Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 09:33 am GMT

PDB ID	:	6HS7
EMDB ID	:	EMD-0264
Title	:	Type VI membrane complex
Authors	:	Rapisarda, C.; Fronzes, R.
Deposited on	:	2018-09-28
Resolution	:	4.60 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:

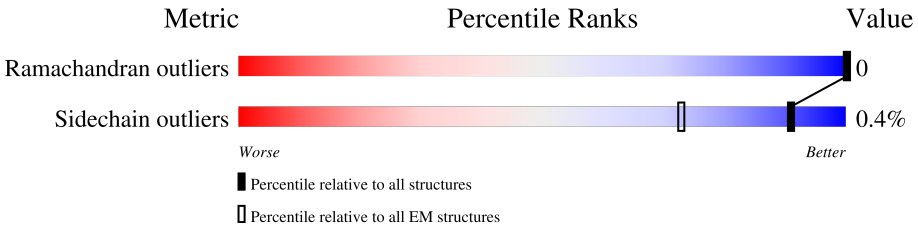
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.60 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.



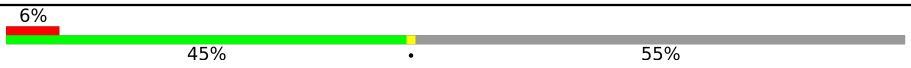
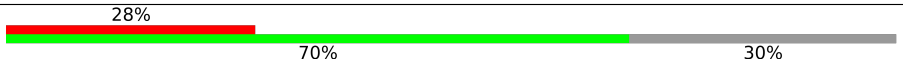
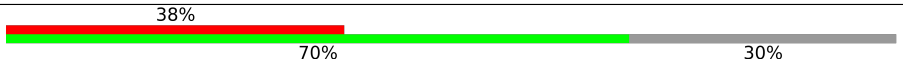
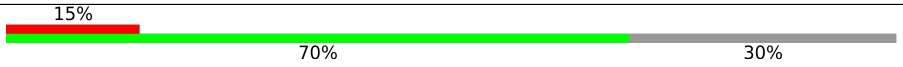
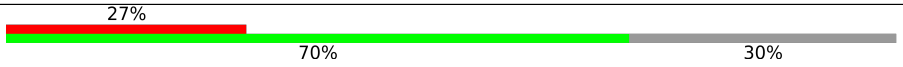
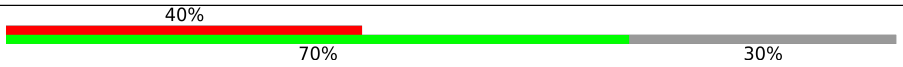
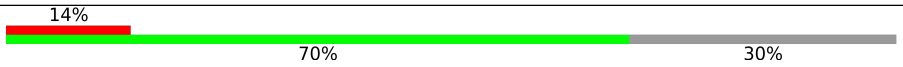
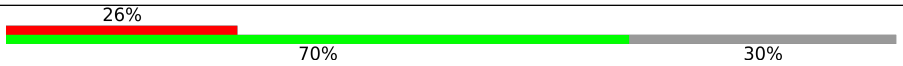
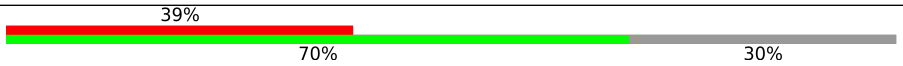
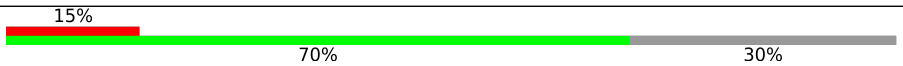
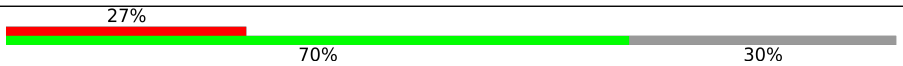
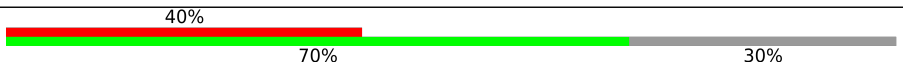
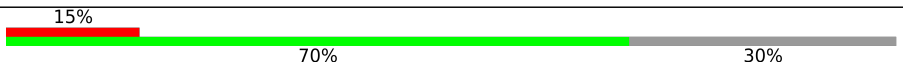
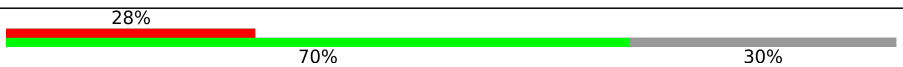
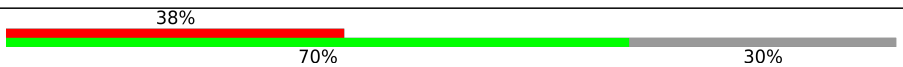
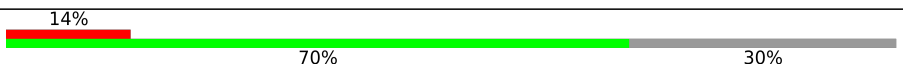
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1129	7% 42% 58%
1	B	1129	7% 42% 58%
1	C	1129	7% 42% 58%
1	D	1129	8% 42% 58%
1	E	1129	7% 42% 58%
1	a	1129	6% 45% 55%
1	b	1129	6% 45% 55%
1	c	1129	6% 45% 55%
1	d	1129	6% 45% 55%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	e	1129	
2	F	186	
2	G	186	
2	H	186	
2	I	186	
2	J	186	
2	K	186	
2	L	186	
2	M	186	
2	N	186	
2	O	186	
2	P	186	
2	Q	186	
2	R	186	
2	S	186	
2	T	186	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 52890 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 ImcF-like family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	478	Total	C	N	O	S	0	0
			3629	2286	648	682	13		
1	B	478	Total	C	N	O	S	0	0
			3629	2286	648	682	13		
1	C	478	Total	C	N	O	S	0	0
			3629	2286	648	682	13		
1	D	478	Total	C	N	O	S	0	0
			3629	2286	648	682	13		
1	E	478	Total	C	N	O	S	0	0
			3629	2286	648	682	13		
1	a	513	Total	C	N	O	S	0	0
			3949	2484	705	745	15		
1	b	513	Total	C	N	O	S	0	0
			3949	2484	705	745	15		
1	c	513	Total	C	N	O	S	0	0
			3949	2484	705	745	15		
1	d	513	Total	C	N	O	S	0	0
			3949	2484	705	745	15		
1	e	513	Total	C	N	O	S	0	0
			3949	2484	705	745	15		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	VAL	ALA	conflict	UNP I2W7L4
B	446	VAL	ALA	conflict	UNP I2W7L4
C	446	VAL	ALA	conflict	UNP I2W7L4
D	446	VAL	ALA	conflict	UNP I2W7L4
E	446	VAL	ALA	conflict	UNP I2W7L4
a	446	VAL	ALA	conflict	UNP I2W7L4
b	446	VAL	ALA	conflict	UNP I2W7L4
c	446	VAL	ALA	conflict	UNP I2W7L4
d	446	VAL	ALA	conflict	UNP I2W7L4
e	446	VAL	ALA	conflict	UNP I2W7L4

- Molecule 2 is a protein called Type VI secretion system protein VasD.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	130	Total	C	N	O	S	0	0
			1000	633	171	194	2		
2	G	130	Total	C	N	O	S	0	0
			1000	633	171	194	2		
2	H	130	Total	C	N	O	S	0	0
			1000	633	171	194	2		
2	I	130	Total	C	N	O	S	0	0
			1000	633	171	194	2		
2	J	130	Total	C	N	O	S	0	0
			1000	633	171	194	2		
2	K	130	Total	C	N	O	S	0	0
			1000	633	171	194	2		
2	L	130	Total	C	N	O	S	0	0
			1000	633	171	194	2		
2	M	130	Total	C	N	O	S	0	0
			1000	633	171	194	2		
2	N	130	Total	C	N	O	S	0	0
			1000	633	171	194	2		
2	O	130	Total	C	N	O	S	0	0
			1000	633	171	194	2		
2	P	130	Total	C	N	O	S	0	0
			1000	633	171	194	2		
2	Q	130	Total	C	N	O	S	0	0
			1000	633	171	194	2		
2	R	130	Total	C	N	O	S	0	0
			1000	633	171	194	2		
2	S	130	Total	C	N	O	S	0	0
			1000	633	171	194	2		
2	T	130	Total	C	N	O	S	0	0
			1000	633	171	194	2		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	156	TRP	-	expression tag	UNP H4UNW1
F	157	SER	-	expression tag	UNP H4UNW1
F	158	HIS	-	expression tag	UNP H4UNW1
F	159	PRO	-	expression tag	UNP H4UNW1
F	160	GLN	-	expression tag	UNP H4UNW1
F	161	PHE	-	expression tag	UNP H4UNW1
F	162	GLU	-	expression tag	UNP H4UNW1
F	163	LYS	-	expression tag	UNP H4UNW1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	156	TRP	-	expression tag	UNP H4UNW1
G	157	SER	-	expression tag	UNP H4UNW1
G	158	HIS	-	expression tag	UNP H4UNW1
G	159	PRO	-	expression tag	UNP H4UNW1
G	160	GLN	-	expression tag	UNP H4UNW1
G	161	PHE	-	expression tag	UNP H4UNW1
G	162	GLU	-	expression tag	UNP H4UNW1
G	163	LYS	-	expression tag	UNP H4UNW1
H	156	TRP	-	expression tag	UNP H4UNW1
H	157	SER	-	expression tag	UNP H4UNW1
H	158	HIS	-	expression tag	UNP H4UNW1
H	159	PRO	-	expression tag	UNP H4UNW1
H	160	GLN	-	expression tag	UNP H4UNW1
H	161	PHE	-	expression tag	UNP H4UNW1
H	162	GLU	-	expression tag	UNP H4UNW1
H	163	LYS	-	expression tag	UNP H4UNW1
I	156	TRP	-	expression tag	UNP H4UNW1
I	157	SER	-	expression tag	UNP H4UNW1
I	158	HIS	-	expression tag	UNP H4UNW1
I	159	PRO	-	expression tag	UNP H4UNW1
I	160	GLN	-	expression tag	UNP H4UNW1
I	161	PHE	-	expression tag	UNP H4UNW1
I	162	GLU	-	expression tag	UNP H4UNW1
I	163	LYS	-	expression tag	UNP H4UNW1
J	156	TRP	-	expression tag	UNP H4UNW1
J	157	SER	-	expression tag	UNP H4UNW1
J	158	HIS	-	expression tag	UNP H4UNW1
J	159	PRO	-	expression tag	UNP H4UNW1
J	160	GLN	-	expression tag	UNP H4UNW1
J	161	PHE	-	expression tag	UNP H4UNW1
J	162	GLU	-	expression tag	UNP H4UNW1
J	163	LYS	-	expression tag	UNP H4UNW1
K	156	TRP	-	expression tag	UNP H4UNW1
K	157	SER	-	expression tag	UNP H4UNW1
K	158	HIS	-	expression tag	UNP H4UNW1
K	159	PRO	-	expression tag	UNP H4UNW1
K	160	GLN	-	expression tag	UNP H4UNW1
K	161	PHE	-	expression tag	UNP H4UNW1
K	162	GLU	-	expression tag	UNP H4UNW1
K	163	LYS	-	expression tag	UNP H4UNW1
L	156	TRP	-	expression tag	UNP H4UNW1
L	157	SER	-	expression tag	UNP H4UNW1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	158	HIS	-	expression tag	UNP H4UNW1
L	159	PRO	-	expression tag	UNP H4UNW1
L	160	GLN	-	expression tag	UNP H4UNW1
L	161	PHE	-	expression tag	UNP H4UNW1
L	162	GLU	-	expression tag	UNP H4UNW1
L	163	LYS	-	expression tag	UNP H4UNW1
M	156	TRP	-	expression tag	UNP H4UNW1
M	157	SER	-	expression tag	UNP H4UNW1
M	158	HIS	-	expression tag	UNP H4UNW1
M	159	PRO	-	expression tag	UNP H4UNW1
M	160	GLN	-	expression tag	UNP H4UNW1
M	161	PHE	-	expression tag	UNP H4UNW1
M	162	GLU	-	expression tag	UNP H4UNW1
M	163	LYS	-	expression tag	UNP H4UNW1
N	156	TRP	-	expression tag	UNP H4UNW1
N	157	SER	-	expression tag	UNP H4UNW1
N	158	HIS	-	expression tag	UNP H4UNW1
N	159	PRO	-	expression tag	UNP H4UNW1
N	160	GLN	-	expression tag	UNP H4UNW1
N	161	PHE	-	expression tag	UNP H4UNW1
N	162	GLU	-	expression tag	UNP H4UNW1
N	163	LYS	-	expression tag	UNP H4UNW1
O	156	TRP	-	expression tag	UNP H4UNW1
O	157	SER	-	expression tag	UNP H4UNW1
O	158	HIS	-	expression tag	UNP H4UNW1
O	159	PRO	-	expression tag	UNP H4UNW1
O	160	GLN	-	expression tag	UNP H4UNW1
O	161	PHE	-	expression tag	UNP H4UNW1
O	162	GLU	-	expression tag	UNP H4UNW1
O	163	LYS	-	expression tag	UNP H4UNW1
P	156	TRP	-	expression tag	UNP H4UNW1
P	157	SER	-	expression tag	UNP H4UNW1
P	158	HIS	-	expression tag	UNP H4UNW1
P	159	PRO	-	expression tag	UNP H4UNW1
P	160	GLN	-	expression tag	UNP H4UNW1
P	161	PHE	-	expression tag	UNP H4UNW1
P	162	GLU	-	expression tag	UNP H4UNW1
P	163	LYS	-	expression tag	UNP H4UNW1
Q	156	TRP	-	expression tag	UNP H4UNW1
Q	157	SER	-	expression tag	UNP H4UNW1
Q	158	HIS	-	expression tag	UNP H4UNW1
Q	159	PRO	-	expression tag	UNP H4UNW1

Continued on next page...

Continued from previous page...

