Full wwPDB EM Validation Report (i)

Mar 11, 2024 – 02:14 AM EDT

PDB ID	:	6U5F
EMDB ID	:	EMD-20644
Title	:	CryoEM Structure of Pyocin R2 - precontracted - collar
Authors	:	Ge, P.; Avaylon, J.; Scholl, D.; Shneider, M.M.; Browning, C.; Buth, S.A.; Plattner, M.; Ding, K.; Leiman, P.G.; Miller, J.F.; Zhou, Z.H.
Deposited on	:	2019-08-27
Resolution	:	3.80 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 (i) 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 (i)) were used in the production of this report:

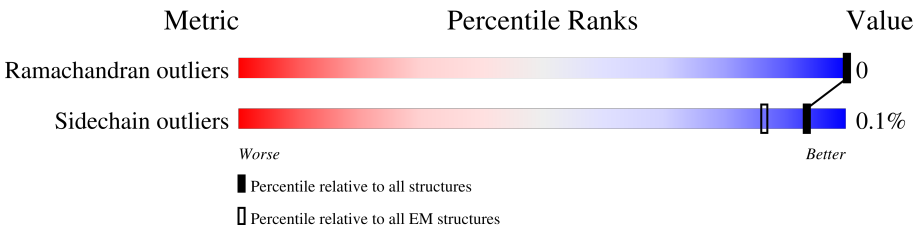
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	171	43% 97%
1	B	171	43% 97%
1	C	171	44% 97%
1	D	171	42% 97%
1	E	171	44% 97%
1	F	171	42% 97%
2	G	386	54% 99%
2	H	386	54% 99%
2	I	386	54% 99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	386	53% 99%
2	K	386	55% 99%
2	L	386	54% 99%
2	S	386	41% 100%
2	T	386	41% 100%
2	U	386	40% 100%
2	V	386	41% 100%
2	W	386	40% 100%
2	X	386	41% 100%
2	g	386	37% 100%
2	h	386	37% 100%
2	i	386	37% 100%
2	j	386	37% 100%
2	k	386	37% 100%
2	l	386	37% 100%
2	s	386	37% 100%
2	t	386	36% 100%
2	u	386	38% 100%
2	v	386	36% 100%
2	w	386	36% 100%
2	x	386	37% 100%
3	0	167	27% 100%
3	1	167	24% 100%
3	2	167	28% 100%
3	3	167	26% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	4	167	25% 100%
3	5	167	27% 100%
3	M	167	28% 99%
3	N	167	29% 99%
3	O	167	30% 99%
3	P	167	28% 99%
3	Q	167	29% 99%
3	R	167	29% 99%
3	a	167	25% 100%
3	b	167	26% 100%
3	c	167	26% 100%
3	d	167	25% 100%
3	e	167	26% 100%
3	f	167	25% 100%
3	m	167	25% 100%
3	n	167	26% 100%
3	o	167	25% 100%
3	p	167	26% 100%
3	q	167	25% 100%
3	r	167	25% 100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 107550 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 PA0615.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	167	1306	830	227	245	4	0	0
1	B	167	1306	830	227	245	4	0	0
1	C	167	1306	830	227	245	4	0	0
1	D	167	1306	830	227	245	4	0	0
1	E	167	1306	830	227	245	4	0	0
1	F	167	1306	830	227	245	4	0	0

- Molecule 2 is a protein called Sheath PA0622.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	383	2884	1817	504	555	8	0	0
2	H	383	2884	1817	504	555	8	0	0
2	I	383	2884	1817	504	555	8	0	0
2	J	383	2884	1817	504	555	8	0	0
2	K	383	2884	1817	504	555	8	0	0
2	L	383	2884	1817	504	555	8	0	0
2	S	385	2897	1825	506	558	8	0	0
2	g	385	2897	1825	506	558	8	0	0
2	s	385	2897	1825	506	558	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	T	385	2897	1825	506	558	8	0	0
2	h	385	2897	1825	506	558	8	0	0
2	t	385	2897	1825	506	558	8	0	0
2	U	385	2897	1825	506	558	8	0	0
2	i	385	2897	1825	506	558	8	0	0
2	u	385	2897	1825	506	558	8	0	0
2	V	385	2897	1825	506	558	8	0	0
2	j	385	2897	1825	506	558	8	0	0
2	v	385	2897	1825	506	558	8	0	0
2	W	385	2897	1825	506	558	8	0	0
2	k	385	2897	1825	506	558	8	0	0
2	w	385	2897	1825	506	558	8	0	0
2	X	385	2897	1825	506	558	8	0	0
2	l	385	2897	1825	506	558	8	0	0
2	x	385	2897	1825	506	558	8	0	0

- Molecule 3 is a protein called Tube PA0623.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	M	166	1255	795	214	242	4	0	0
3	N	166	1255	795	214	242	4	0	0
3	O	166	1255	795	214	242	4	0	0
3	P	166	1255	795	214	242	4	0	0

Continued on next page...

Continued from previous page...

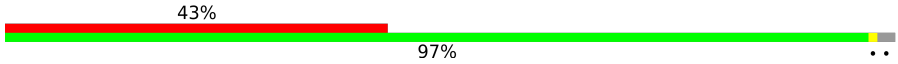
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Q	166	1255	795	214	242	4	0	0
			Total	C	N	O	S		
3	R	166	1255	795	214	242	4	0	0
			Total	C	N	O	S		
3	a	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	0	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	e	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	d	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	m	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	b	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	n	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	1	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	c	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	o	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	2	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	p	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	3	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	q	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	4	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	f	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	r	167	1263	800	215	243	5	0	0
			Total	C	N	O	S		
3	5	167	1263	800	215	243	5	0	0

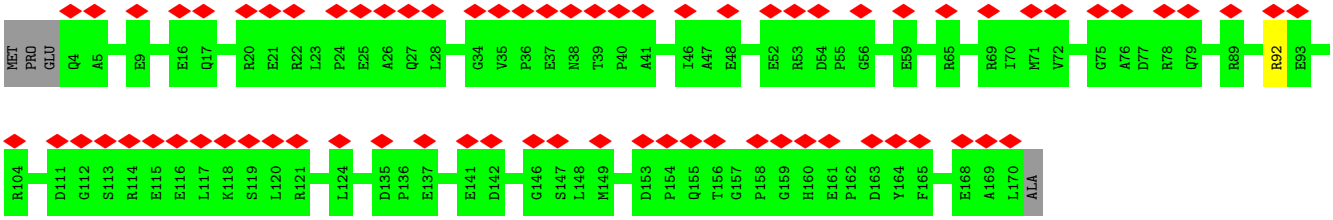
3 Residue-property plots (i)

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 PA0615

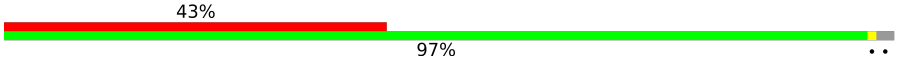
Chain A:

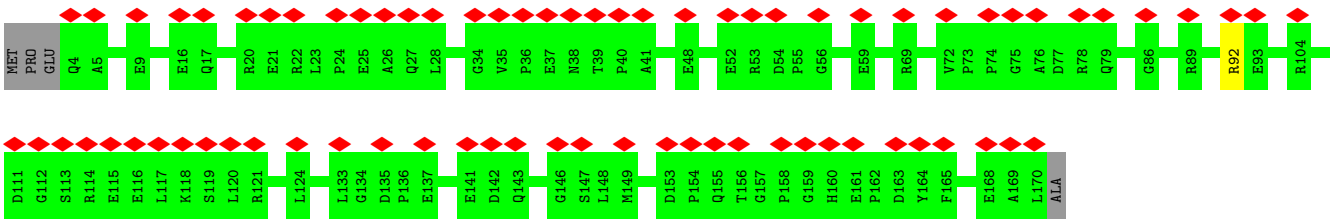




- Molecule 1: Collar PA0615

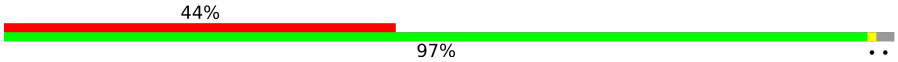
Chain B:

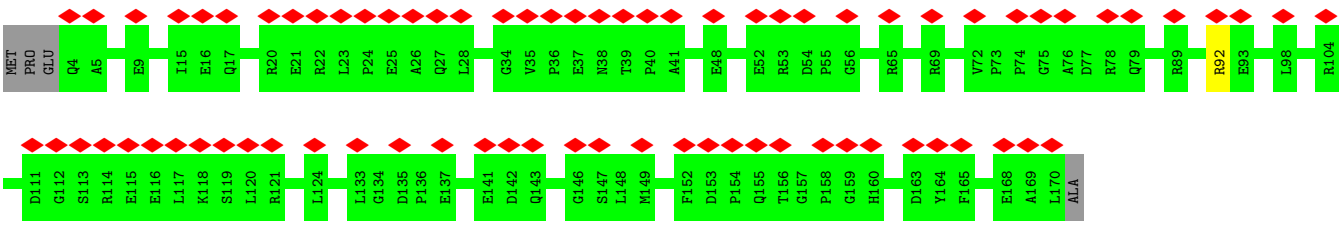




- Molecule 1: Collar PA0615

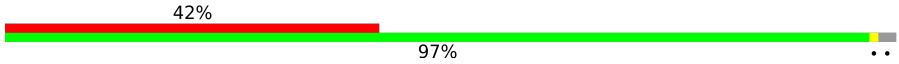
Chain C:

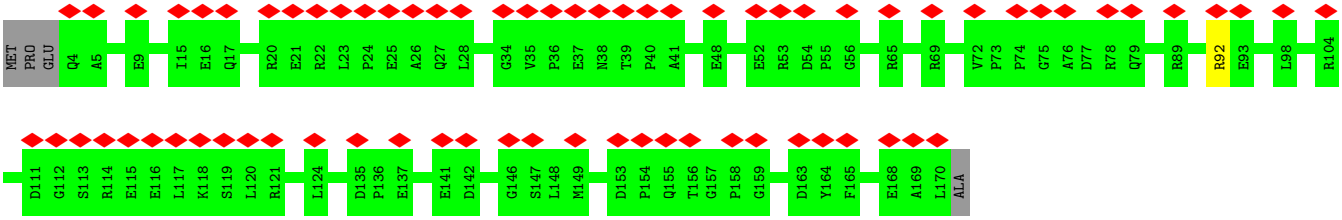




- Molecule 1: Collar PA0615

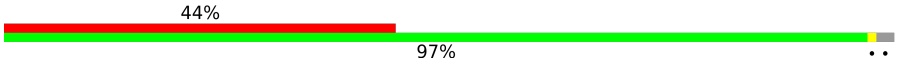
Chain D:

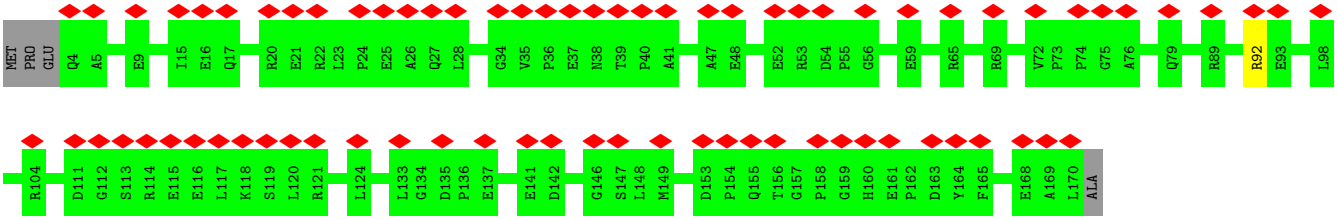




- Molecule 1: Collar PA0615

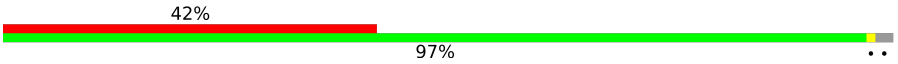
Chain E:

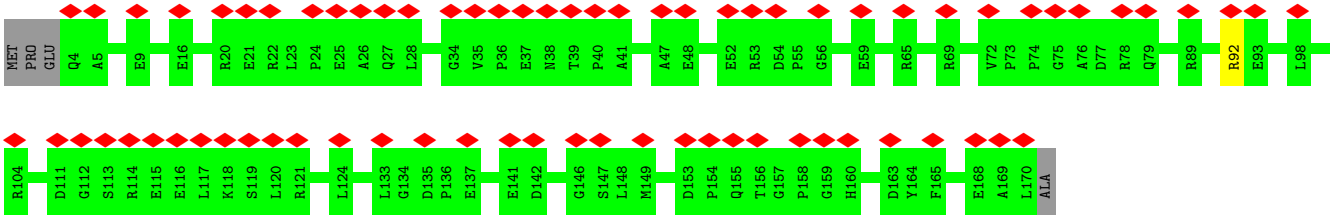




- Molecule 1: Collar PA0615

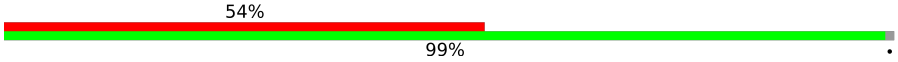
Chain F:

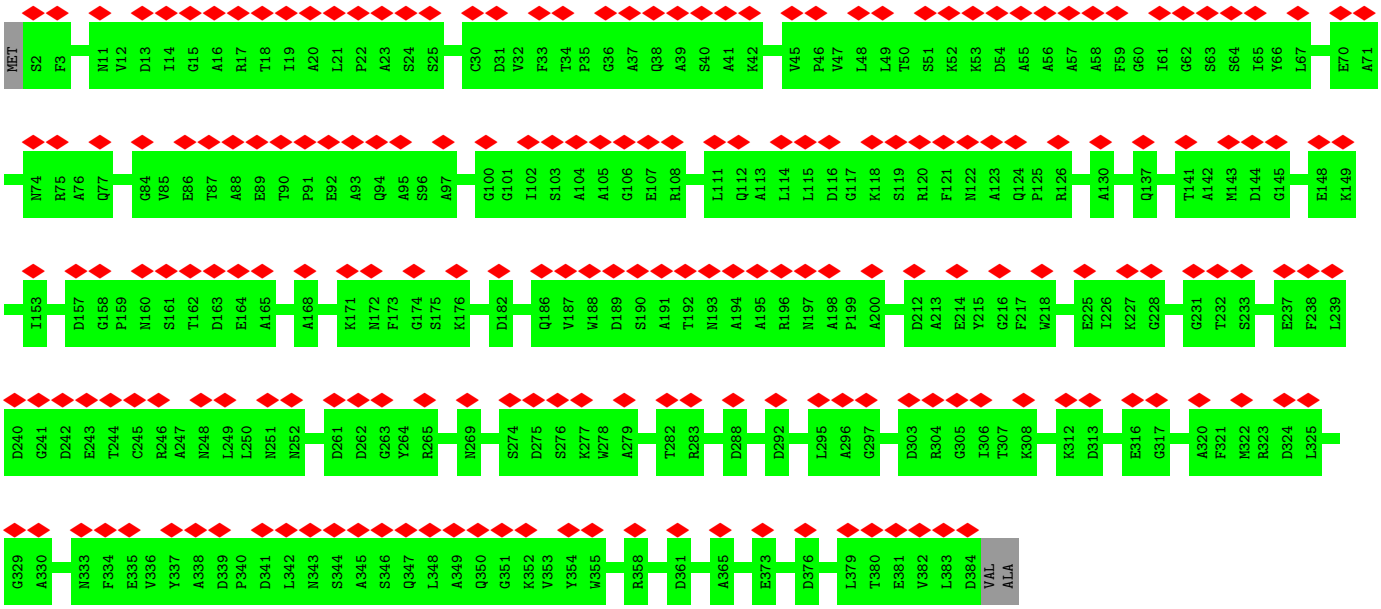




- Molecule 2: Sheath PA0622

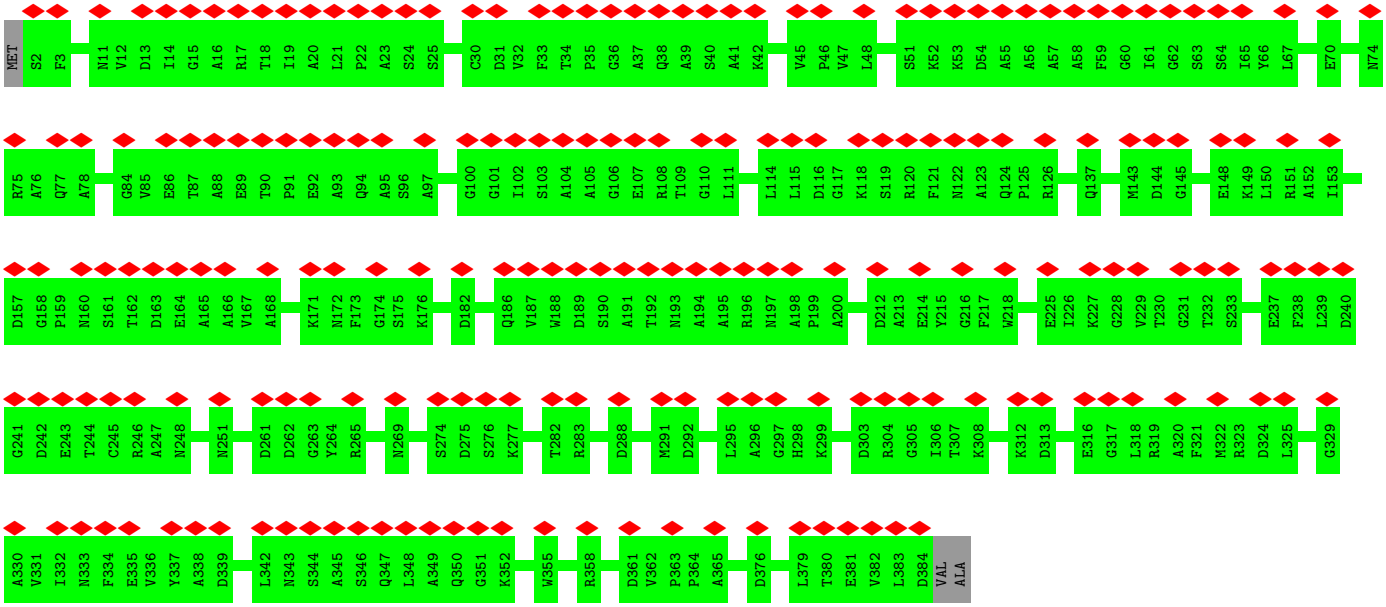
Chain G:





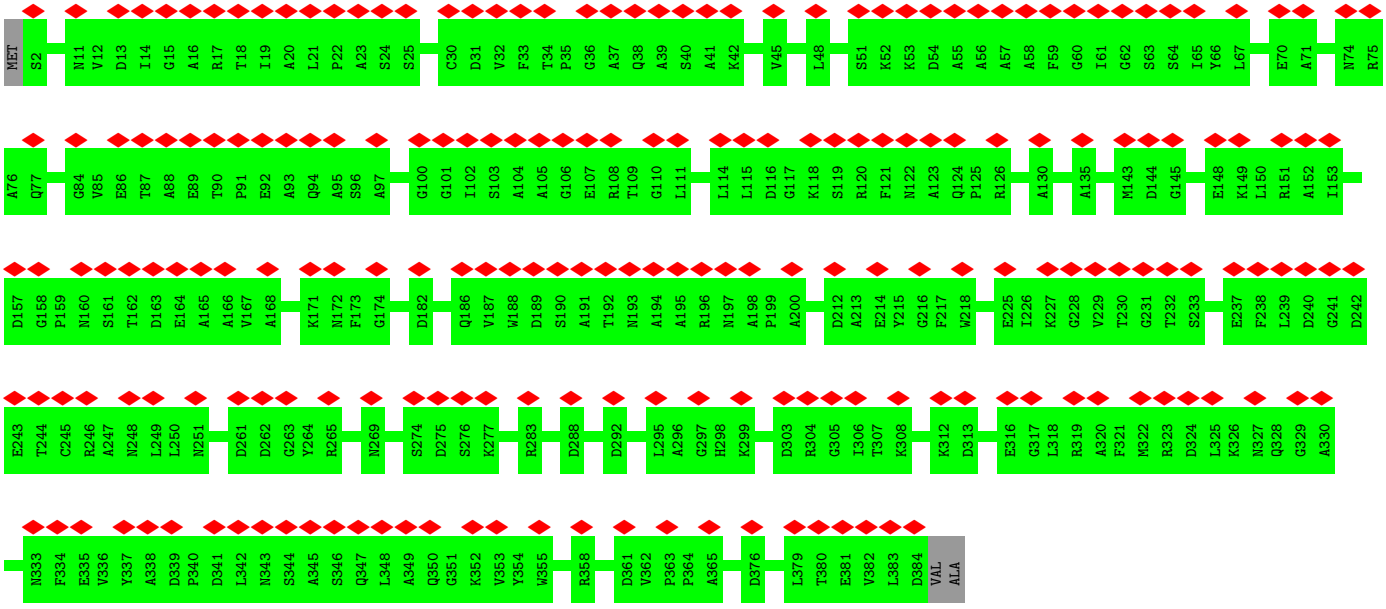
- Molecule 2: Sheath PA0622

Chain H: 54% 99%



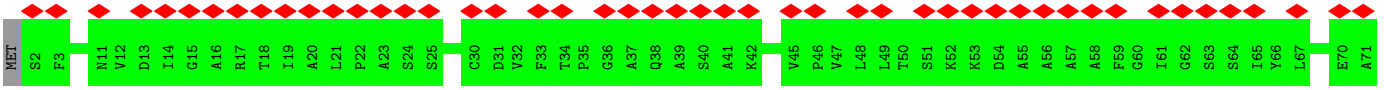
- Molecule 2: Sheath PA0622

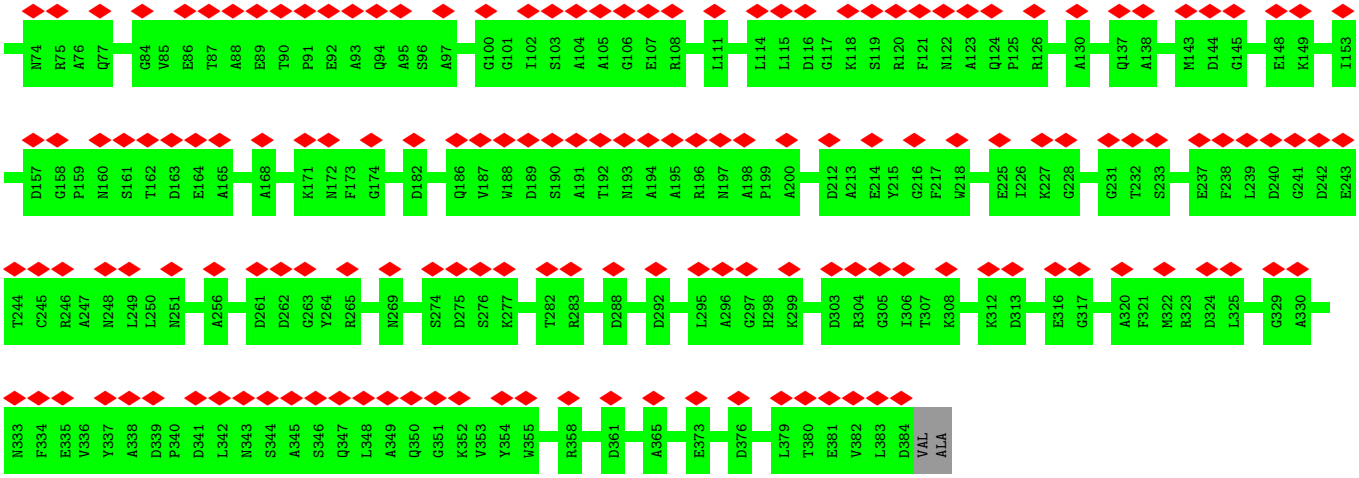
Chain I: 54% 99%



- Molecule 2: Sheath PA0622

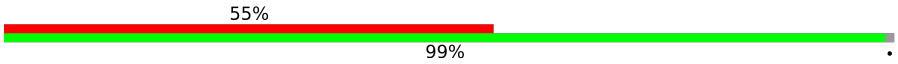
Chain J: 53% 99%





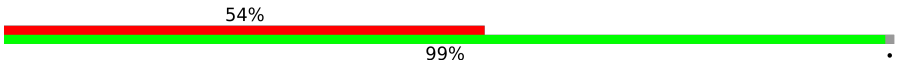
- Molecule 2: Sheath PA0622

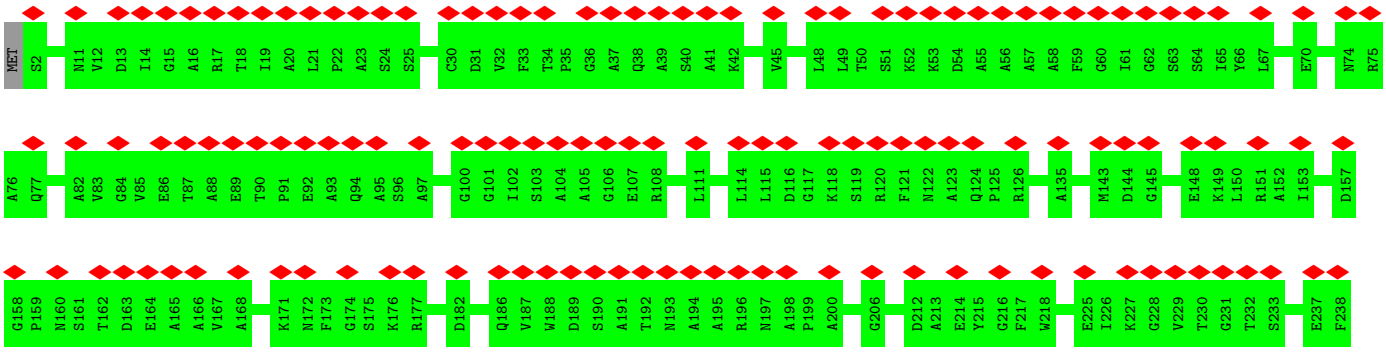
Chain K:

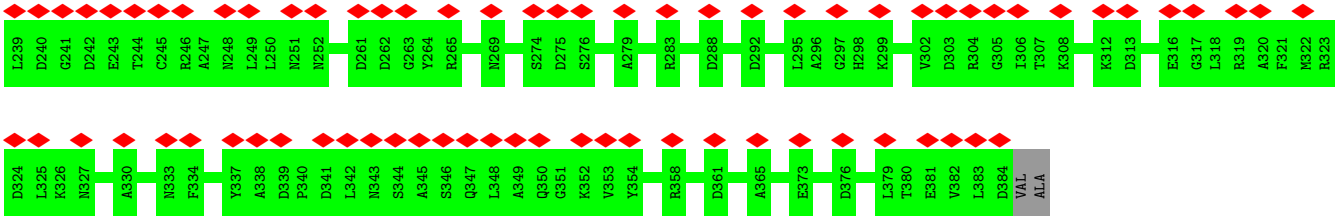


- Molecule 2: Sheath PA0622

Chain L:

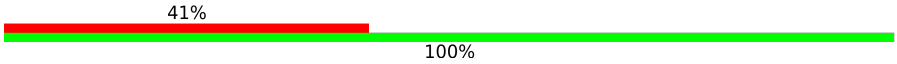


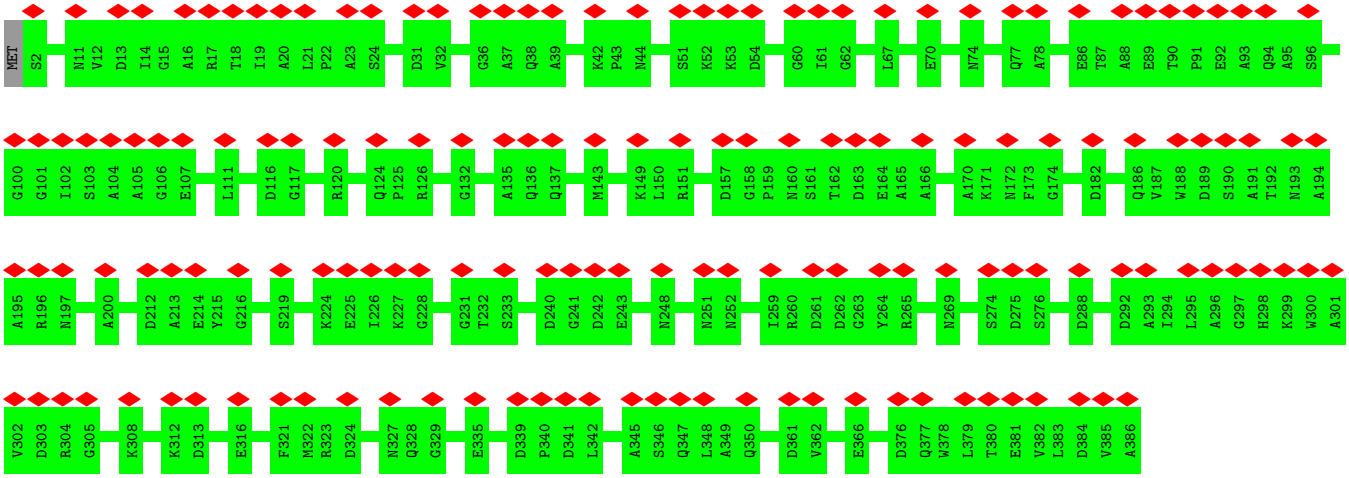




- Molecule 2: Sheath PA0622

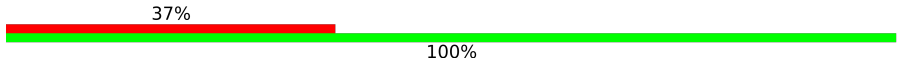
Chain S:

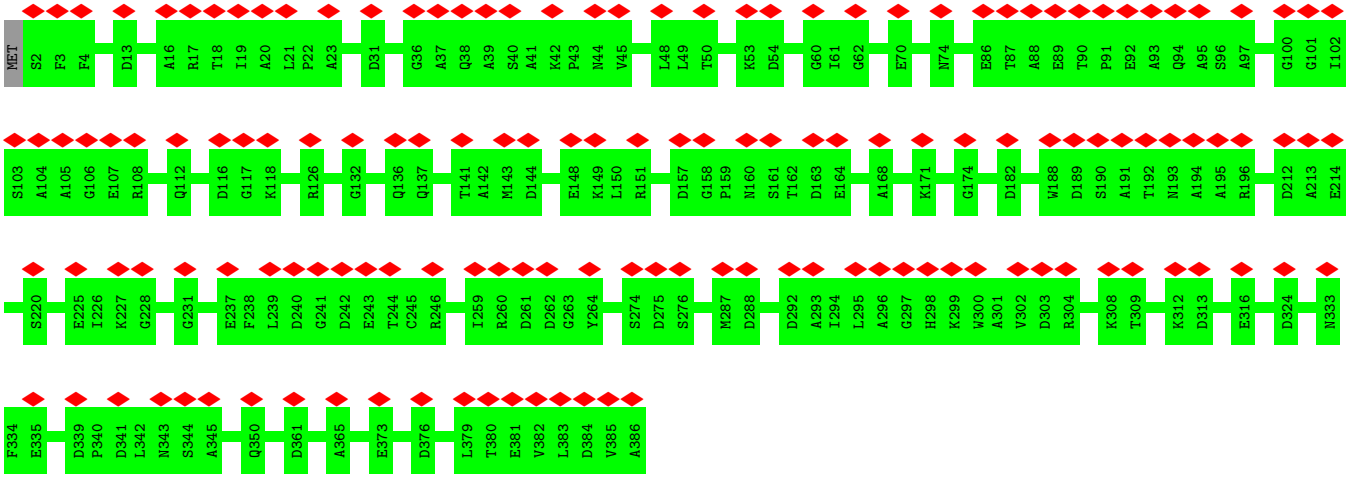




- Molecule 2: Sheath PA0622

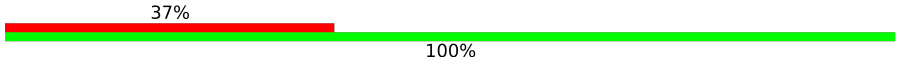
Chain g:

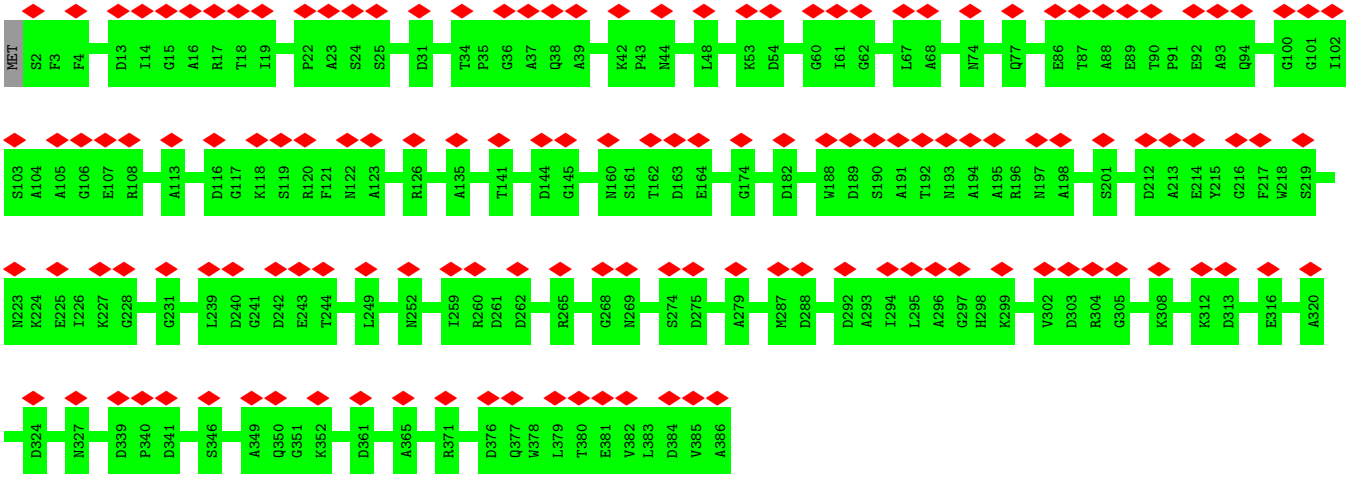




- Molecule 2: Sheath PA0622

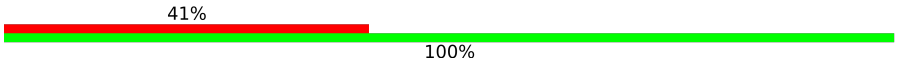
Chain s:

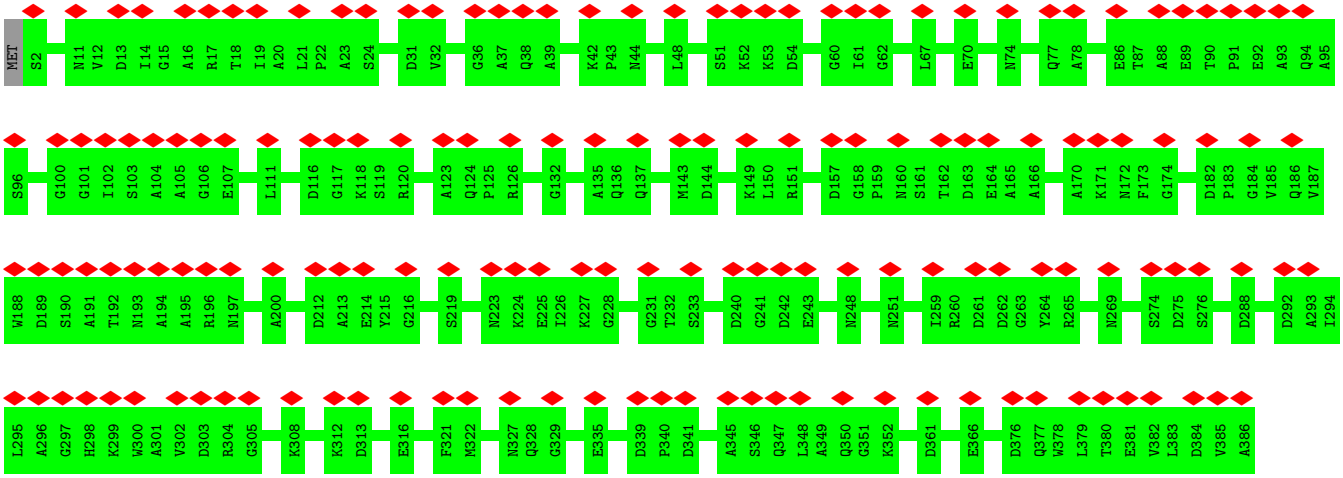




- Molecule 2: Sheath PA0622

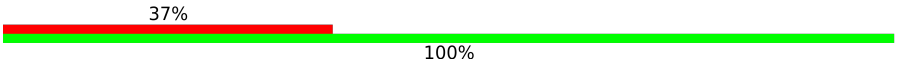
Chain T:

