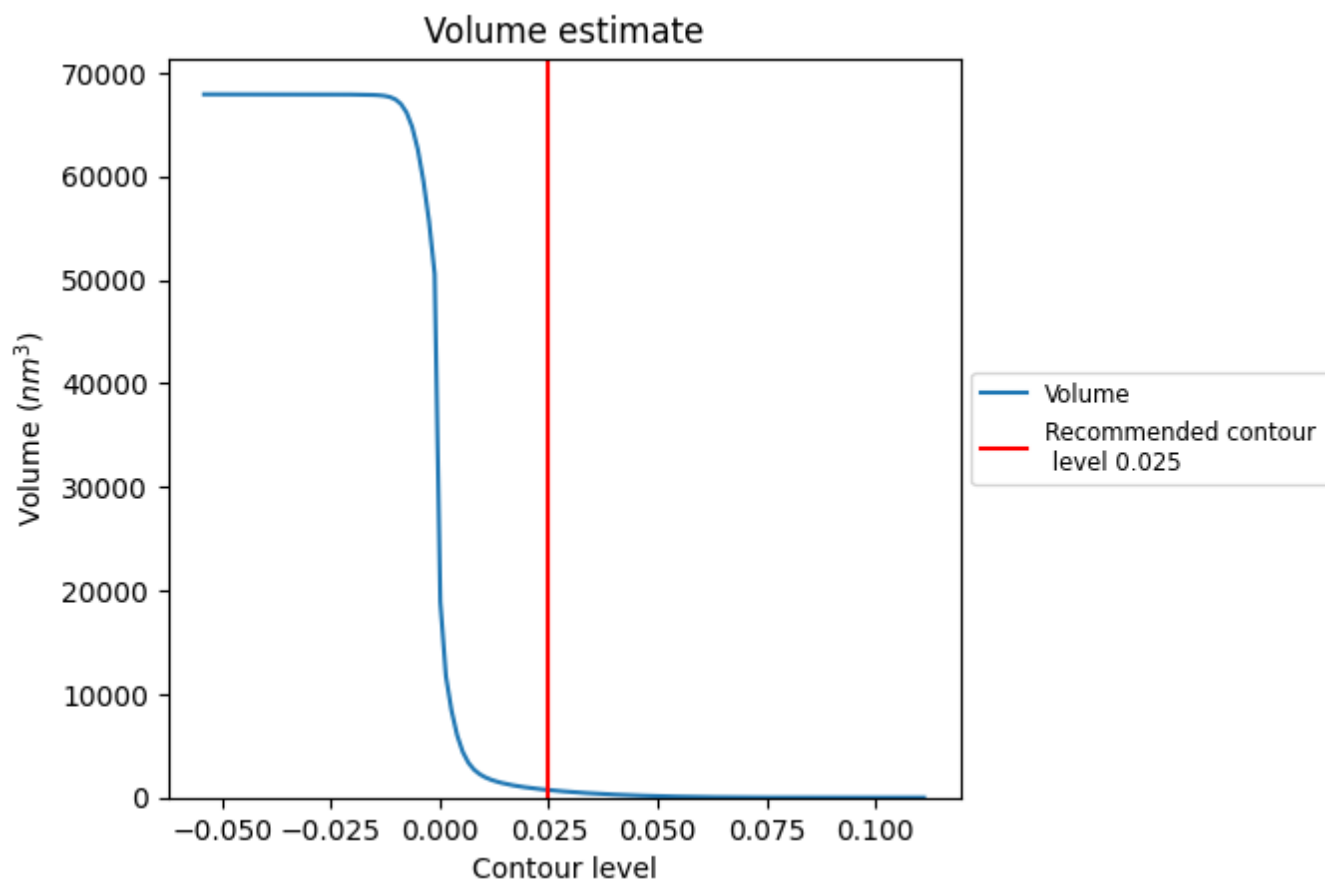
This section contains the results of statistical analysis of the map.

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.