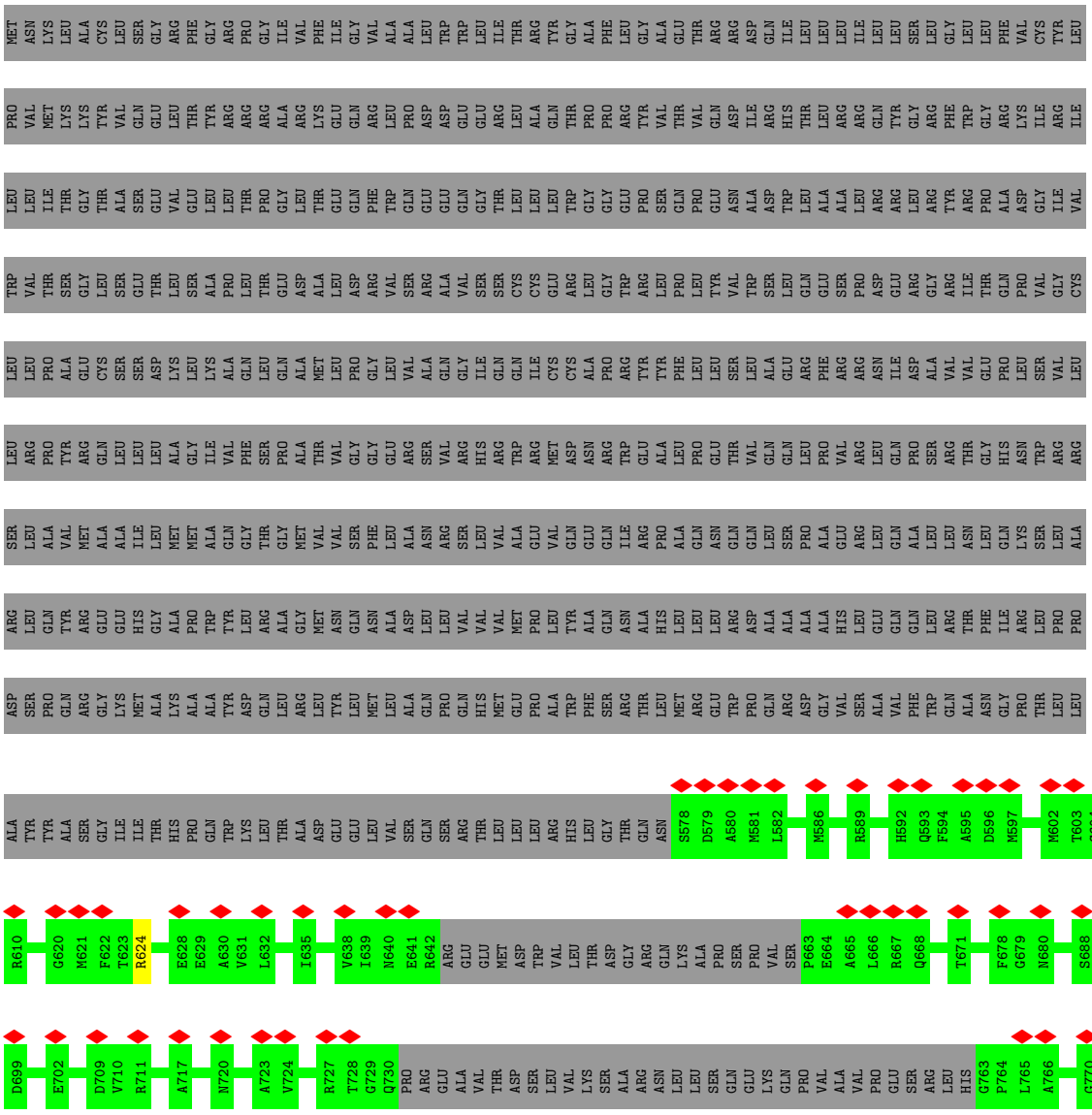
Chain	Residue	Modelled	Actual	Comment	Reference
Q	160	GLN	-	expression tag	UNP H4UNW1
Q	161	PHE	-	expression tag	UNP H4UNW1
Q	162	GLU	-	expression tag	UNP H4UNW1
Q	163	LYS	-	expression tag	UNP H4UNW1
R	156	TRP	-	expression tag	UNP H4UNW1
R	157	SER	-	expression tag	UNP H4UNW1
R	158	HIS	-	expression tag	UNP H4UNW1
R	159	PRO	-	expression tag	UNP H4UNW1
R	160	GLN	-	expression tag	UNP H4UNW1
R	161	PHE	-	expression tag	UNP H4UNW1
R	162	GLU	-	expression tag	UNP H4UNW1
R	163	LYS	-	expression tag	UNP H4UNW1
S	156	TRP	-	expression tag	UNP H4UNW1
S	157	SER	-	expression tag	UNP H4UNW1
S	158	HIS	-	expression tag	UNP H4UNW1
S	159	PRO	-	expression tag	UNP H4UNW1
S	160	GLN	-	expression tag	UNP H4UNW1
S	161	PHE	-	expression tag	UNP H4UNW1
S	162	GLU	-	expression tag	UNP H4UNW1
S	163	LYS	-	expression tag	UNP H4UNW1
T	156	TRP	-	expression tag	UNP H4UNW1
T	157	SER	-	expression tag	UNP H4UNW1
T	158	HIS	-	expression tag	UNP H4UNW1
T	159	PRO	-	expression tag	UNP H4UNW1
T	160	GLN	-	expression tag	UNP H4UNW1
T	161	PHE	-	expression tag	UNP H4UNW1
T	162	GLU	-	expression tag	UNP H4UNW1
T	163	LYS	-	expression tag	UNP H4UNW1

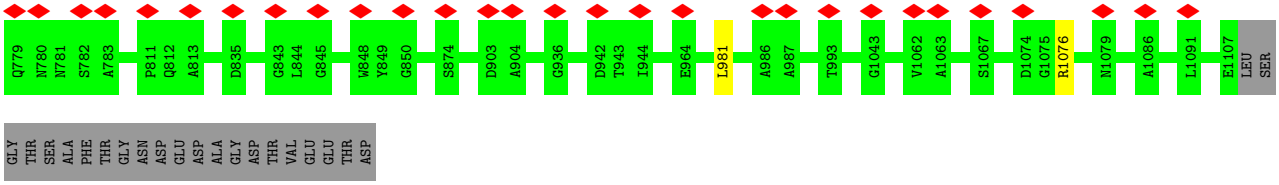
3 Residue-property plots (i)

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.

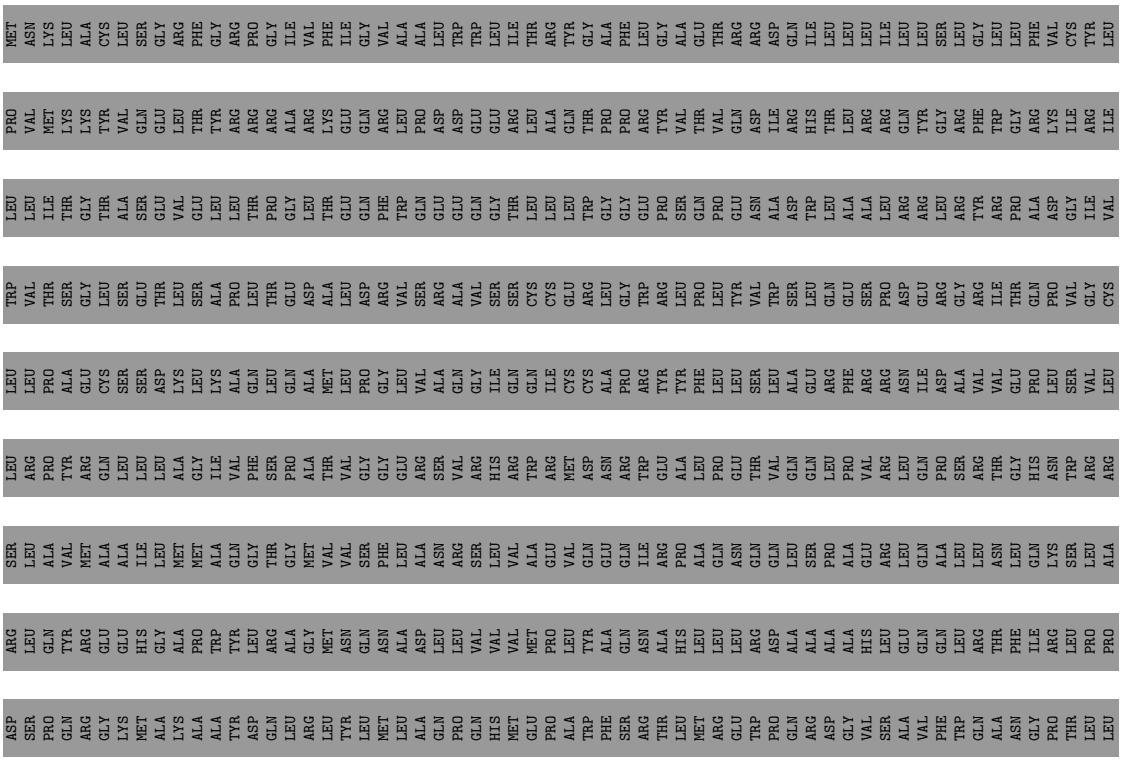
- Molecule 1: ImcF-like family protein

Chain A:



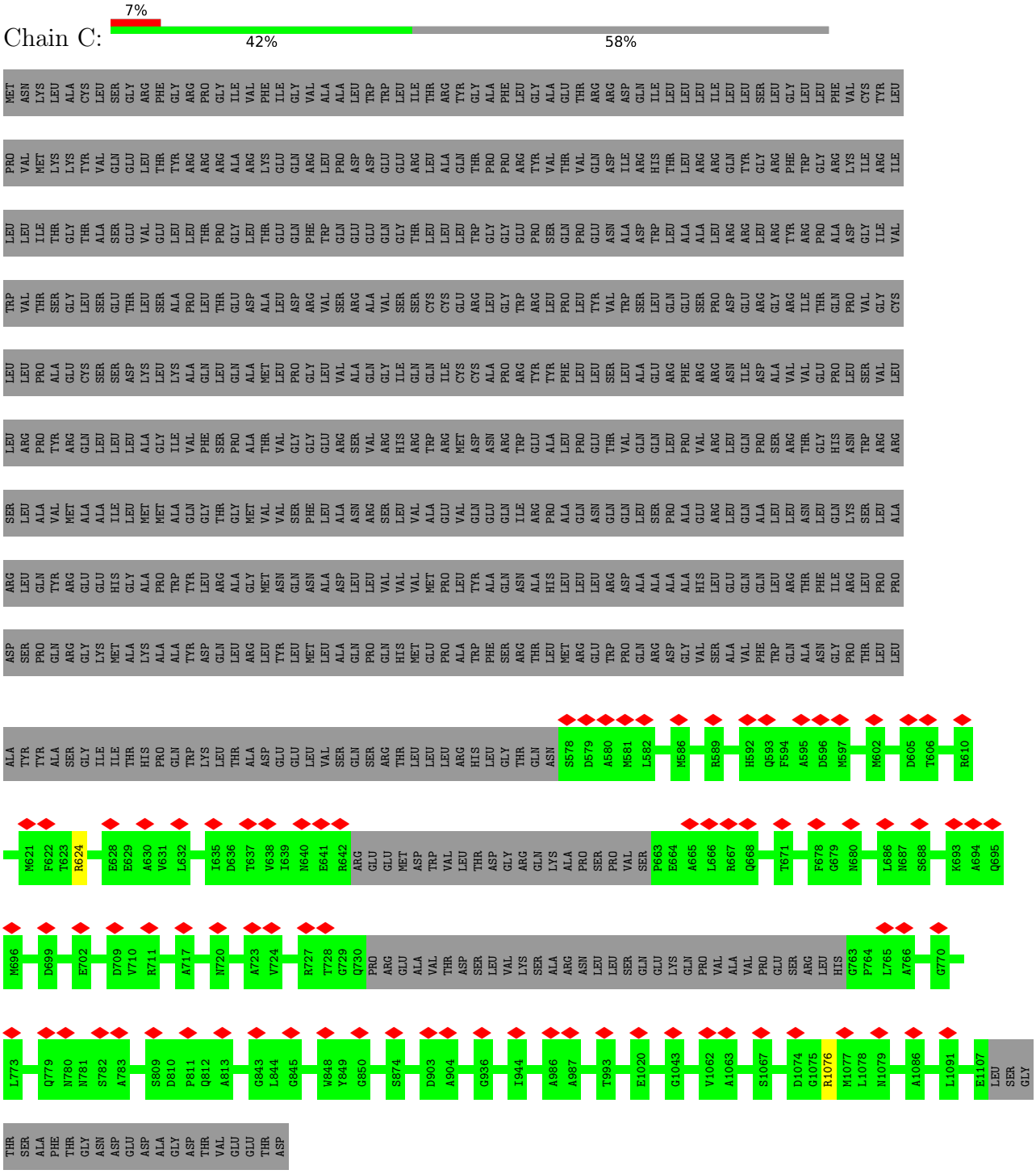


• Molecule 1: ImcF-like family protein



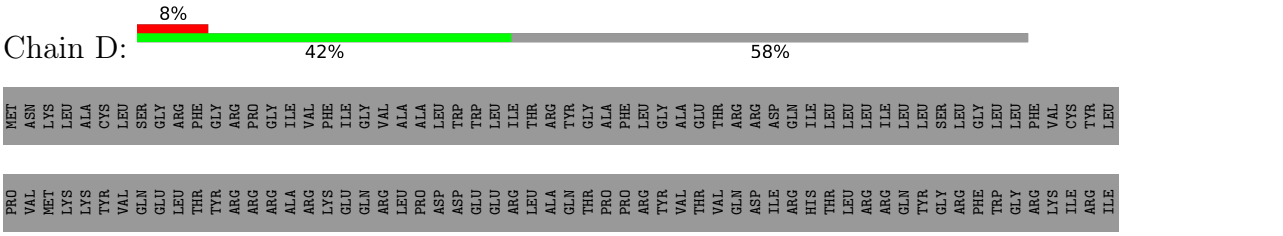
• Molecule 1: ImcF-like family protein

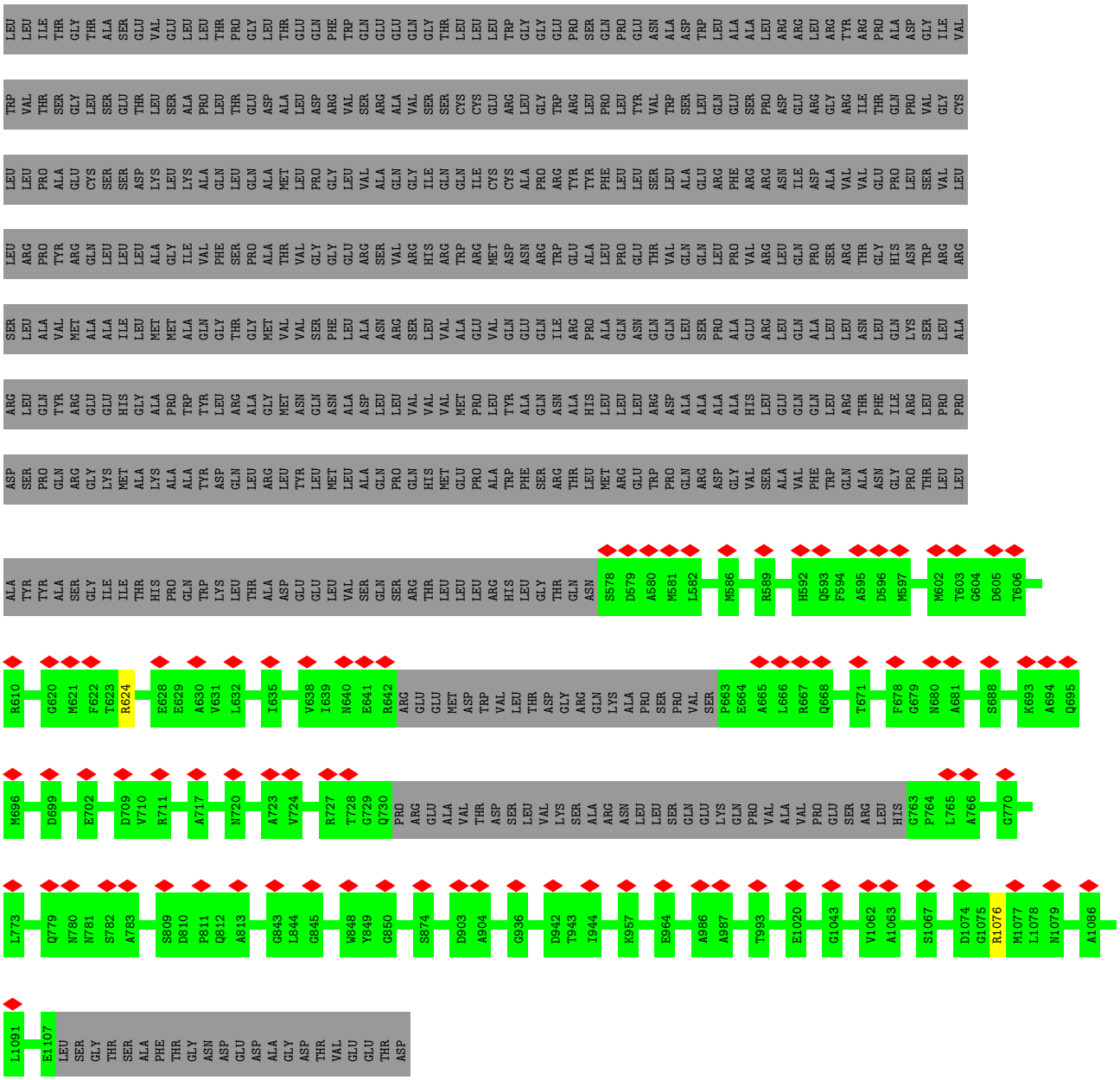
Chain C:



• Molecule 1: ImcF-like family protein

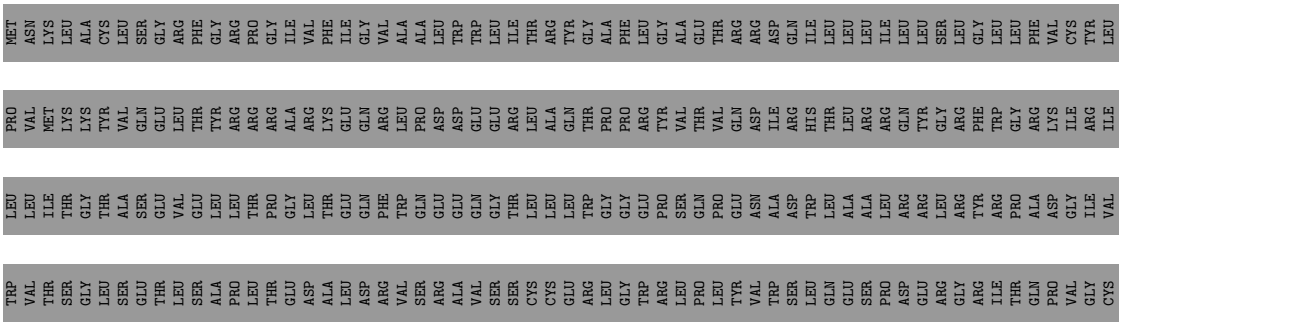
Chain D:

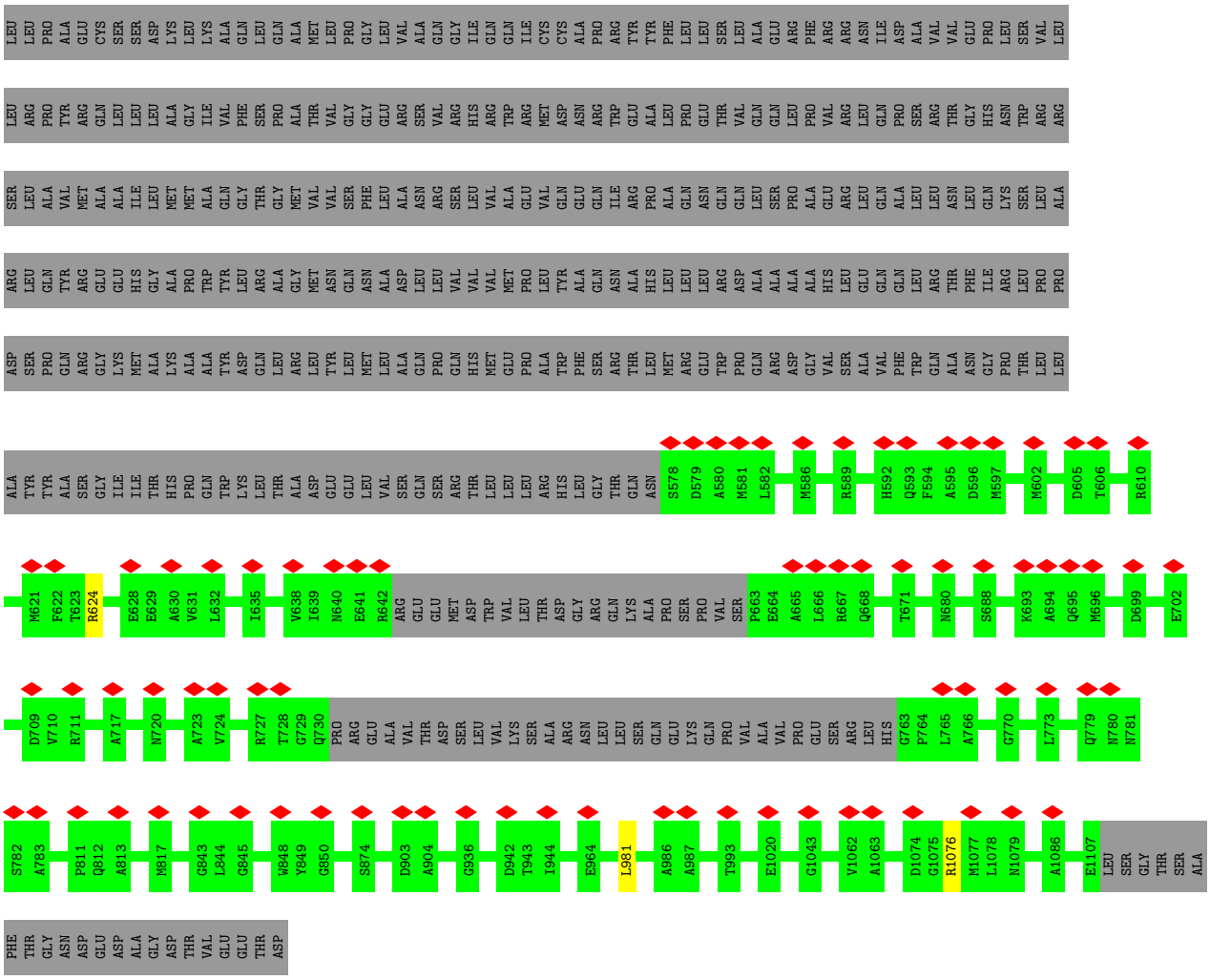




• Molecule 1: ImcF-like family protein

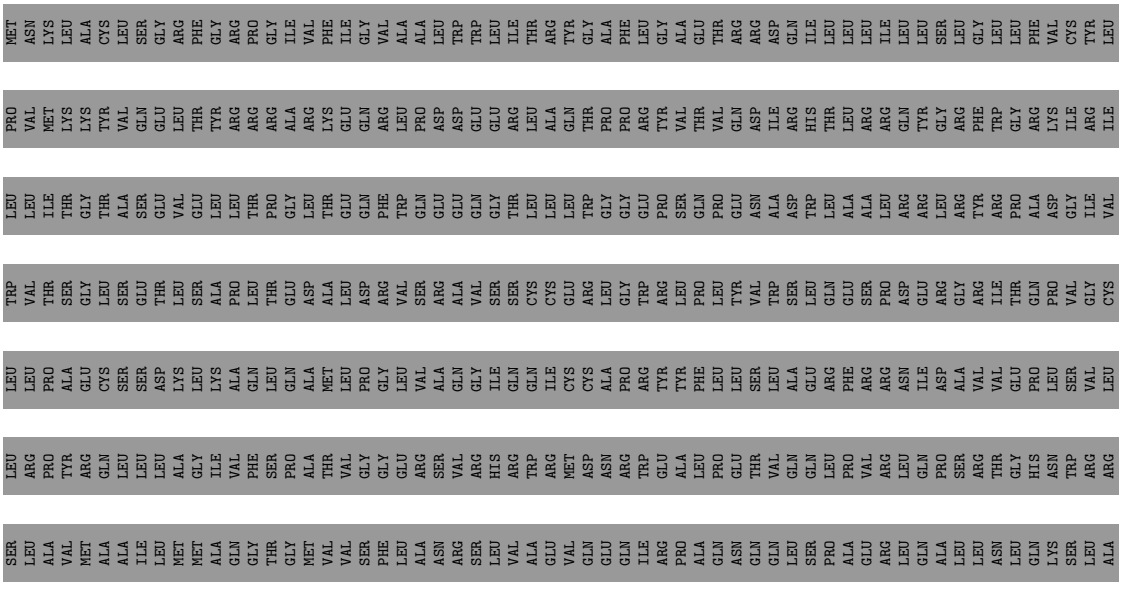
Chain E:

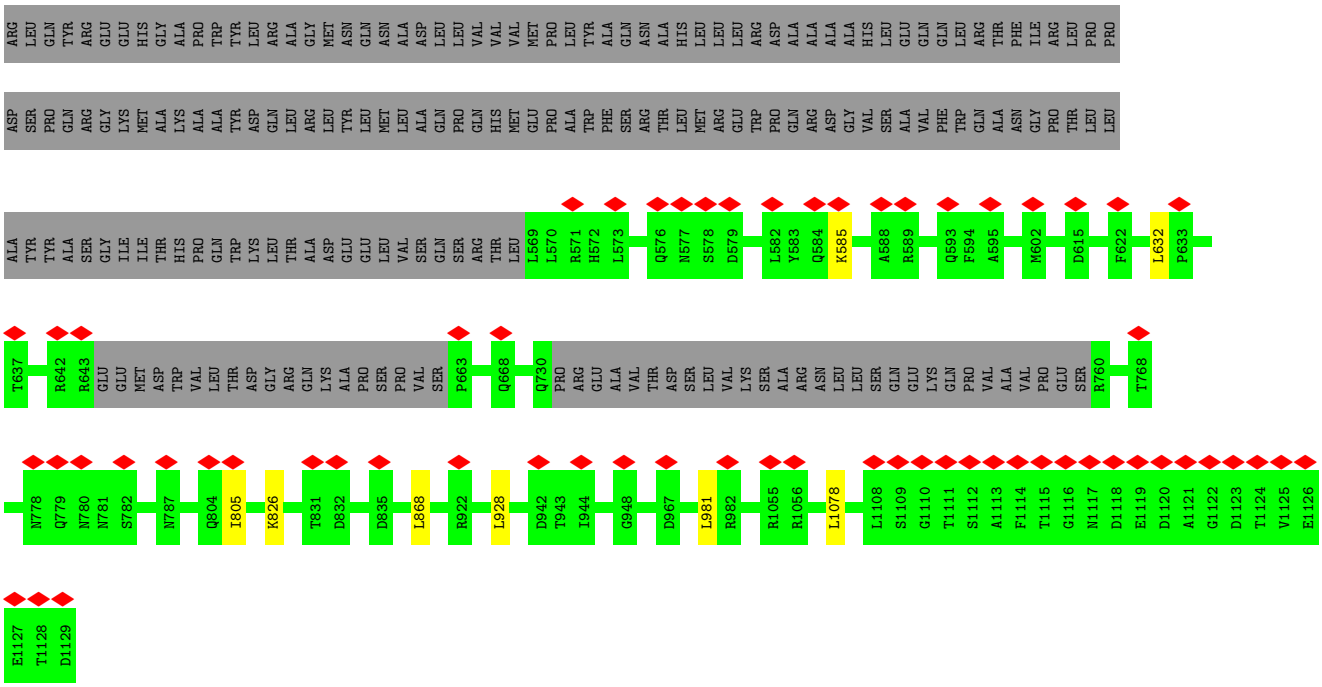




• Molecule 1: ImcF-like family protein

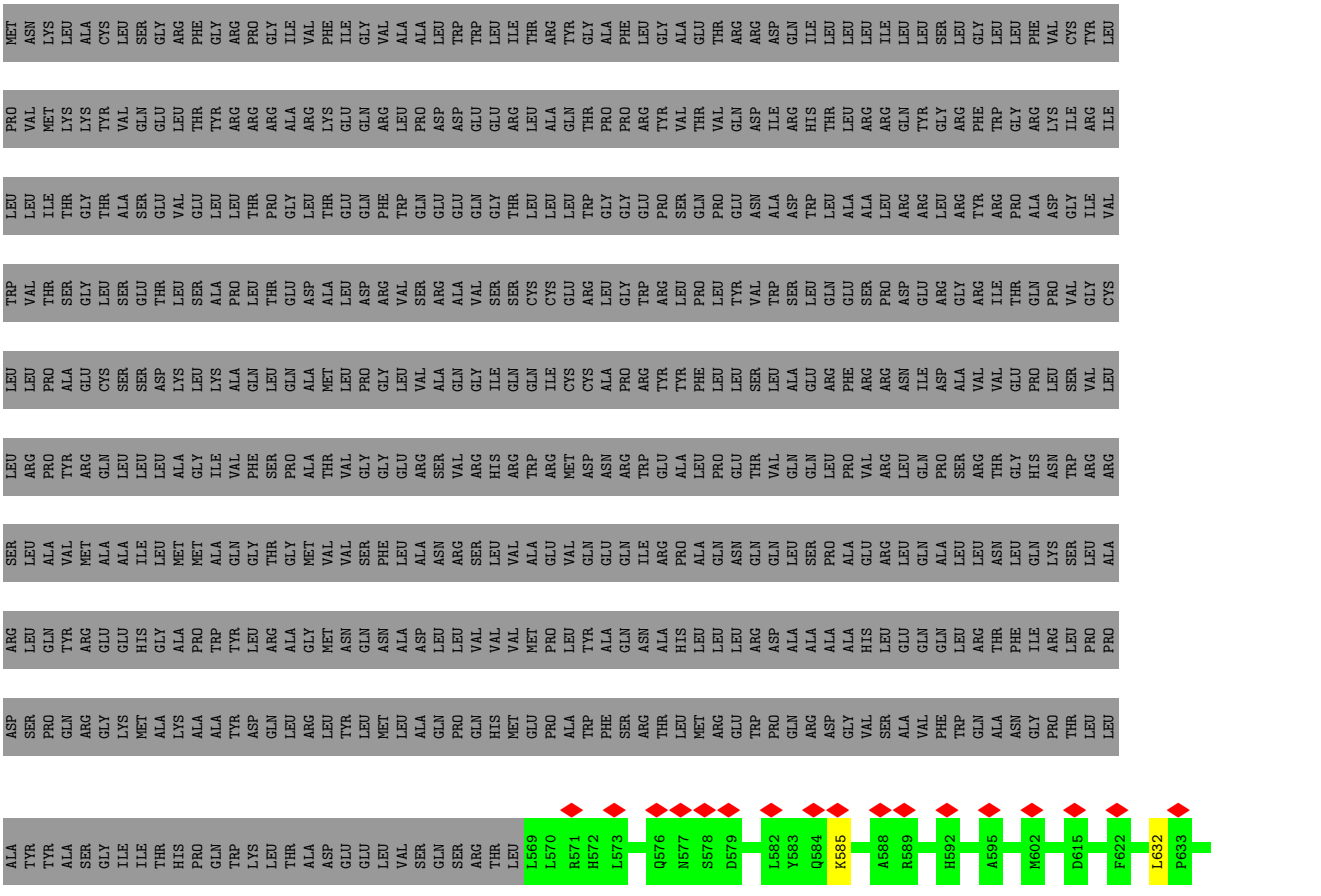
Chain a:

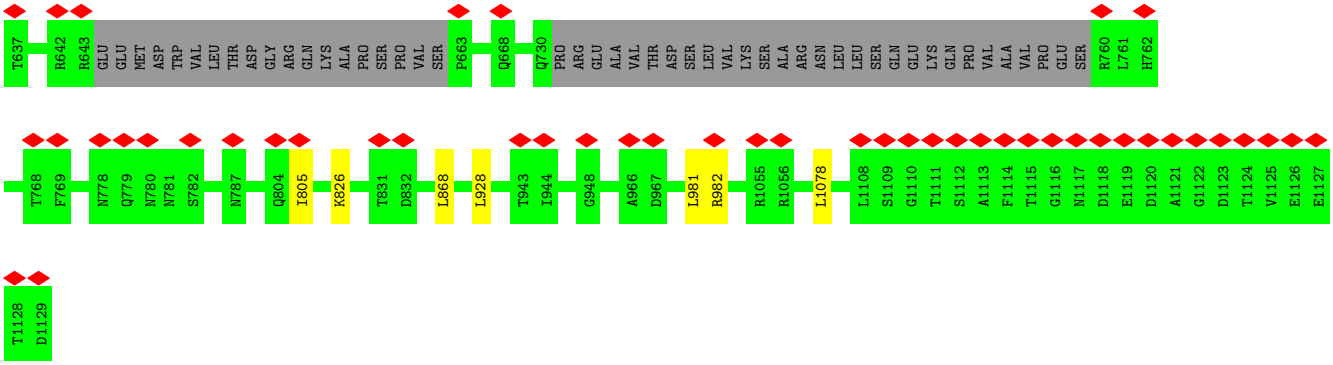




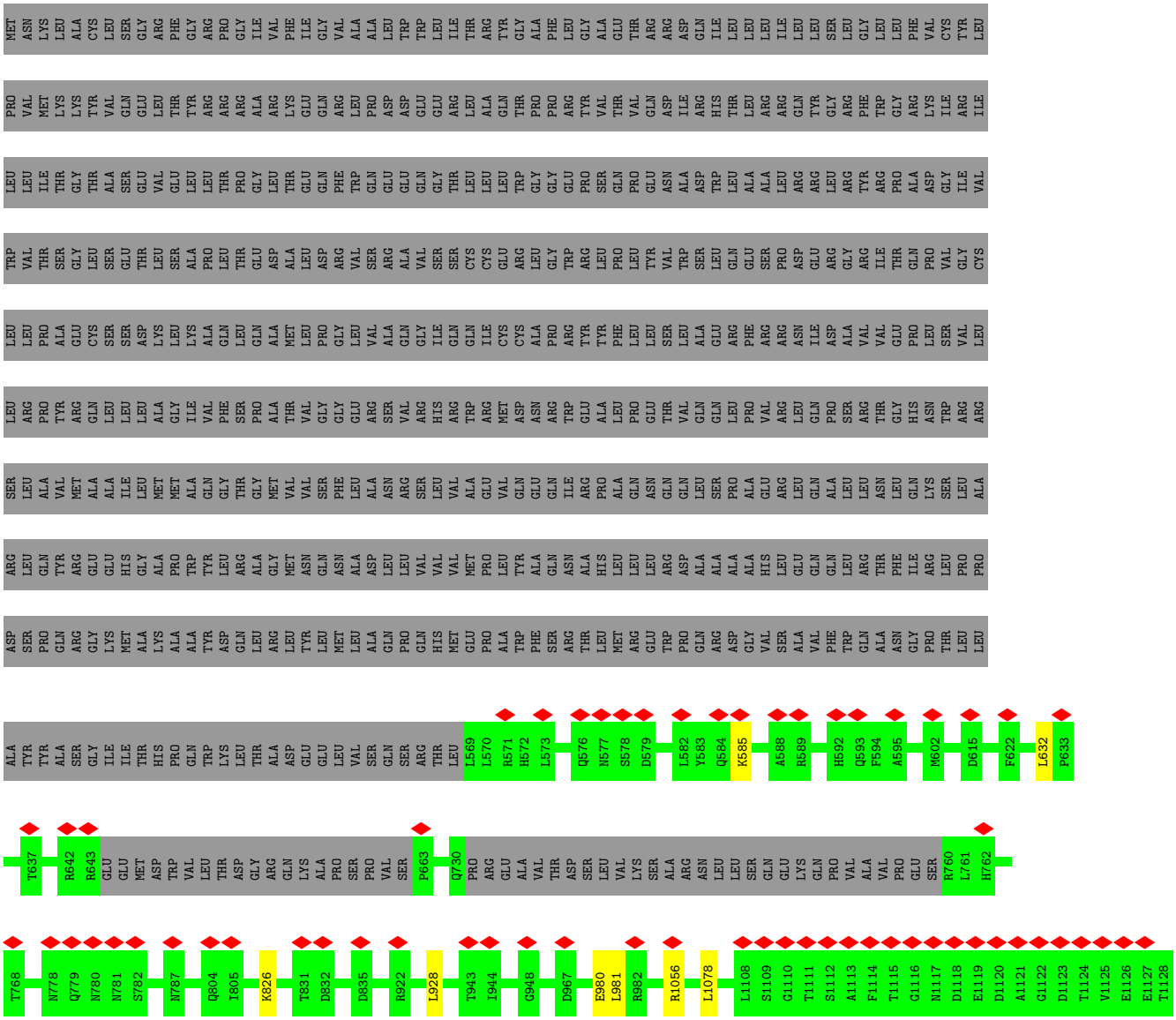
• Molecule 1: ImcF-like family protein

Chain b:



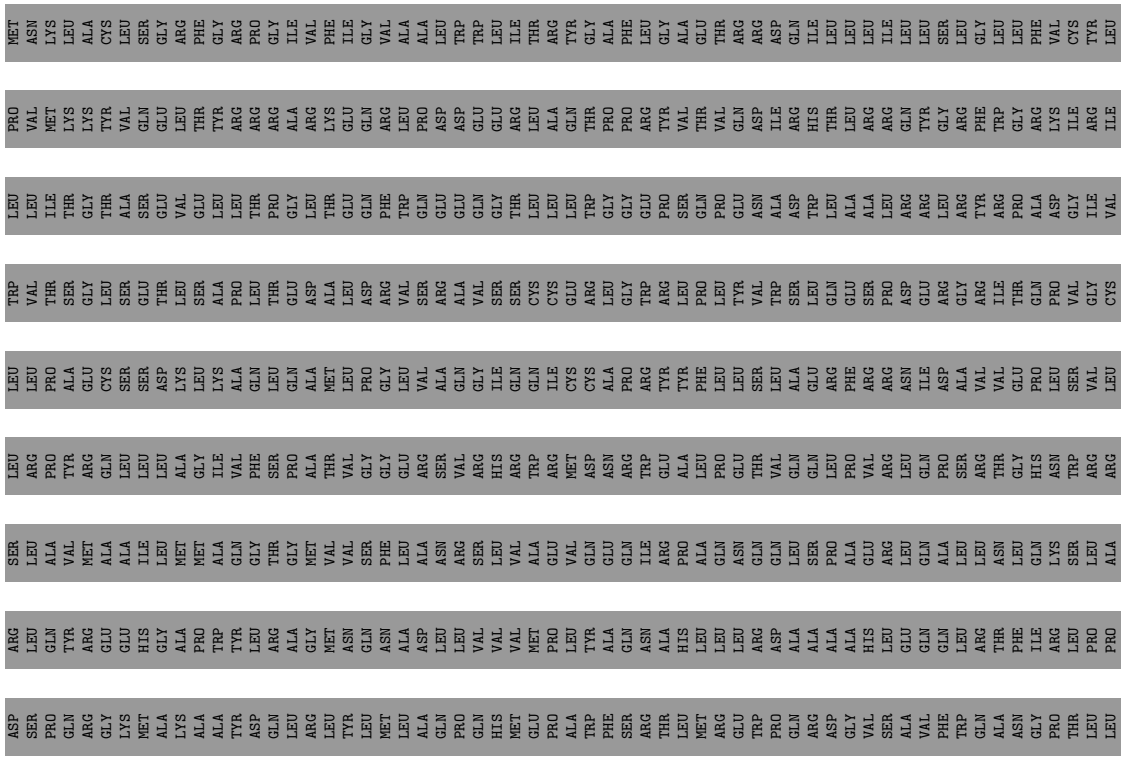


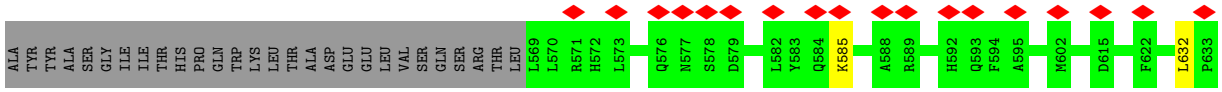
• Molecule 1: ImcF-like family protein

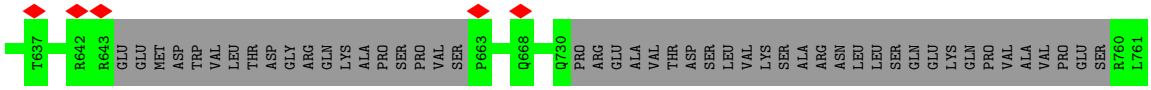


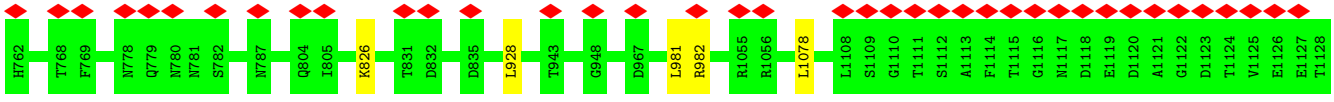
• Molecule 1: ImcF-like family protein

Chain d:



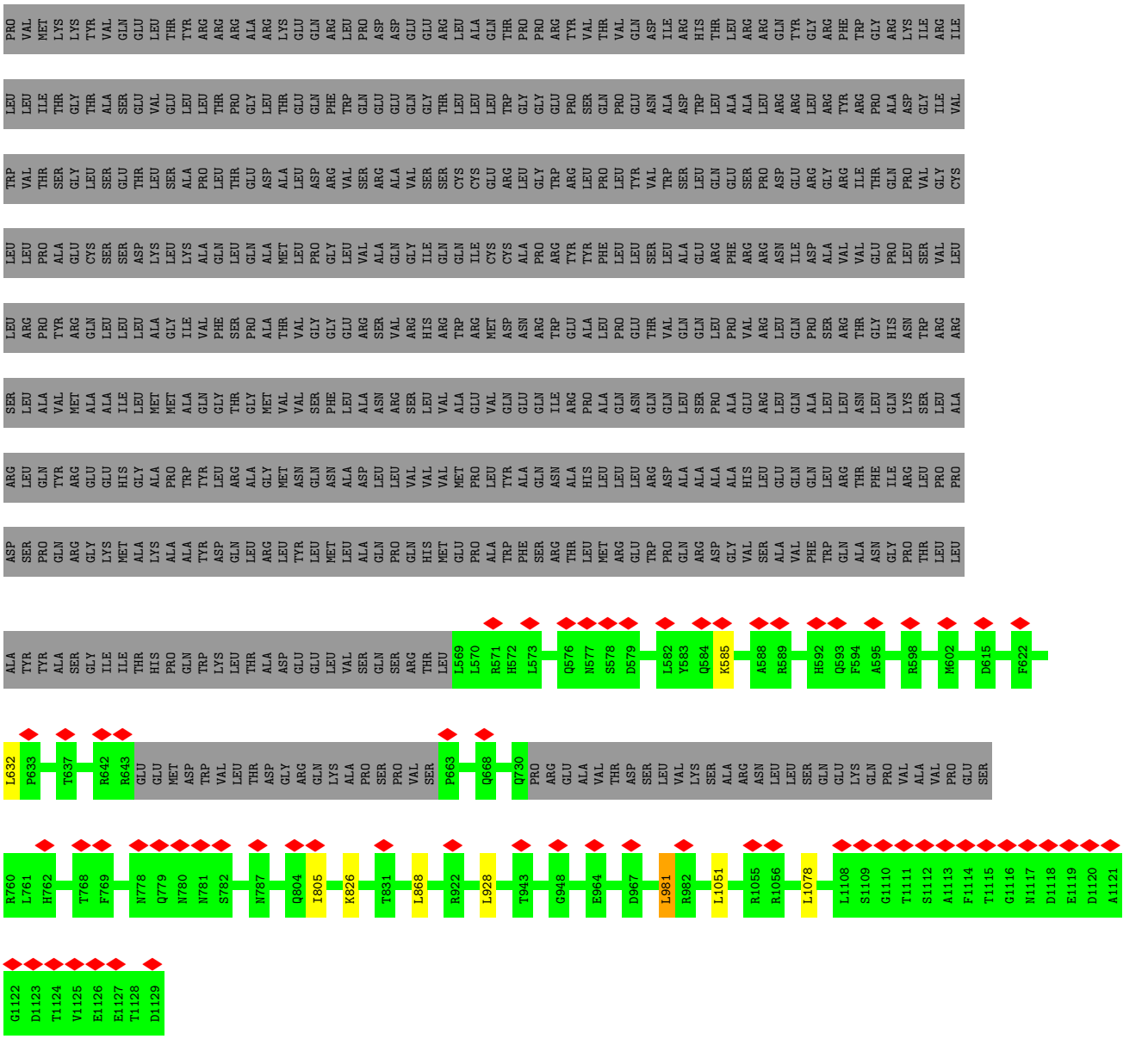




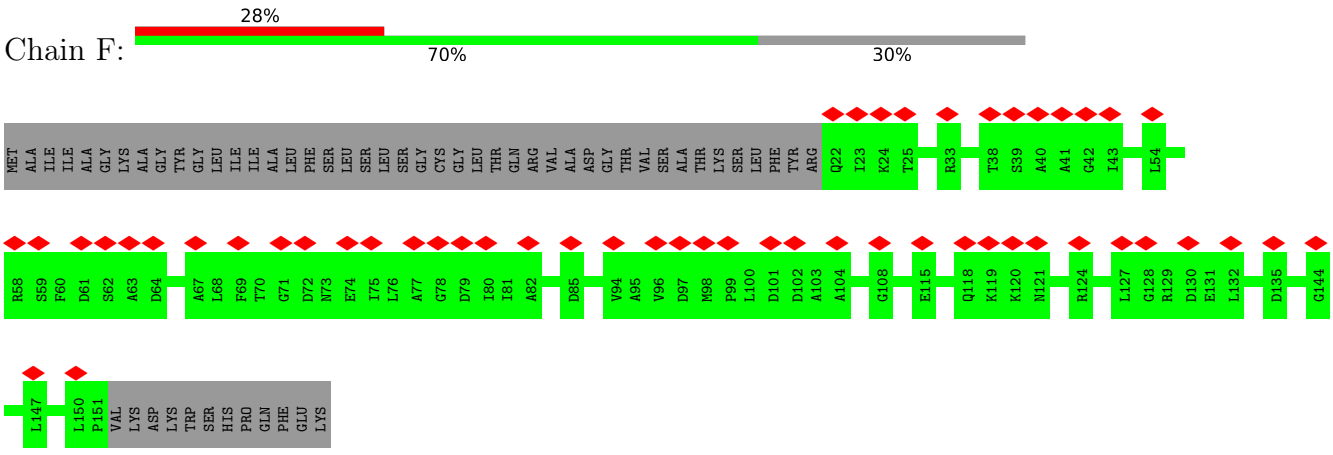


• Molecule 1: ImcF-like family protein

Chain e:

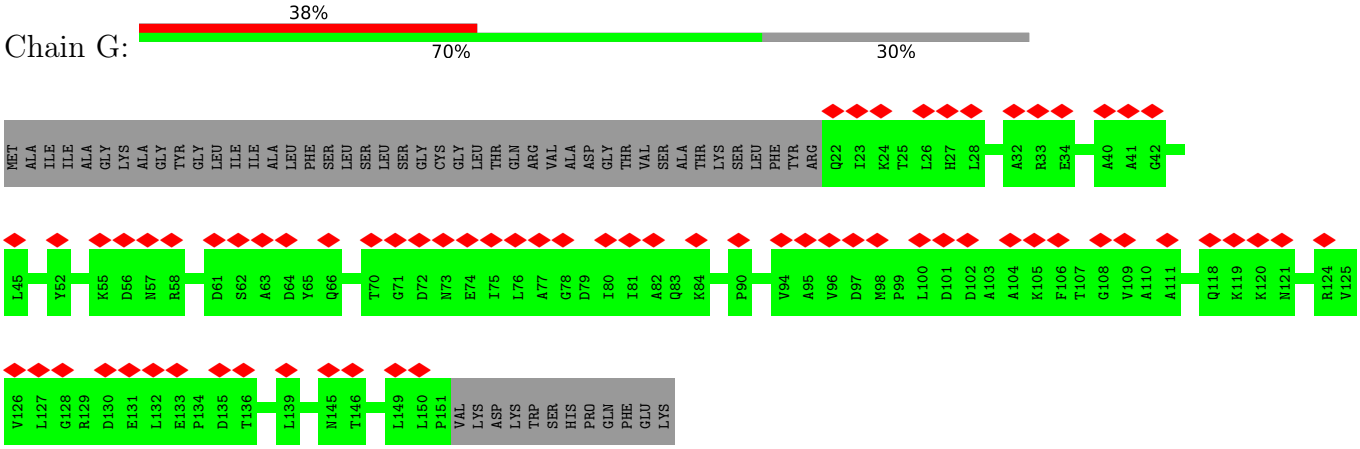


• Molecule 2: Type VI secretion system protein VasD



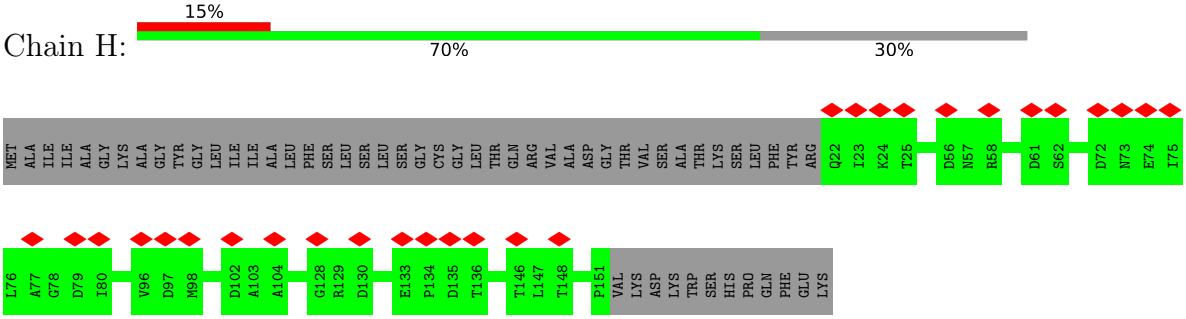
• Molecule 2: Type VI secretion system protein VasD