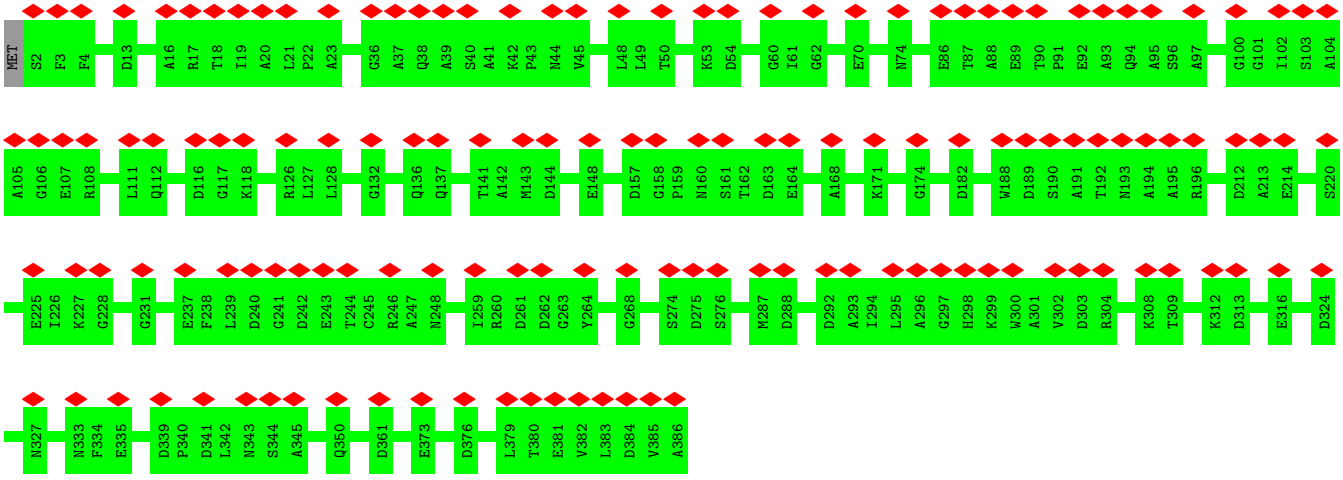




- Molecule 2: Sheath PA0622

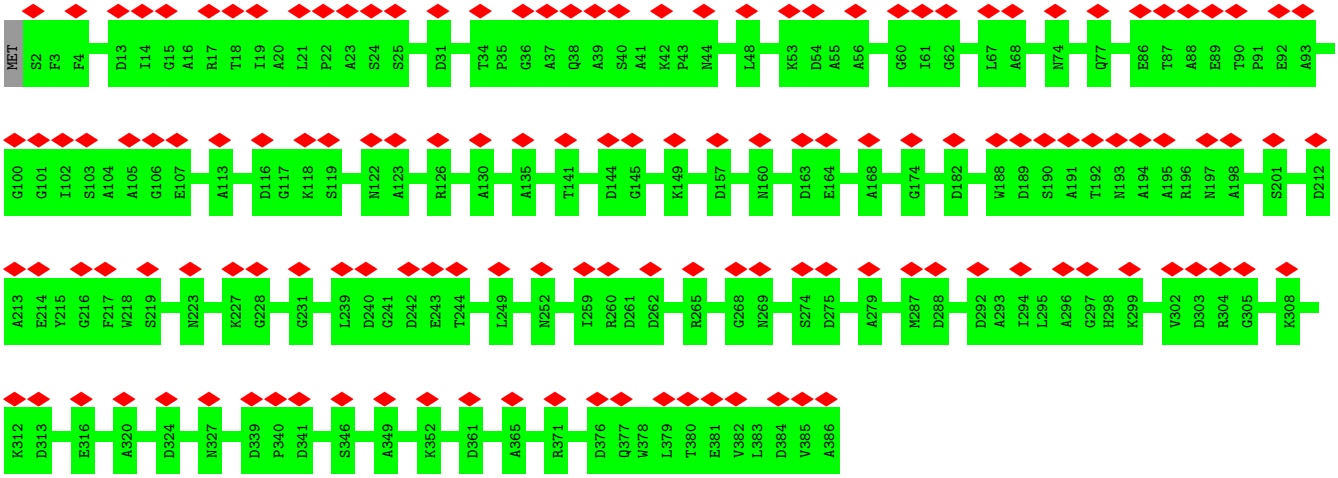
Chain h:





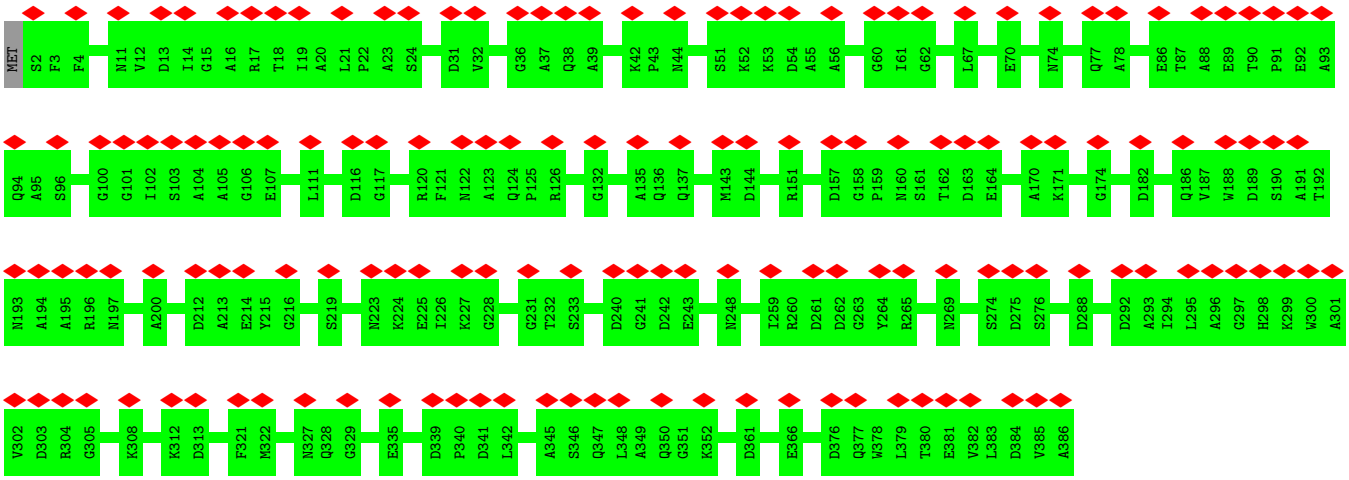
- Molecule 2: Sheath PA0622

Chain t: 36% 100%



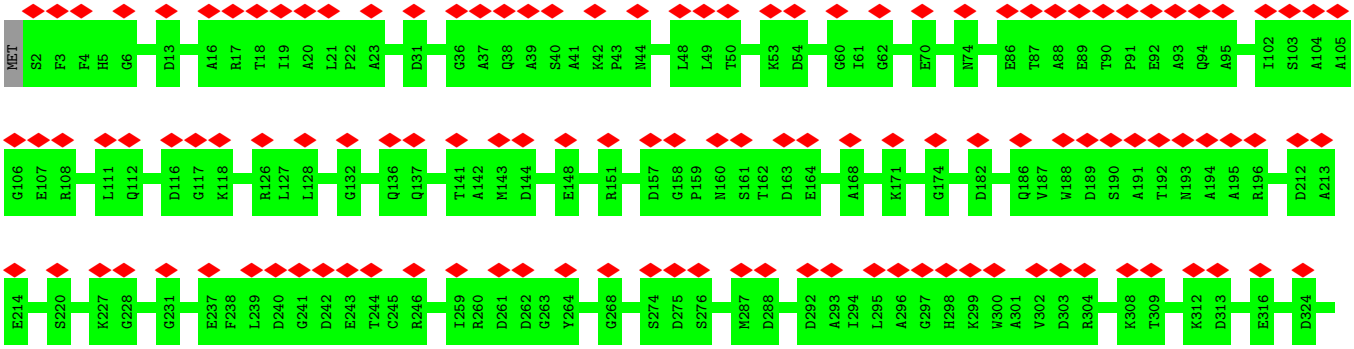
- Molecule 2: Sheath PA0622

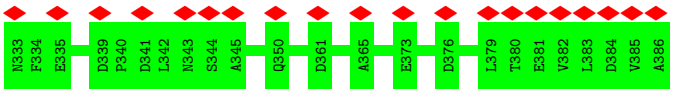
Chain U: 40% 100%



- Molecule 2: Sheath PA0622

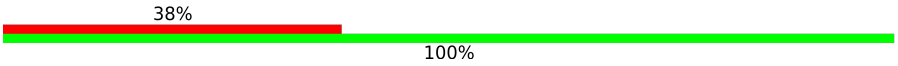
Chain i: 37% 100%

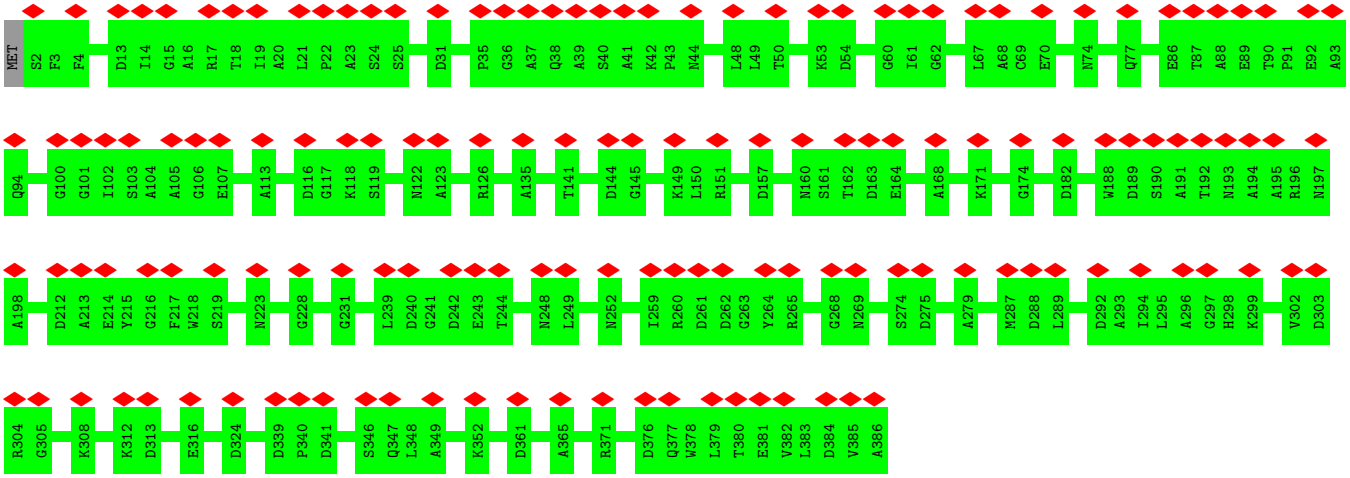




- Molecule 2: Sheath PA0622

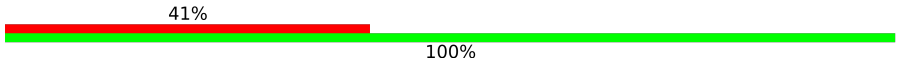
Chain u:

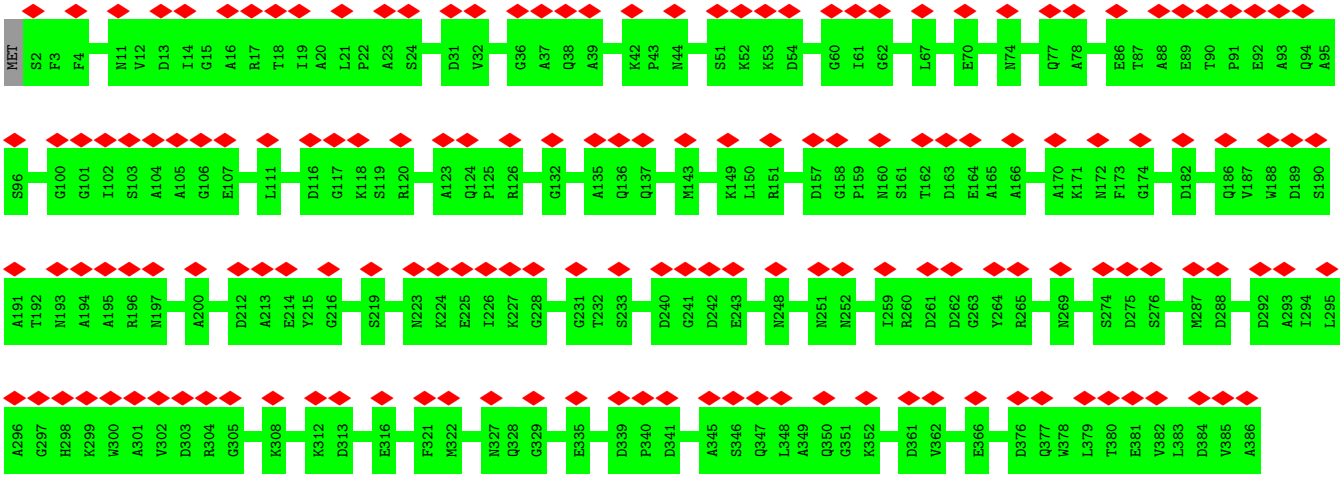




- Molecule 2: Sheath PA0622

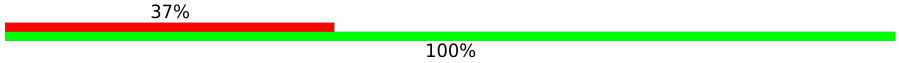
Chain V:

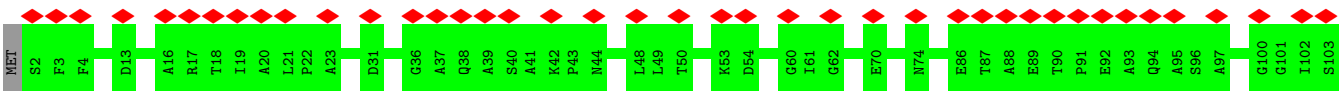


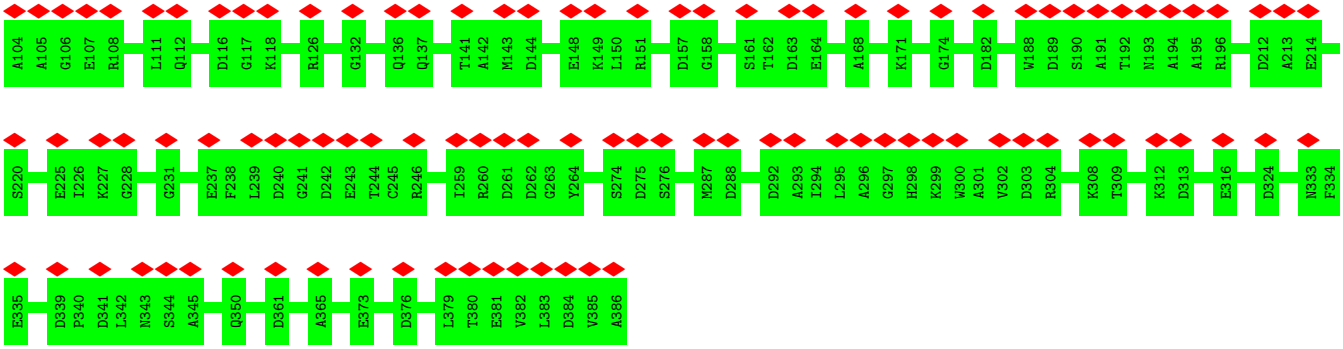


- Molecule 2: Sheath PA0622

Chain j:

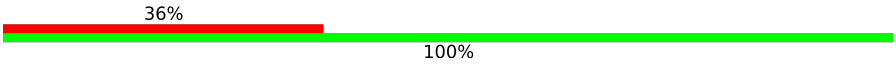


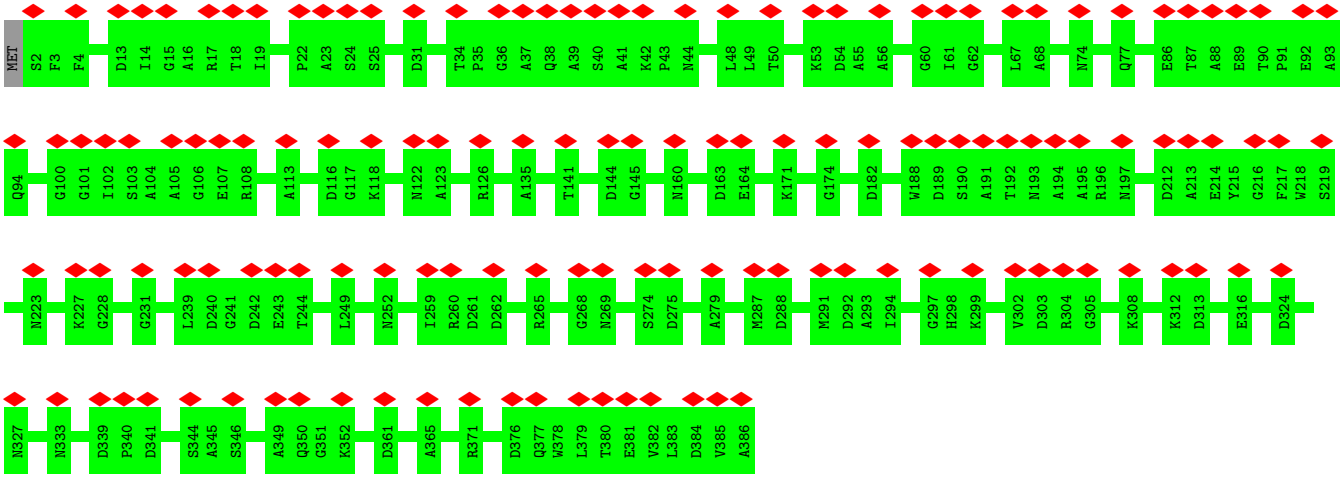




- Molecule 2: Sheath PA0622

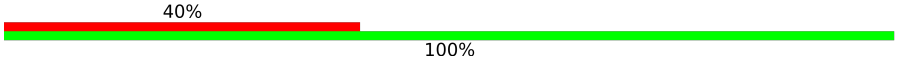
Chain v:

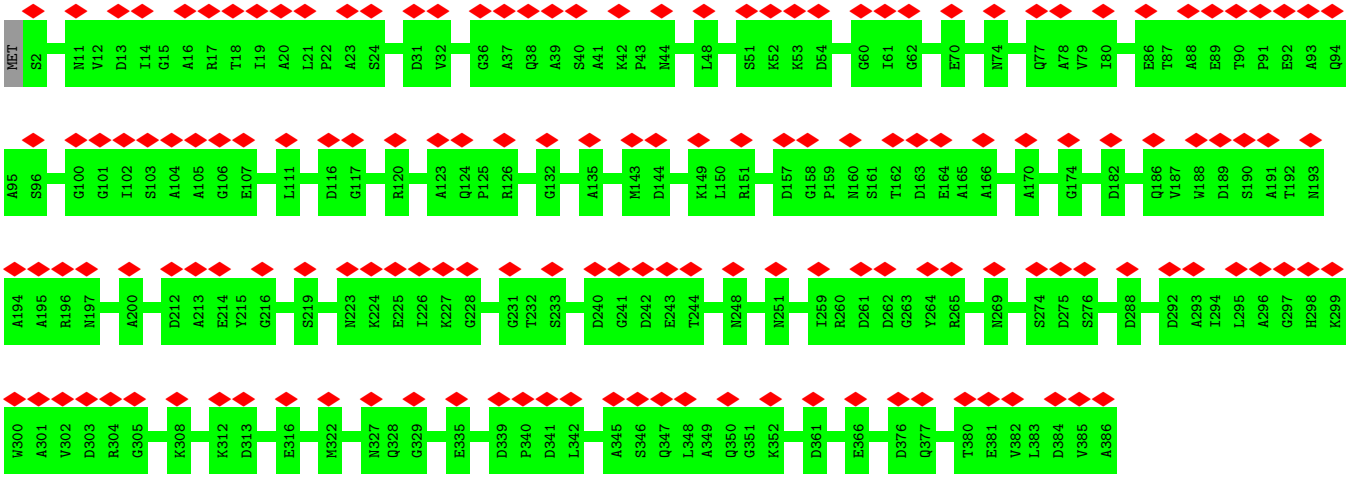




- Molecule 2: Sheath PA0622

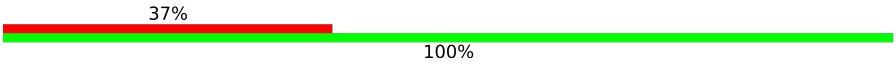
Chain W:

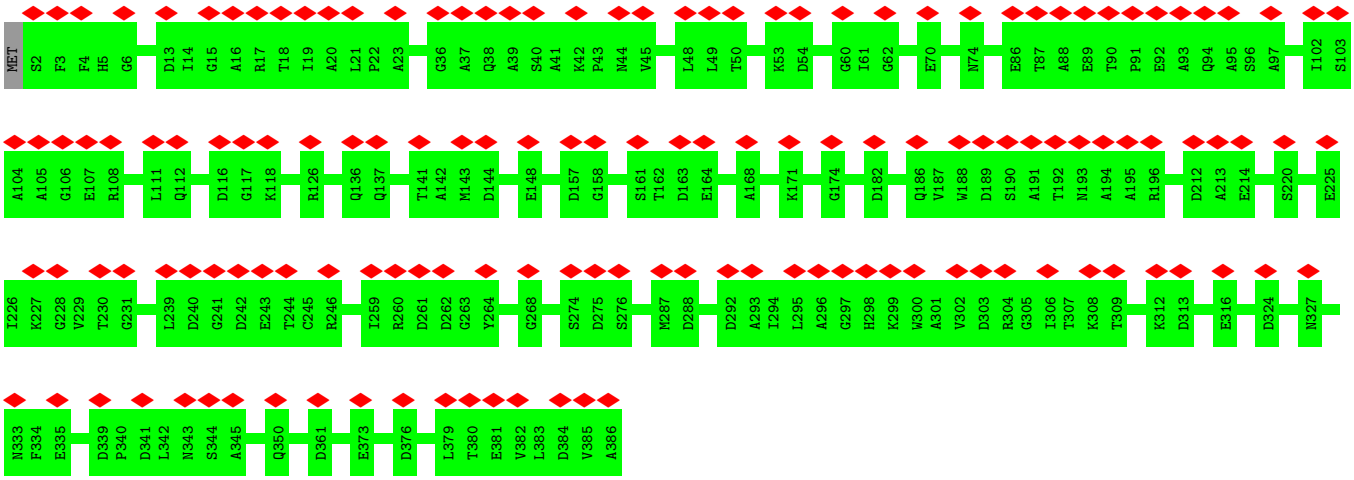




- Molecule 2: Sheath PA0622

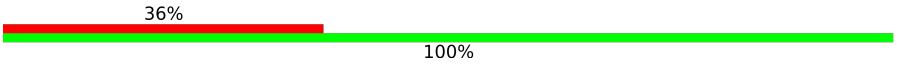
Chain k:

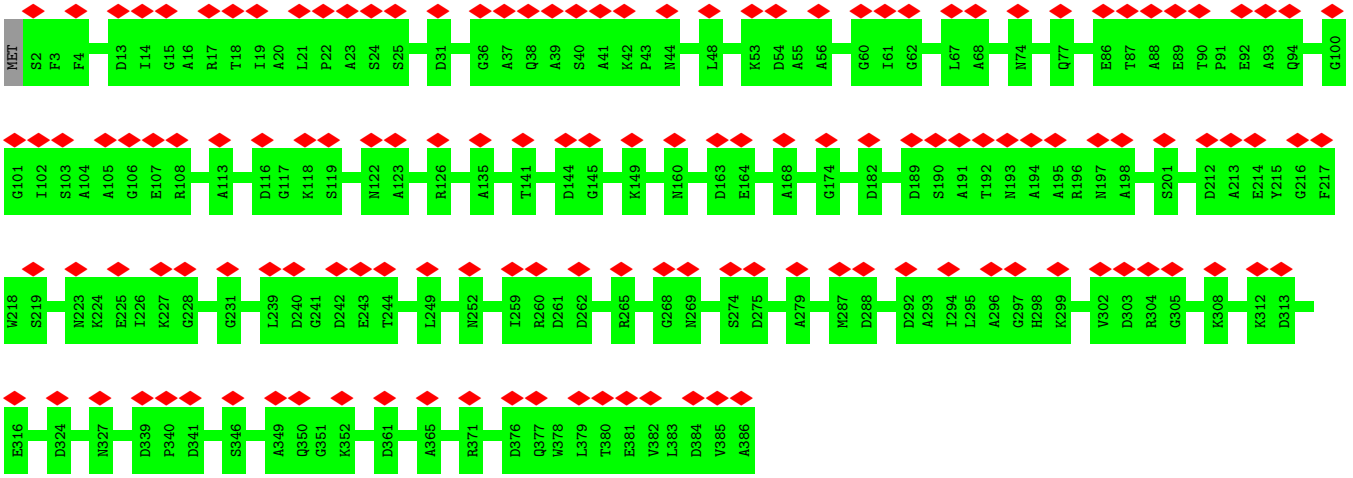




- Molecule 2: Sheath PA0622

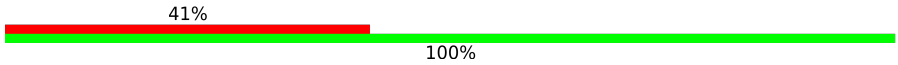
Chain w:

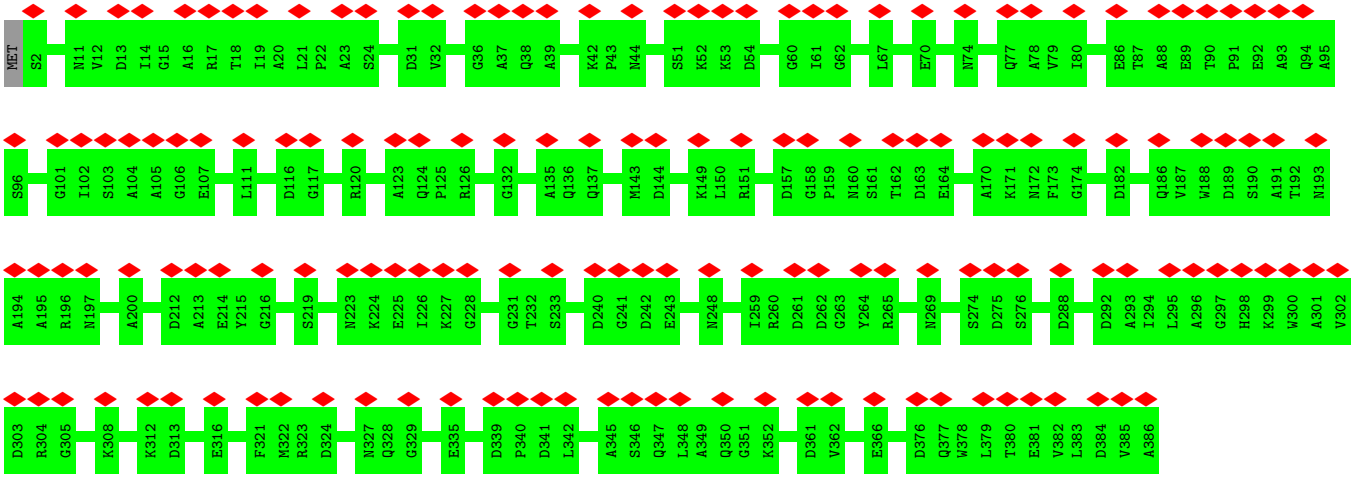




- Molecule 2: Sheath PA0622

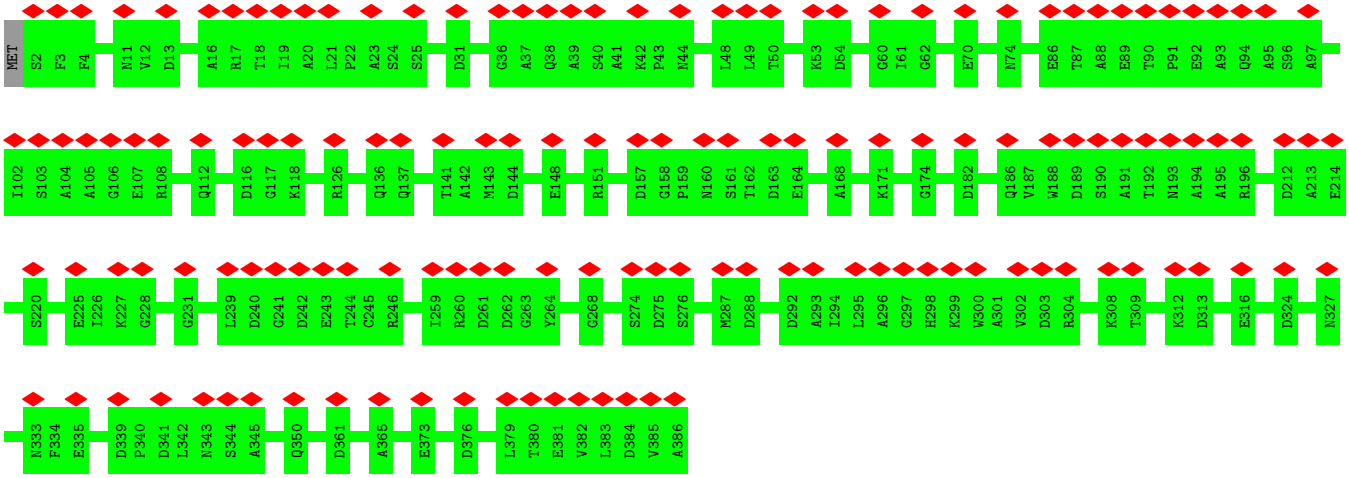
Chain X:





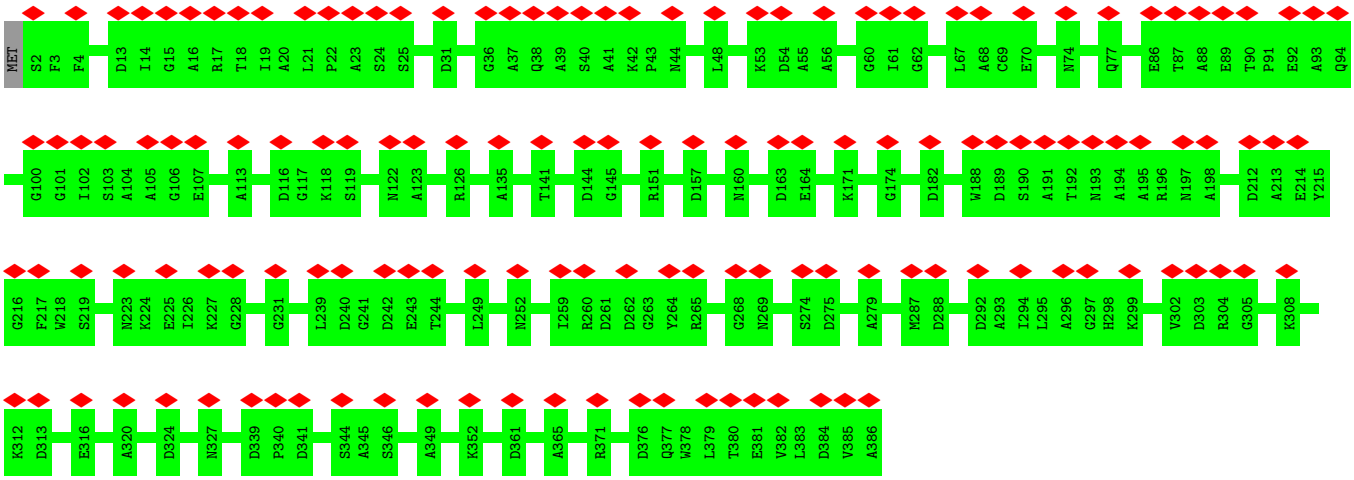
- Molecule 2: Sheath PA0622

Chain l: 37% 100%



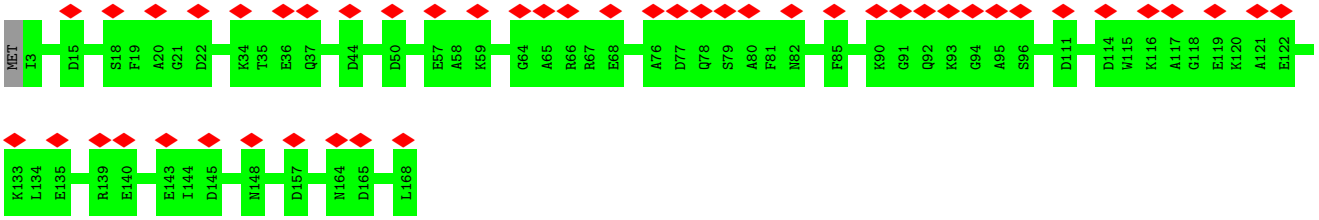
- Molecule 2: Sheath PA0622

Chain x: 37% 100%



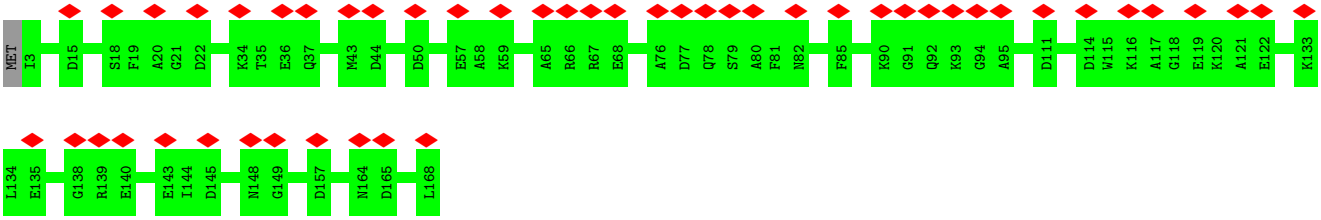
- Molecule 3: Tube PA0623

Chain M: 28% 99%



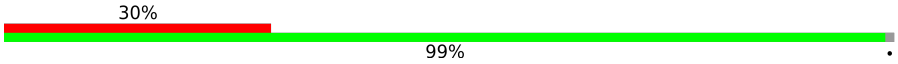
- Molecule 3: Tube PA0623

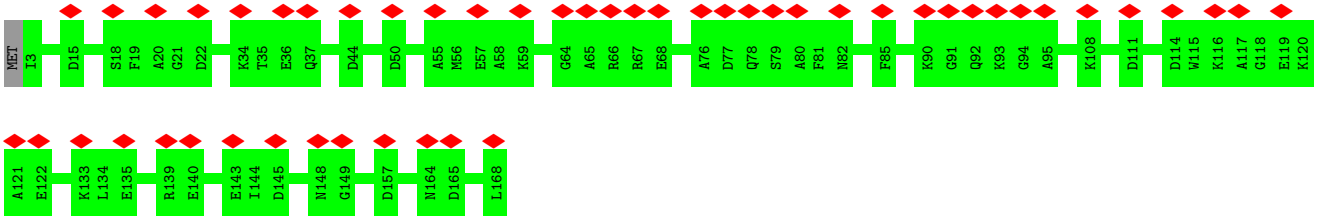
Chain N: 29% 99%



• Molecule 3: Tube PA0623

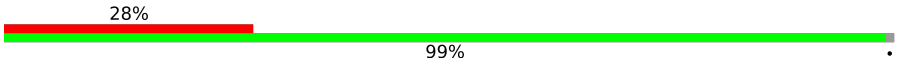
Chain O:

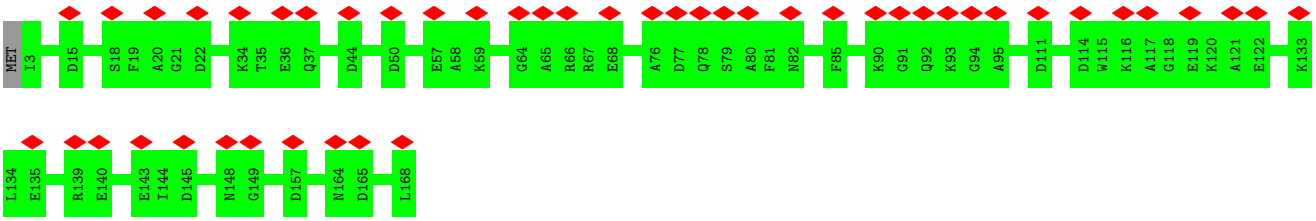




• Molecule 3: Tube PA0623

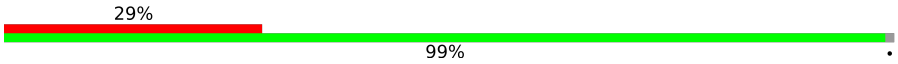
Chain P:

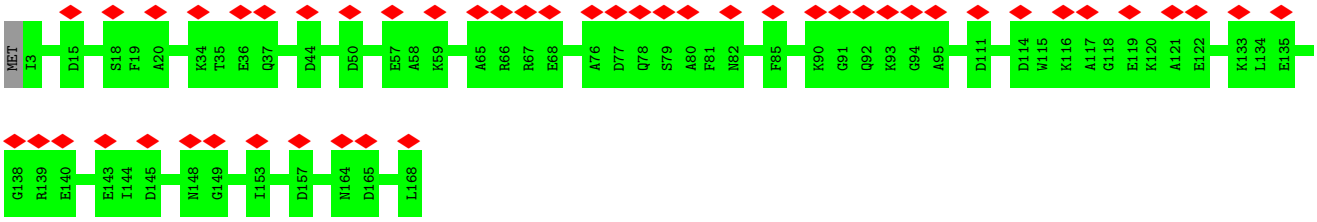




• Molecule 3: Tube PA0623

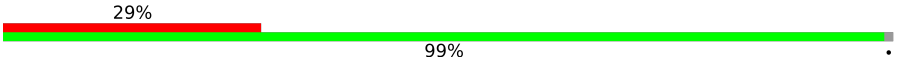
Chain Q:

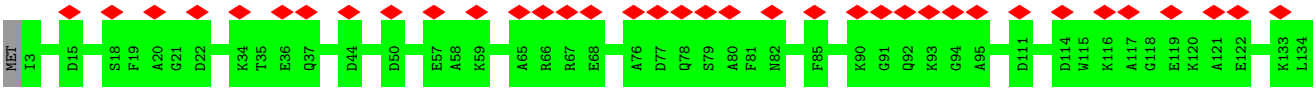


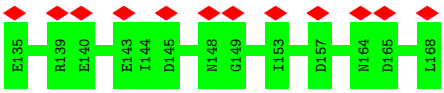


• Molecule 3: Tube PA0623

Chain R:

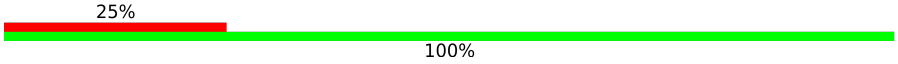


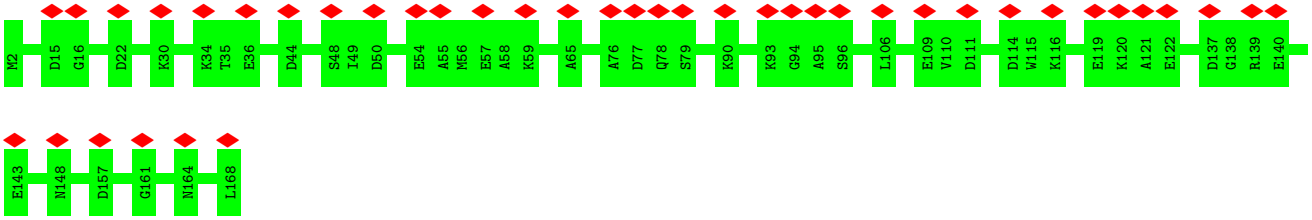




• Molecule 3: Tube PA0623

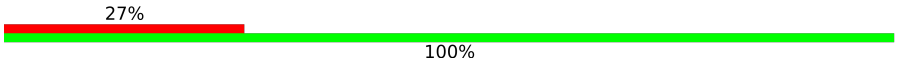
Chain a:

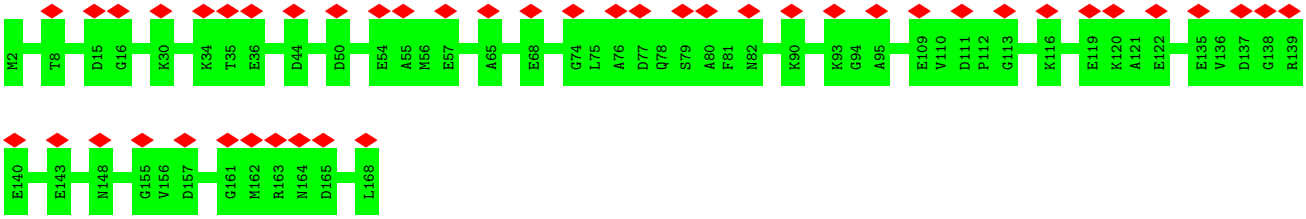




• Molecule 3: Tube PA0623

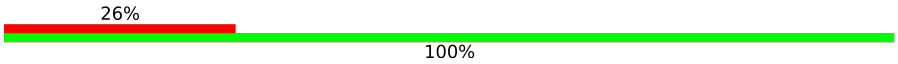
Chain 0:

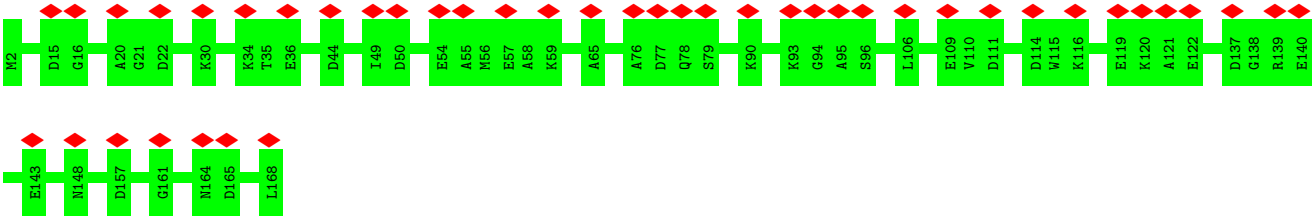




• Molecule 3: Tube PA0623

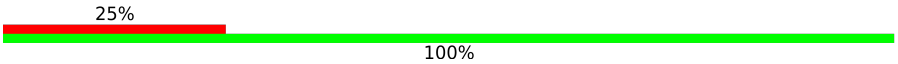
Chain e:

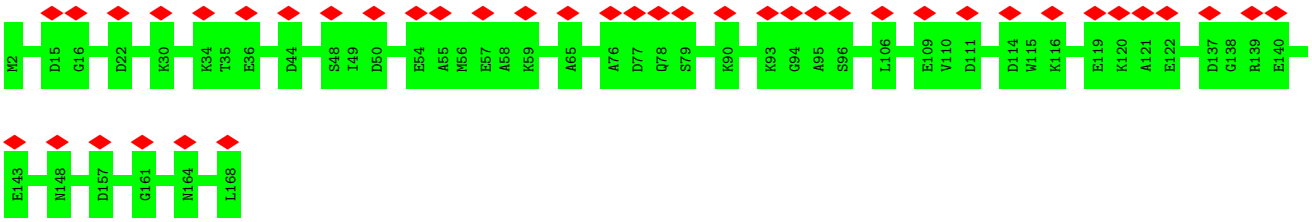




• Molecule 3: Tube PA0623

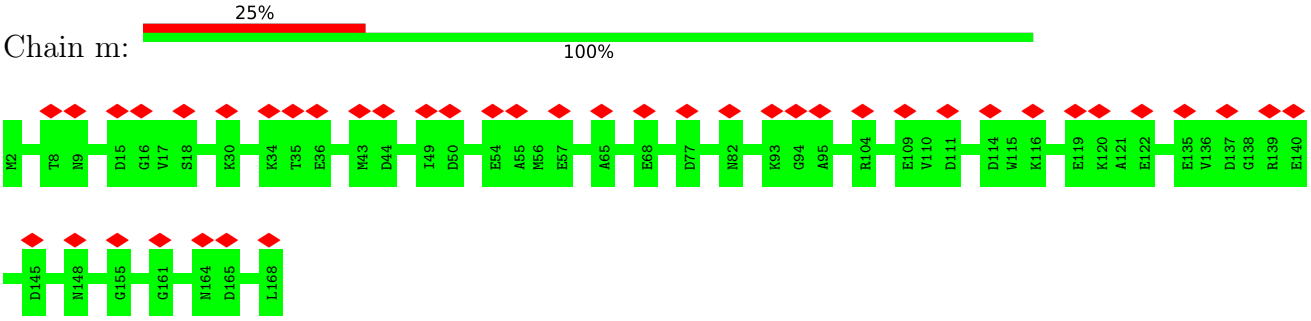
Chain d:





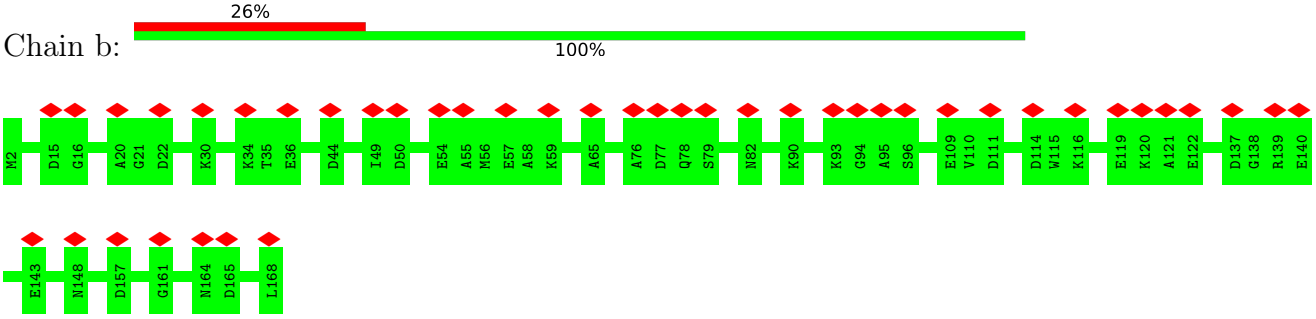
• Molecule 3: Tube PA0623

Chain m:



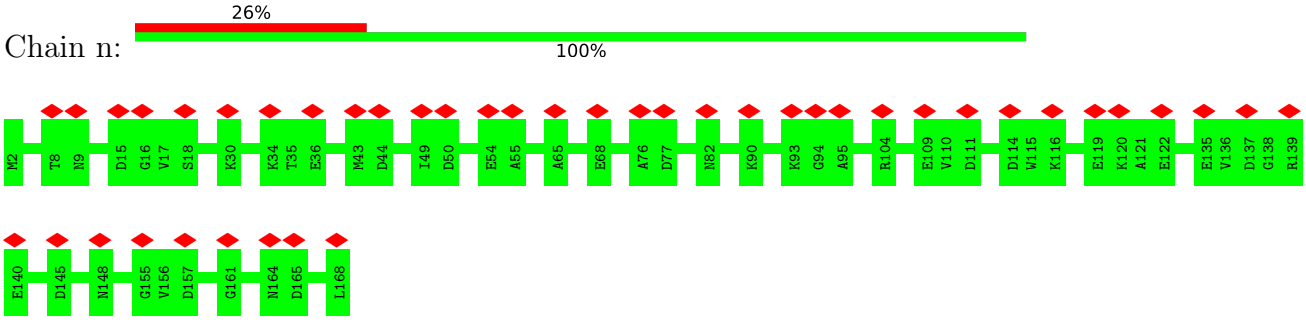
- Molecule 3: Tube PA0623

Chain b:



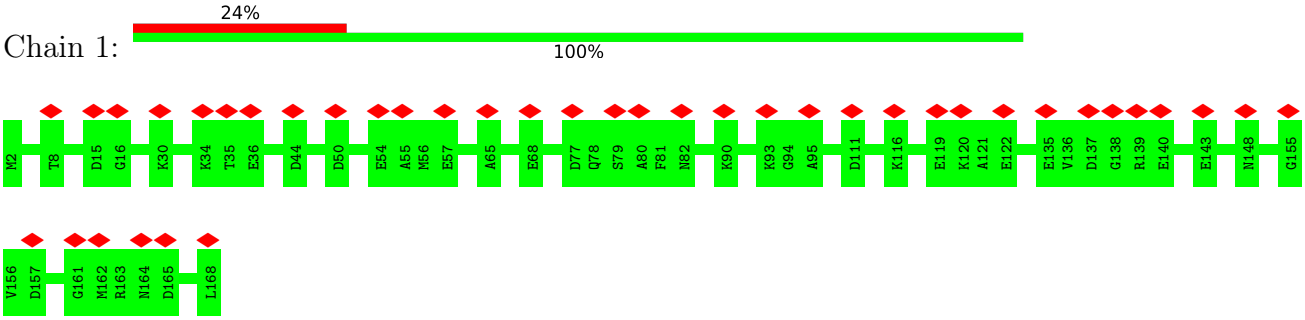
- Molecule 3: Tube PA0623

Chain n:



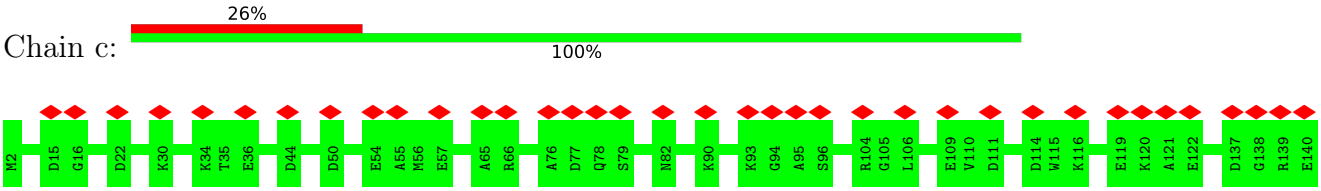
- Molecule 3: Tube PA0623

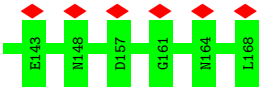
Chain 1:



- Molecule 3: Tube PA0623

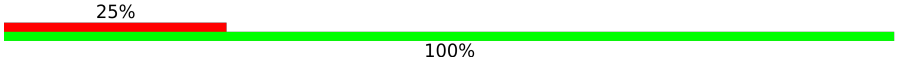
Chain c:

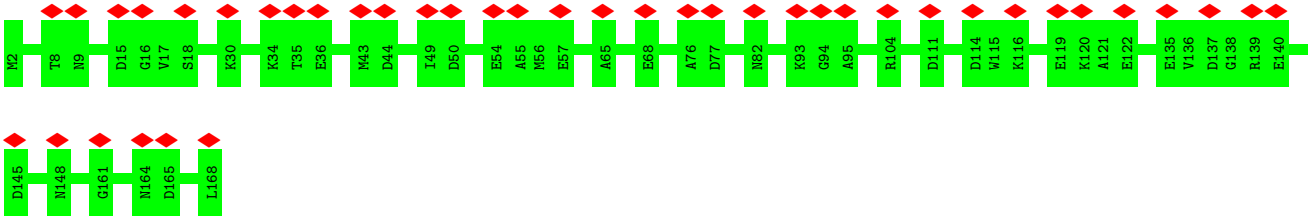




• Molecule 3: Tube PA0623

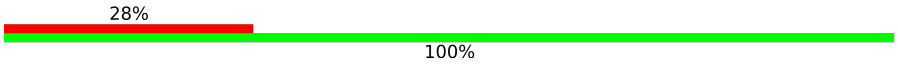
Chain o:

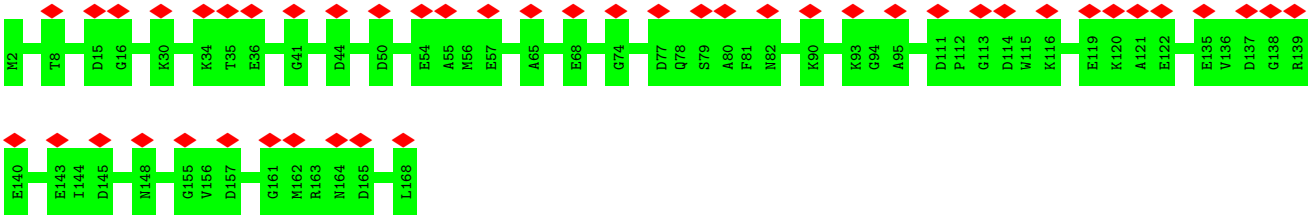




• Molecule 3: Tube PA0623

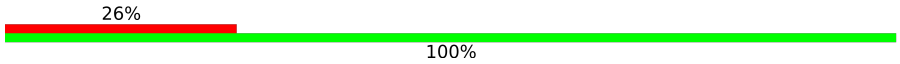
Chain 2:

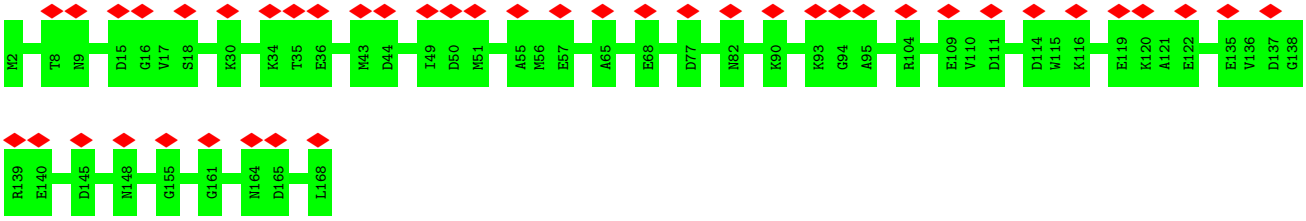




• Molecule 3: Tube PA0623

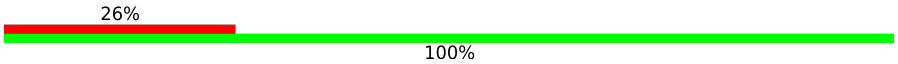
Chain p:

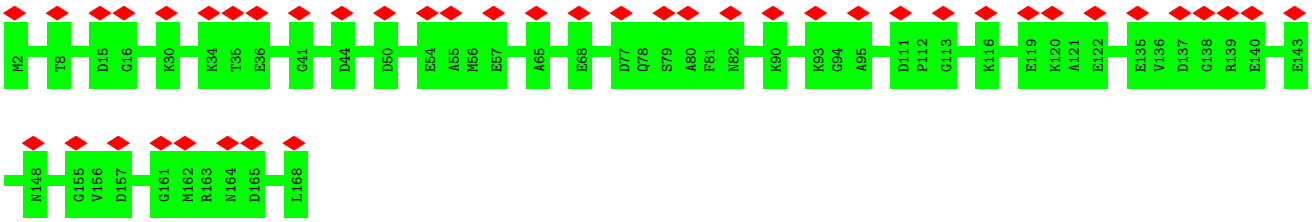




• Molecule 3: Tube PA0623

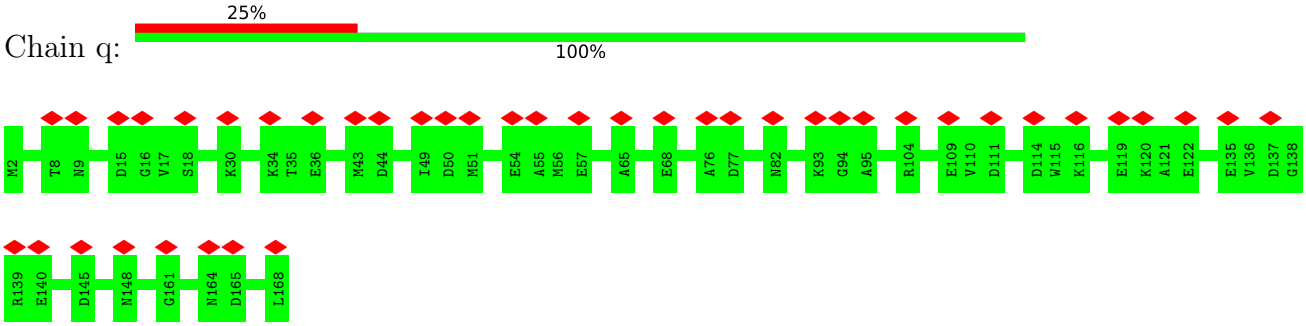
Chain 3:





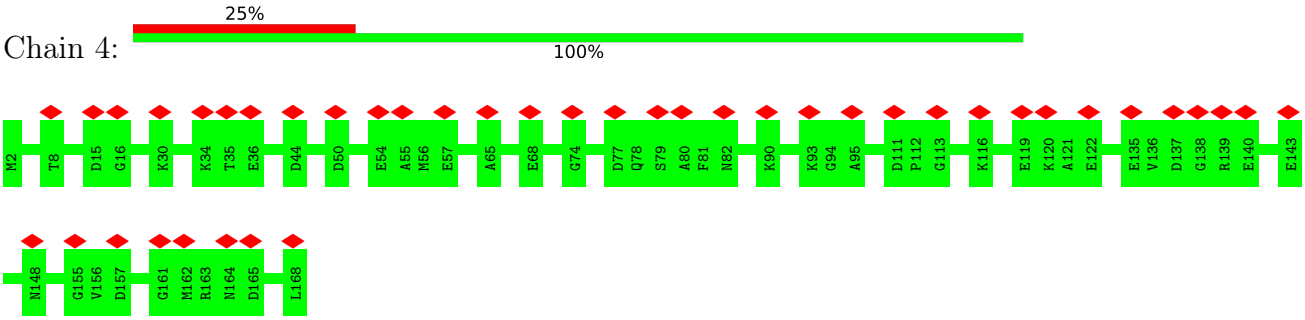
• Molecule 3: Tube PA0623

Chain q:



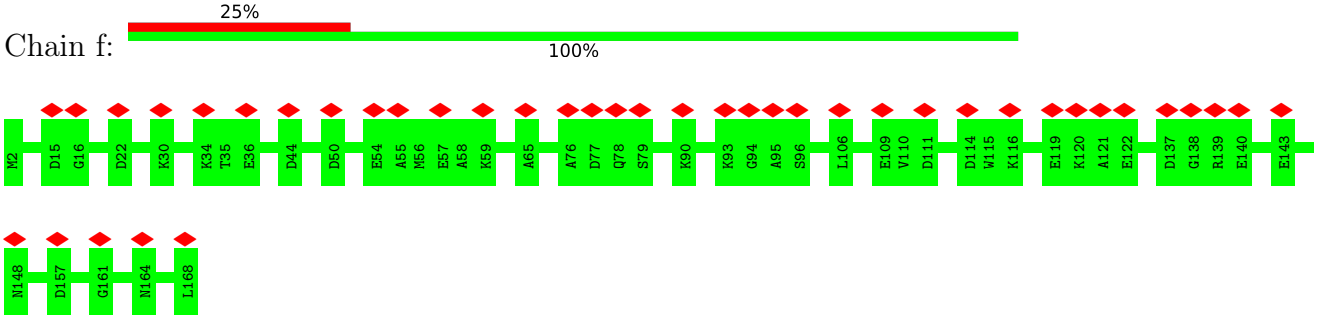
- Molecule 3: Tube PA0623

Chain 4:



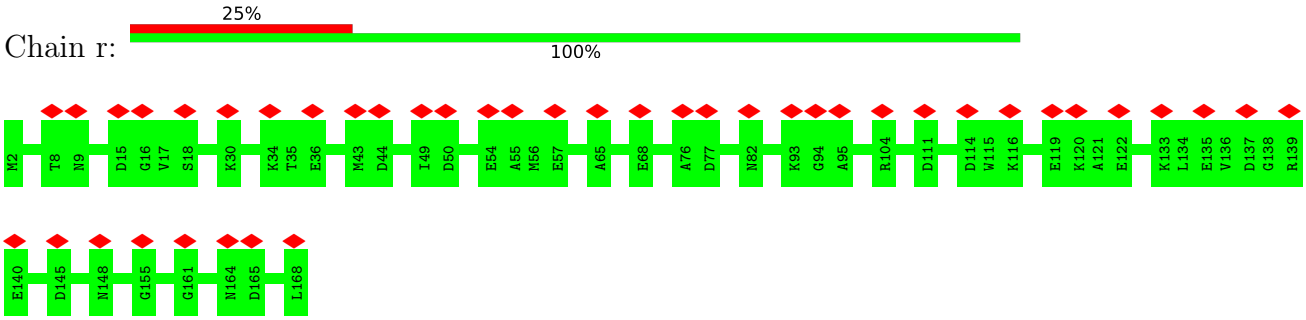
- Molecule 3: Tube PA0623

Chain f:



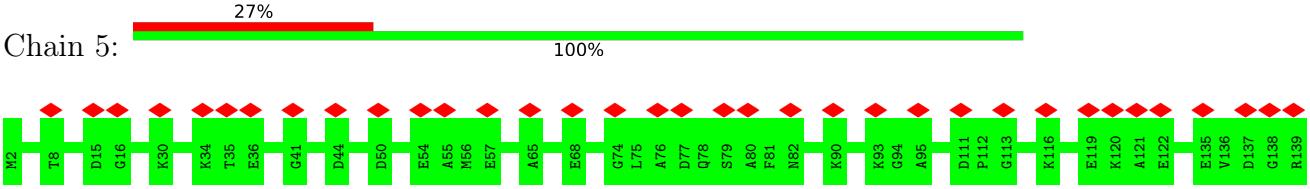
- Molecule 3: Tube PA0623

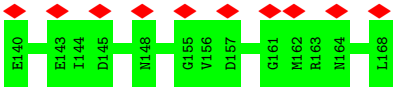
Chain r:



- Molecule 3: Tube PA0623

Chain 5:




E140
E143
I144
D145
N148
G155
V156
D157
G161
M162
R163
N164
L168

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	4110	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.098	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.037	Depositor
Map size (Å)	333.12, 333.12, 333.12	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.041, 1.041, 1.041	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	A	0.37	0/1340	0.62	0/1833
1	B	0.37	0/1340	0.62	0/1833
1	C	0.37	0/1340	0.62	0/1833
1	D	0.37	0/1340	0.62	0/1833
1	E	0.37	0/1340	0.62	0/1833
1	F	0.37	0/1340	0.62	0/1833
2	G	0.36	0/2942	0.59	0/4010
2	H	0.36	0/2942	0.59	0/4010
2	I	0.36	0/2942	0.59	0/4010
2	J	0.36	0/2942	0.59	0/4010
2	K	0.36	0/2942	0.59	0/4010
2	L	0.36	0/2942	0.59	0/4010
2	S	0.37	0/2955	0.58	0/4027
2	T	0.37	0/2955	0.59	0/4027
2	U	0.37	0/2955	0.59	0/4027
2	V	0.37	0/2955	0.59	0/4027
2	W	0.37	0/2955	0.58	0/4027
2	X	0.37	0/2955	0.59	0/4027
2	g	0.38	0/2955	0.60	0/4027
2	h	0.38	0/2955	0.60	0/4027
2	i	0.38	0/2955	0.60	0/4027
2	j	0.38	0/2955	0.60	0/4027
2	k	0.38	0/2955	0.60	0/4027
2	l	0.38	0/2955	0.60	0/4027
2	s	0.36	0/2955	0.59	0/4027
2	t	0.36	0/2955	0.60	0/4027
2	u	0.36	0/2955	0.59	0/4027
2	v	0.36	0/2955	0.59	0/4027
2	w	0.36	0/2955	0.59	0/4027
2	x	0.36	0/2955	0.59	0/4027
3	0	0.44	0/1285	0.64	0/1734
3	1	0.44	0/1285	0.64	0/1734
3	2	0.44	0/1285	0.64	0/1734
3	3	0.44	0/1285	0.64	0/1734

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	4	0.44	0/1285	0.64	0/1734
3	5	0.44	0/1285	0.64	0/1734
3	M	0.39	0/1277	0.59	0/1724
3	N	0.39	0/1277	0.59	0/1724
3	O	0.39	0/1277	0.59	0/1724
3	P	0.39	0/1277	0.59	0/1724
3	Q	0.39	0/1277	0.59	0/1724
3	R	0.39	0/1277	0.59	0/1724
3	a	0.44	0/1285	0.64	0/1734
3	b	0.44	0/1285	0.64	0/1734
3	c	0.44	0/1285	0.64	0/1734
3	d	0.44	0/1285	0.64	0/1734
3	e	0.44	0/1285	0.64	0/1734
3	f	0.44	0/1285	0.64	0/1734
3	m	0.48	0/1285	0.63	0/1734
3	n	0.48	0/1285	0.63	0/1734
3	o	0.48	0/1285	0.63	0/1734
3	p	0.48	0/1285	0.63	0/1734
3	q	0.48	0/1285	0.63	0/1734
3	r	0.48	0/1285	0.63	0/1734
All	All	0.39	0/109674	0.60	0/149100

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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	165/171 (96%)	150 (91%)	15 (9%)	0	100	100
1	B	165/171 (96%)	150 (91%)	15 (9%)	0	100	100
1	C	165/171 (96%)	149 (90%)	16 (10%)	0	100	100
1	D	165/171 (96%)	149 (90%)	16 (10%)	0	100	100
1	E	165/171 (96%)	149 (90%)	16 (10%)	0	100	100
1	F	165/171 (96%)	150 (91%)	15 (9%)	0	100	100
2	G	381/386 (99%)	340 (89%)	41 (11%)	0	100	100
2	H	381/386 (99%)	340 (89%)	41 (11%)	0	100	100
2	I	381/386 (99%)	340 (89%)	41 (11%)	0	100	100
2	J	381/386 (99%)	340 (89%)	41 (11%)	0	100	100
2	K	381/386 (99%)	340 (89%)	41 (11%)	0	100	100
2	L	381/386 (99%)	340 (89%)	41 (11%)	0	100	100
2	S	383/386 (99%)	338 (88%)	45 (12%)	0	100	100
2	T	383/386 (99%)	338 (88%)	45 (12%)	0	100	100
2	U	383/386 (99%)	339 (88%)	44 (12%)	0	100	100
2	V	383/386 (99%)	338 (88%)	45 (12%)	0	100	100
2	W	383/386 (99%)	338 (88%)	45 (12%)	0	100	100
2	X	383/386 (99%)	338 (88%)	45 (12%)	0	100	100
2	g	383/386 (99%)	343 (90%)	40 (10%)	0	100	100
2	h	383/386 (99%)	343 (90%)	40 (10%)	0	100	100
2	i	383/386 (99%)	343 (90%)	40 (10%)	0	100	100
2	j	383/386 (99%)	343 (90%)	40 (10%)	0	100	100
2	k	383/386 (99%)	343 (90%)	40 (10%)	0	100	100
2	l	383/386 (99%)	343 (90%)	40 (10%)	0	100	100
2	s	383/386 (99%)	351 (92%)	32 (8%)	0	100	100
2	t	383/386 (99%)	348 (91%)	35 (9%)	0	100	100
2	u	383/386 (99%)	349 (91%)	34 (9%)	0	100	100
2	v	383/386 (99%)	350 (91%)	33 (9%)	0	100	100
2	w	383/386 (99%)	350 (91%)	33 (9%)	0	100	100
2	x	383/386 (99%)	349 (91%)	34 (9%)	0	100	100
3	0	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
3	1	165/167 (99%)	147 (89%)	18 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
3	3	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
3	4	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
3	5	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
3	M	164/167 (98%)	137 (84%)	27 (16%)	0	100	100
3	N	164/167 (98%)	137 (84%)	27 (16%)	0	100	100
3	O	164/167 (98%)	138 (84%)	26 (16%)	0	100	100
3	P	164/167 (98%)	137 (84%)	27 (16%)	0	100	100
3	Q	164/167 (98%)	138 (84%)	26 (16%)	0	100	100
3	R	164/167 (98%)	137 (84%)	27 (16%)	0	100	100
3	a	165/167 (99%)	144 (87%)	21 (13%)	0	100	100
3	b	165/167 (99%)	145 (88%)	20 (12%)	0	100	100
3	c	165/167 (99%)	144 (87%)	21 (13%)	0	100	100
3	d	165/167 (99%)	144 (87%)	21 (13%)	0	100	100
3	e	165/167 (99%)	144 (87%)	21 (13%)	0	100	100
3	f	165/167 (99%)	144 (87%)	21 (13%)	0	100	100
3	m	165/167 (99%)	146 (88%)	19 (12%)	0	100	100
3	n	165/167 (99%)	146 (88%)	19 (12%)	0	100	100
3	o	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
3	p	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
3	q	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
3	r	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
All	All	14124/14298 (99%)	12572 (89%)	1552 (11%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	138/141 (98%)	137 (99%)	1 (1%)	84	91
1	B	138/141 (98%)	137 (99%)	1 (1%)	84	91
1	C	138/141 (98%)	137 (99%)	1 (1%)	84	91
1	D	138/141 (98%)	137 (99%)	1 (1%)	84	91
1	E	138/141 (98%)	137 (99%)	1 (1%)	84	91
1	F	138/141 (98%)	137 (99%)	1 (1%)	84	91
2	G	296/298 (99%)	296 (100%)	0	100	100
2	H	296/298 (99%)	296 (100%)	0	100	100
2	I	296/298 (99%)	296 (100%)	0	100	100
2	J	296/298 (99%)	296 (100%)	0	100	100
2	K	296/298 (99%)	296 (100%)	0	100	100
2	L	296/298 (99%)	296 (100%)	0	100	100
2	S	297/298 (100%)	297 (100%)	0	100	100
2	T	297/298 (100%)	297 (100%)	0	100	100
2	U	297/298 (100%)	297 (100%)	0	100	100
2	V	297/298 (100%)	297 (100%)	0	100	100
2	W	297/298 (100%)	297 (100%)	0	100	100
2	X	297/298 (100%)	297 (100%)	0	100	100
2	g	297/298 (100%)	297 (100%)	0	100	100
2	h	297/298 (100%)	297 (100%)	0	100	100
2	i	297/298 (100%)	297 (100%)	0	100	100
2	j	297/298 (100%)	297 (100%)	0	100	100
2	k	297/298 (100%)	297 (100%)	0	100	100
2	l	297/298 (100%)	297 (100%)	0	100	100
2	s	297/298 (100%)	297 (100%)	0	100	100
2	t	297/298 (100%)	297 (100%)	0	100	100
2	u	297/298 (100%)	297 (100%)	0	100	100
2	v	297/298 (100%)	297 (100%)	0	100	100
2	w	297/298 (100%)	297 (100%)	0	100	100
2	x	297/298 (100%)	297 (100%)	0	100	100
3	0	130/130 (100%)	130 (100%)	0	100	100
3	1	130/130 (100%)	130 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2	130/130 (100%)	130 (100%)	0	100	100
3	3	130/130 (100%)	130 (100%)	0	100	100
3	4	130/130 (100%)	130 (100%)	0	100	100
3	5	130/130 (100%)	130 (100%)	0	100	100
3	M	129/130 (99%)	129 (100%)	0	100	100
3	N	129/130 (99%)	129 (100%)	0	100	100
3	O	129/130 (99%)	129 (100%)	0	100	100
3	P	129/130 (99%)	129 (100%)	0	100	100
3	Q	129/130 (99%)	129 (100%)	0	100	100
3	R	129/130 (99%)	129 (100%)	0	100	100
3	a	130/130 (100%)	130 (100%)	0	100	100
3	b	130/130 (100%)	130 (100%)	0	100	100
3	c	130/130 (100%)	130 (100%)	0	100	100
3	d	130/130 (100%)	130 (100%)	0	100	100
3	e	130/130 (100%)	130 (100%)	0	100	100
3	f	130/130 (100%)	130 (100%)	0	100	100
3	m	130/130 (100%)	130 (100%)	0	100	100
3	n	130/130 (100%)	130 (100%)	0	100	100
3	o	130/130 (100%)	130 (100%)	0	100	100
3	p	130/130 (100%)	130 (100%)	0	100	100
3	q	130/130 (100%)	130 (100%)	0	100	100
3	r	130/130 (100%)	130 (100%)	0	100	100
All	All	11064/11118 (100%)	11058 (100%)	6 (0%)	93	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ARG
1	B	92	ARG
1	C	92	ARG
1	D	92	ARG
1	E	92	ARG
1	F	92	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	356	ASN
3	M	71	ASN
2	H	251	ASN
2	I	251	ASN
2	J	251	ASN
2	K	251	ASN
2	L	251	ASN
3	N	71	ASN
3	O	71	ASN
3	O	154	ASN
3	P	71	ASN
3	Q	71	ASN
3	R	71	ASN
2	S	74	ASN
2	S	94	GLN
2	S	328	GLN
3	e	9	ASN
3	d	9	ASN
3	m	71	ASN
3	b	9	ASN
3	n	71	ASN
3	o	71	ASN
3	p	71	ASN
3	q	71	ASN
3	f	9	ASN
3	f	71	ASN
3	r	71	ASN
2	g	94	GLN
2	g	172	ASN
2	s	74	ASN
2	s	252	ASN
2	T	74	ASN
2	T	94	GLN
2	T	328	GLN
2	h	94	GLN
2	h	172	ASN
2	t	74	ASN
2	U	74	ASN
2	U	94	GLN
2	U	252	ASN
2	U	328	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	i	94	GLN
2	i	172	ASN
2	u	74	ASN
2	u	252	ASN
2	V	74	ASN
2	V	94	GLN
2	V	328	GLN
2	j	94	GLN
2	j	172	ASN
2	v	74	ASN
2	W	74	ASN
2	W	94	GLN
2	W	328	GLN
2	k	94	GLN
2	k	172	ASN
2	w	74	ASN
2	X	74	ASN
2	X	94	GLN
2	X	252	ASN
2	X	328	GLN
2	l	94	GLN
2	l	172	ASN
2	x	74	ASN
2	x	252	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