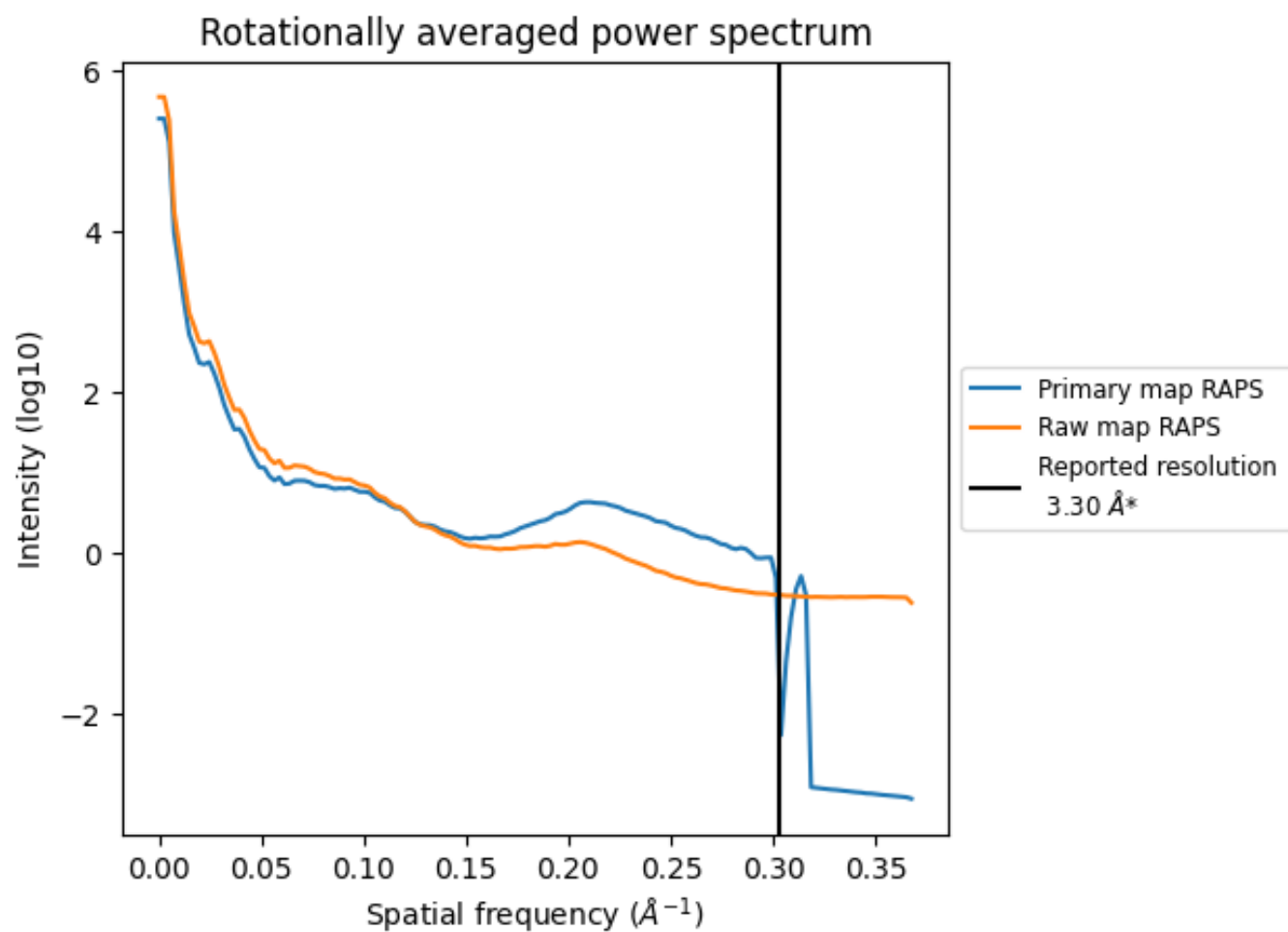
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 727 nm³; this corresponds to an approximate mass of 657 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 ⓘ

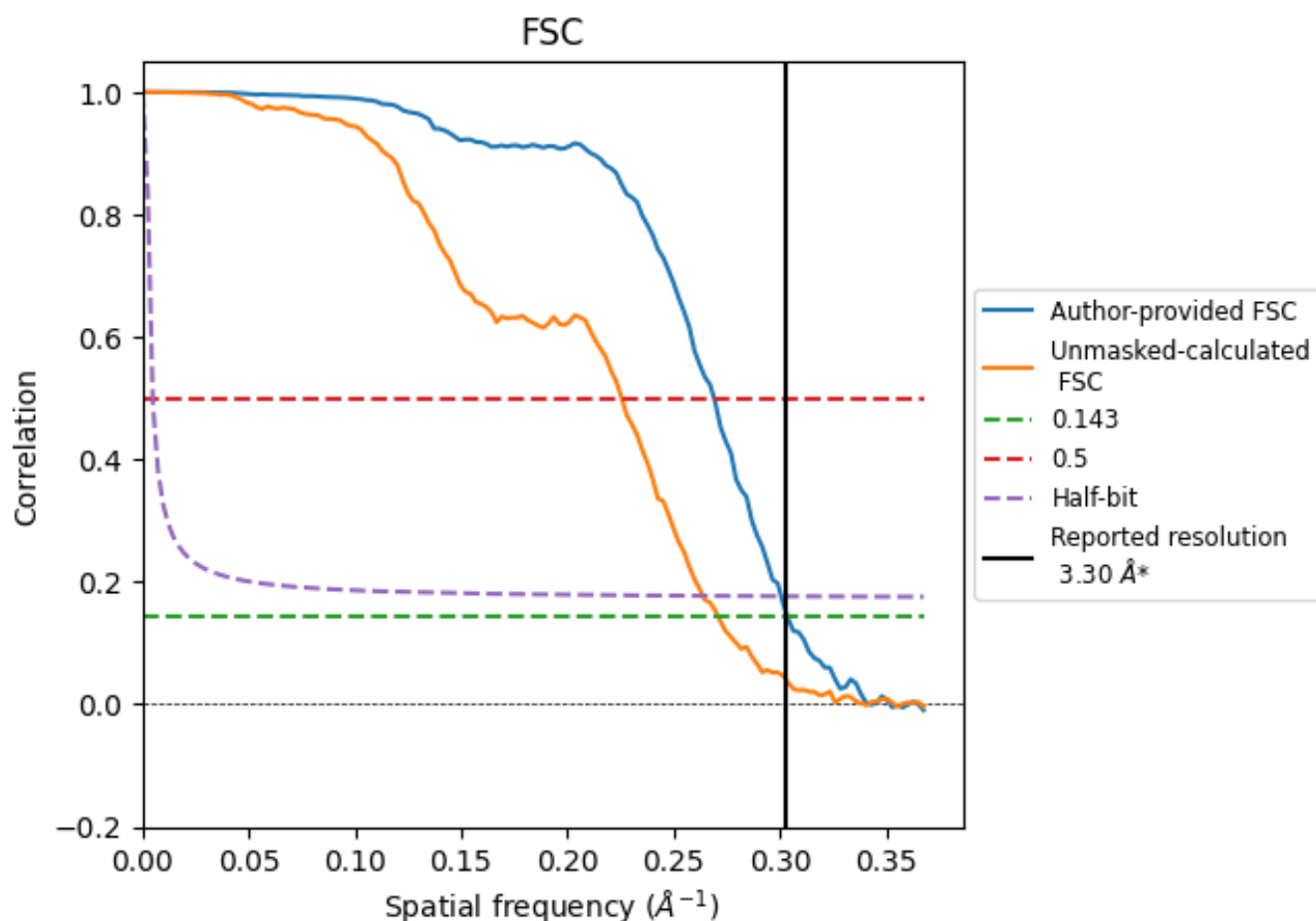


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

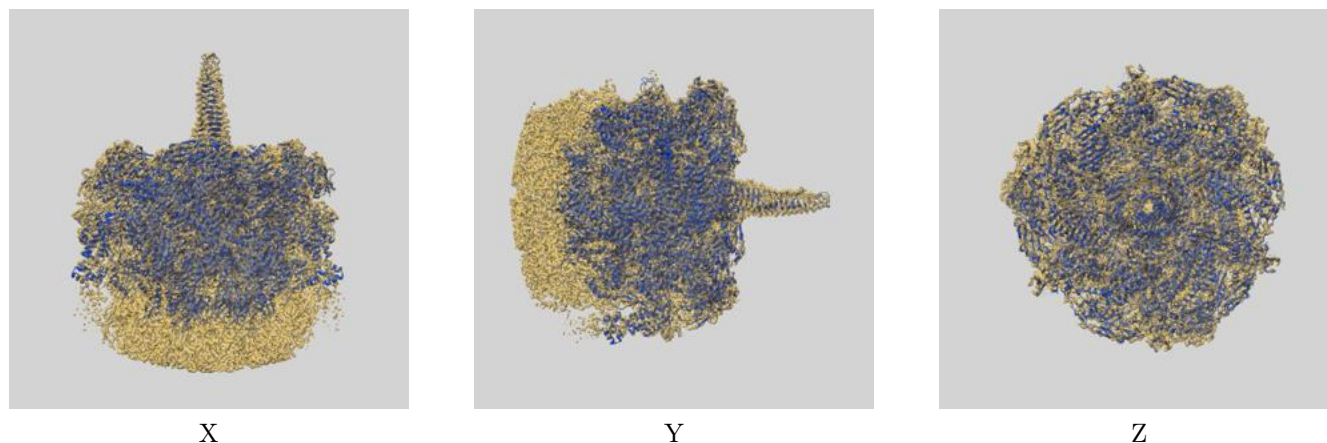
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.72	3.33
Unmasked-calculated*	3.69	4.43	3.79

