Full wwPDB EM Validation Report ⓘ

Jun 12, 2024 – 05:00 pm BST

PDB ID	:	8RTD
EMDB ID	:	EMD-19488
Title	:	Stalk-Arches-IMC structure from the fully-assembled R388 type IV secretion system determined by cryo-EM.
Authors	:	Mace, K.; Waksman, G.
Deposited on	:	2024-01-25
Resolution	:	4.33 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:

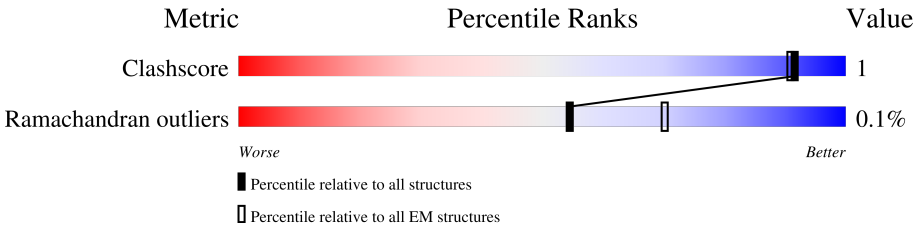
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.33 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	229	16% 86% 14%
1	B	229	14% 85% 14%
1	C	229	16% 86% 14%
1	E	229	17% 86% 14%
1	K	229	17% 86% 14%
2	D	231	6% 16% 84%
2	F	231	12% 88%
2	G	231	6% 94%
2	Q	231	50% 84% 14%

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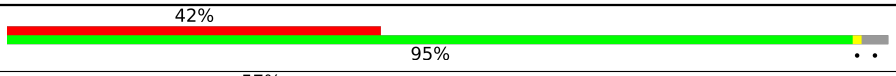
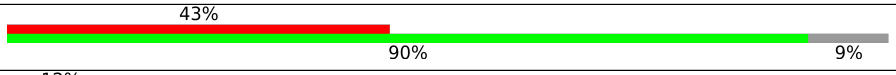
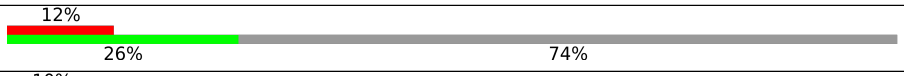
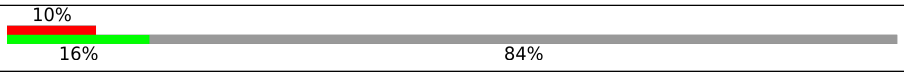
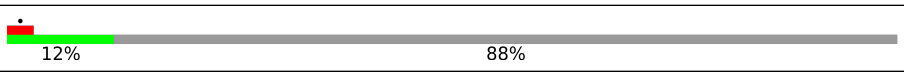
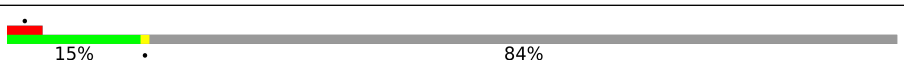
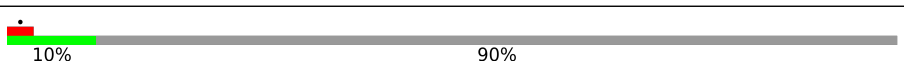
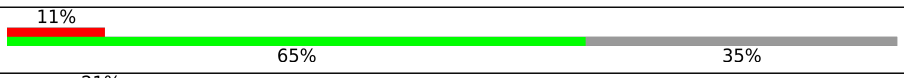
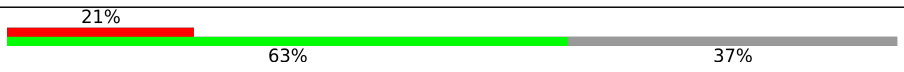
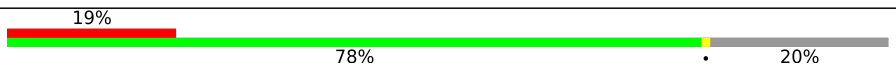
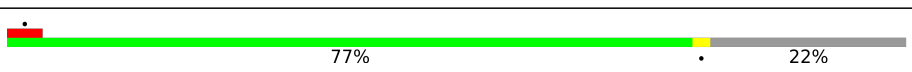
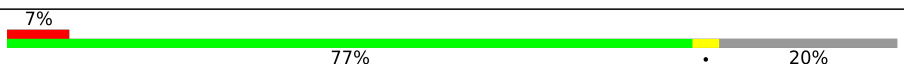
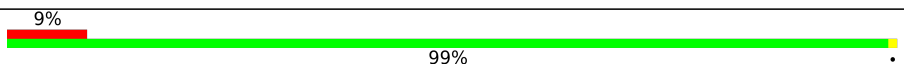
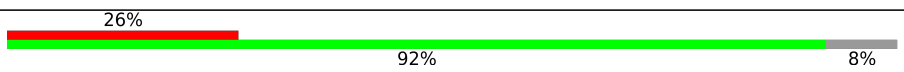
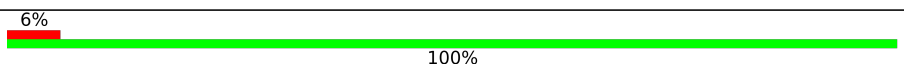
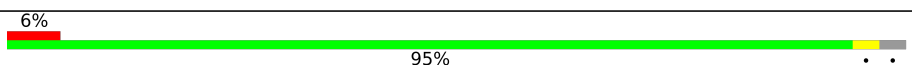
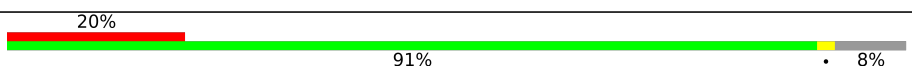
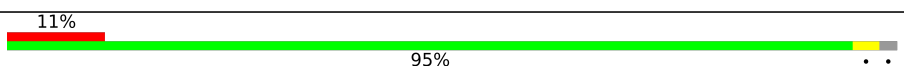
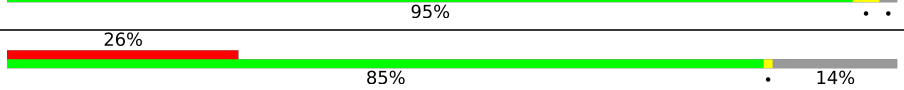
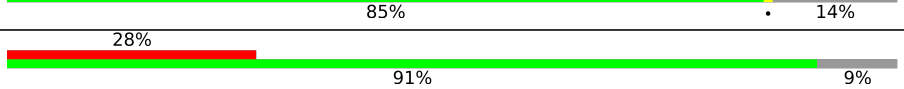
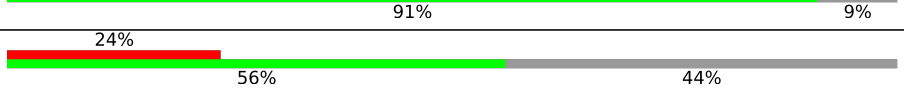
Mol	Chain	Length	Quality of chain
2	S	231	
2	U	231	
2	X	231	
2	Y	231	
2	b	231	
2	c	231	
2	d	231	
2	i	231	
3	Z	395	
3	a	395	
3	e	395	
4	H	342	
4	I	342	
4	J	342	
4	L	342	
4	M	342	
5	R	104	
5	f	104	
5	j	104	
6	O	823	
6	P	823	
6	T	823	
6	V	823	
6	g	823	
6	h	823	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 40078 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 TrwJ protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	197	Total 969	C 575	N 197	O 197	0	0
1	B	197	Total 969	C 575	N 197	O 197	0	0
1	C	197	Total 969	C 575	N 197	O 197	0	0
1	K	197	Total 969	C 575	N 197	O 197	0	0
1	E	197	Total 969	C 575	N 197	O 197	0	0

- Molecule 2 is a protein called TrwG protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	37	Total 183	C 109	N 37	O 37	0	0
2	F	28	Total 138	C 82	N 28	O 28	0	0
2	G	13	Total 64	C 38	N 13	O 13	0	0
2	Q	198	Total 855	C 459	N 198	O 198	0	0
2	S	223	Total 973	C 527	N 223	O 223	0	0
2	U	193	Total 839	C 453	N 193	O 193	0	0
2	X	61	Total 297	C 175	N 61	O 61	0	0
2	Y	188	Total 814	C 438	N 188	O 188	0	0
2	b	210	Total 912	C 492	N 210	O 210	0	0
2	c	59	Total 287	C 169	N 59	O 59	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
2	d	38	Total C N O 184 108 38 38	0	0
2	i	28	Total C N O 138 82 28 28	0	0

- Molecule 3 is a protein called TrwE protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	a	49	Total C N O 242 144 49 49	0	0
3	Z	62	Total C N O 306 182 62 62	0	0
3	e	39	Total C N O 193 115 39 39	0	0

- Molecule 4 is a protein called TrwI protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	L	268	Total C N O 1311 775 268 268	0	0
4	M	272	Total C N O 1330 786 272 272	1	0
4	H	222	Total C N O 1087 643 222 222	1	0
4	I	217	Total C N O 1062 628 217 217	1	0
4	J	272	Total C N O 1330 786 272 272	1	0

- Molecule 5 is a protein called TrwM protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	j	104	Total C N O 515 307 104 104	0	0
5	R	104	Total C N O 515 307 104 104	0	0
5	f	96	Total C N O 475 283 96 96	0	0

- Molecule 6 is a protein called Type IV secretion system protein virB4.

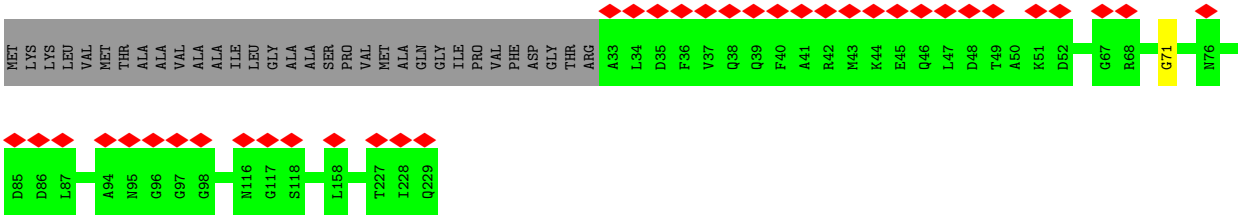
Mol	Chain	Residues	Atoms				AltConf	Trace
6	O	799	Total 3947	C 2349	N 799	O 799	0	0
6	P	760	Total 3754	C 2234	N 760	O 760	0	0
6	T	808	Total 3992	C 2376	N 808	O 808	0	0
6	V	711	Total 3512	C 2090	N 711	O 711	0	0
6	g	753	Total 3719	C 2213	N 753	O 753	0	0
6	h	457	Total 2259	C 1345	N 457	O 457	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

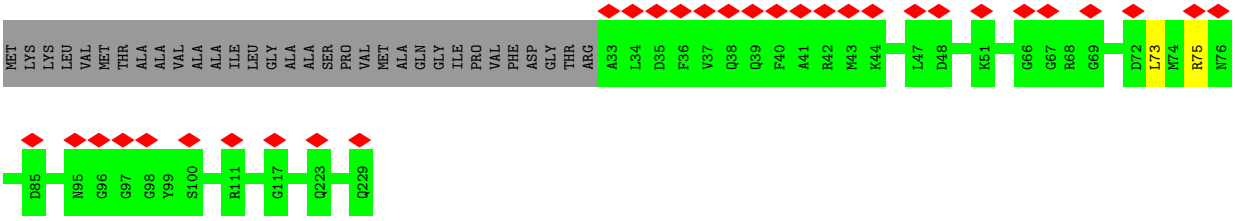
• Molecule 1: TrwJ protein

Chain A:



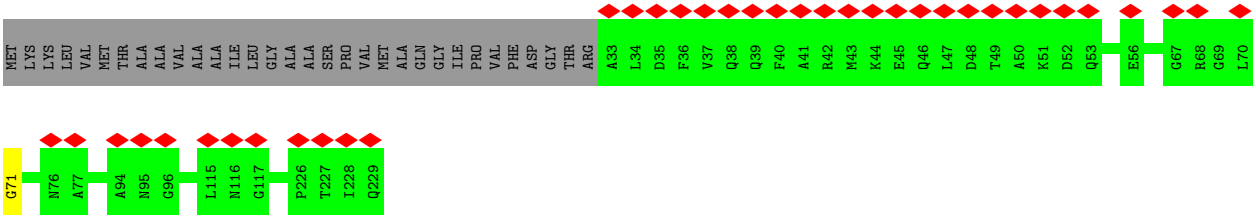
• Molecule 1: TrwJ protein

Chain B:



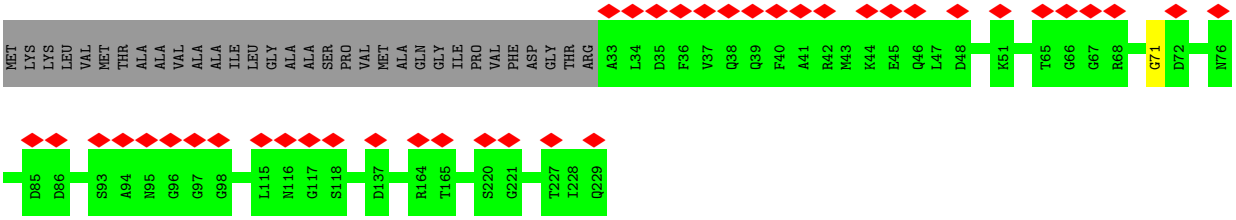
• Molecule 1: TrwJ protein

Chain C:



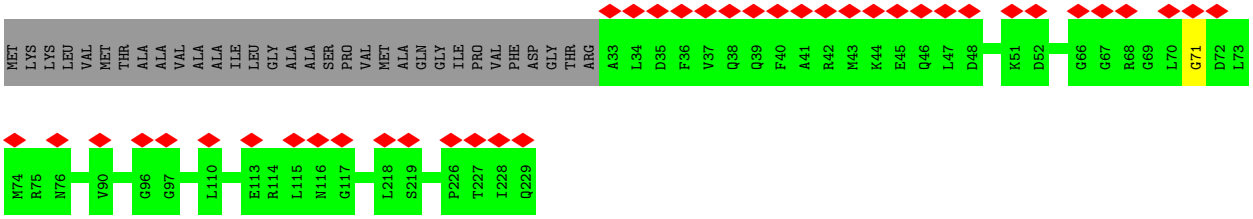
• Molecule 1: TrwJ protein

Chain K:



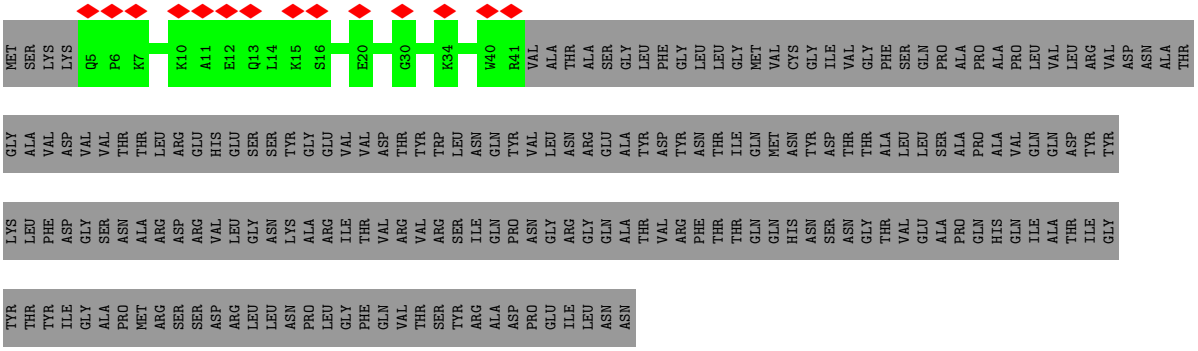
• Molecule 1: TrwJ protein

Chain E:



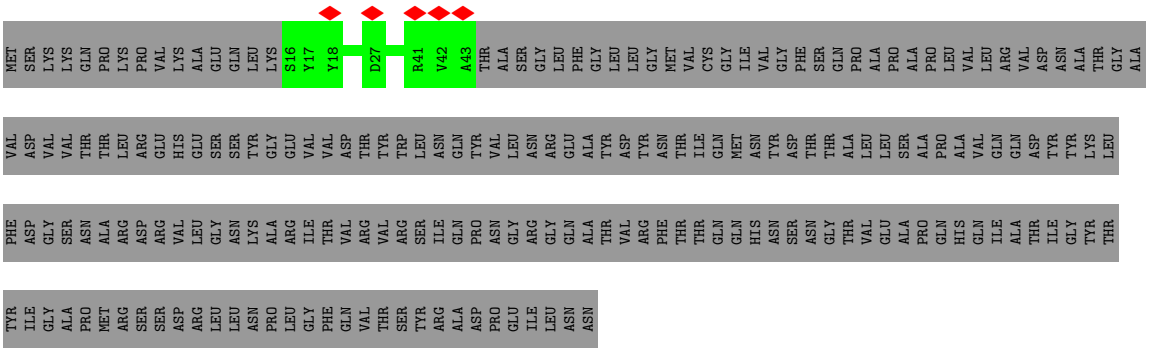
• Molecule 2: TrwG protein

Chain D:



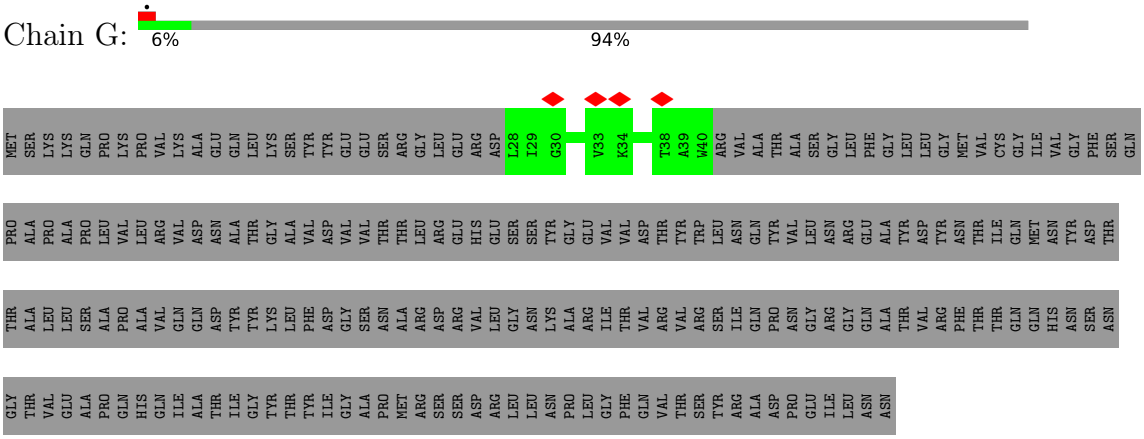
• Molecule 2: TrwG protein

Chain F:



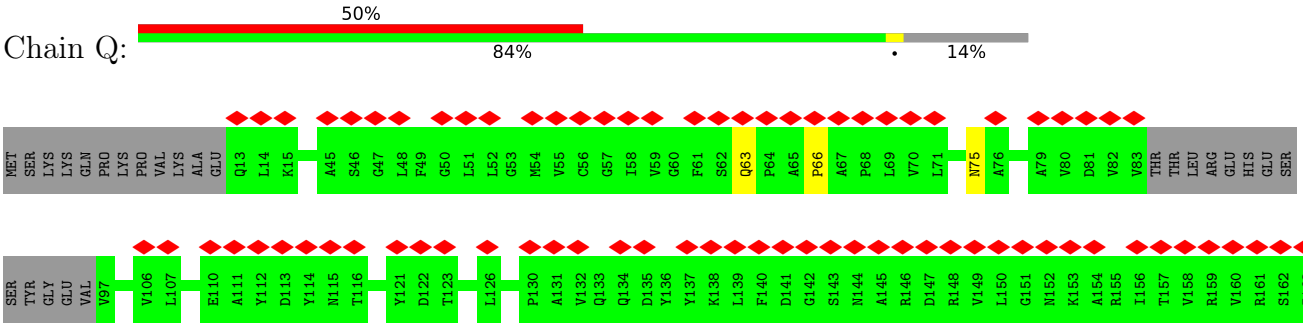
• Molecule 2: TrwG protein

Chain G:



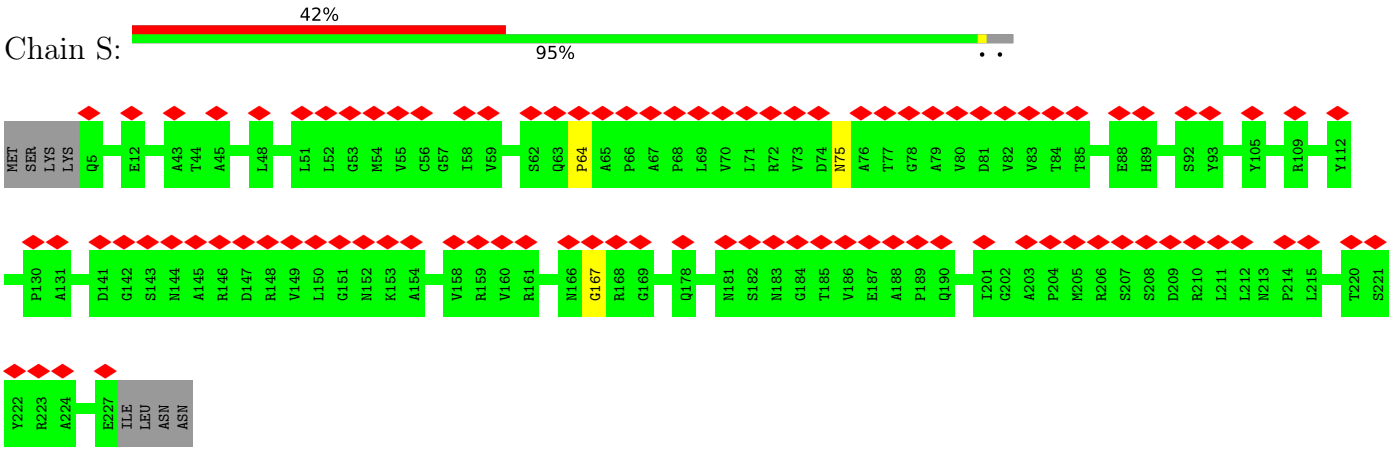
• Molecule 2: TrwG protein

Chain Q:



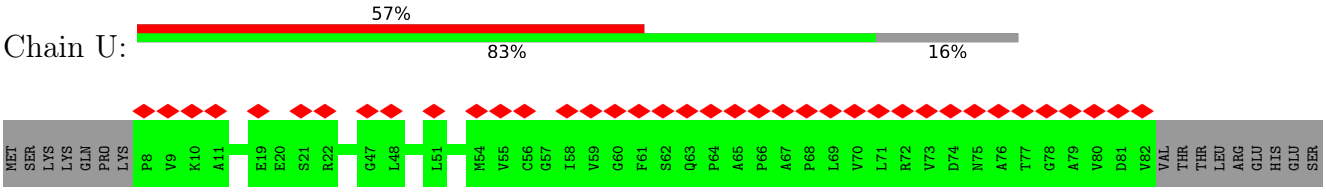
• Molecule 2: TrwG protein

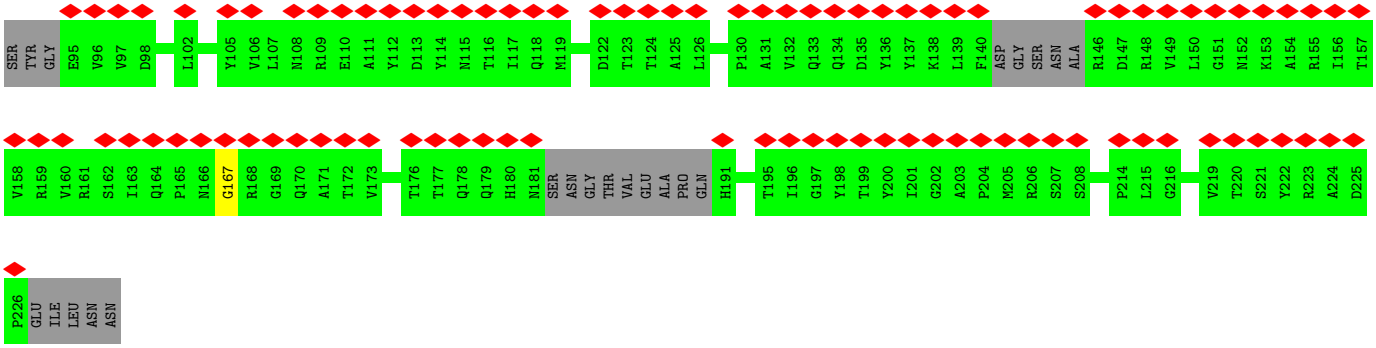
Chain S:



• Molecule 2: TrwG protein

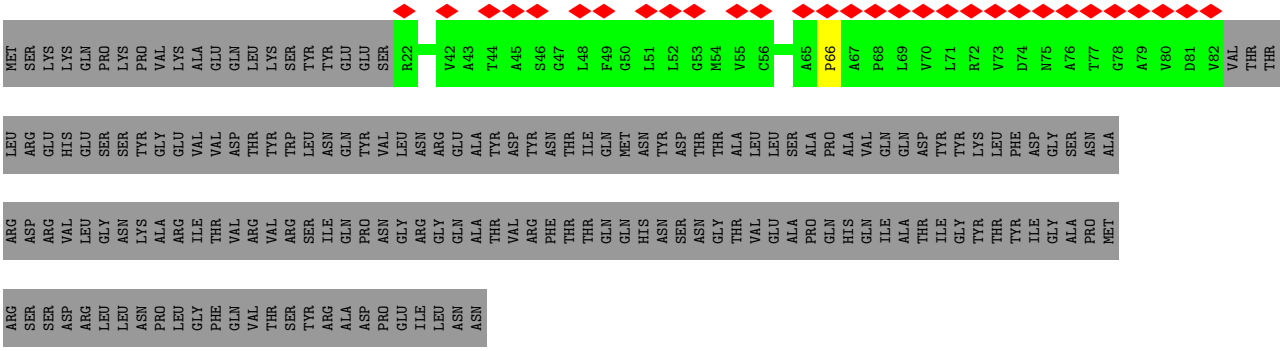
Chain U:





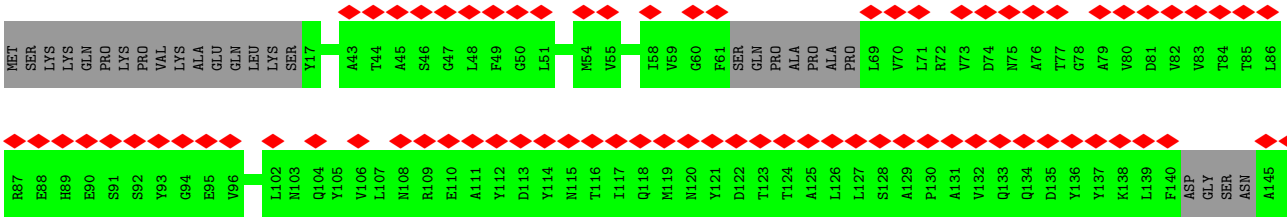
• Molecule 2: TrwG protein

Chain X:



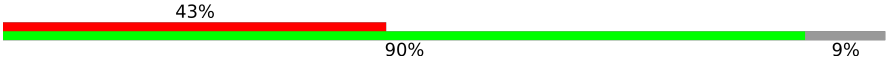
• Molecule 2: TrwG protein

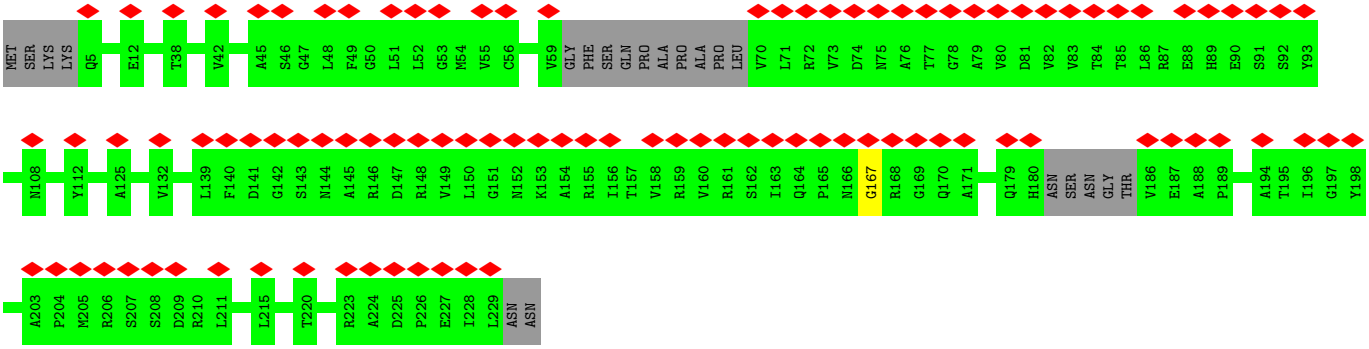
Chain Y:



• Molecule 2: TrwG protein

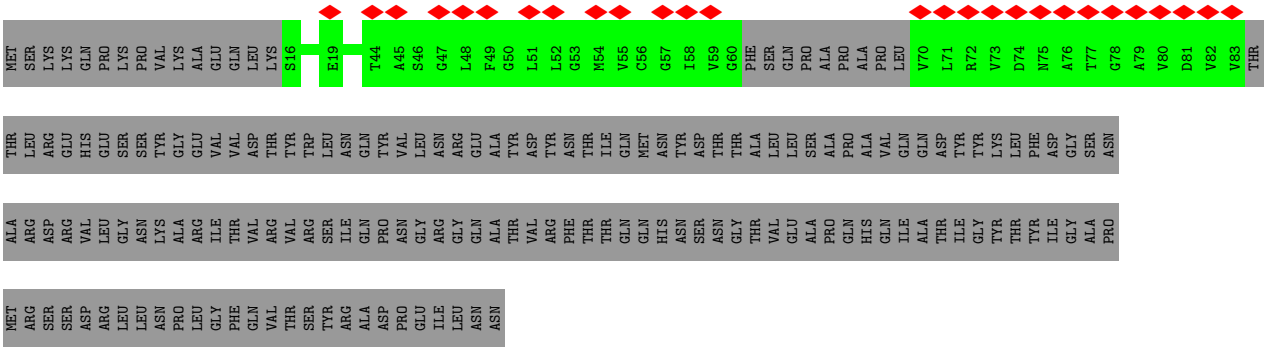
Chain b:





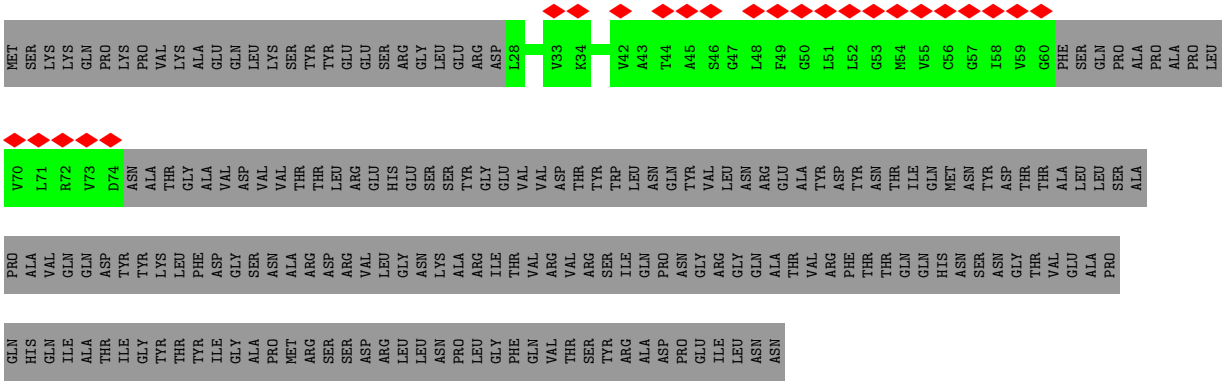
• Molecule 2: TrwG protein

Chain c:



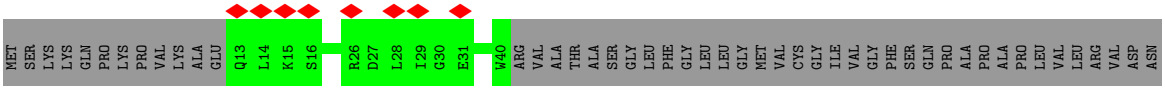
• Molecule 2: TrwG protein

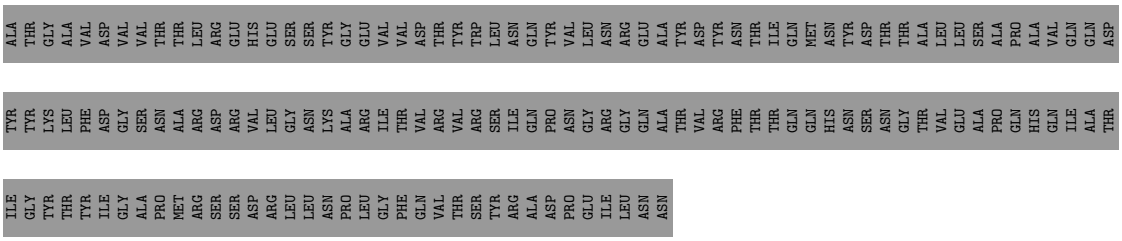
Chain d:



• Molecule 2: TrwG protein

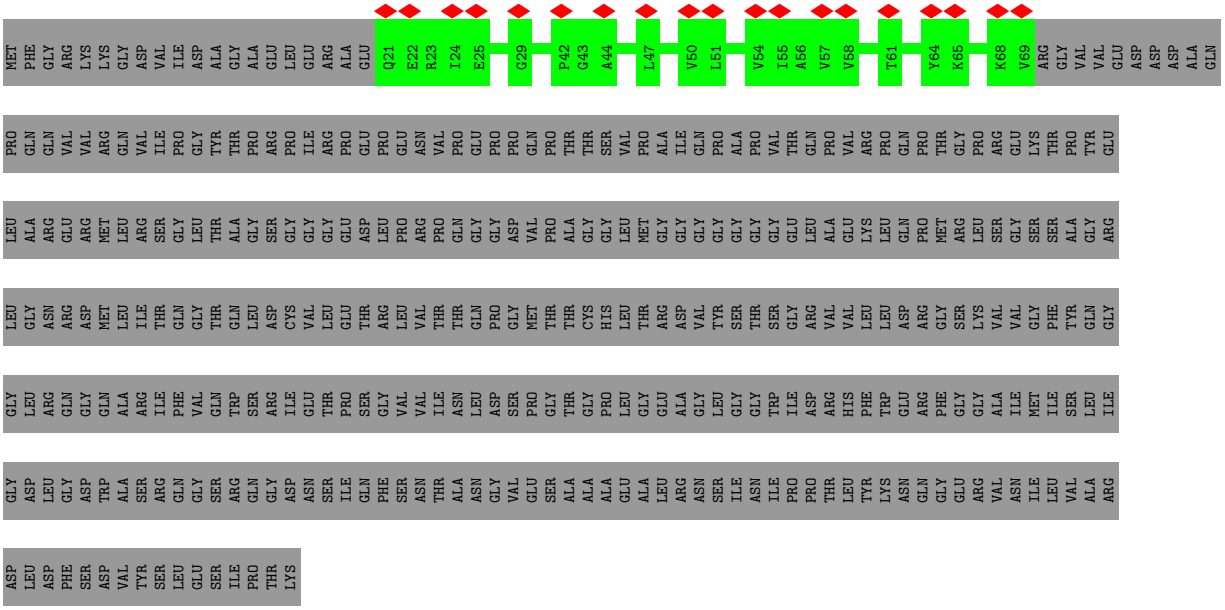
Chain i:





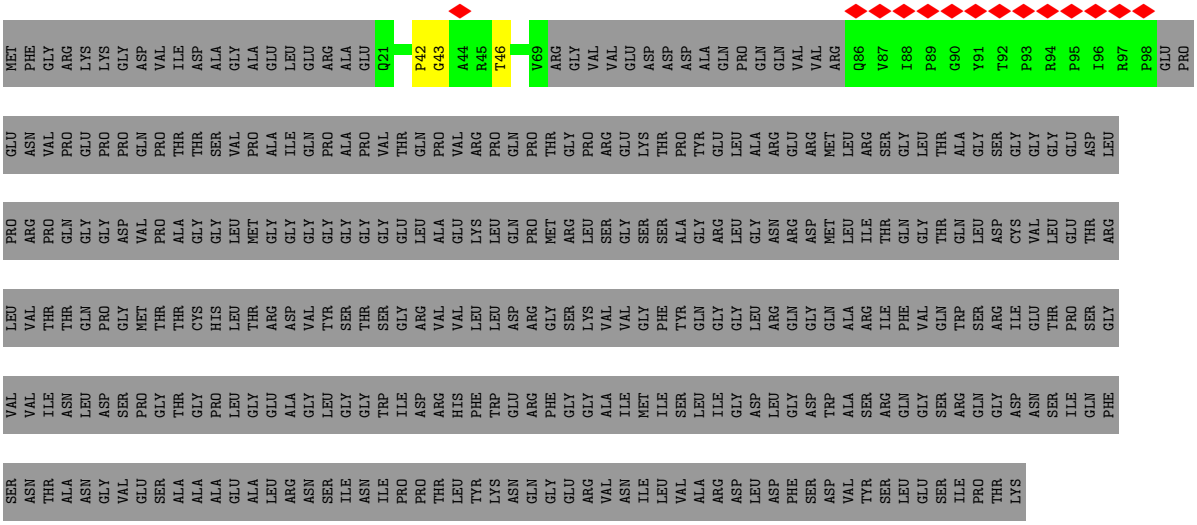
• Molecule 3: TrwE protein

Chain a:



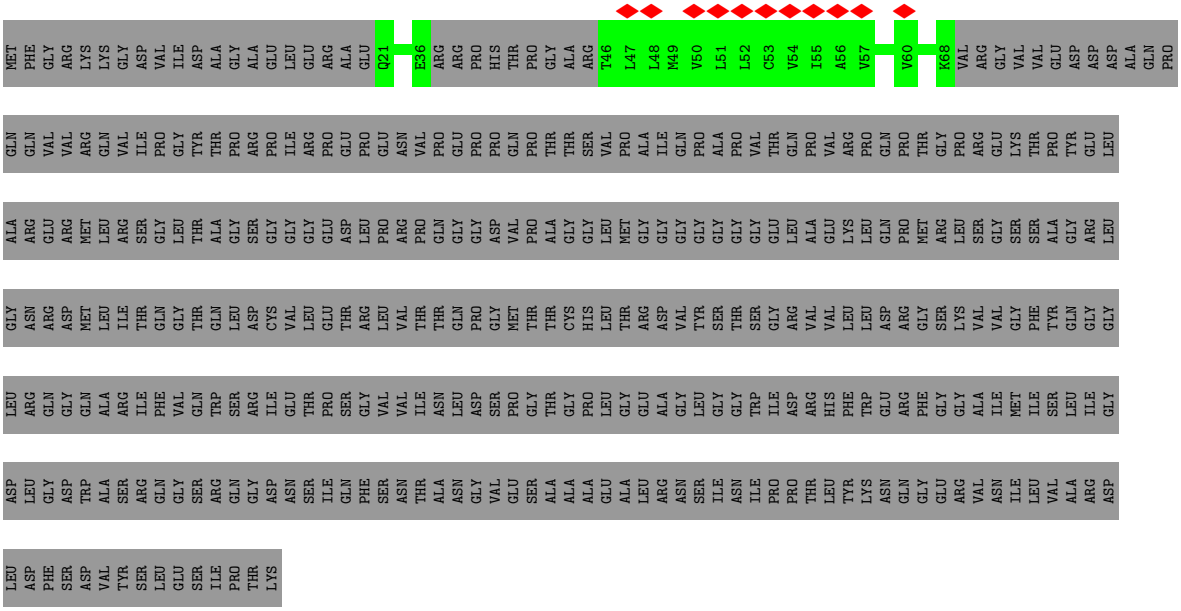
• Molecule 3: TrwE protein

Chain Z:



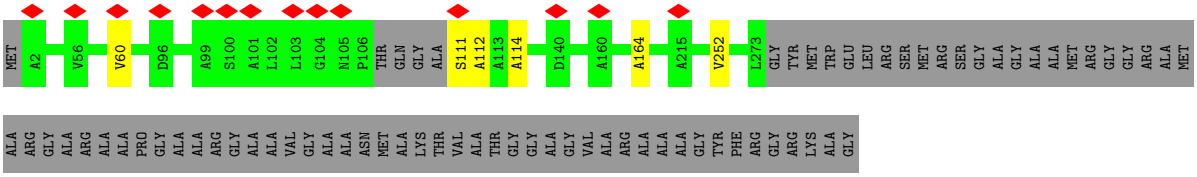
• Molecule 3: TrwE protein

Chain e:



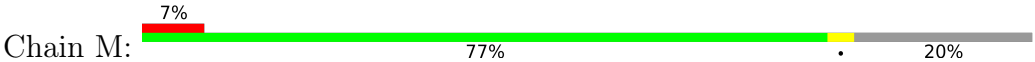
• Molecule 4: TrwI protein

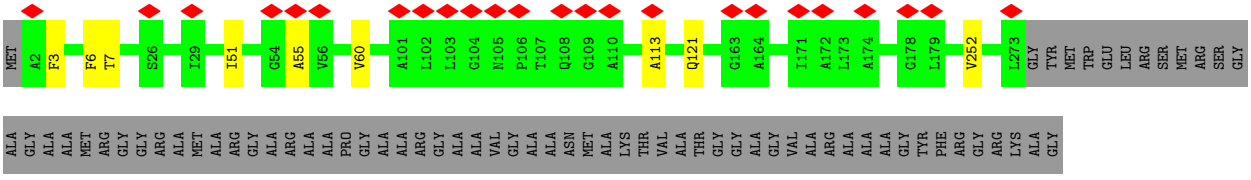
Chain L:



• Molecule 4: TrwI protein

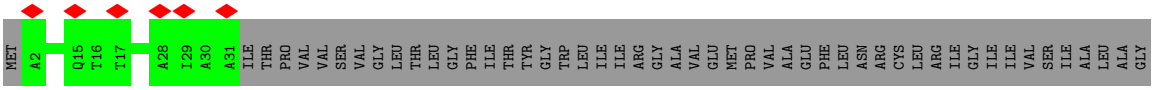
Chain M:

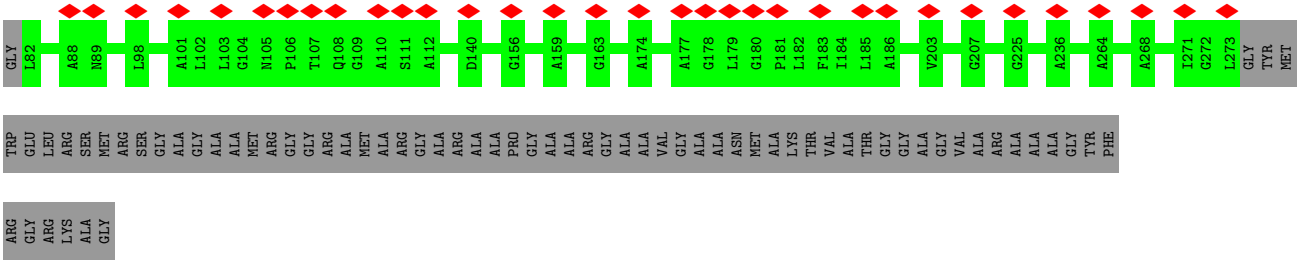




• Molecule 4: TrwI protein

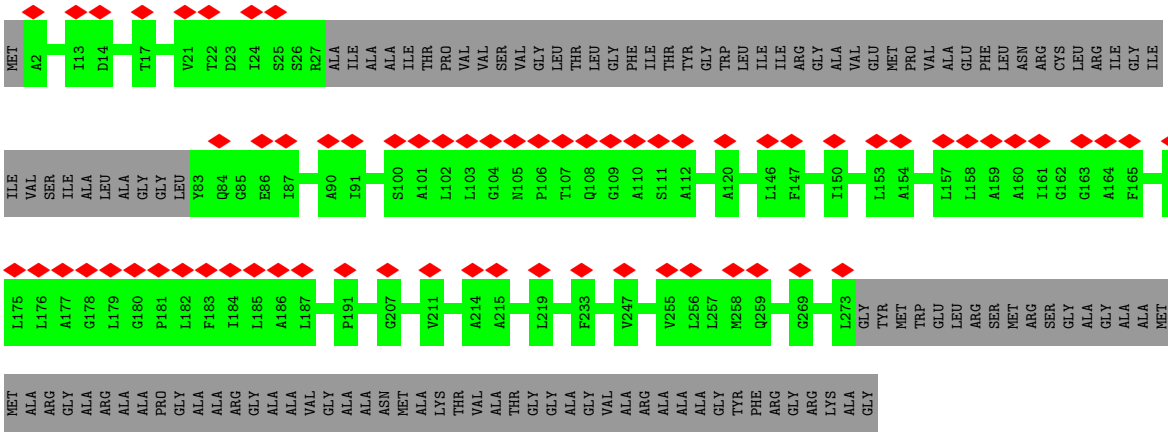
Chain H:





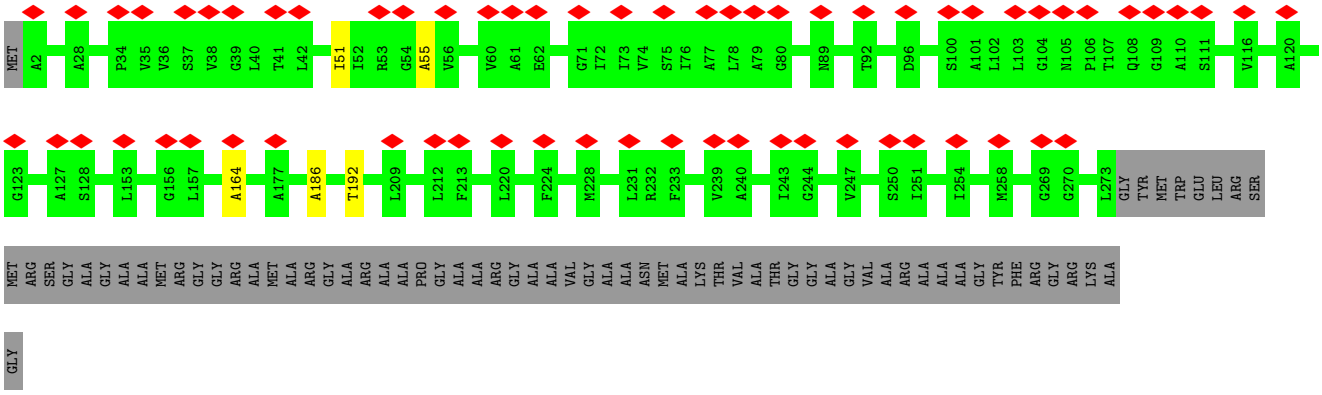
• Molecule 4: TrwI protein

Chain I:



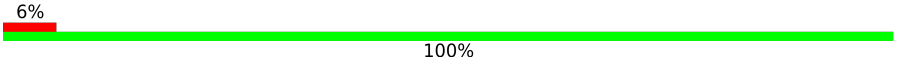
• Molecule 4: TrwI protein

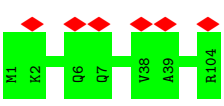
Chain J:



• Molecule 5: TrwM protein

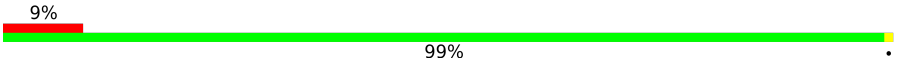
Chain j:

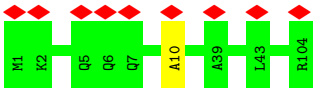




• Molecule 5: TrwM protein

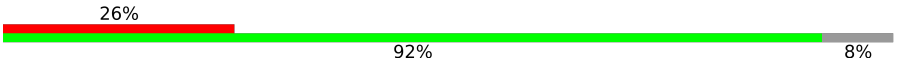
Chain R:

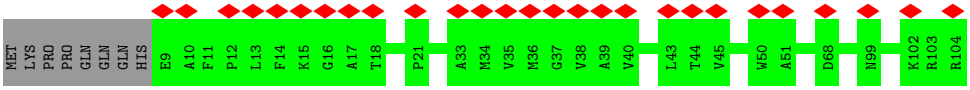




• Molecule 5: TrwM protein

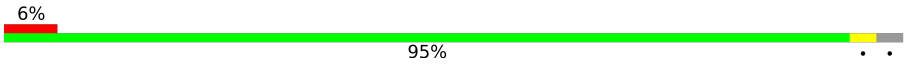
Chain f:

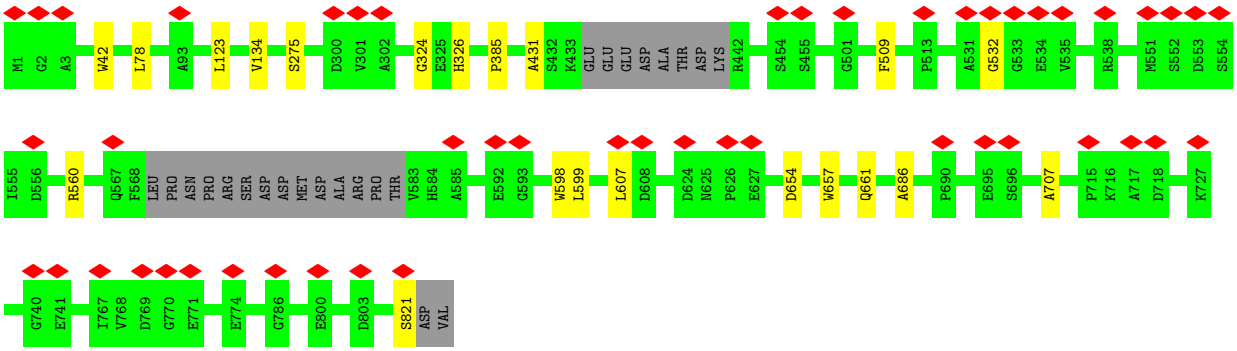




• Molecule 6: Type IV secretion system protein virB4

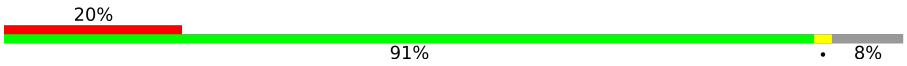
Chain O:

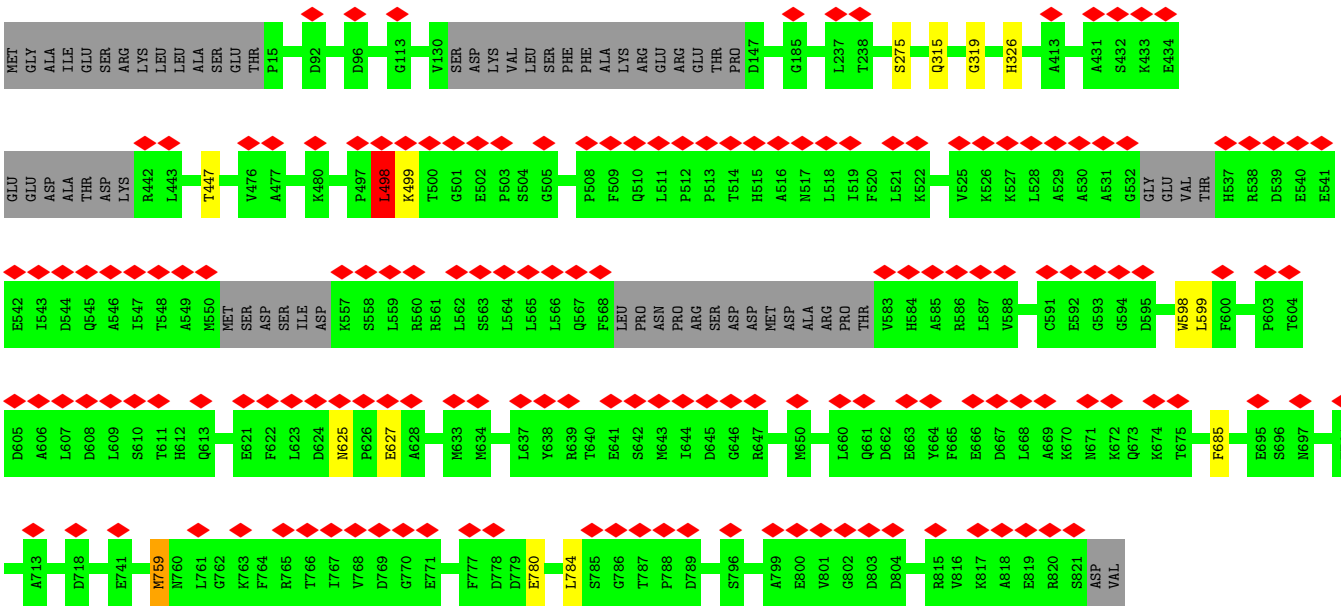




• Molecule 6: Type IV secretion system protein virB4

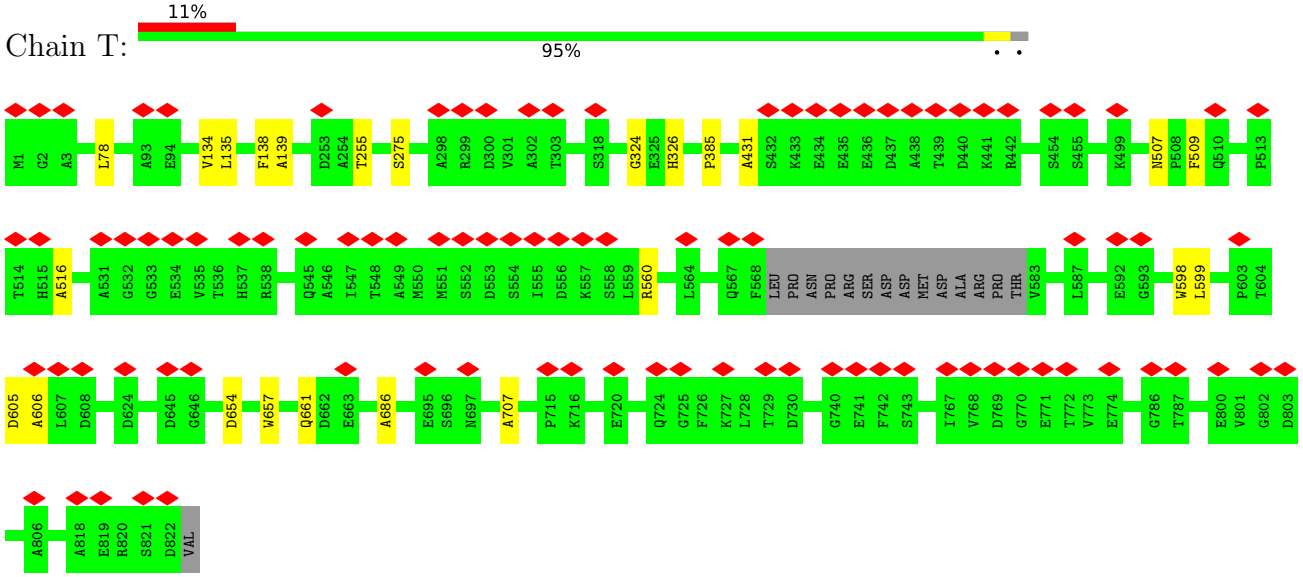
Chain P:





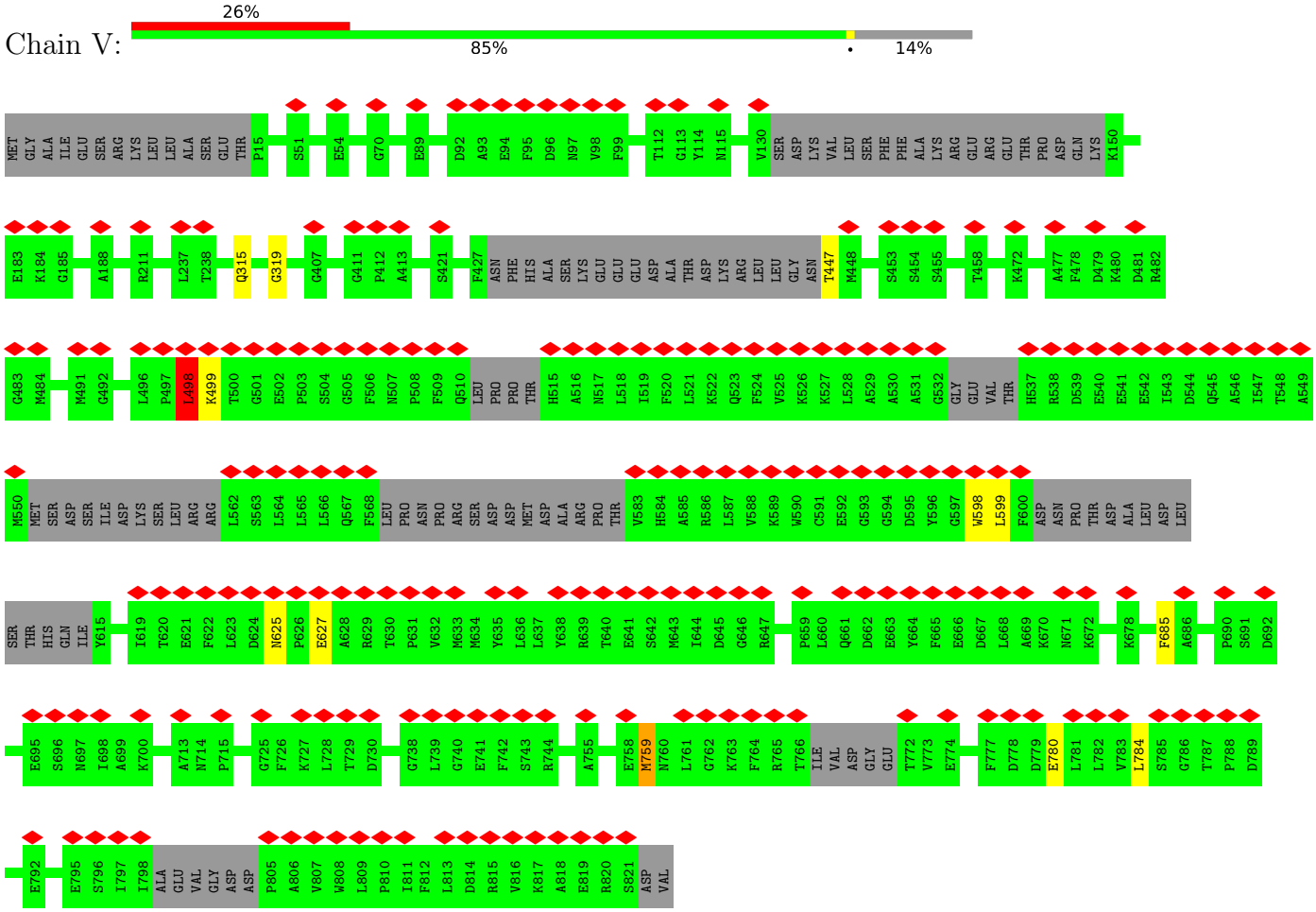
• Molecule 6: Type IV secretion system protein virB4

Chain T:



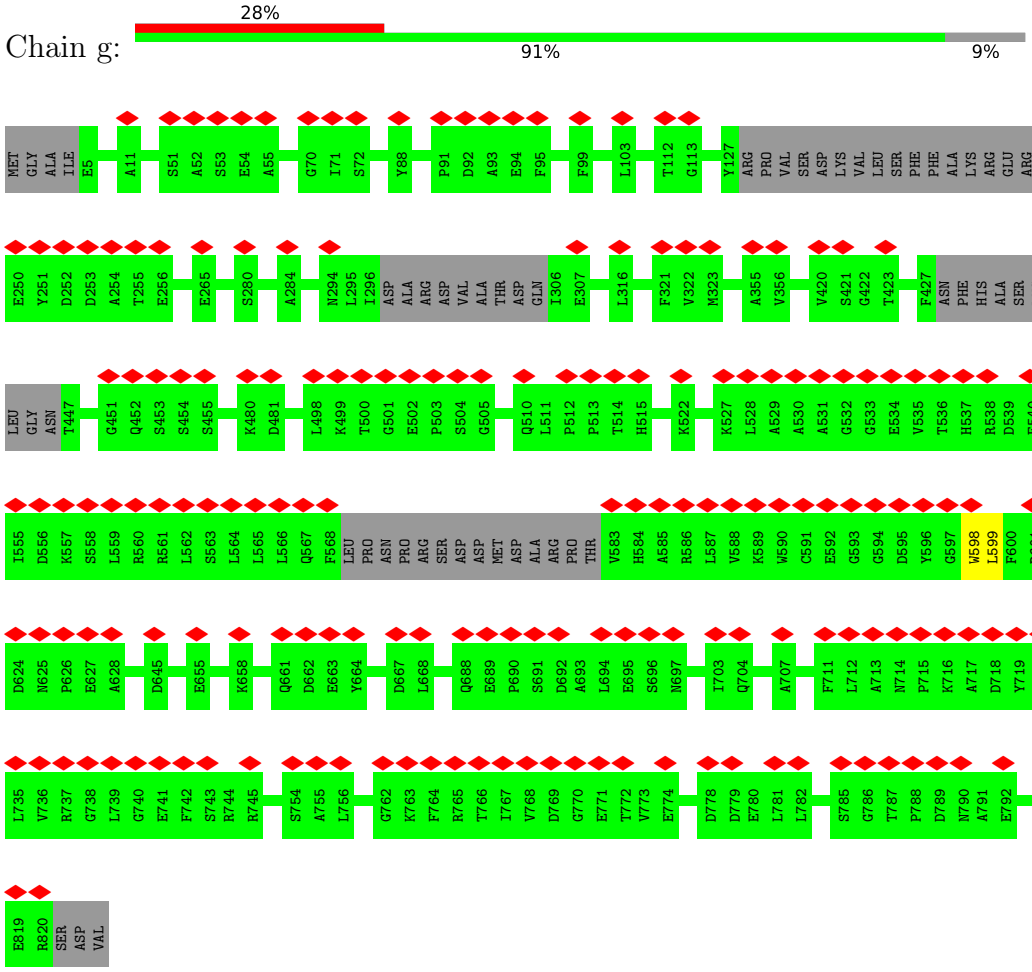
• Molecule 6: Type IV secretion system protein virB4