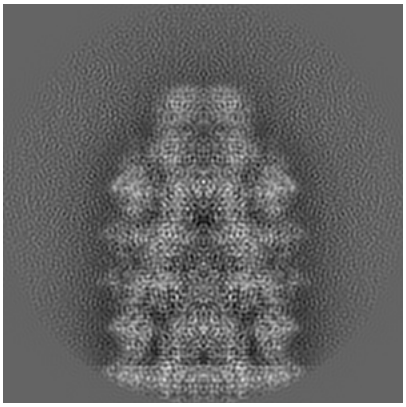
6 Map visualisation (i)

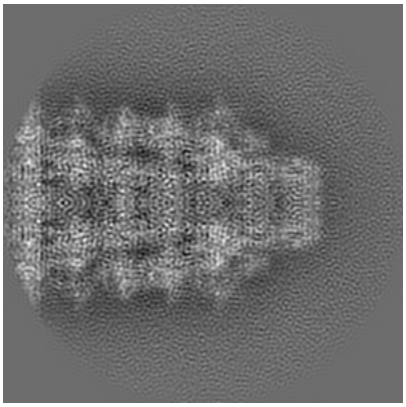
This section contains visualisations of the EMDB entry EMD-20644. These allow visual inspection of the internal detail of the map and identification of artifacts.

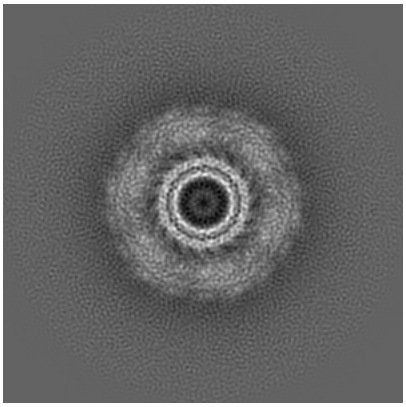
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

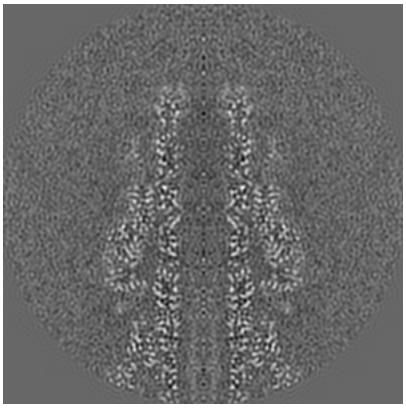

Y

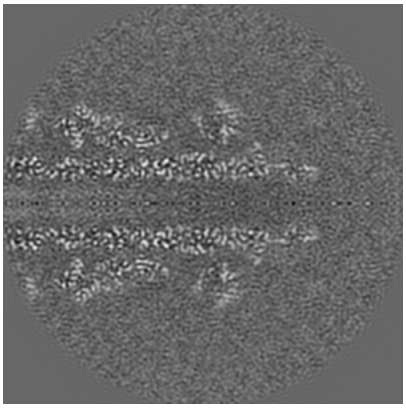

Z

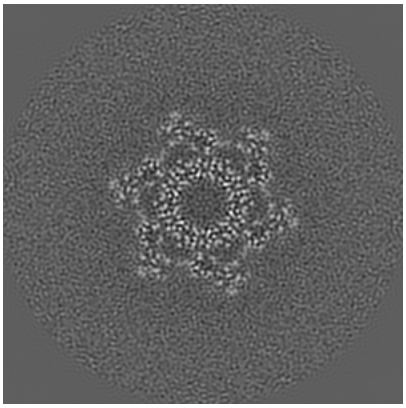
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 160

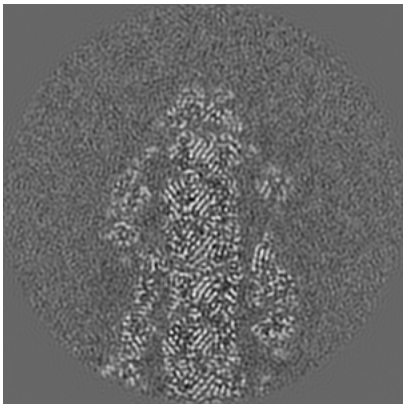

Y Index: 160

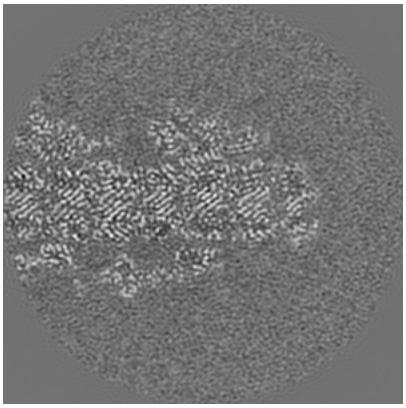

Z Index: 160

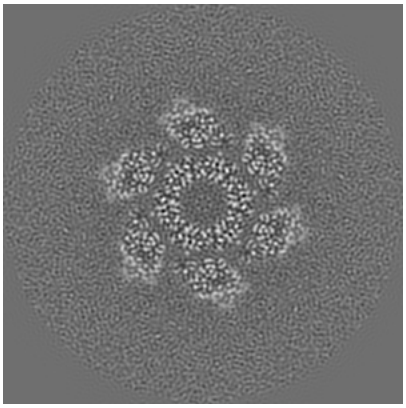
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 183

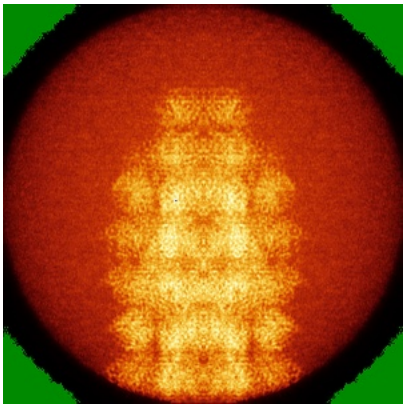

Y Index: 138

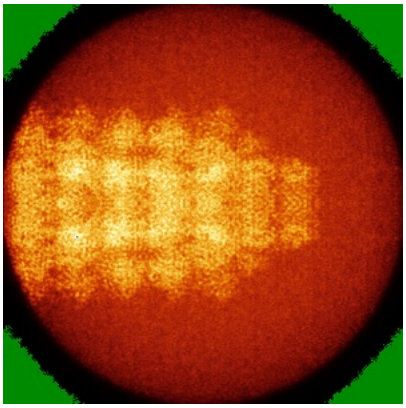

Z Index: 133

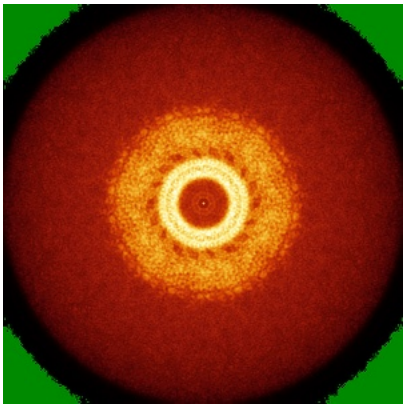
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

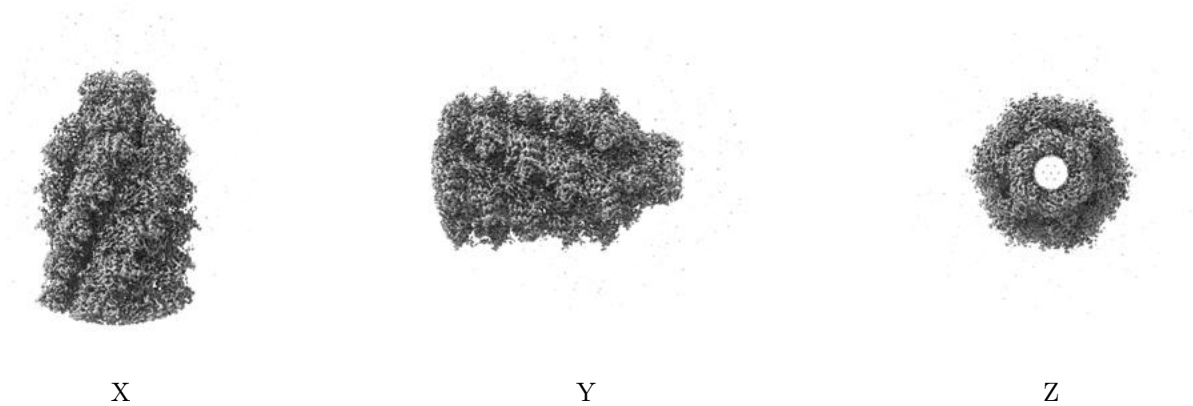

Y


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.037. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

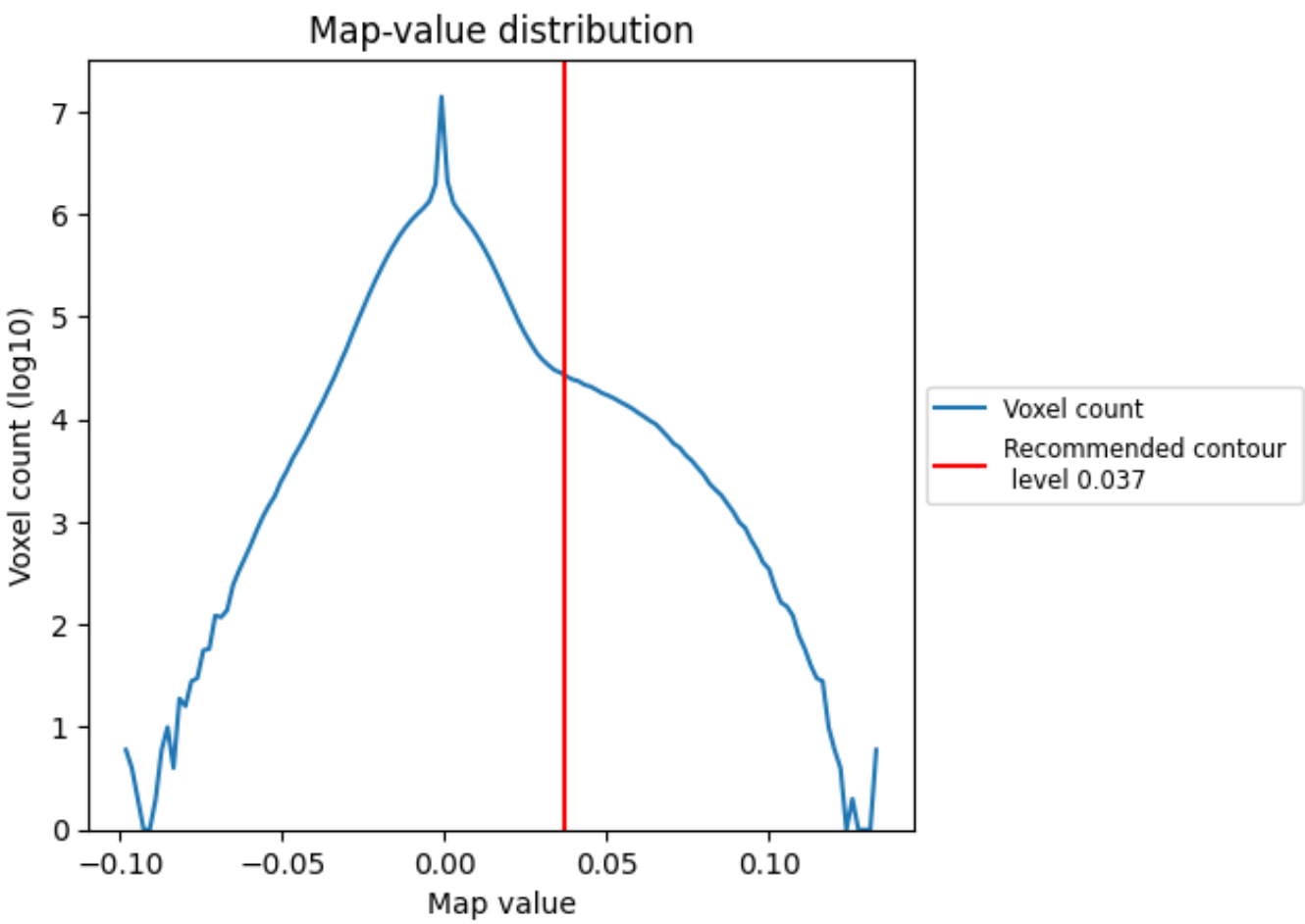
6.6 Mask visualisation (i)

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

7 Map analysis (i)

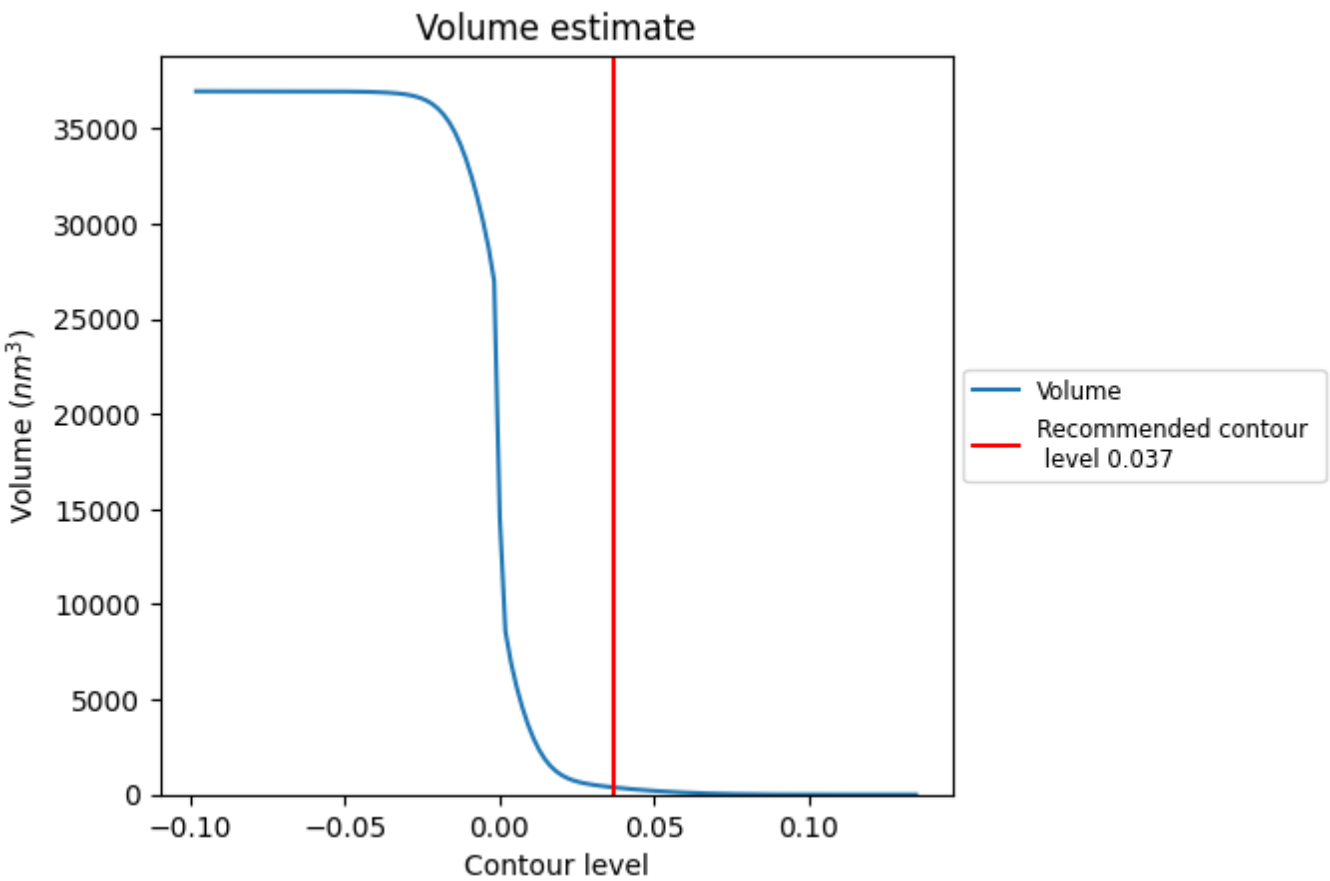
This section contains the results of statistical analysis of the map.