*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 3.69 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

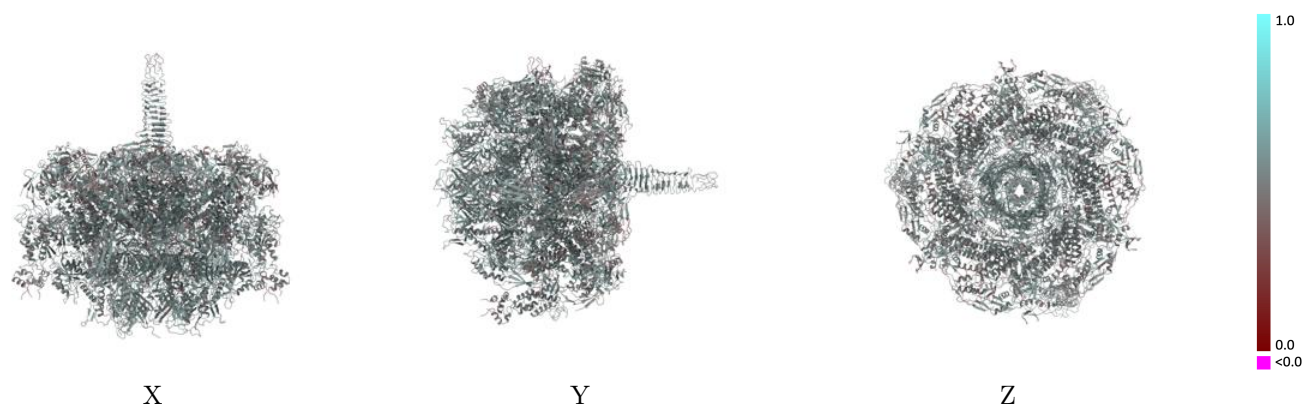
This section contains information regarding the fit between EMDB map EMD-62362 and PDB model 9KI1. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



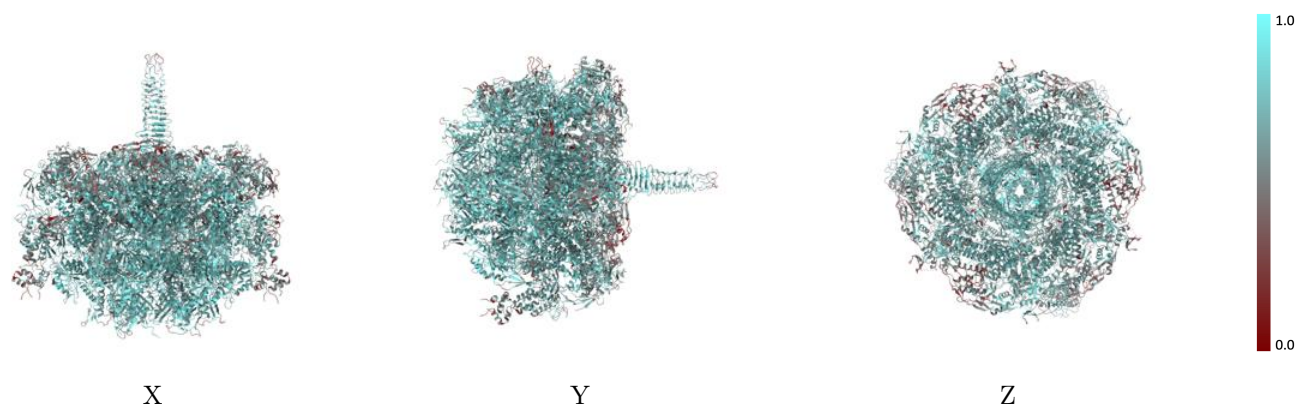
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