Chain G:



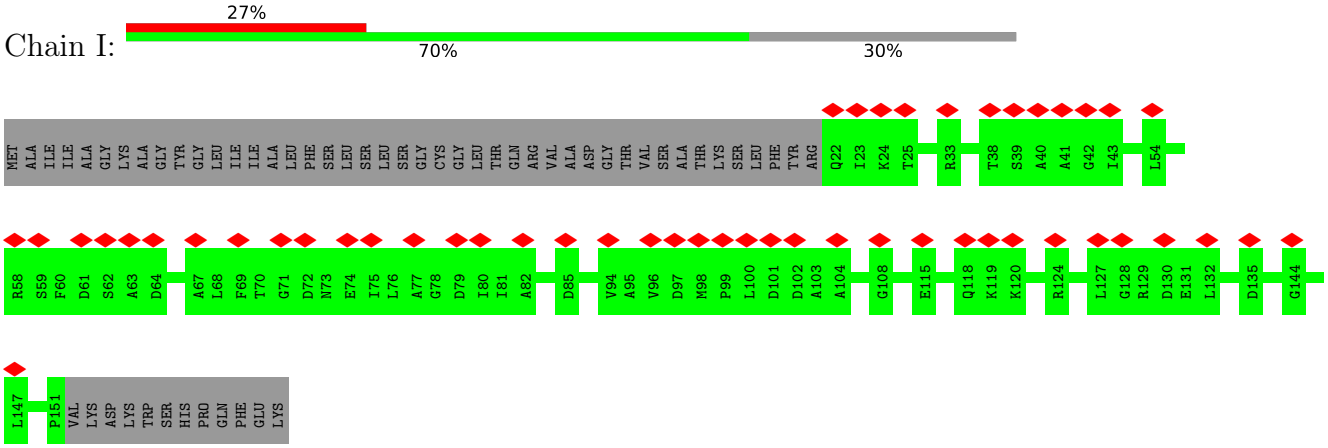
• Molecule 2: Type VI secretion system protein VasD

Chain H:



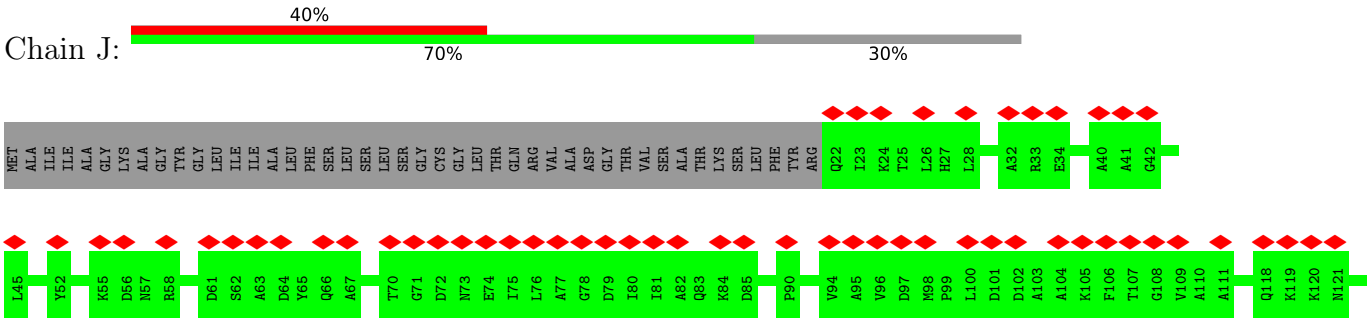
• Molecule 2: Type VI secretion system protein VasD

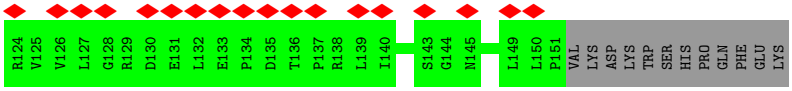
Chain I:



• Molecule 2: Type VI secretion system protein VasD

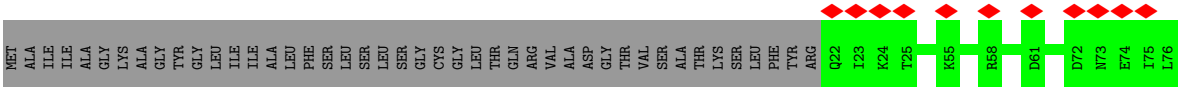
Chain J:

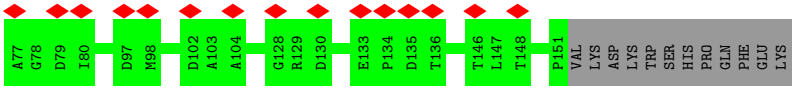




• Molecule 2: Type VI secretion system protein VasD

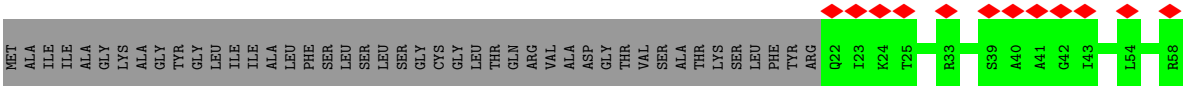
Chain K:

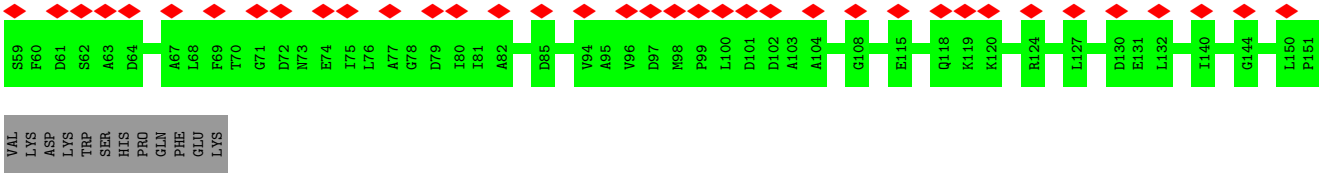




• Molecule 2: Type VI secretion system protein VasD

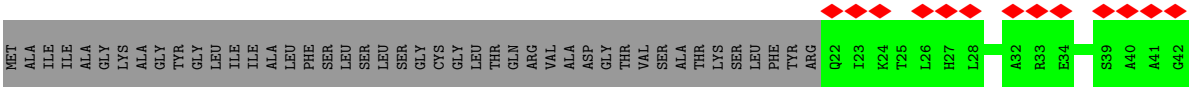
Chain L:

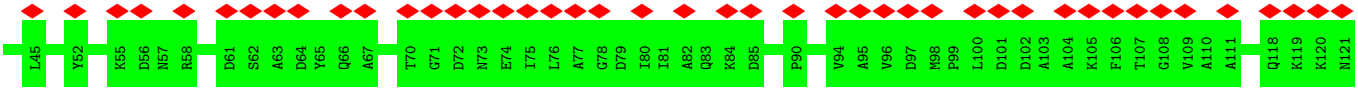


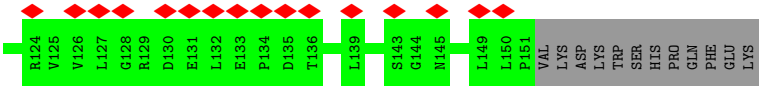


• Molecule 2: Type VI secretion system protein VasD

Chain M:

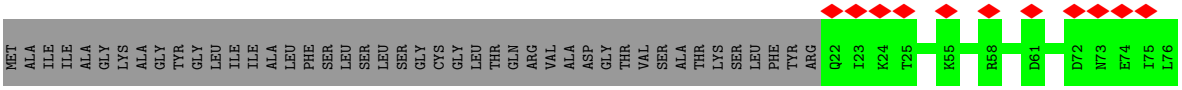


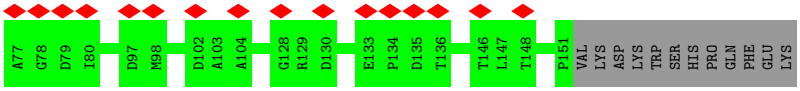




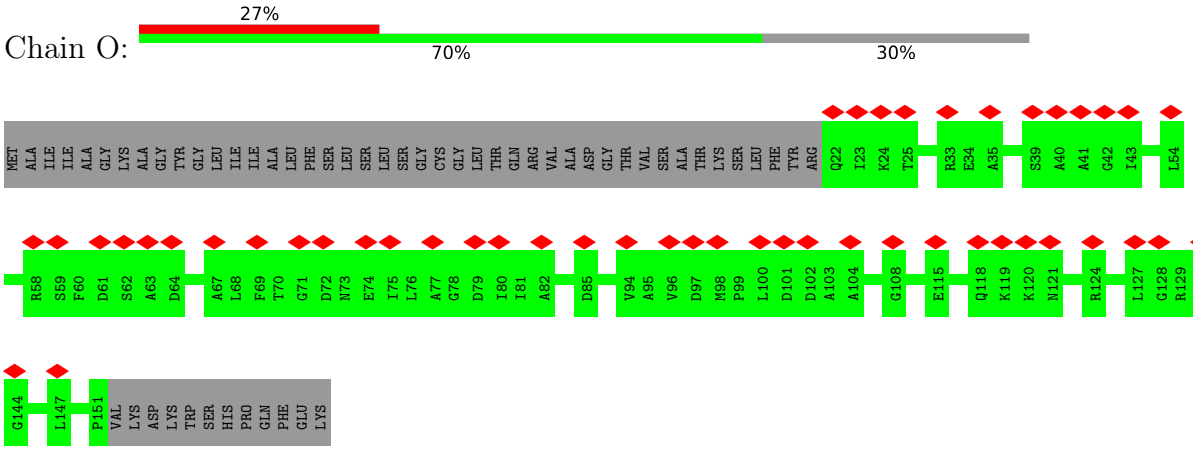
• Molecule 2: Type VI secretion system protein VasD

Chain N:

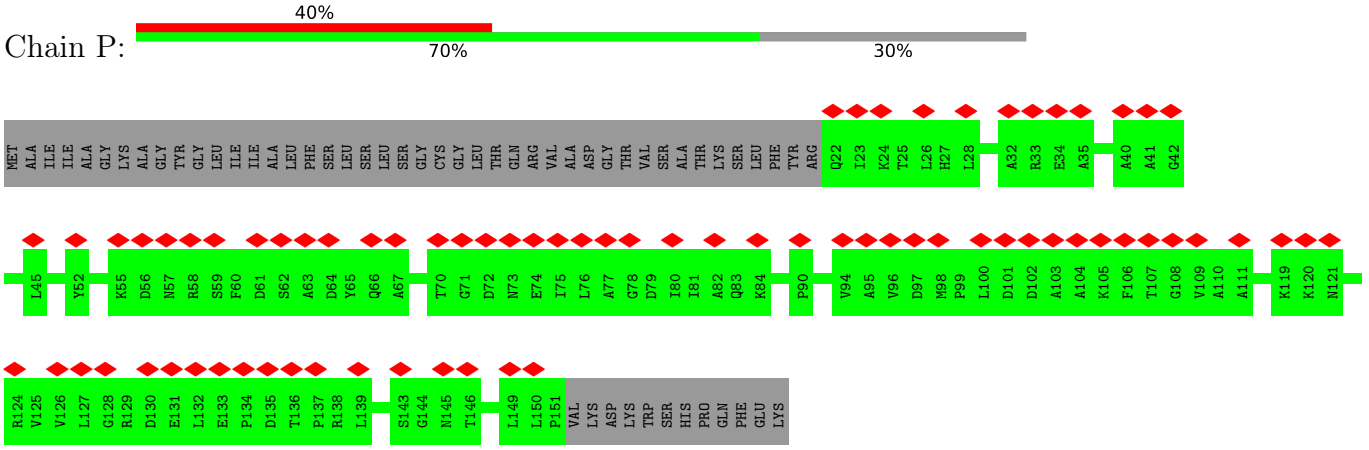




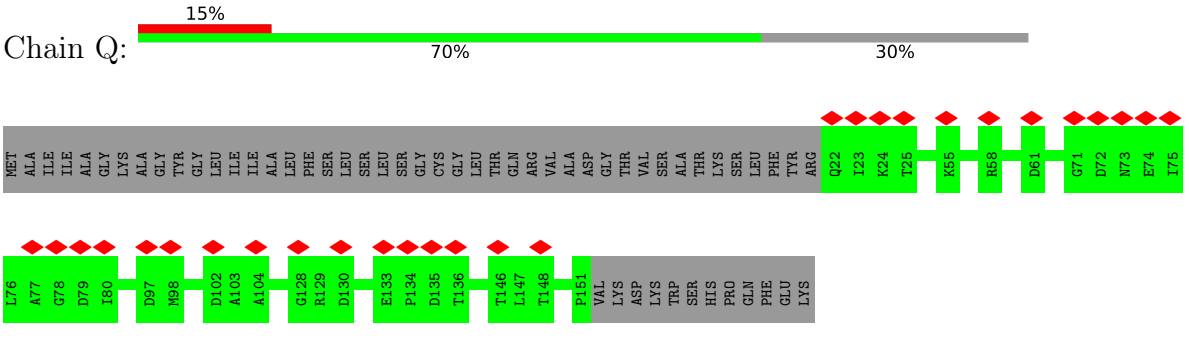
• Molecule 2: Type VI secretion system protein VasD



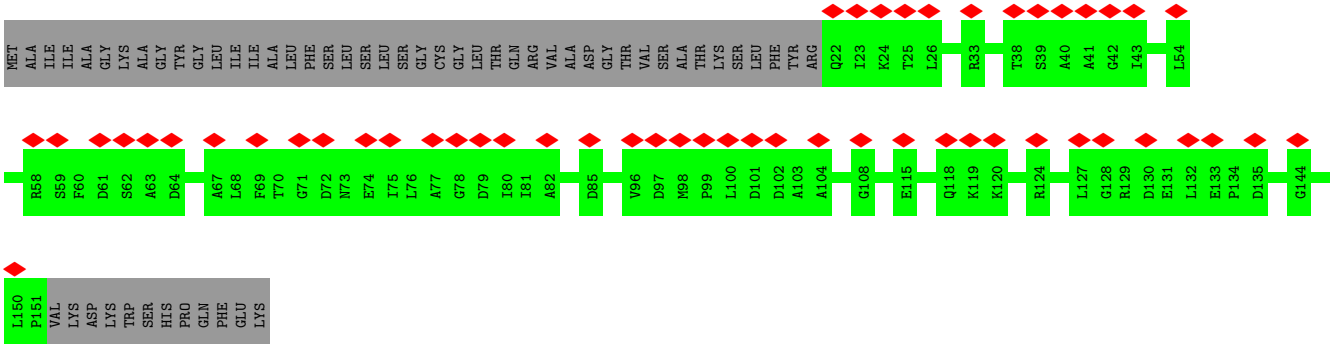
• Molecule 2: Type VI secretion system protein VasD