Chain V:



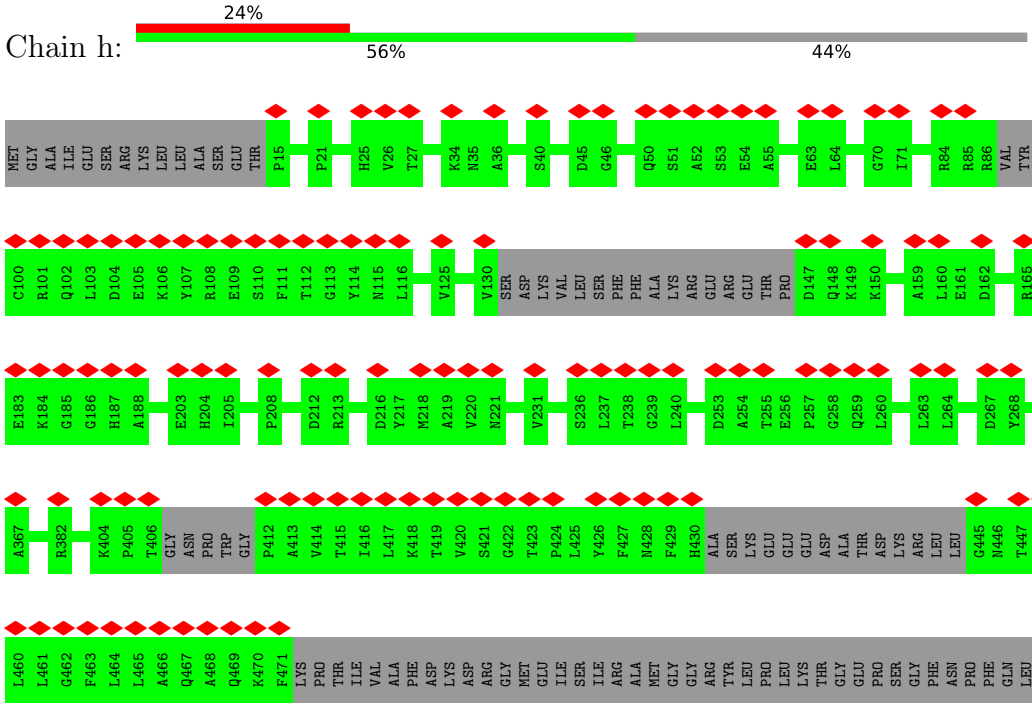
• Molecule 6: Type IV secretion system protein virB4

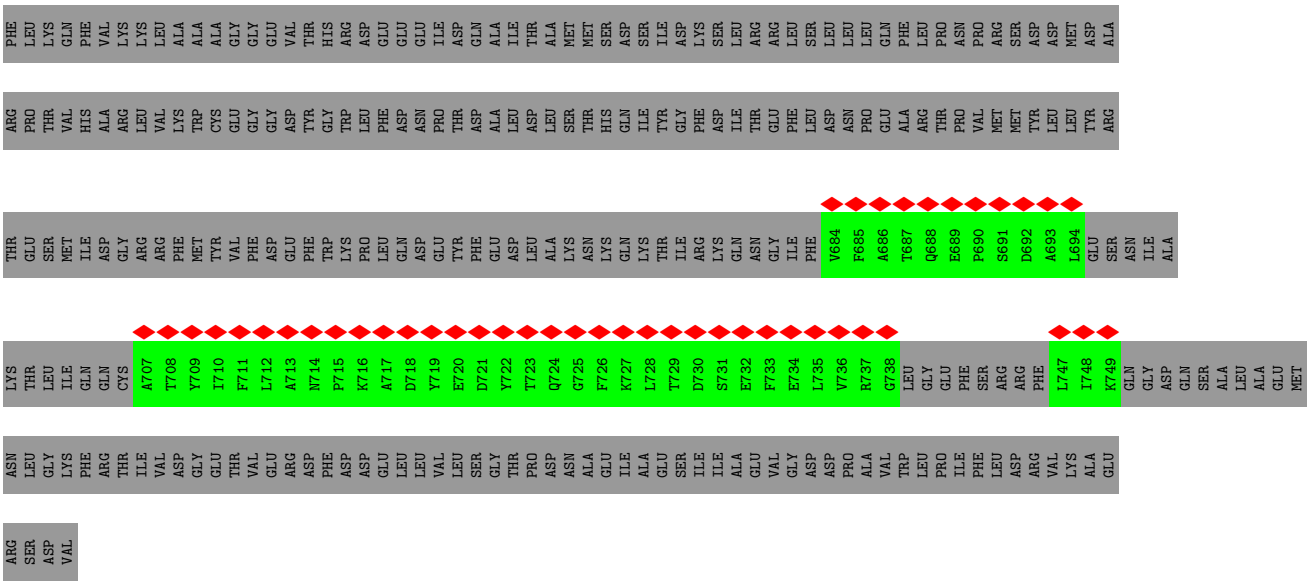
Chain g:



• Molecule 6: Type IV secretion system protein virB4

Chain h:




PHE LEU LYS GLN PHE VAL LYS LYS LEU ALA ALA ALA GLY GLY GLU VAL THR HIS ARG ASP GLU GLU GLU ILE ASP GLN ALA ILE THR ALA MET MET SER ASP SER ILE ASP LYS SER LEU ARG ARG LEU SER LEU LEU LEU GLN PHE LEU PRO ASN PRO ARG SER ASP ASP MET ASP ALA
ARG PRO THR VAL HIS ALA ARG LEU VAL LYS TRP CYS GLU GLY GLY GLY ASP TYR GLY TRP LEU PHE ASP ASN PRO THR ASP ALA LEU ASP LEU SER THR HIS GLN ILE TYR GLY PHE ASP ILE THR GLU PHE LEU ASP ASN PRO GLU ALA ALA ARG THR PRO VAL MET MET TYR LEU LEU TYR ARG
THR GLU SER MET ILE ASP GLY ARG ARG PHE MET TYR VAL PHE ASP GLU PHE TRP LYS PRO LEU GLN ASP GLU TYR PHE GLU ASP LEU ALA LYS ASN LYS GLN LYS THR ILE ARG LYS GLN ASN GLY ILE PHE V684 F685 A686 T687 Q688 E689 P690 S691 D692 A693 L694 GLU SER ASN ILE ALA
LYS THR LEU ILE GLN GLN CYS A707 T708 Y709 I710 F711 L712 A713 N714 P715 K716 A717 D718 Y719 E720 D721 Y722 T723 Q724 G725 F726 K727 L728 T729 D730 S731 E732 F733 E734 L735 V736 R737 G738 LEU GLY GLU PHE SER ARG ARG PHE L747 I748 K749 GLN GLY ASP GLN SER ALA LEU ALA GLU MET
ASN LEU GLY LYS PHE ARG THR ILE VAL ASP GLY GLU THR VAL GLU ARG ASP PHE ASP ASP GLU LEU LEU VAL LEU SER GLY THR PRO ASP ASN ALA GLU ILE ALA GLU SER ILE ILE ALA GLU VAL GLY ASP ASP PRO ALA VAL TRP LEU PRO ILE PHE LEU ASP ARG VAL LYS ALA GLU
ARG SER ASP VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65173	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	57.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.997	Depositor
Minimum map value	-0.718	Depositor
Average map value	0.027	Depositor
Map value standard deviation	0.091	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	546.304, 546.304, 546.304	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.40	0/968	0.47	0/1344
1	B	0.41	0/968	0.50	0/1344
1	C	0.41	0/968	0.47	0/1344
1	E	0.39	0/968	0.47	0/1344
1	K	0.38	0/968	0.47	0/1344
2	D	0.26	0/182	0.49	0/252
2	F	0.54	0/137	0.62	0/189
2	G	0.21	0/63	0.46	0/86
2	Q	0.44	0/852	0.79	1/1107 (0.1%)
2	S	0.45	0/972	0.75	1/1274 (0.1%)
2	U	0.52	0/835	0.78	1/1087 (0.1%)
2	X	0.51	0/296	0.56	0/408
2	Y	0.47	0/810	0.80	1/1052 (0.1%)
2	b	0.43	0/909	0.74	1/1185 (0.1%)
2	c	0.53	0/285	0.61	0/391
2	d	0.38	0/182	0.49	0/248
2	i	0.25	0/137	0.44	0/189
3	Z	0.41	0/304	0.63	0/420
3	a	0.27	0/241	0.48	0/334
3	e	0.27	0/191	0.50	0/263
4	H	0.38	0/1085	0.51	0/1502
4	I	0.37	0/1060	0.48	0/1467
4	J	0.39	0/1329	0.51	0/1841
4	L	0.36	0/1309	0.48	0/1812
4	M	0.35	0/1329	0.46	0/1841
5	R	0.29	0/514	0.49	0/715
5	f	0.29	0/474	0.49	0/659
5	j	0.29	0/514	0.49	0/715
6	O	0.35	1/3944 (0.0%)	0.52	1/5488 (0.0%)
6	P	0.40	1/3748 (0.0%)	0.81	7/5210 (0.1%)
6	T	0.35	1/3990 (0.0%)	0.52	1/5554 (0.0%)
6	V	0.38	1/3502 (0.0%)	0.82	7/4861 (0.1%)
6	g	0.36	1/3713 (0.0%)	0.52	1/5161 (0.0%)
6	h	0.29	0/2251	0.49	0/3123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.38	5/39998 (0.0%)	0.60	22/55154 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
1	K	0	1
6	P	0	2
6	V	0	2
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	599	LEU	C-N	6.17	1.48	1.34
6	O	599	LEU	C-N	6.14	1.48	1.34
6	g	599	LEU	C-N	6.13	1.48	1.34
6	P	599	LEU	C-N	6.13	1.48	1.34
6	T	599	LEU	C-N	6.12	1.48	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	759	MET	O-C-N	-31.29	72.64	122.70
6	V	759	MET	O-C-N	-31.25	72.70	122.70
6	V	759	MET	CA-C-N	19.98	161.15	117.20
6	P	759	MET	CA-C-N	19.97	161.14	117.20
6	V	498	LEU	O-C-N	-13.40	101.25	122.70
6	P	498	LEU	O-C-N	-13.40	101.26	122.70
2	S	167	GLY	C-N-CA	13.29	154.94	121.70
2	b	167	GLY	C-N-CA	13.29	154.93	121.70
2	U	167	GLY	C-N-CA	13.28	154.89	121.70
2	Y	167	GLY	C-N-CA	13.25	154.83	121.70
2	Q	167	GLY	C-N-CA	13.24	154.80	121.70
6	V	759	MET	C-N-CA	12.96	154.11	121.70
6	P	759	MET	C-N-CA	12.94	154.04	121.70
6	V	498	LEU	C-N-CA	-8.77	99.79	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	498	LEU	C-N-CA	-8.76	99.80	121.70
6	V	498	LEU	CA-C-N	-7.91	99.79	117.20
6	P	498	LEU	CA-C-N	-7.89	99.84	117.20
6	P	598	TRP	O-C-N	-5.32	114.19	122.70
6	g	598	TRP	O-C-N	-5.32	114.20	122.70
6	T	598	TRP	O-C-N	-5.31	114.20	122.70
6	V	598	TRP	O-C-N	-5.31	114.20	122.70
6	O	598	TRP	O-C-N	-5.31	114.21	122.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	71	GLY	Peptide
1	C	71	GLY	Peptide
1	E	71	GLY	Peptide
1	K	71	GLY	Peptide
6	P	498	LEU	Mainchain
6	P	759	MET	Mainchain
6	V	498	LEU	Mainchain
6	V	759	MET	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	969	0	479	0	0
1	B	969	0	479	2	0
1	C	969	0	479	0	0
1	E	969	0	479	0	0
1	K	969	0	479	0	0
2	D	183	0	79	0	0
2	F	138	0	63	0	0
2	G	64	0	29	0	0
2	Q	855	0	300	1	0
2	S	973	0	349	1	0
2	U	839	0	299	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	297	0	147	0	0
2	Y	814	0	284	0	0
2	b	912	0	318	0	0
2	c	287	0	139	0	0
2	d	184	0	89	0	0
2	i	138	0	60	0	0
3	Z	306	0	135	6	0
3	a	242	0	113	0	0
3	e	193	0	90	0	0
4	H	1087	0	563	0	0
4	I	1062	0	544	0	0
4	J	1330	0	681	3	0
4	L	1311	0	669	8	0
4	M	1330	0	681	11	0
5	R	515	0	236	1	0
5	f	475	0	219	0	0
5	j	515	0	236	0	0
6	O	3947	0	1786	13	0
6	P	3754	0	1693	6	0
6	T	3992	0	1808	23	0
6	V	3512	0	1583	5	0
6	g	3719	0	1670	0	0
6	h	2259	0	1015	0	0
All	All	40078	0	18273	62	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:821:SER:O	6:T:516:ALA:HB1	1.49	1.12
6:T:139:ALA:HB2	3:Z:42:PRO:O	1.49	1.12
4:M:7:THR:N	4:M:113:ALA:HB1	1.67	1.08
4:M:6:PHE:C	4:M:113:ALA:HB1	1.80	1.00
6:O:821:SER:O	6:T:516:ALA:CB	2.15	0.95
6:T:139:ALA:CB	3:Z:42:PRO:O	2.21	0.88
6:P:498:LEU:O	6:P:499:LYS:CB	2.16	0.87
6:V:498:LEU:O	6:V:499:LYS:CB	2.15	0.85
4:J:186:ALA:HB1	4:J:192[A]:THR:O	1.86	0.76
4:M:7:THR:CA	4:M:113:ALA:HB1	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:7:THR:HA	4:M:113:ALA:CB	2.19	0.73
4:L:60:VAL:HA	6:T:134:VAL:CB	2.22	0.70
6:T:138:PHE:CB	3:Z:46:THR:CB	2.76	0.63
6:T:135:LEU:O	3:Z:43:GLY:HA3	2.01	0.61
6:O:821:SER:C	6:T:516:ALA:HB1	2.20	0.61
4:M:6:PHE:C	4:M:113:ALA:CB	2.64	0.59
4:M:7:THR:CA	4:M:113:ALA:CB	2.80	0.59
6:O:654:ASP:HA	6:O:686:ALA:HB3	1.85	0.58
6:T:139:ALA:CA	3:Z:42:PRO:O	2.51	0.58
6:T:654:ASP:HA	6:T:686:ALA:HB3	1.85	0.58
4:L:112:ALA:C	4:L:114:ALA:H	2.09	0.56
4:M:7:THR:HA	4:M:113:ALA:HB3	1.87	0.55
6:O:431:ALA:HB3	6:O:707:ALA:HB1	1.89	0.54
6:T:657:TRP:O	6:T:661:GLN:N	2.41	0.54
6:T:431:ALA:HB3	6:T:707:ALA:HB1	1.89	0.54
6:O:657:TRP:O	6:O:661:GLN:N	2.41	0.53
4:M:51:ILE:HA	4:M:55:ALA:HB3	1.91	0.53
4:L:60:VAL:CB	6:T:134:VAL:CB	2.87	0.53
6:T:507:ASN:O	6:T:605:ASP:CB	2.58	0.52
4:J:51:ILE:HA	4:J:55:ALA:HB3	1.92	0.51
4:L:111:SER:O	4:L:114:ALA:HB3	2.11	0.51
6:T:78:LEU:O	6:T:275:SER:HA	2.11	0.51
6:O:78:LEU:O	6:O:275:SER:HA	2.11	0.50
6:O:821:SER:C	6:T:516:ALA:CB	2.80	0.49
4:M:60:VAL:CB	6:O:134:VAL:CB	2.90	0.49
6:V:315:GLN:O	6:V:319:GLY:N	2.37	0.49
2:Q:75:ASN:H	2:S:75:ASN:CB	2.25	0.48
6:T:324:GLY:O	6:T:385:PRO:HA	2.13	0.48
1:B:73:LEU:C	1:B:75:ARG:H	2.15	0.48
6:O:324:GLY:O	6:O:385:PRO:HA	2.13	0.47
4:M:3:PHE:CB	4:M:121:GLN:CB	2.93	0.46
5:R:10:ALA:HB1	6:T:255:THR:H	1.79	0.46
6:T:135:LEU:O	3:Z:43:GLY:CA	2.64	0.46
4:L:164:ALA:HB2	4:M:252:VAL:HA	1.97	0.45
1:B:73:LEU:C	1:B:75:ARG:N	2.69	0.45
6:V:447:THR:O	6:V:685:PHE:N	2.49	0.45
6:P:315:GLN:O	6:P:319:GLY:N	2.37	0.44
6:O:275:SER:O	6:O:326:HIS:HA	2.18	0.44
4:L:60:VAL:CA	6:T:134:VAL:CB	2.93	0.43
6:P:447:THR:O	6:P:685:PHE:N	2.49	0.43
6:T:275:SER:O	6:T:326:HIS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:625:ASN:O	6:P:627:GLU:N	2.51	0.43
6:V:625:ASN:O	6:V:627:GLU:N	2.51	0.43
6:T:605:ASP:O	6:T:606:ALA:C	2.58	0.42
4:L:112:ALA:C	4:L:114:ALA:N	2.72	0.42
6:P:780:GLU:O	6:P:784:LEU:N	2.53	0.42
4:L:252:VAL:HA	4:J:164:ALA:HB2	2.02	0.42
6:T:509:PHE:CB	6:T:560:ARG:O	2.68	0.42
6:O:509:PHE:CB	6:O:560:ARG:O	2.68	0.41
6:O:42:TRP:N	6:O:123:LEU:O	2.52	0.41
6:P:275:SER:O	6:P:326:HIS:HA	2.21	0.41
6:V:780:GLU:O	6:V:784:LEU:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	195/229 (85%)	194 (100%)	1 (0%)	0	100	100
1	B	195/229 (85%)	193 (99%)	2 (1%)	0	100	100
1	C	195/229 (85%)	194 (100%)	1 (0%)	0	100	100
1	E	195/229 (85%)	194 (100%)	1 (0%)	0	100	100
1	K	195/229 (85%)	193 (99%)	2 (1%)	0	100	100
2	D	35/231 (15%)	32 (91%)	3 (9%)	0	100	100
2	F	26/231 (11%)	25 (96%)	1 (4%)	0	100	100
2	G	11/231 (5%)	8 (73%)	3 (27%)	0	100	100
2	Q	192/231 (83%)	184 (96%)	6 (3%)	2 (1%)	15	54
2	S	221/231 (96%)	209 (95%)	11 (5%)	1 (0%)	29	68
2	U	185/231 (80%)	178 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	59/231 (26%)	49 (83%)	9 (15%)	1 (2%)	9	43
2	Y	180/231 (78%)	177 (98%)	3 (2%)	0	100	100
2	b	204/231 (88%)	195 (96%)	9 (4%)	0	100	100
2	c	55/231 (24%)	54 (98%)	1 (2%)	0	100	100
2	d	34/231 (15%)	28 (82%)	6 (18%)	0	100	100
2	i	26/231 (11%)	25 (96%)	1 (4%)	0	100	100
3	Z	58/395 (15%)	54 (93%)	4 (7%)	0	100	100
3	a	47/395 (12%)	45 (96%)	2 (4%)	0	100	100
3	e	35/395 (9%)	35 (100%)	0	0	100	100
4	H	218/342 (64%)	209 (96%)	9 (4%)	0	100	100
4	I	213/342 (62%)	207 (97%)	6 (3%)	0	100	100
4	J	270/342 (79%)	258 (96%)	12 (4%)	0	100	100
4	L	264/342 (77%)	255 (97%)	9 (3%)	0	100	100
4	M	270/342 (79%)	257 (95%)	13 (5%)	0	100	100
5	R	102/104 (98%)	91 (89%)	11 (11%)	0	100	100
5	f	94/104 (90%)	84 (89%)	10 (11%)	0	100	100
5	j	102/104 (98%)	91 (89%)	11 (11%)	0	100	100
6	O	793/823 (96%)	736 (93%)	55 (7%)	2 (0%)	41	76
6	P	748/823 (91%)	705 (94%)	43 (6%)	0	100	100
6	T	804/823 (98%)	745 (93%)	59 (7%)	0	100	100
6	V	691/823 (84%)	653 (94%)	38 (6%)	0	100	100
6	g	741/823 (90%)	689 (93%)	52 (7%)	0	100	100
6	h	441/823 (54%)	415 (94%)	26 (6%)	0	100	100
All	All	8094/12062 (67%)	7661 (95%)	427 (5%)	6 (0%)	54	85