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.

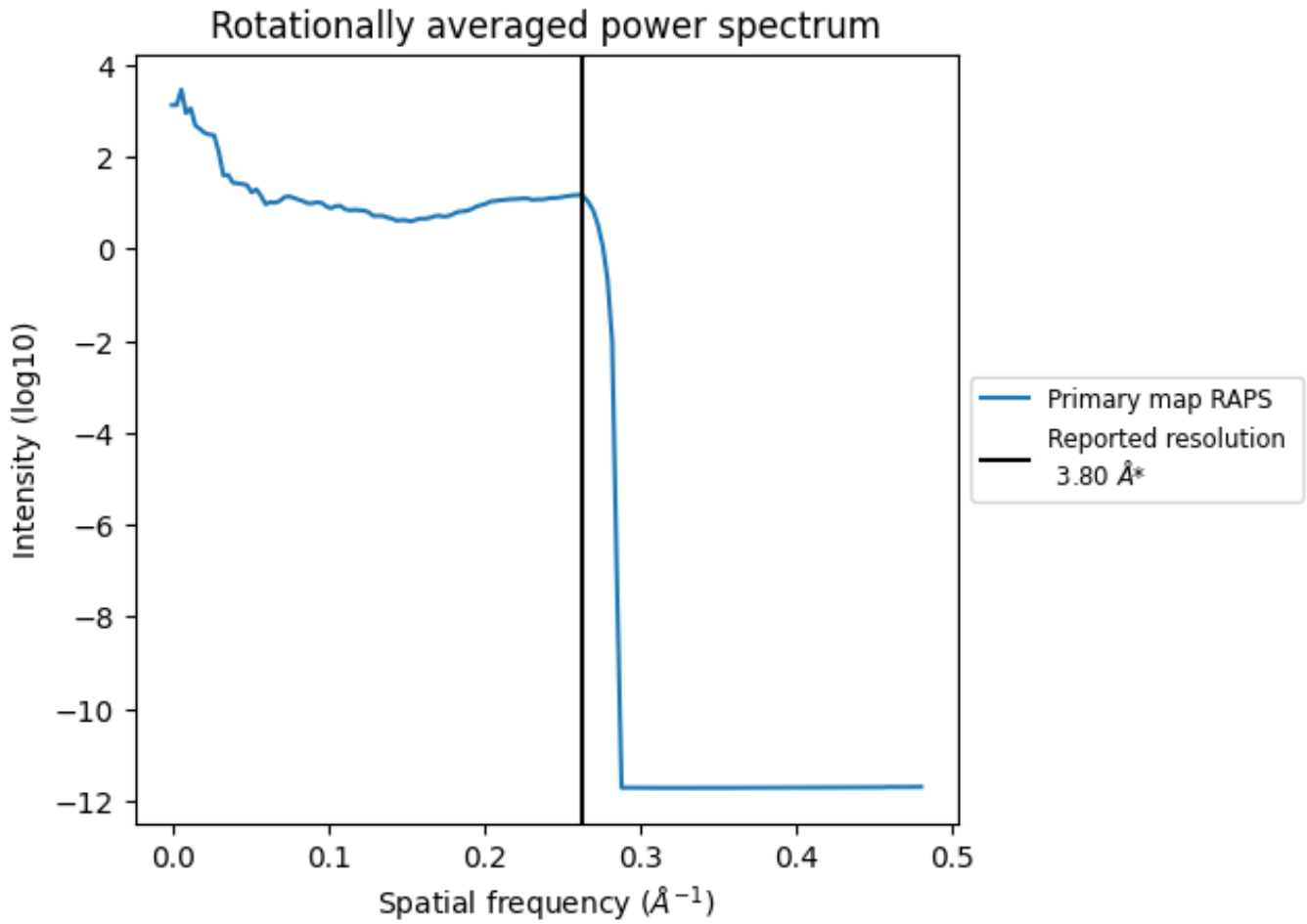
7.2 Volume estimate (i)



The volume at the recommended contour level is 375 nm^3; this corresponds to an approximate mass of 339 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

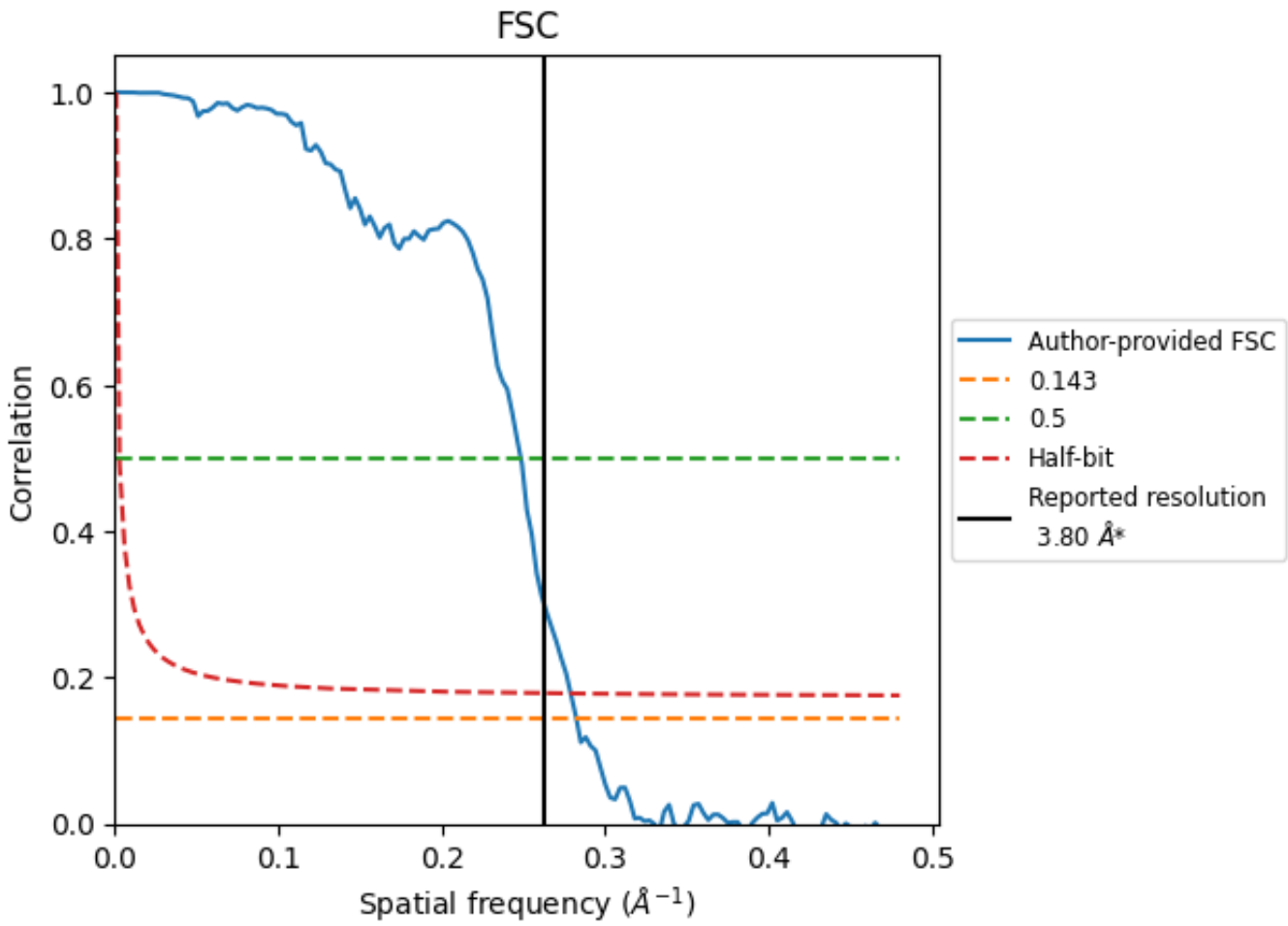


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

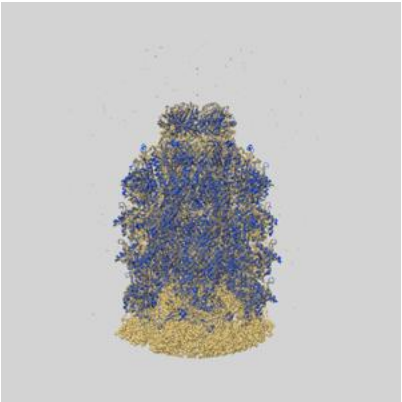
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.54	4.03	3.59
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

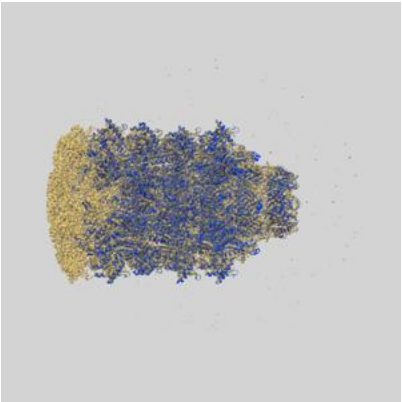
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20644 and PDB model 6U5F. Per-residue inclusion information can be found in section 3 on page 8.

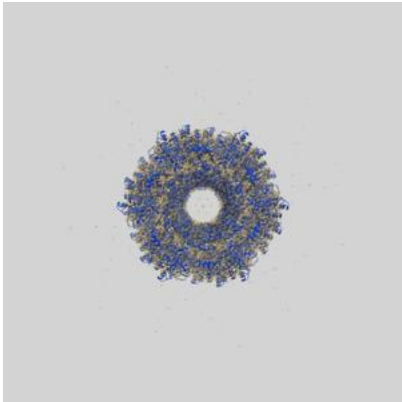
9.1 Map-model overlay (i)



X



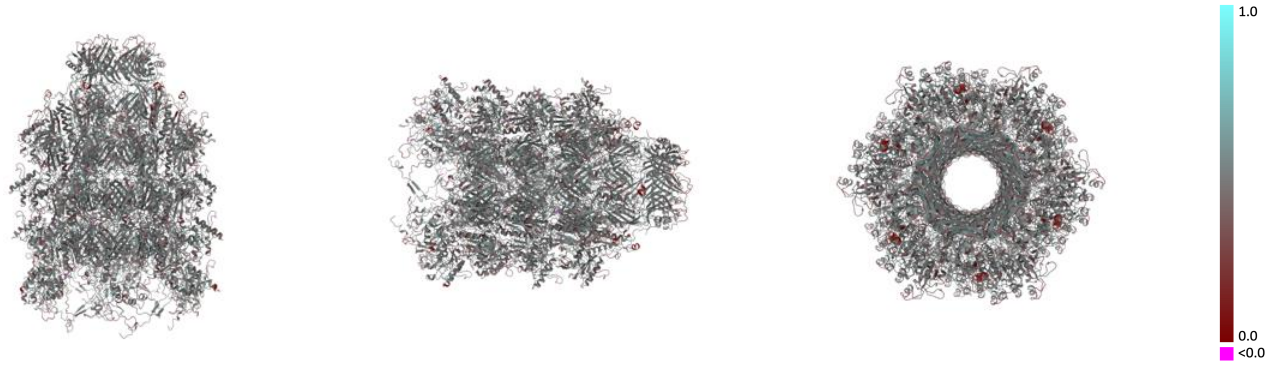
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.037 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.

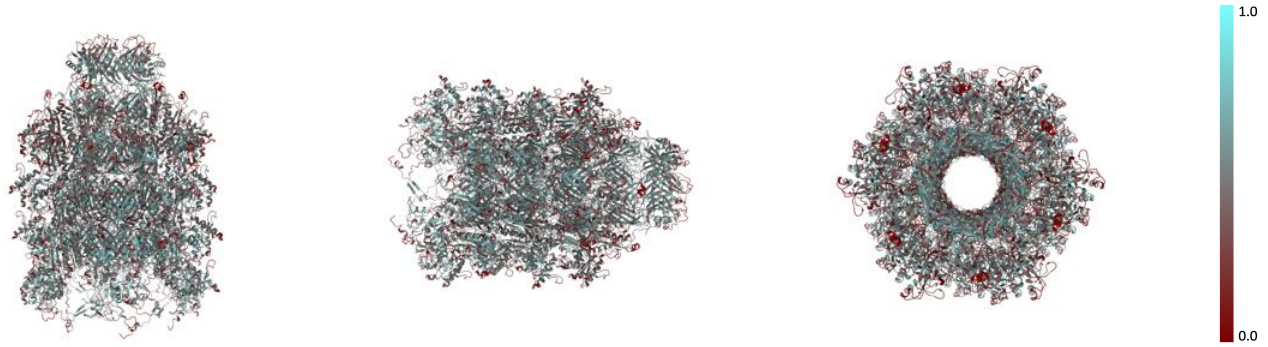
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

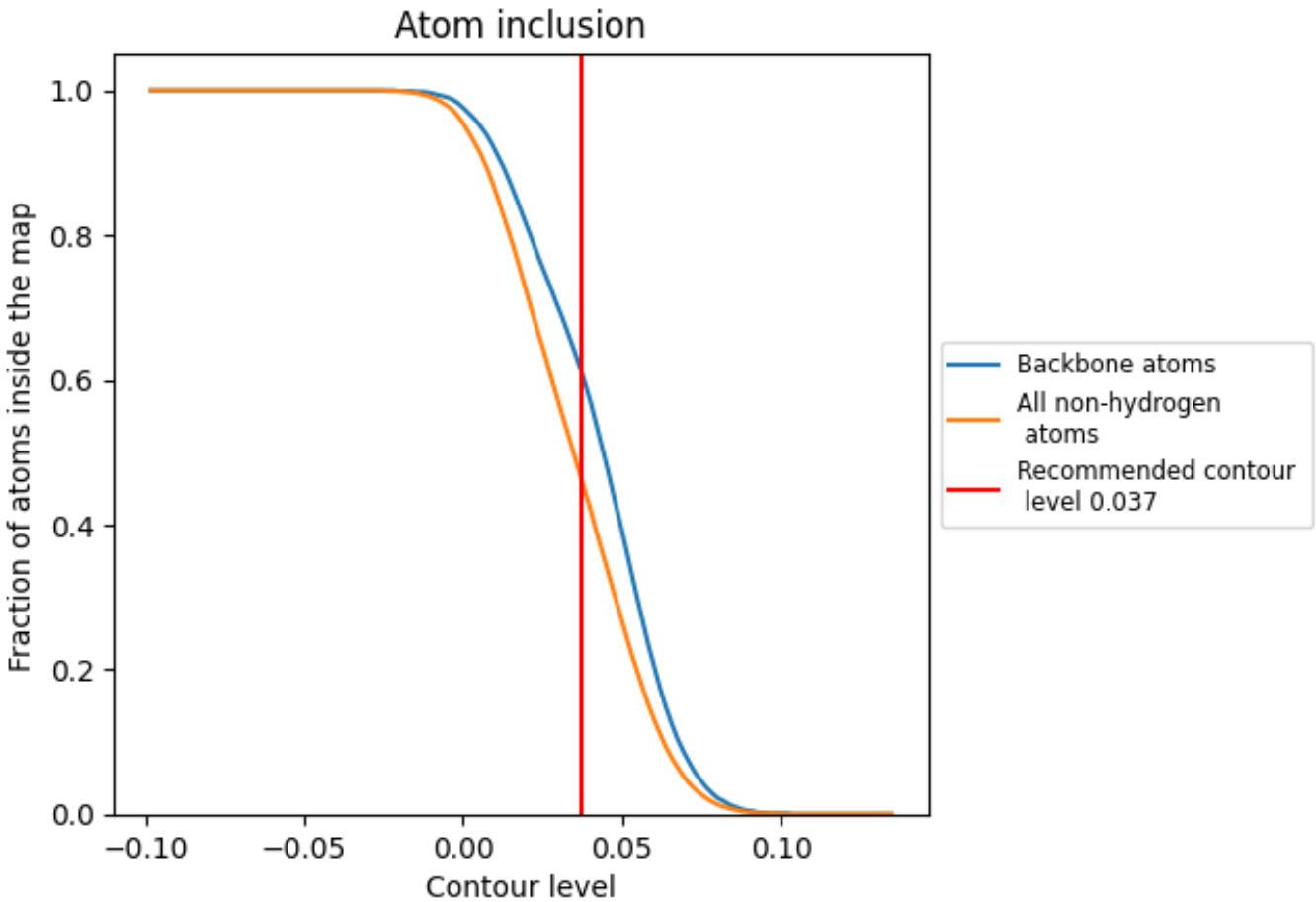
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.037).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4670	0.4640
0	0.5400	0.4960
1	0.5380	0.4930
2	0.5370	0.4940
3	0.5460	0.4930
4	0.5410	0.4930
5	0.5370	0.4910
A	0.4230	0.4380
B	0.4200	0.4380
C	0.4230	0.4390
D	0.4250	0.4420
E	0.4190	0.4410
F	0.4300	0.4400
G	0.3910	0.4400
H	0.3850	0.4390
I	0.3870	0.4390
J	0.3890	0.4410
K	0.3810	0.4390
L	0.3860	0.4380
M	0.5170	0.4890
N	0.5050	0.4880
O	0.5110	0.4880
P	0.5110	0.4890
Q	0.5110	0.4880
R	0.5160	0.4910
S	0.4520	0.4630
T	0.4500	0.4630
U	0.4530	0.4630
V	0.4500	0.4630
W	0.4510	0.4640
X	0.4530	0.4650
a	0.5370	0.4970
b	0.5350	0.4990
c	0.5330	0.4980
d	0.5350	0.4990

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	0.5370	0.4990
f	0.5330	0.4970
g	0.4700	0.4530
h	0.4720	0.4520
i	0.4680	0.4520
j	0.4710	0.4520
k	0.4700	0.4530
l	0.4680	0.4530
m	0.5450	0.4950
n	0.5490	0.4940
o	0.5520	0.4950
p	0.5450	0.4940
q	0.5450	0.4950
r	0.5450	0.4950
s	0.4660	0.4590
t	0.4660	0.4590
u	0.4590	0.4580
v	0.4680	0.4600
w	0.4670	0.4600
x	0.4610	0.4600