• Molecule 2: Type VI secretion system protein VasD

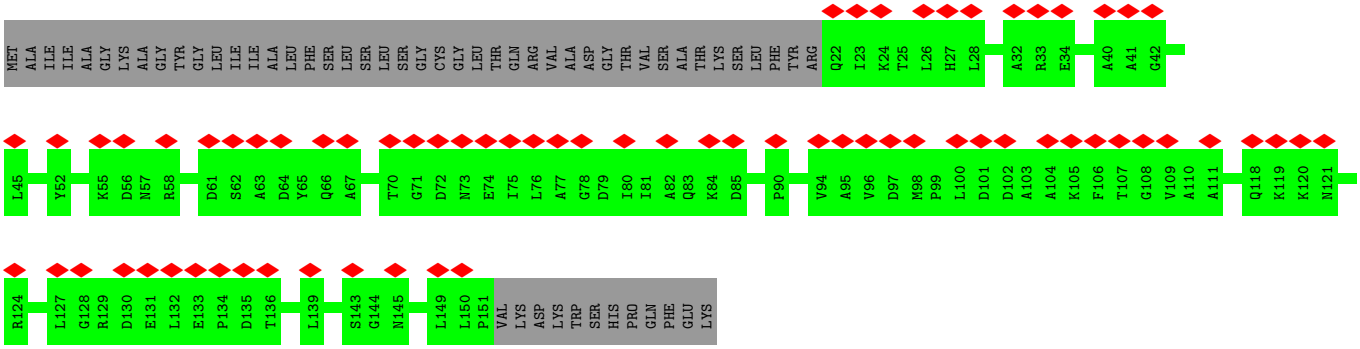


• Molecule 2: Type VI secretion system protein VasD



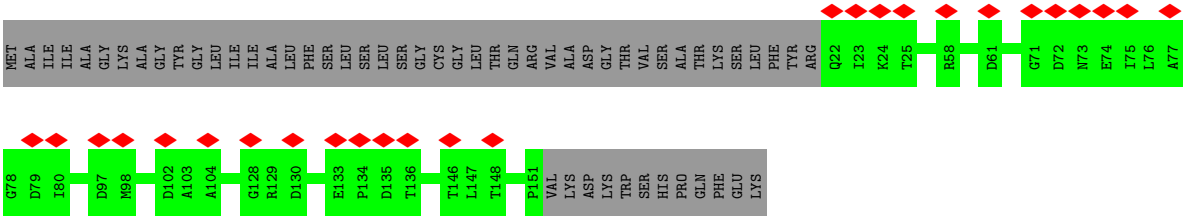
• Molecule 2: Type VI secretion system protein VasD

Chain S:



• Molecule 2: Type VI secretion system protein VasD

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	36828	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	120	Depositor
Minimum defocus (nm)	0.5	Depositor
Maximum defocus (nm)	3	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.316	Depositor
Minimum map value	-0.003	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	620.0, 620.0, 620.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	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	0.33	0/3701	0.59	1/5047 (0.0%)
1	B	0.33	0/3701	0.58	1/5047 (0.0%)
1	C	0.32	0/3701	0.57	0/5047
1	D	0.33	0/3701	0.57	0/5047
1	E	0.33	0/3701	0.58	1/5047 (0.0%)
1	a	0.38	0/4028	0.65	5/5485 (0.1%)
1	b	0.37	0/4028	0.64	5/5485 (0.1%)
1	c	0.37	0/4028	0.65	3/5485 (0.1%)
1	d	0.38	0/4028	0.65	3/5485 (0.1%)
1	e	0.38	0/4028	0.67	6/5485 (0.1%)
2	F	0.28	0/1017	0.46	0/1384
2	G	0.28	0/1017	0.46	0/1384
2	H	0.28	0/1017	0.46	0/1384
2	I	0.28	0/1017	0.46	0/1384
2	J	0.28	0/1017	0.46	0/1384
2	K	0.28	0/1017	0.46	0/1384
2	L	0.28	0/1017	0.46	0/1384
2	M	0.28	0/1017	0.46	0/1384
2	N	0.28	0/1017	0.46	0/1384
2	O	0.28	0/1017	0.46	0/1384
2	P	0.28	0/1017	0.46	0/1384
2	Q	0.28	0/1017	0.46	0/1384
2	R	0.28	0/1017	0.46	0/1384
2	S	0.28	0/1017	0.46	0/1384
2	T	0.28	0/1017	0.46	0/1384
All	All	0.34	0/53900	0.58	25/73420 (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.

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	1
1	b	0	2
1	c	0	3
1	d	0	1
1	e	0	2
All	All	0	9

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	b	1078	LEU	CA-CB-CG	6.73	130.78	115.30
1	d	1078	LEU	CA-CB-CG	6.53	130.32	115.30
1	e	981	LEU	CA-CB-CG	6.40	130.03	115.30
1	d	981	LEU	CA-CB-CG	6.29	129.77	115.30
1	a	981	LEU	CA-CB-CG	6.21	129.59	115.30
1	e	1078	LEU	CA-CB-CG	6.21	129.59	115.30
1	c	1078	LEU	CA-CB-CG	6.10	129.33	115.30
1	a	1078	LEU	CA-CB-CG	5.95	128.99	115.30
1	c	928	LEU	CA-CB-CG	5.87	128.80	115.30
1	a	928	LEU	CA-CB-CG	5.80	128.64	115.30
1	E	981	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	b	928	LEU	CA-CB-CG	5.76	128.55	115.30
1	e	1051	LEU	CA-CB-CG	5.75	128.53	115.30
1	b	981	LEU	CA-CB-CG	5.69	128.39	115.30
1	B	1041	LEU	CA-CB-CG	5.57	128.12	115.30
1	d	928	LEU	CA-CB-CG	5.46	127.86	115.30
1	b	805	ILE	CG1-CB-CG2	-5.45	99.40	111.40
1	e	928	LEU	CA-CB-CG	5.44	127.81	115.30
1	a	868	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	981	LEU	CB-CG-CD1	-5.34	101.93	111.00
1	a	805	ILE	CG1-CB-CG2	-5.32	99.69	111.40
1	c	981	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	e	868	LEU	CA-CB-CG	5.17	127.19	115.30
1	e	805	ILE	CG1-CB-CG2	-5.16	100.06	111.40
1	b	868	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	632	LEU	Peptide
1	b	632	LEU	Peptide
1	b	982	ARG	Peptide
1	c	1056	ARG	Peptide
1	c	632	LEU	Peptide
1	c	980	GLU	Peptide
1	d	632	LEU	Peptide
1	e	632	LEU	Peptide
1	e	981	LEU	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	472/1129 (42%)	425 (90%)	47 (10%)	0	100	100
1	B	472/1129 (42%)	425 (90%)	47 (10%)	0	100	100
1	C	472/1129 (42%)	423 (90%)	49 (10%)	0	100	100
1	D	472/1129 (42%)	425 (90%)	47 (10%)	0	100	100
1	E	472/1129 (42%)	422 (89%)	50 (11%)	0	100	100
1	a	507/1129 (45%)	439 (87%)	68 (13%)	0	100	100
1	b	507/1129 (45%)	435 (86%)	72 (14%)	0	100	100
1	c	507/1129 (45%)	425 (84%)	82 (16%)	0	100	100
1	d	507/1129 (45%)	426 (84%)	81 (16%)	0	100	100
1	e	507/1129 (45%)	437 (86%)	70 (14%)	0	100	100
2	F	128/186 (69%)	121 (94%)	7 (6%)	0	100	100
2	G	128/186 (69%)	121 (94%)	7 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	128/186 (69%)	121 (94%)	7 (6%)	0	100	100
2	I	128/186 (69%)	121 (94%)	7 (6%)	0	100	100
2	J	128/186 (69%)	121 (94%)	7 (6%)	0	100	100
2	K	128/186 (69%)	121 (94%)	7 (6%)	0	100	100
2	L	128/186 (69%)	121 (94%)	7 (6%)	0	100	100
2	M	128/186 (69%)	121 (94%)	7 (6%)	0	100	100
2	N	128/186 (69%)	121 (94%)	7 (6%)	0	100	100
2	O	128/186 (69%)	121 (94%)	7 (6%)	0	100	100
2	P	128/186 (69%)	121 (94%)	7 (6%)	0	100	100
2	Q	128/186 (69%)	121 (94%)	7 (6%)	0	100	100
2	R	128/186 (69%)	121 (94%)	7 (6%)	0	100	100
2	S	128/186 (69%)	121 (94%)	7 (6%)	0	100	100
2	T	128/186 (69%)	121 (94%)	7 (6%)	0	100	100
All	All	6815/14080 (48%)	6097 (90%)	718 (10%)	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	368/950 (39%)	366 (100%)	2 (0%)	88	93
1	B	368/950 (39%)	366 (100%)	2 (0%)	88	93
1	C	368/950 (39%)	366 (100%)	2 (0%)	88	93
1	D	368/950 (39%)	366 (100%)	2 (0%)	88	93
1	E	368/950 (39%)	366 (100%)	2 (0%)	88	93
1	a	410/950 (43%)	408 (100%)	2 (0%)	88	93
1	b	410/950 (43%)	408 (100%)	2 (0%)	88	93
1	c	410/950 (43%)	408 (100%)	2 (0%)	88	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	d	410/950 (43%)	407 (99%)	3 (1%)	84 90
1	e	410/950 (43%)	408 (100%)	2 (0%)	88 93
2	F	108/153 (71%)	108 (100%)	0	100 100
2	G	108/153 (71%)	108 (100%)	0	100 100
2	H	108/153 (71%)	108 (100%)	0	100 100
2	I	108/153 (71%)	108 (100%)	0	100 100
2	J	108/153 (71%)	108 (100%)	0	100 100
2	K	108/153 (71%)	108 (100%)	0	100 100
2	L	108/153 (71%)	108 (100%)	0	100 100
2	M	108/153 (71%)	108 (100%)	0	100 100
2	N	108/153 (71%)	108 (100%)	0	100 100
2	O	108/153 (71%)	108 (100%)	0	100 100
2	P	108/153 (71%)	108 (100%)	0	100 100
2	Q	108/153 (71%)	108 (100%)	0	100 100
2	R	108/153 (71%)	108 (100%)	0	100 100
2	S	108/153 (71%)	108 (100%)	0	100 100
2	T	108/153 (71%)	108 (100%)	0	100 100
All	All	5510/11795 (47%)	5489 (100%)	21 (0%)	91 94

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	624	ARG
1	A	1076	ARG
1	B	624	ARG
1	B	1076	ARG
1	C	624	ARG
1	C	1076	ARG
1	D	624	ARG
1	D	1076	ARG
1	E	624	ARG
1	E	1076	ARG
1	a	585	LYS
1	a	826	LYS
1	b	585	LYS
1	b	826	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	c	585	LYS
1	c	826	LYS
1	d	585	LYS
1	d	826	LYS
1	d	982	ARG
1	e	585	LYS
1	e	826	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	668	GLN
1	A	687	ASN
1	A	712	GLN
1	A	816	GLN
1	A	978	HIS
1	A	999	GLN
1	B	687	ASN
1	B	712	GLN
1	B	816	GLN
1	B	824	GLN
1	B	945	ASN
1	B	999	GLN
1	C	687	ASN
1	C	712	GLN
1	C	816	GLN
1	C	978	HIS
1	C	999	GLN
1	D	668	GLN
1	D	687	ASN
1	D	712	GLN
1	D	816	GLN
1	D	824	GLN
1	D	999	GLN
1	E	668	GLN
1	E	687	ASN
1	E	712	GLN
1	E	816	GLN
1	E	820	GLN
1	E	999	GLN
2	G	89	GLN
2	J	89	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	89	GLN
1	a	720	ASN
1	a	866	GLN
1	a	998	ASN
1	b	593	GLN
1	b	684	ASN
1	b	762	HIS
1	b	804	GLN
1	b	812	GLN
1	b	816	GLN
1	b	866	GLN
1	c	593	GLN
1	c	684	ASN
1	c	762	HIS
1	c	804	GLN
1	c	812	GLN
1	c	866	GLN
1	c	998	ASN
1	d	593	GLN
1	d	762	HIS
1	d	797	GLN
1	d	804	GLN
1	d	812	GLN
1	d	866	GLN
1	d	998	ASN
1	e	593	GLN
1	e	762	HIS
1	e	804	GLN
1	e	812	GLN
1	e	820	GLN
1	e	846	GLN
1	e	866	GLN
1	e	998	ASN

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 (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.

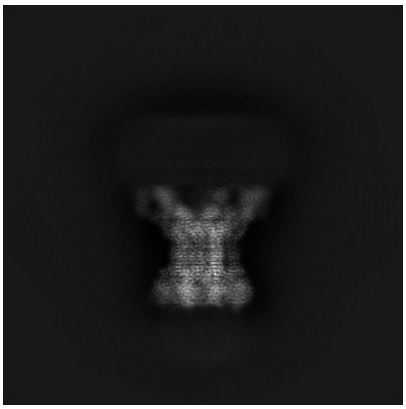
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0264. These allow visual inspection of the internal detail of the map and identification of artifacts.

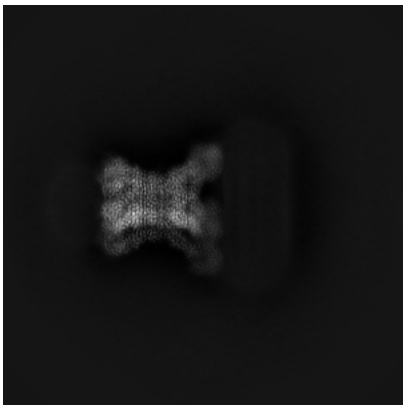
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

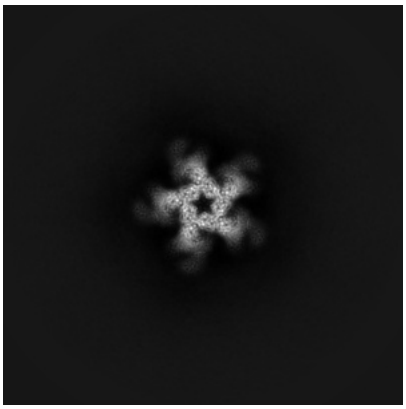
6.1.1 Primary map



X

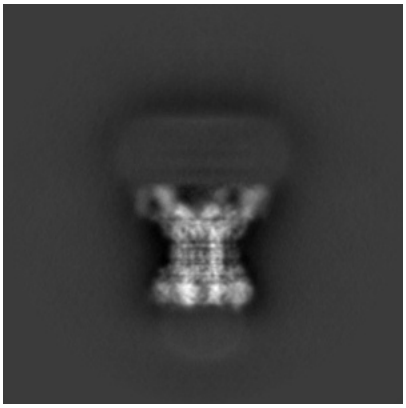


Y

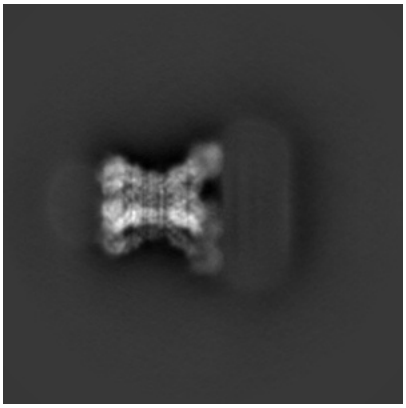


Z

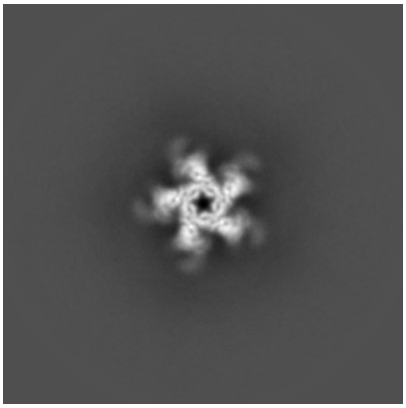
6.1.2 Raw map



X



Y



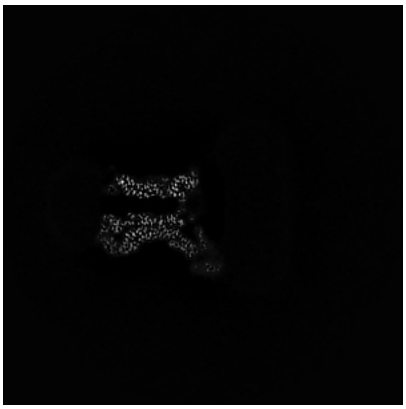
Z

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

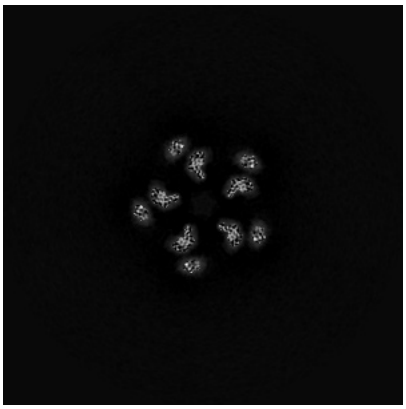
6.2 Central slices (i)