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Q	63	GLN
2	S	64	PRO
6	O	607	LEU
2	Q	66	PRO
2	X	66	PRO
6	O	532	GLY

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

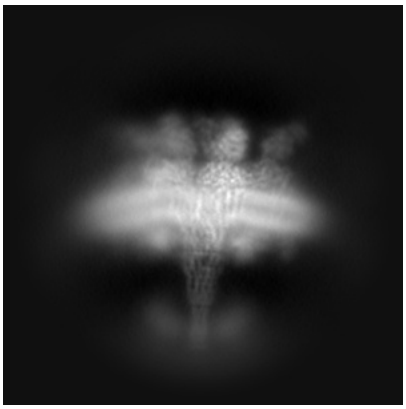
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19488. These allow visual inspection of the internal detail of the map and identification of artifacts.

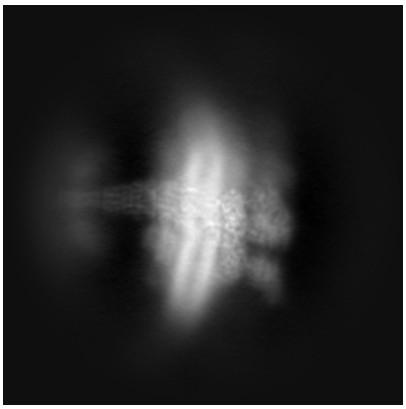
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

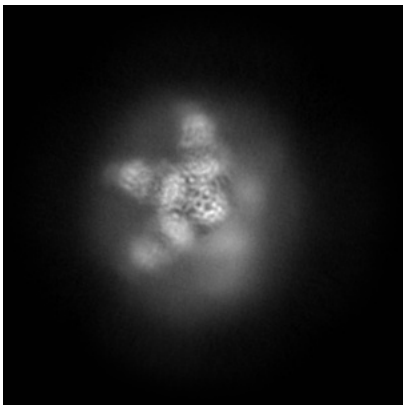
6.1.1 Primary map



X



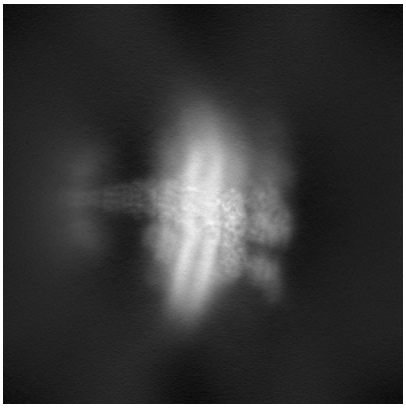
Y



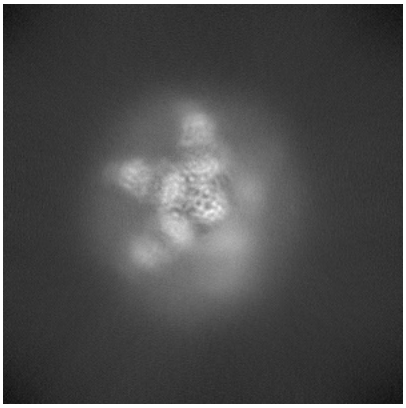
Z

6.1.2 Raw map

X



Y

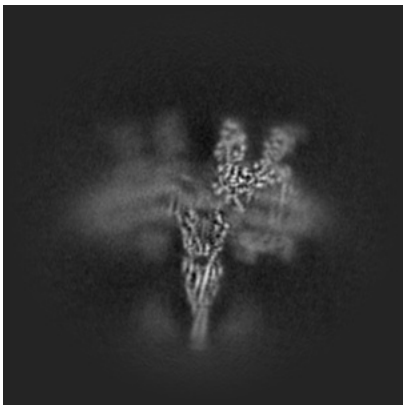


Z

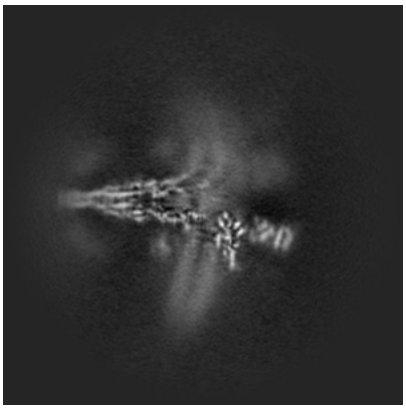
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

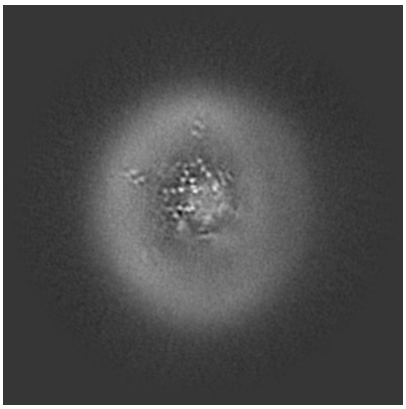
6.2.1 Primary map



X Index: 256

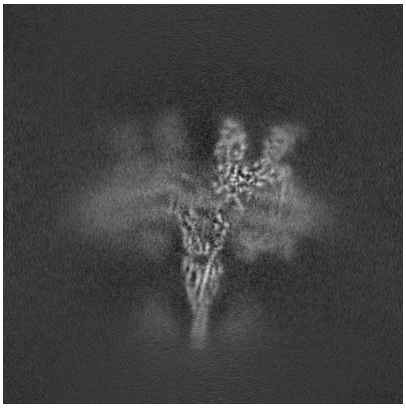


Y Index: 256

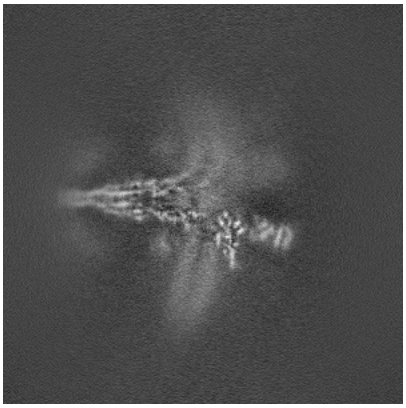


Z Index: 256

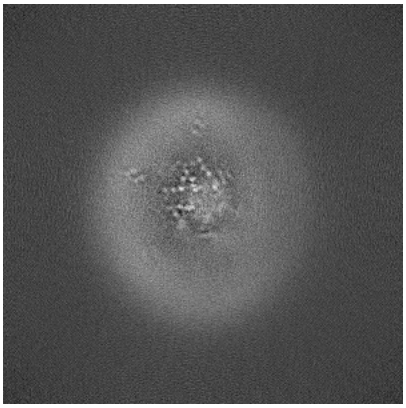
6.2.2 Raw map



X Index: 256



Y Index: 256

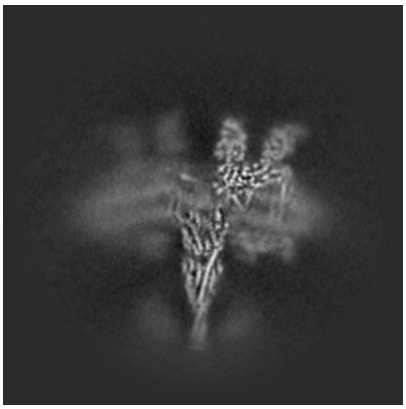


Z Index: 256

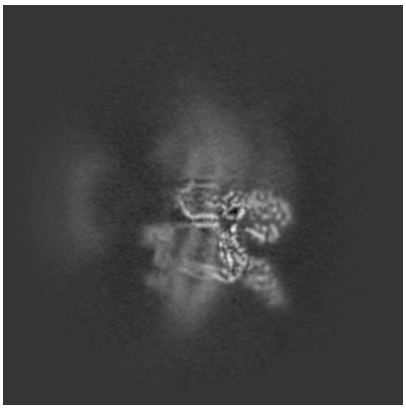
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

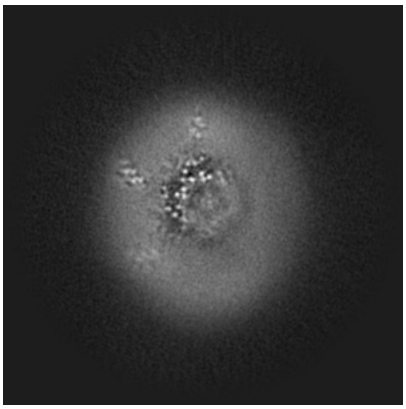
6.3.1 Primary map



X Index: 254

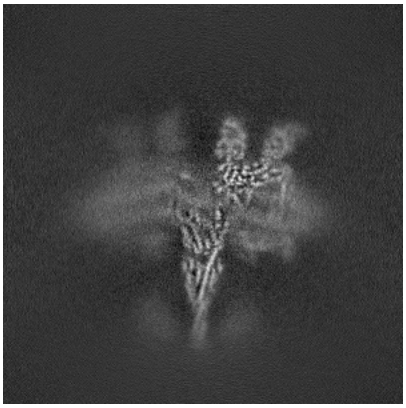


Y Index: 288

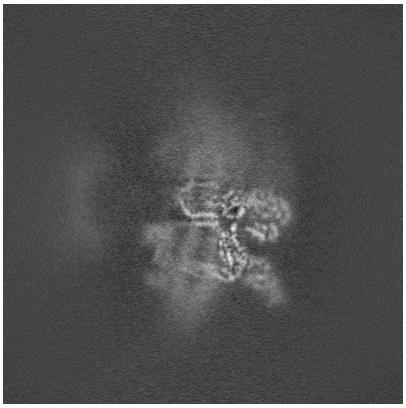


Z Index: 266

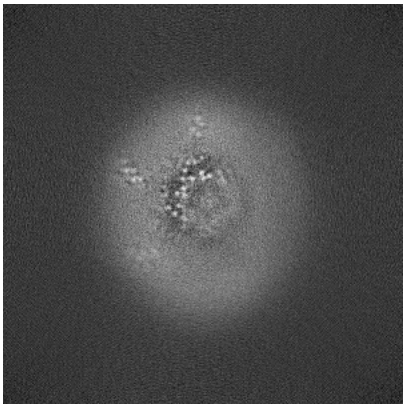
6.3.2 Raw map



X Index: 254



Y Index: 288

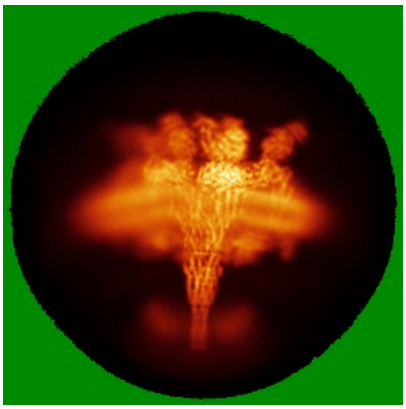


Z Index: 266

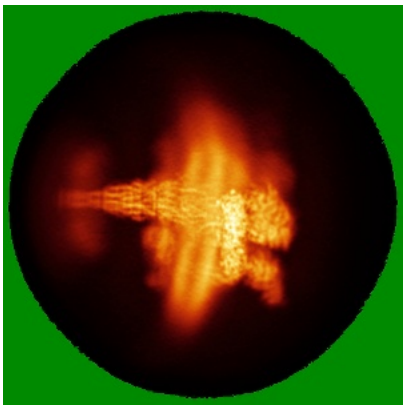
The images above show the largest variance slices of the map in three orthogonal directions.