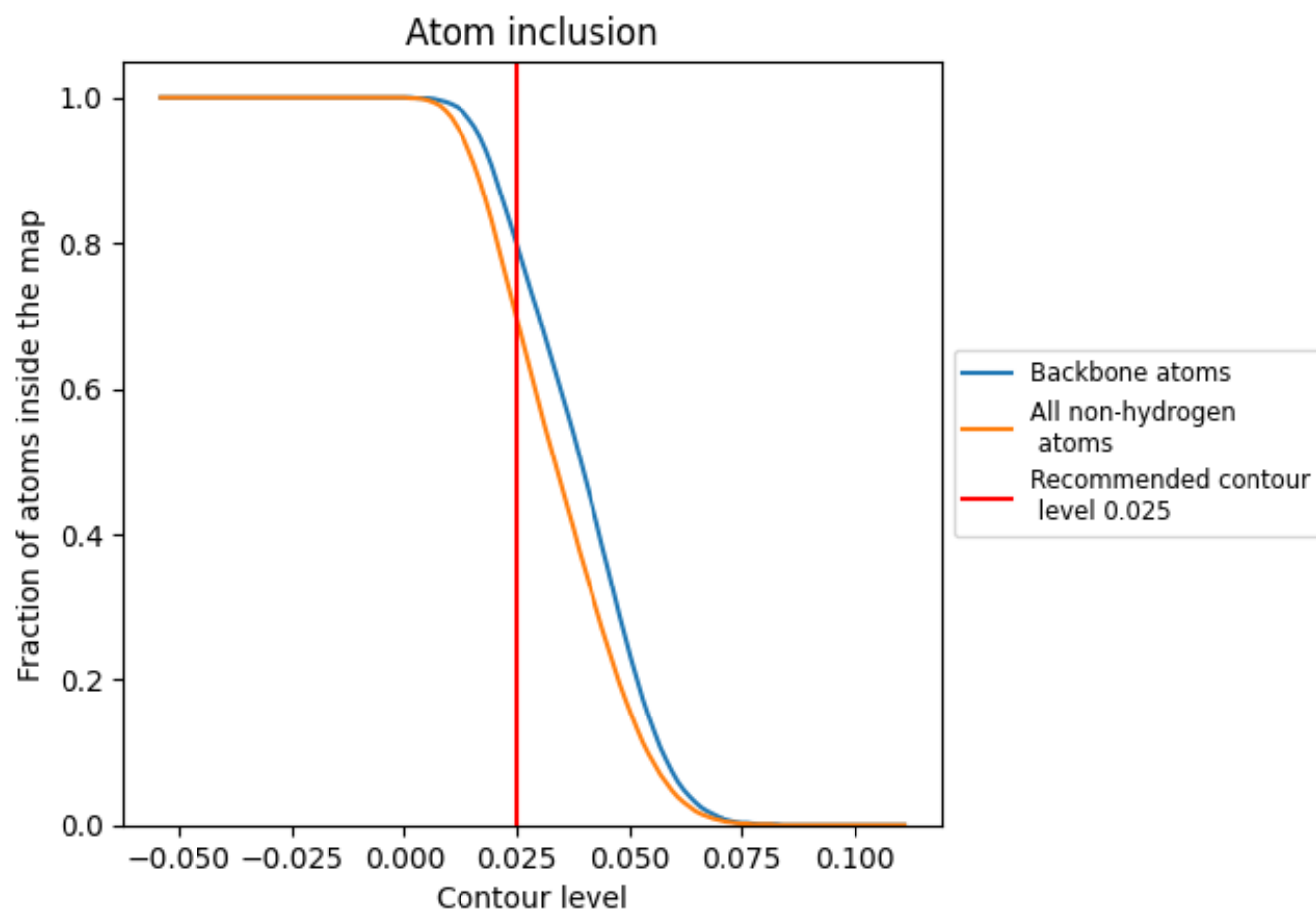
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 70% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6980	 0.5170
0	 0.7320	 0.5190
1	 0.7230	 0.5230
2	 0.7190	 0.5230
3	 0.7220	 0.5230
4	 0.7750	 0.5420
5	 0.7620	 0.5340
6	 0.7670	 0.5430
7	 0.7600	 0.5380
8	 0.7720	 0.5450
9	 0.7760	 0.5320
A	 0.7950	 0.5350
B	 0.7820	 0.5360
C	 0.8010	 0.5400
D	 0.7900	 0.5420
E	 0.8020	 0.5360