6.2.1 Primary map

X Index: 250

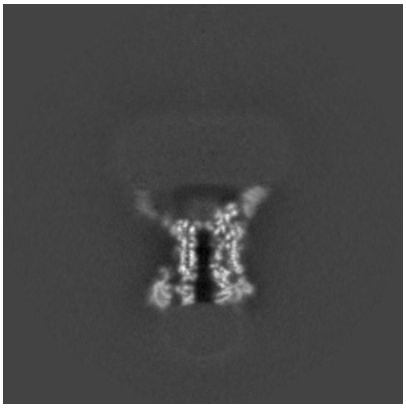


Y Index: 250

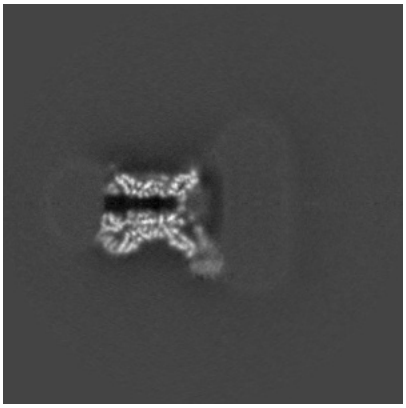


Z Index: 250

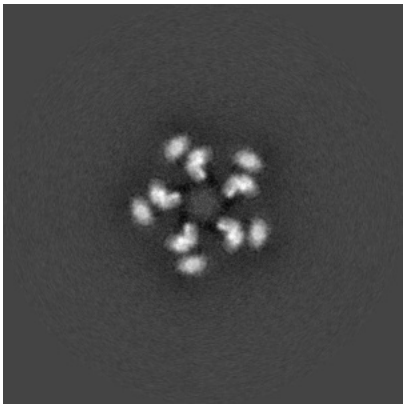
6.2.2 Raw map



X Index: 250



Y Index: 250



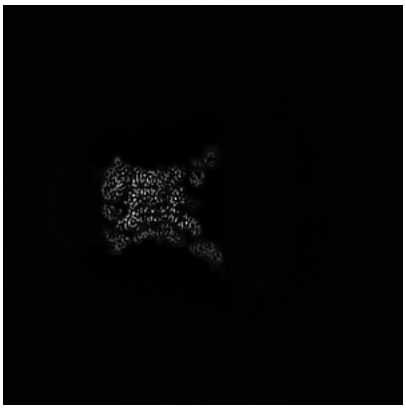
Z Index: 250

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

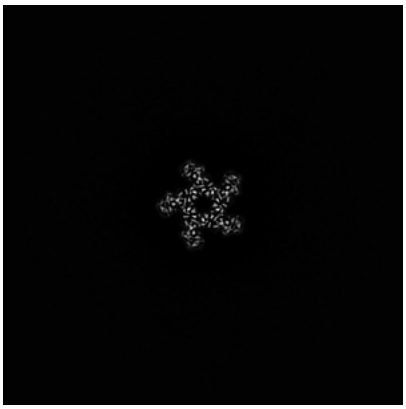
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 239

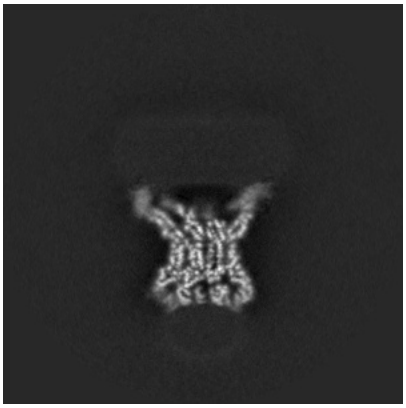


Y Index: 265

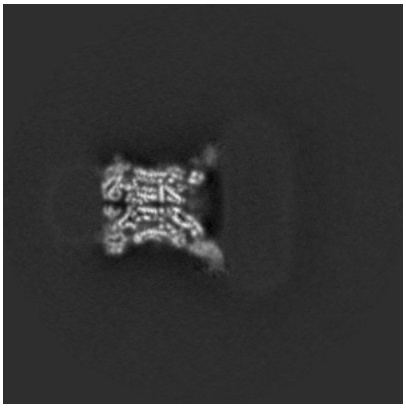


Z Index: 163

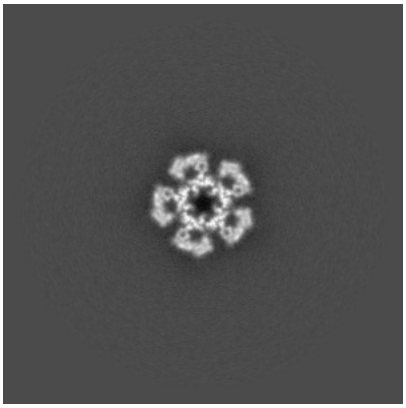
6.3.2 Raw map



X Index: 237



Y Index: 262

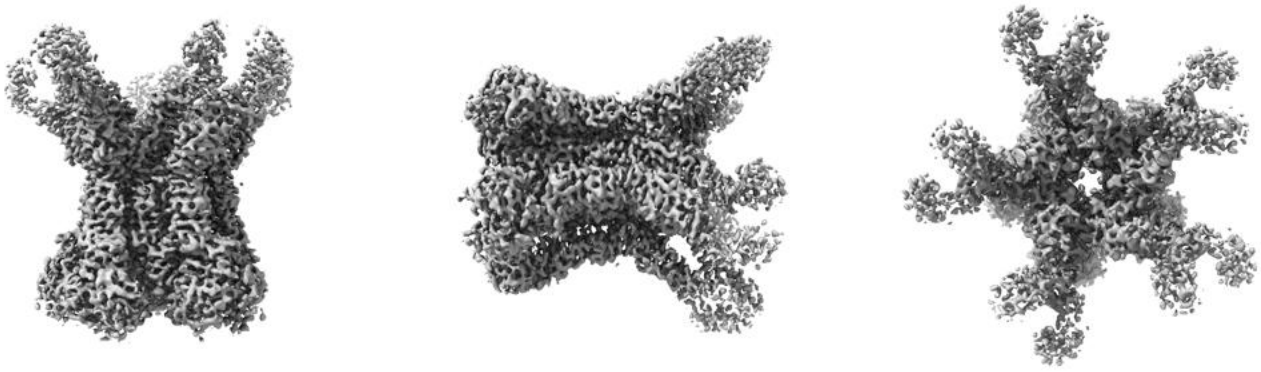


Z Index: 146

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

6.4 Orthogonal surface views (i)

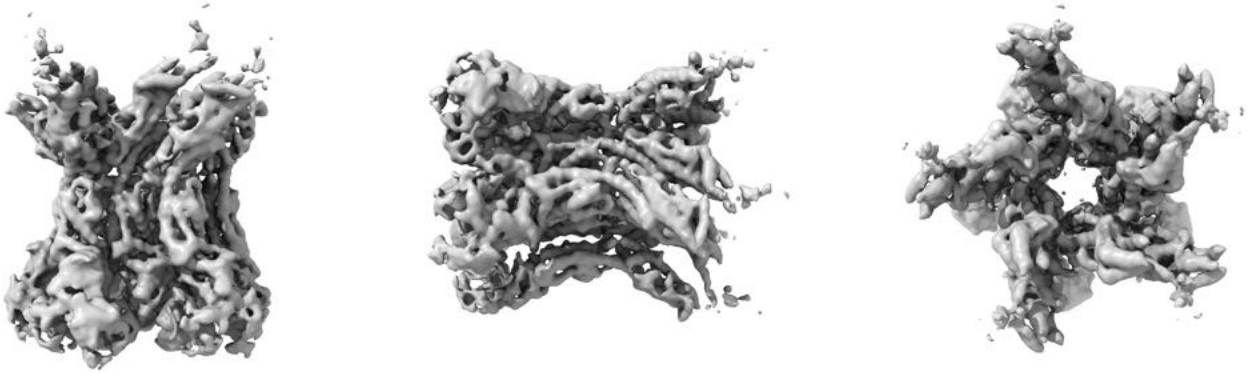
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

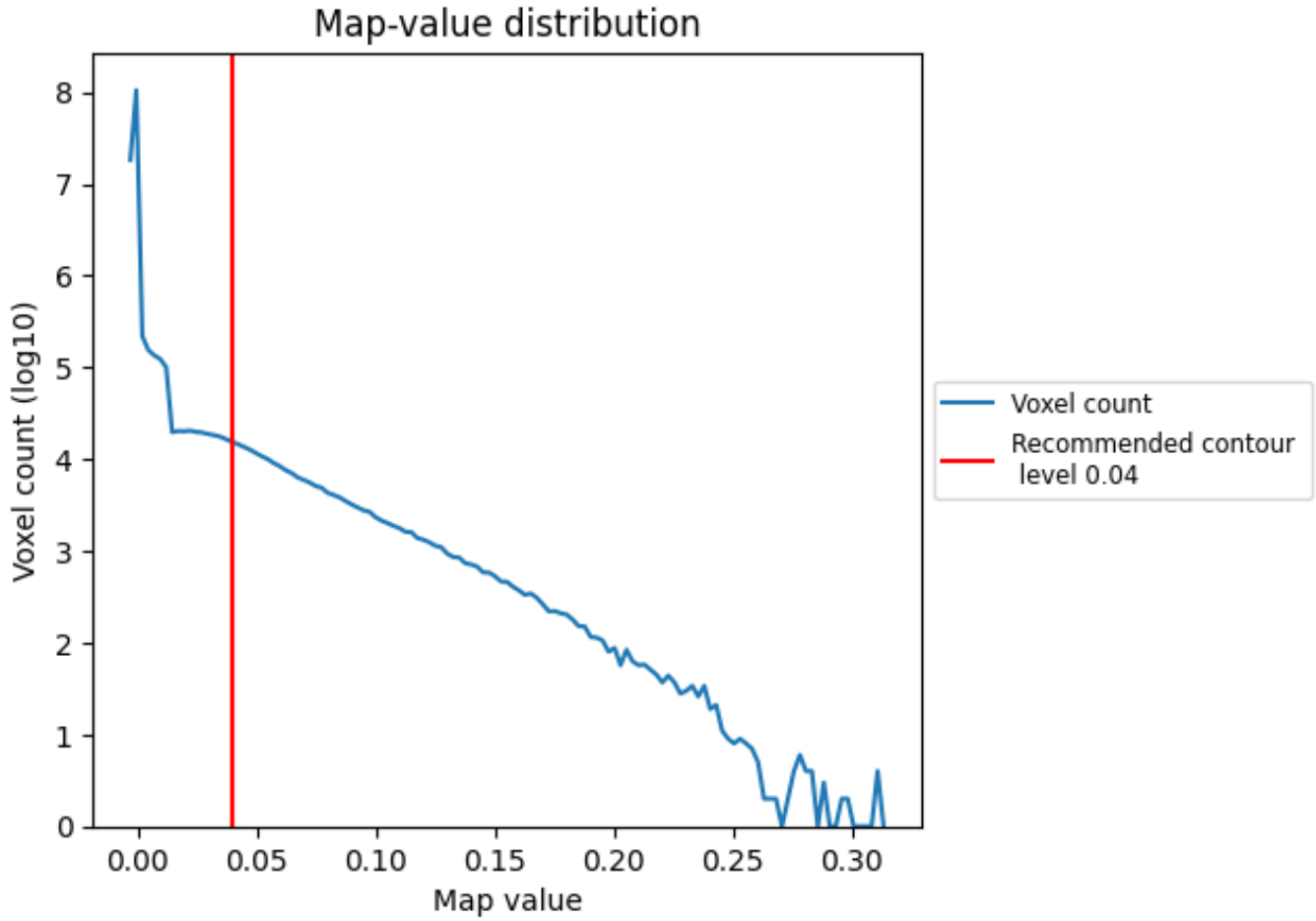
6.5 Mask visualisation (i)

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

7 Map analysis

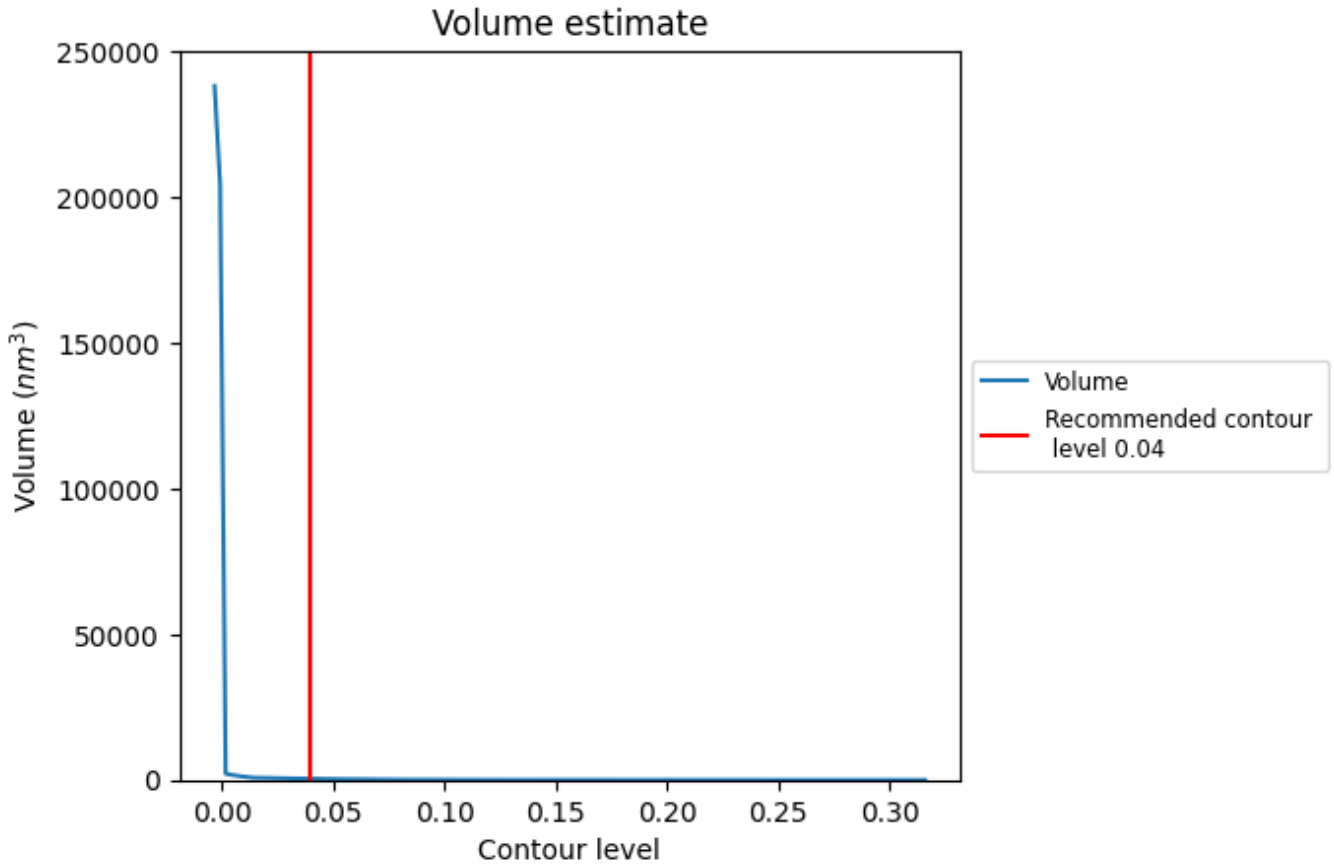
This section contains the results of statistical analysis of the map.

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.