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

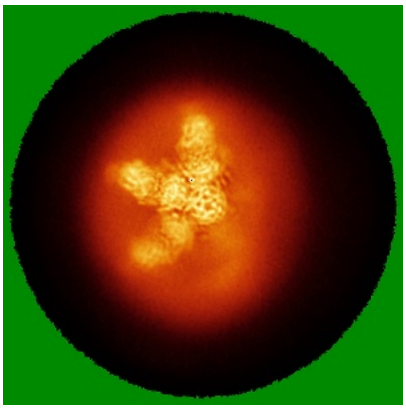
6.4.1 Primary map



X

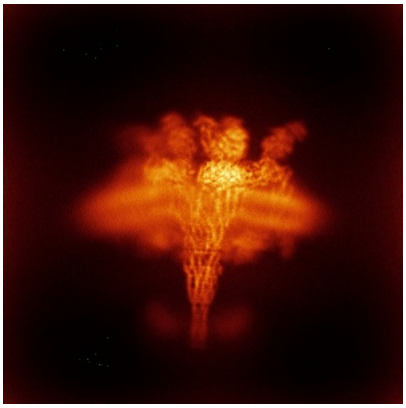


Y

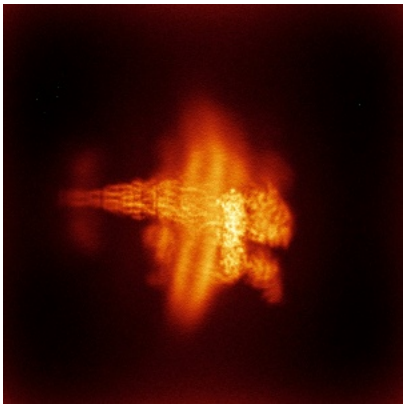


Z

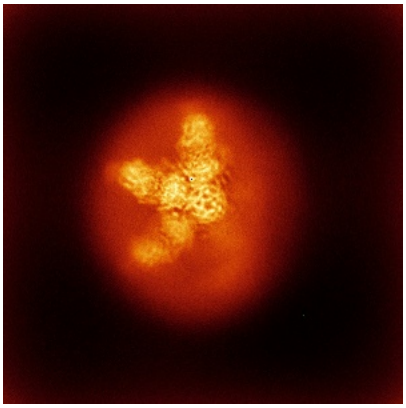
6.4.2 Raw map



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.

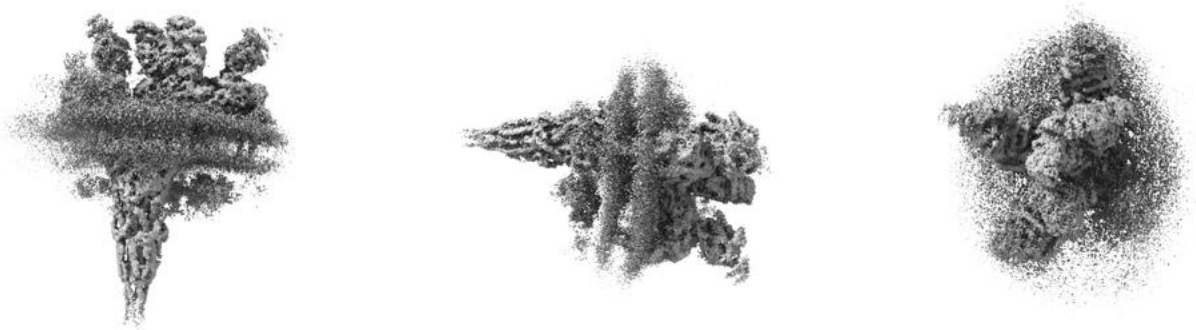
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. 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



X Y Z

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.

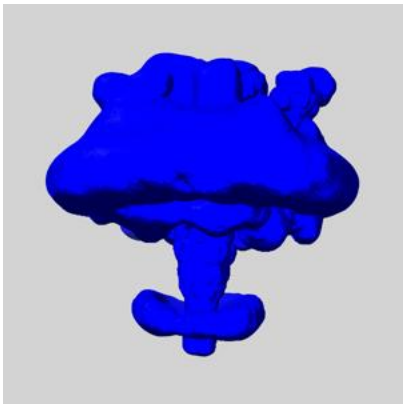
6.6 Mask visualisation (i)

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

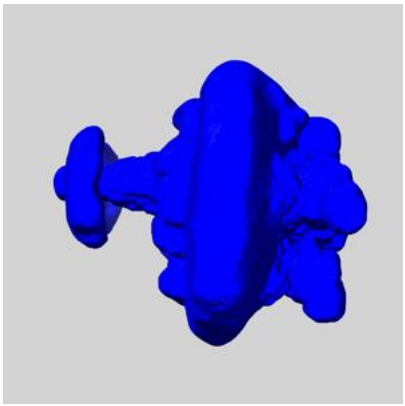
A mask typically either:

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

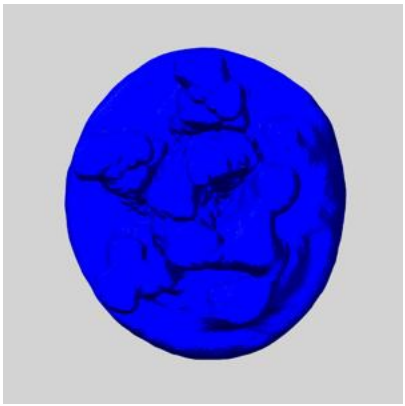
6.6.1 emd_19488_msk_1.map (i)



X



Y

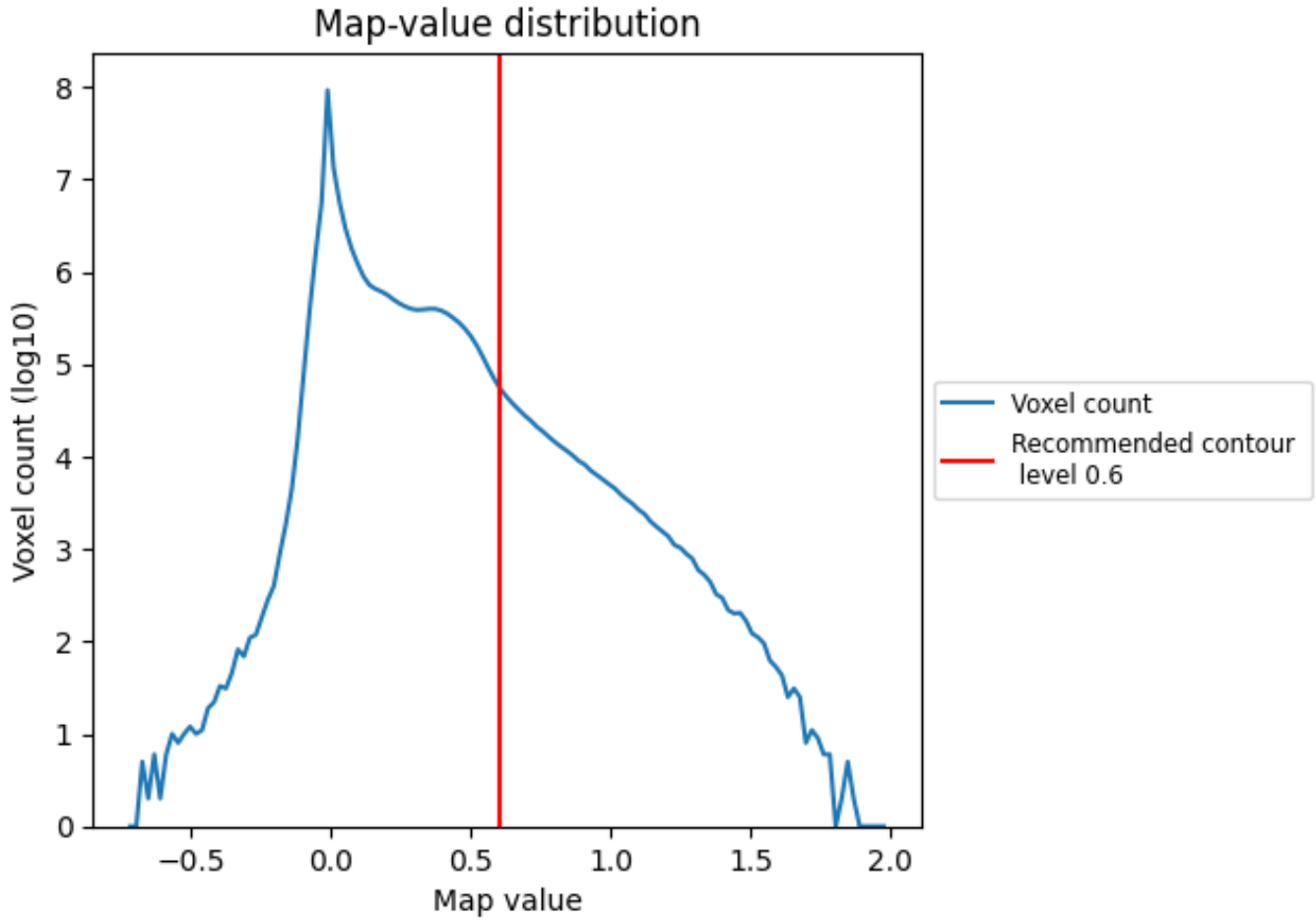


Z

7 Map analysis

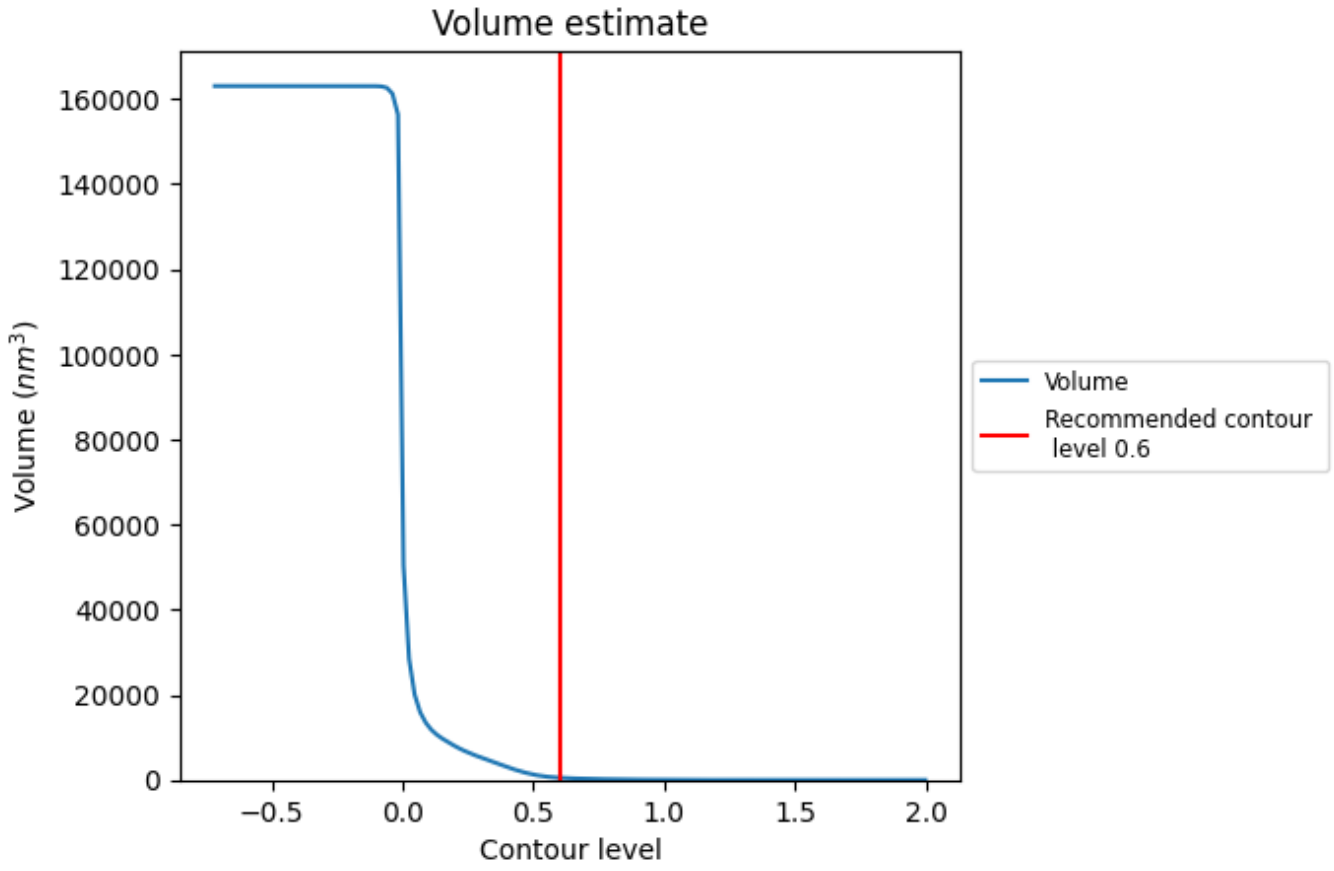
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

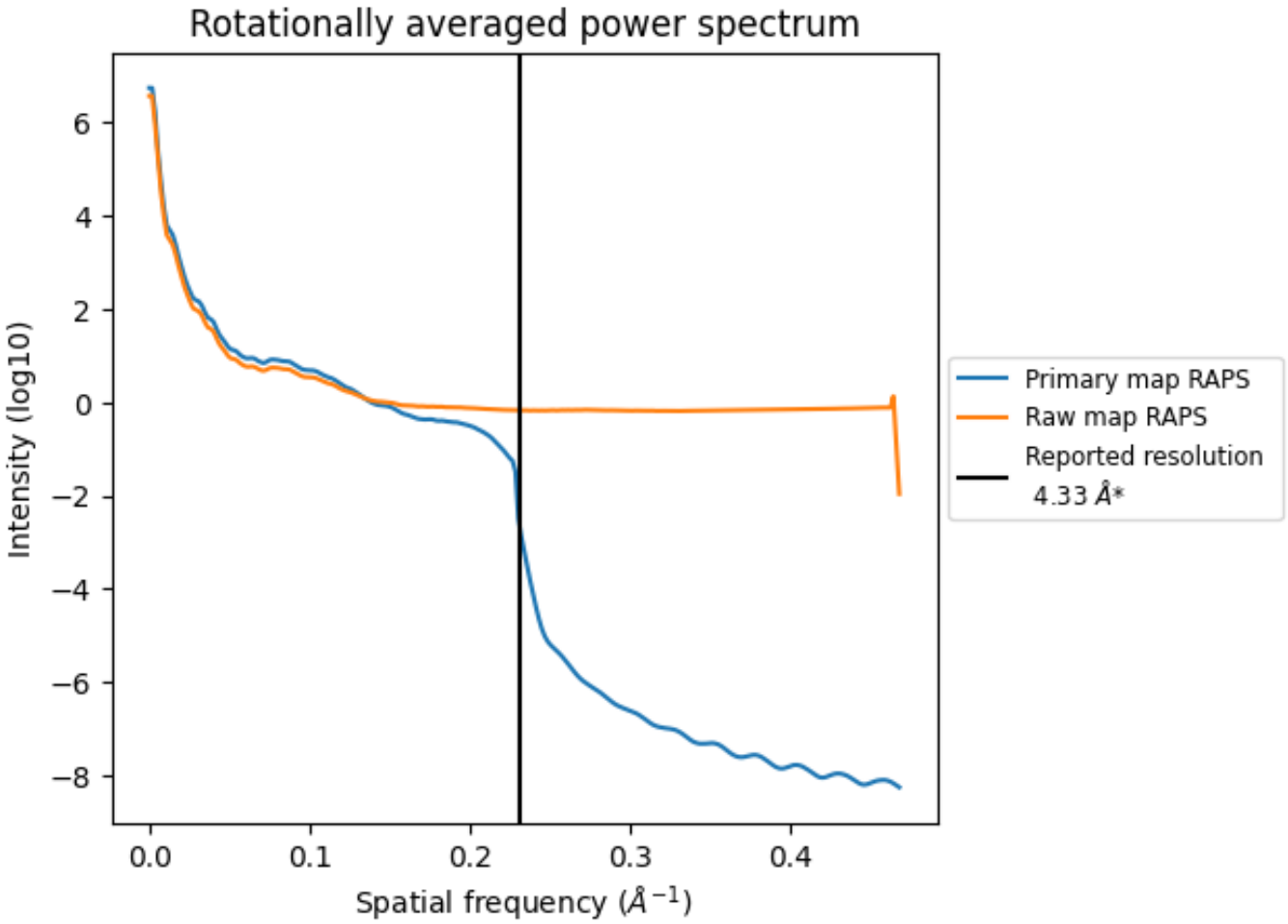
7.2 Volume estimate



The volume at the recommended contour level is 513 nm^3; this corresponds to an approximate mass of 464 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)