F	 0.7900	 0.5410
G	 0.7940	 0.5460
H	 0.6920	 0.5120
I	 0.6960	 0.5150
J	 0.6890	 0.5150
K	 0.5920	 0.4920
L	 0.5890	 0.4910
M	 0.5910	 0.4910
N	 0.7940	 0.5470
O	 0.5790	 0.4970
P	 0.5790	 0.4980
Q	 0.5840	 0.4980
R	 0.6160	 0.4990
S	 0.6100	 0.4980
T	 0.6100	 0.4980
U	 0.7890	 0.5490
V	 0.7330	 0.5320
W	 0.7320	 0.5290
X	 0.7340	 0.5280



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	 0.7200	 0.5200
b	 0.6290	 0.4940
c	 0.7360	 0.5200
d	 0.6320	 0.4870
e	 0.7300	 0.5180
f	 0.6340	 0.4870
g	 0.7010	 0.4910
h	 0.6770	 0.4930
i	 0.6690	 0.4710
j	 0.6200	 0.5070
k	 0.5820	 0.4980
l	 0.6170	 0.5020
m	 0.6250	 0.5060
n	 0.5880	 0.4980
o	 0.6150	 0.5020
p	 0.6120	 0.5130
q	 0.5840	 0.4970
r	 0.6270	 0.5080
s	 0.7360	 0.5210
t	 0.7300	 0.5220
u	 0.7260	 0.5170
v	 0.7340	 0.5180
w	 0.7270	 0.5150
x	 0.7350	 0.5220
y	 0.7430	 0.5220
z	 0.7410	 0.5220