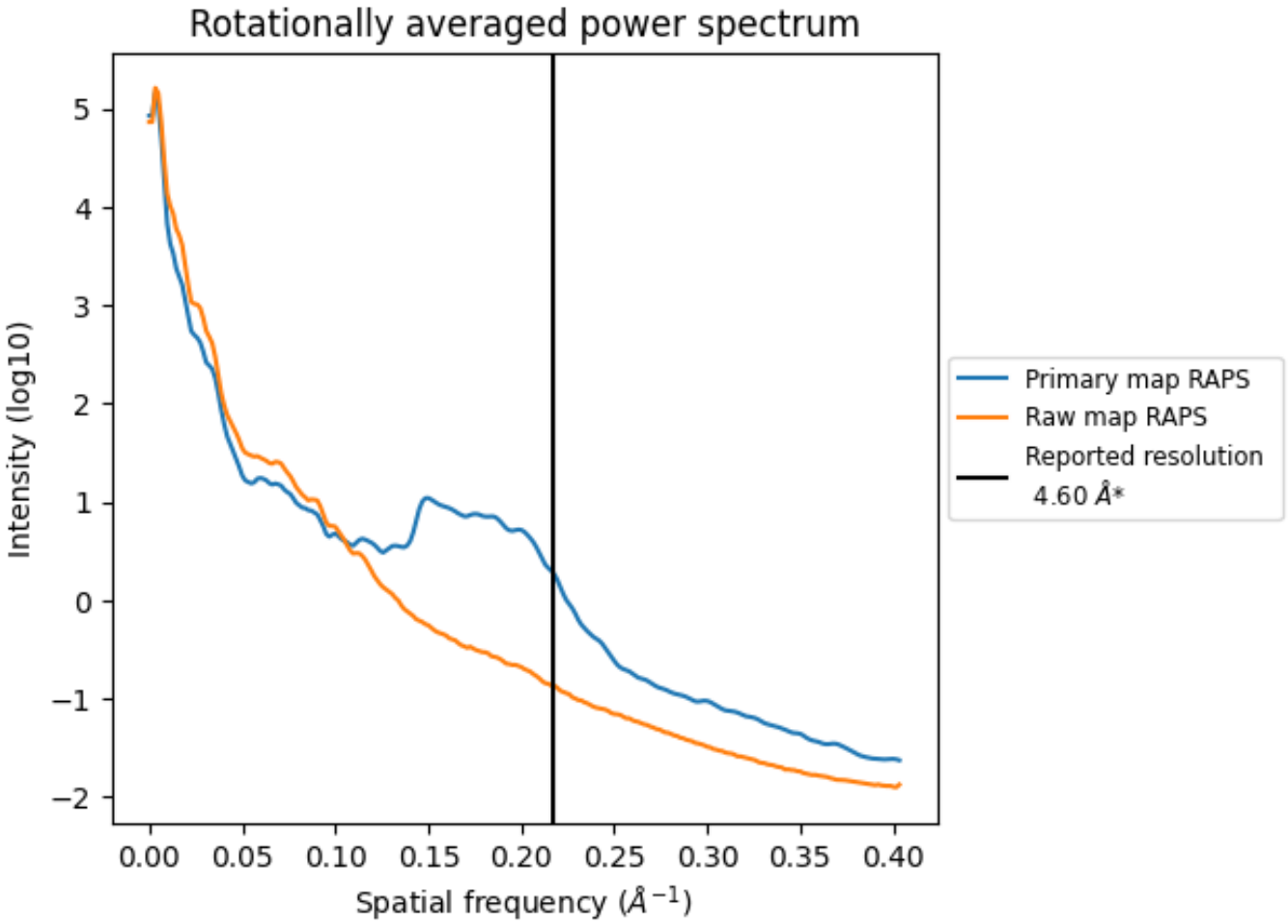
7.2 Volume estimate



The volume at the recommended contour level is 391 nm^3; this corresponds to an approximate mass of 353 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)

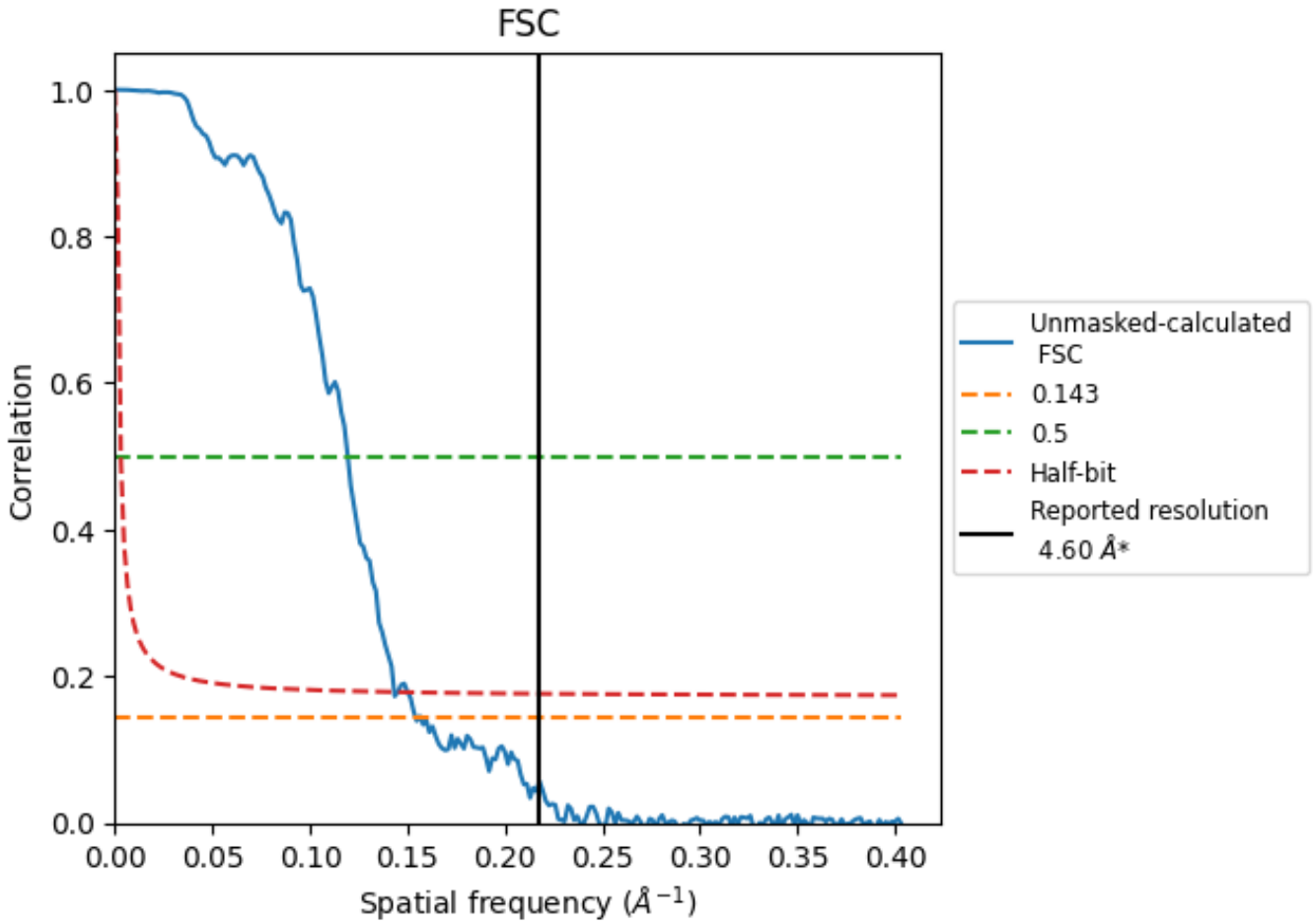


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

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 0.217 Å^{-1}

8.2 Resolution estimates (i)

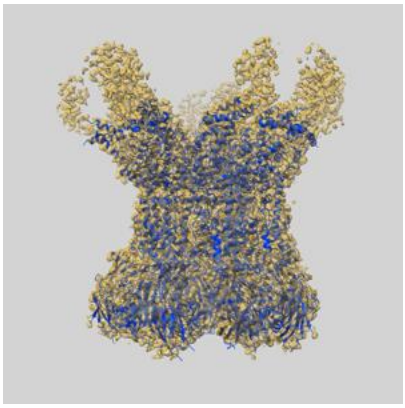
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.48	8.38	6.98

*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 6.48 differs from the reported value 4.6 by more than 10 %

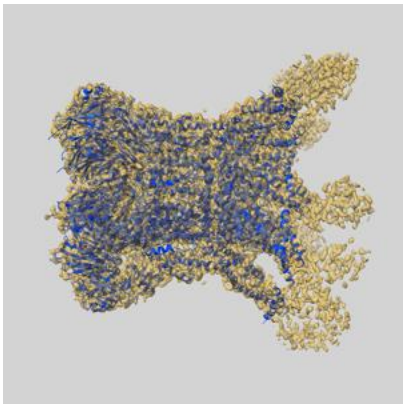
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0264 and PDB model 6HS7. Per-residue inclusion information can be found in section 3 on page 9.

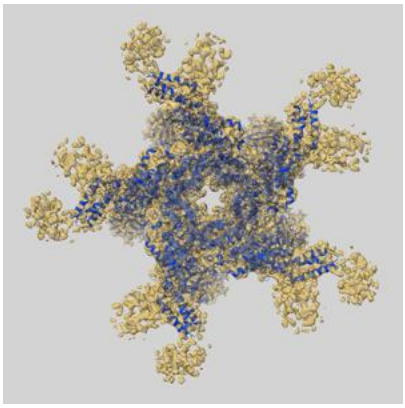
9.1 Map-model overlay



X



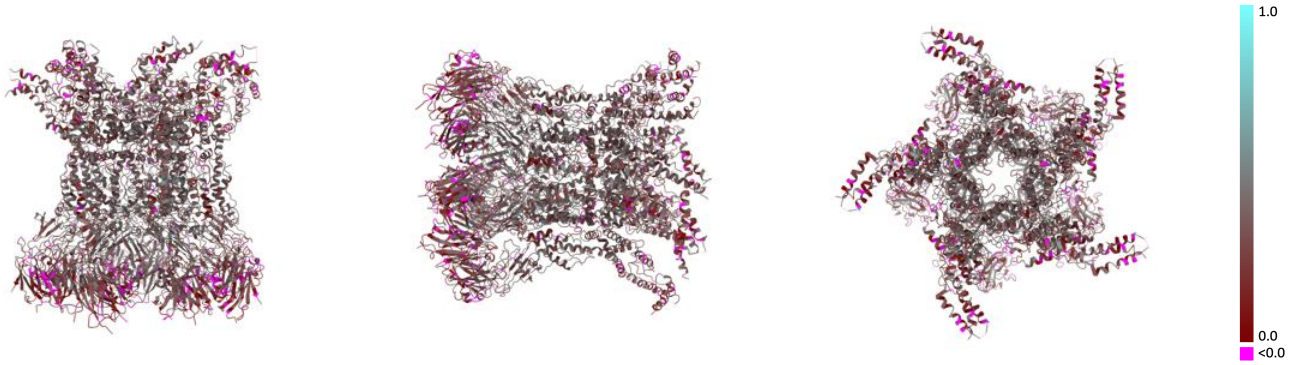
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

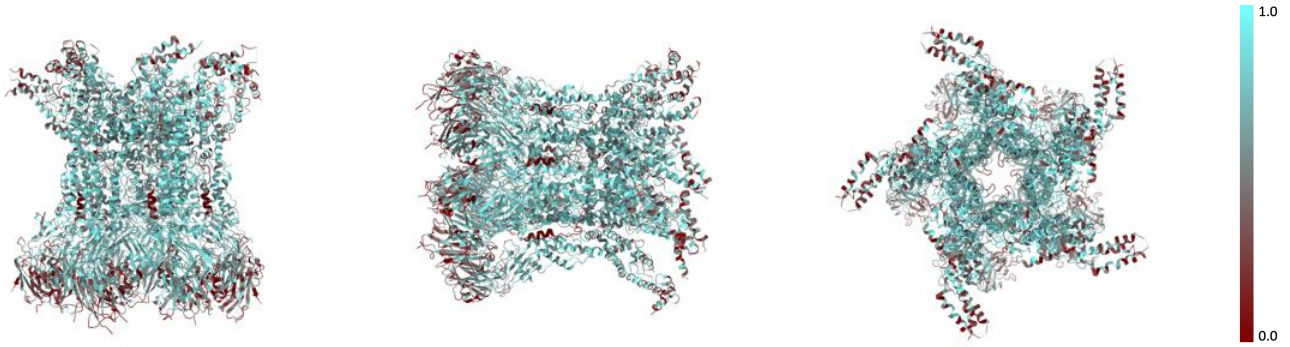
9.2 Q-score mapped to coordinate model (i)



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.

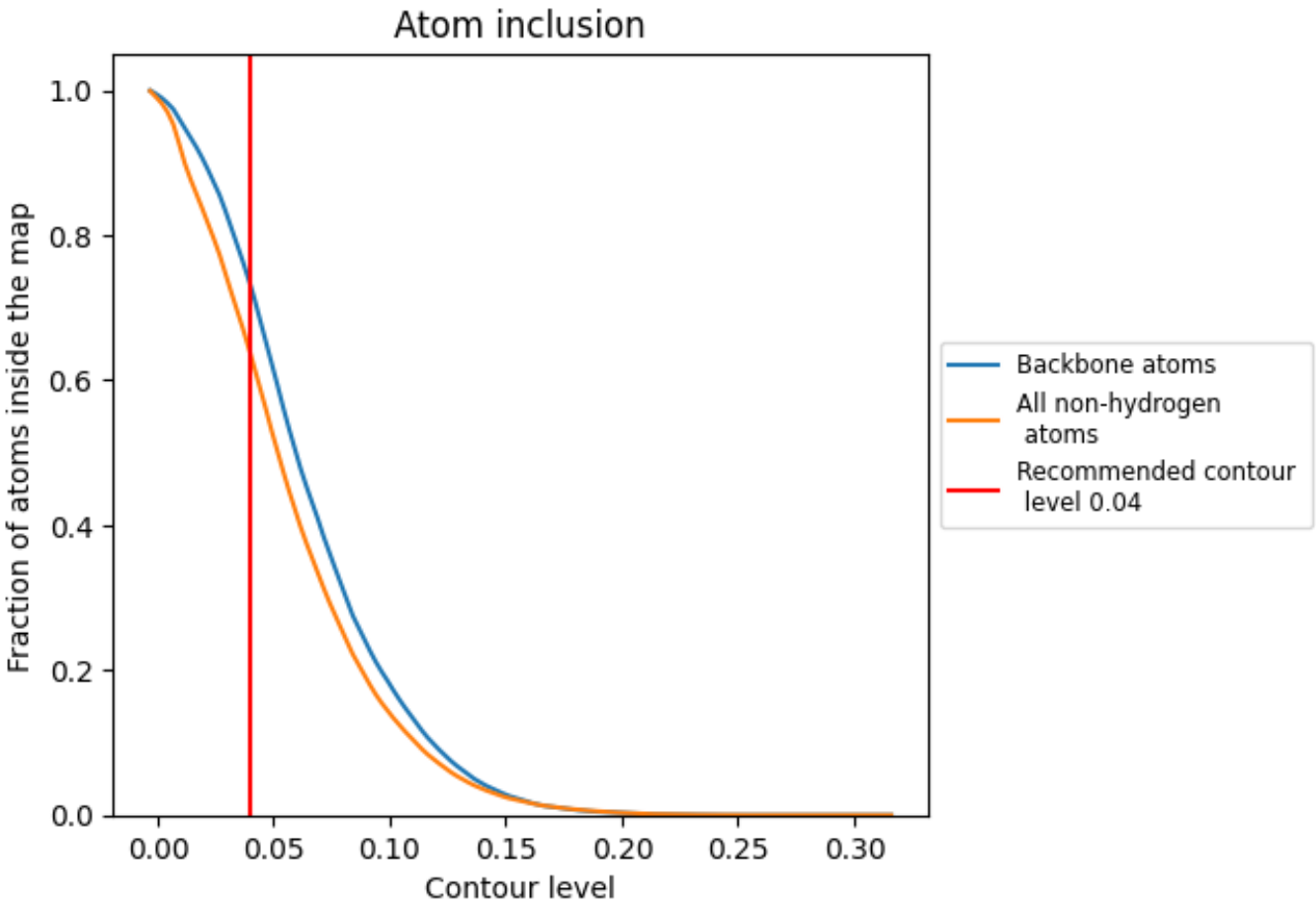
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 64% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6363	0.3120
A	0.6677	0.3320
B	0.6632	0.3320
C	0.6674	0.3300
D	0.6626	0.3340
E	0.6694	0.3330
F	0.4766	0.2280
G	0.3849	0.1800
H	0.6018	0.2900
I	0.4827	0.2260
J	0.3859	0.1810
K	0.6079	0.2930
L	0.4735	0.2290
M	0.3829	0.1890
N	0.6079	0.2910
O	0.4715	0.2230
P	0.3778	0.1760
Q	0.6110	0.2920
R	0.4735	0.2250
S	0.3737	0.1790
T	0.6039	0.2910
a	0.7194	0.3530
b	0.7212	0.3530
c	0.7251	0.3520
d	0.7231	0.3540
e	0.7228	0.3540