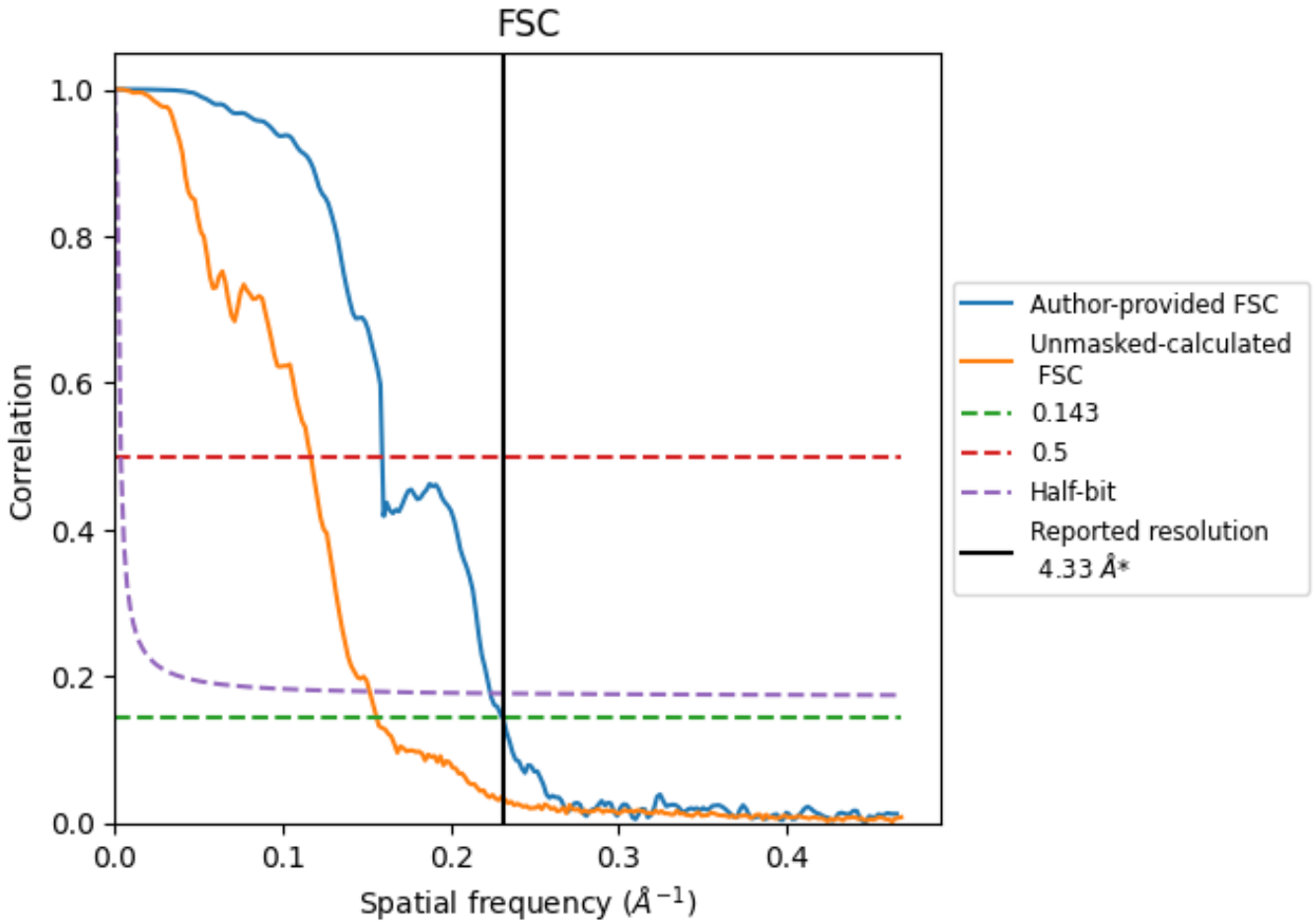


*Reported resolution corresponds to spatial frequency of 0.231 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.231 Å^{-1}

8.2 Resolution estimates (i)

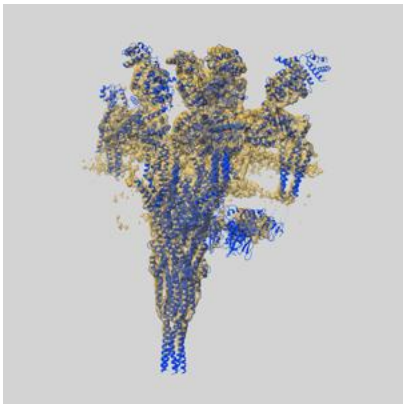
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.33	-	-
Author-provided FSC curve	4.33	6.28	4.47
Unmasked-calculated*	6.41	8.58	6.58

*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 6.41 differs from the reported value 4.33 by more than 10 %

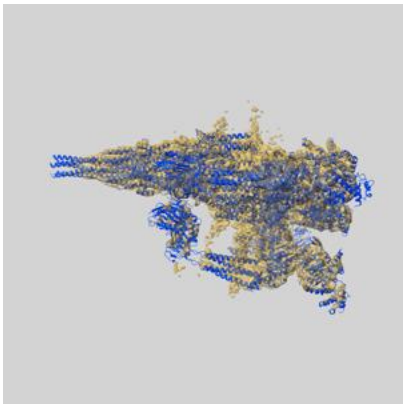
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19488 and PDB model 8RTD. Per-residue inclusion information can be found in section 3 on page 7.

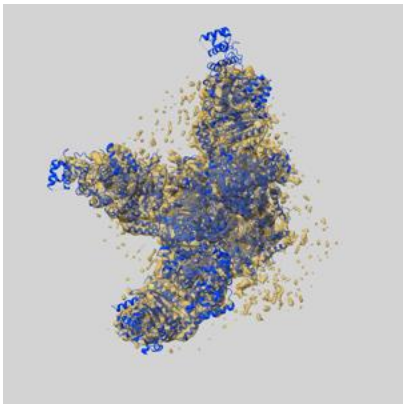
9.1 Map-model overlay



X



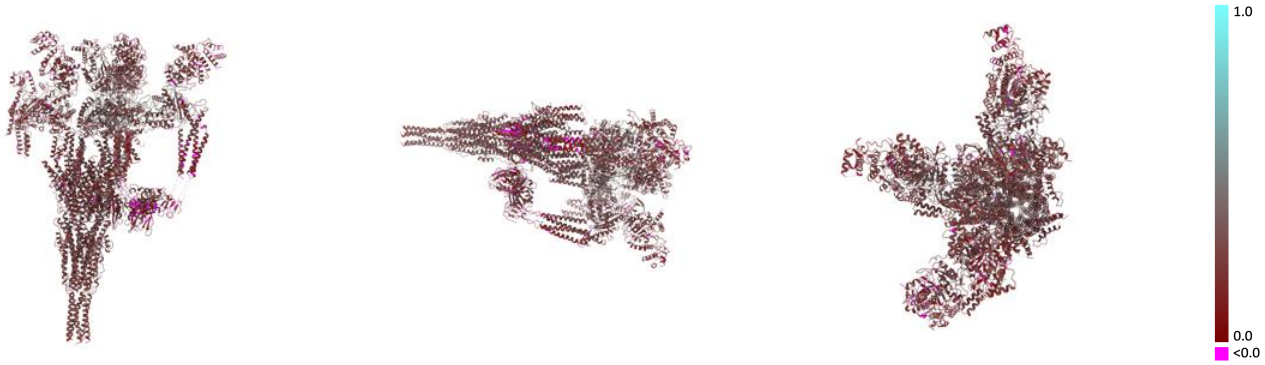
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

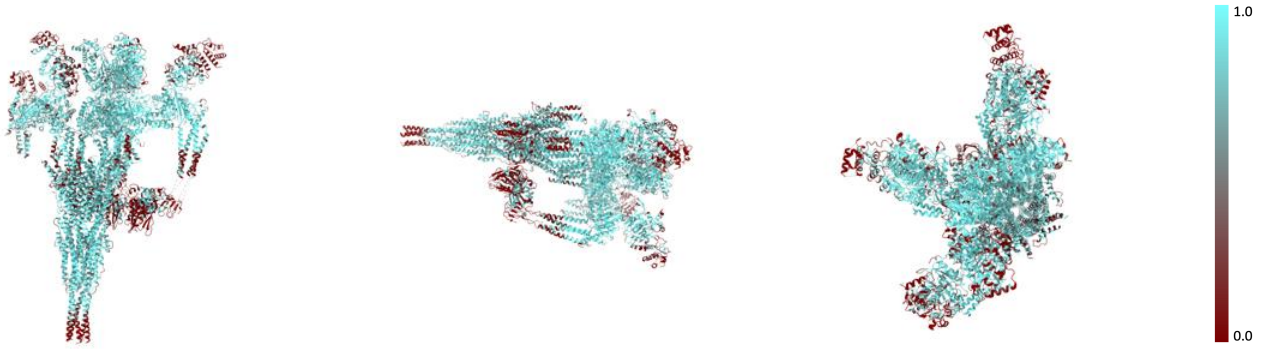
9.2 Q-score mapped to coordinate model (i)



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.

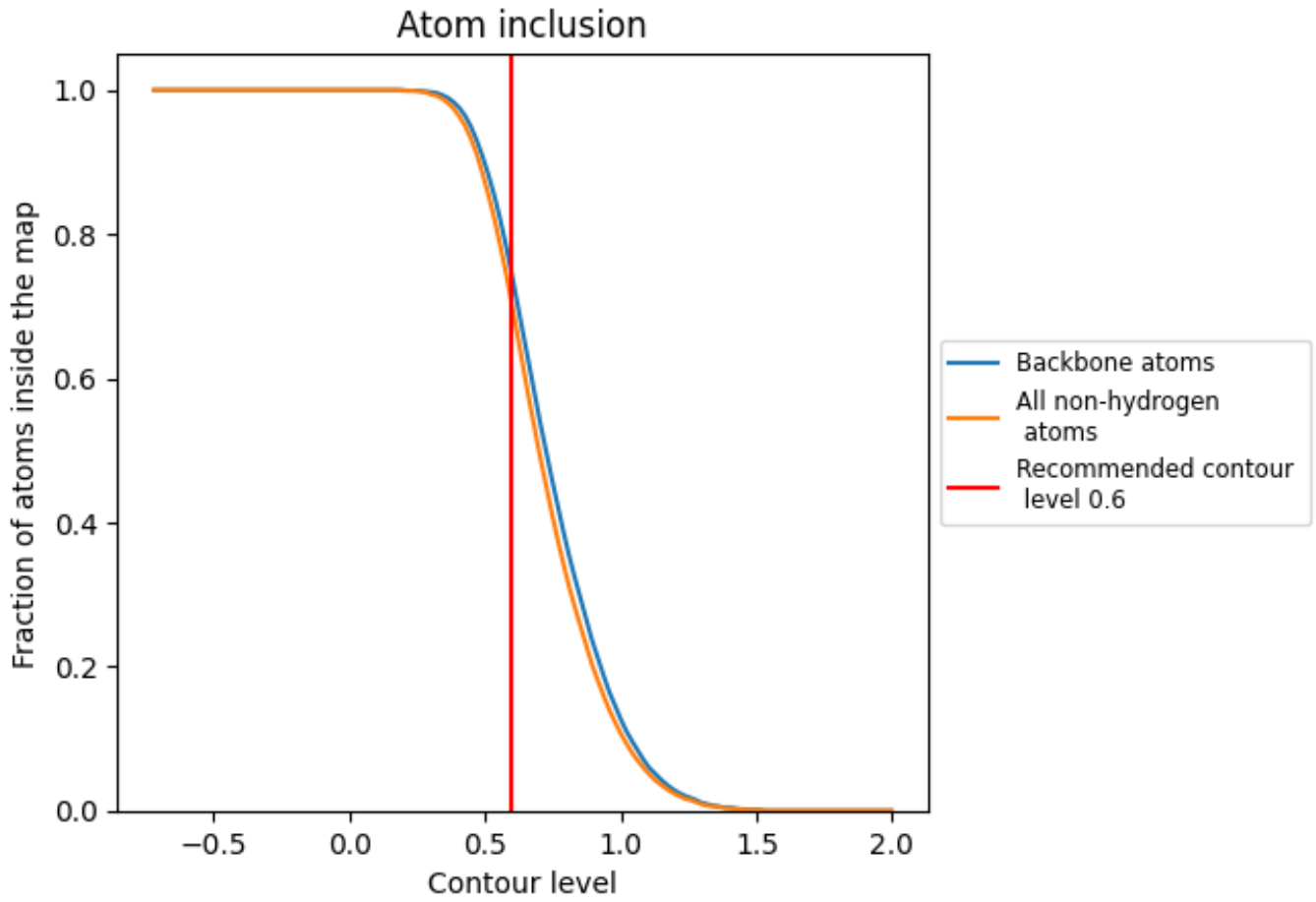
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 74% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7020	0.2670
A	0.7390	0.2840
B	0.7550	0.2990
C	0.7060	0.2950
D	0.6180	0.1890
E	0.7220	0.2770
F	0.7460	0.2080
G	0.7030	0.2230
H	0.7280	0.2590
I	0.6360	0.2490
J	0.7100	0.2510
K	0.7350	0.2820
L	0.8560	0.2990
M	0.8330	0.3000
O	0.8940	0.3280
P	0.7600	0.2720
Q	0.4100	0.2250
R	0.8520	0.3080
S	0.5180	0.2200
T	0.8420	0.3070
U	0.3150	0.1880
V	0.6630	0.2660
X	0.4440	0.1730
Y	0.3210	0.1700
Z	0.7060	0.2860
a	0.5700	0.2590
b	0.4710	0.2070
c	0.5050	0.1330
d	0.3640	0.1210
e	0.5860	0.2780
f	0.6950	0.2640
g	0.6510	0.2500
h	0.5530	0.2110
i	0.6740	0.1940
j	0.8760	0.3330