



wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 12:58 am GMT

PDB ID : 7B9S
EMDB ID : EMD-12105
Title : Structure of the mycobacterial ESX-5 Type VII Secretion System hexameric pore complex
Authors : Chojnowski, G.; Ritter, C.; Beckham, K.S.H.; Mullapudi, E.; Rettel, M.; Savitski, M.M.; Mortensen, S.A.; Ziemianowicz, D.; Kosinski, J.; Wilmanns, M.
Deposited on : 2020-12-14
Resolution : 3.40 Å (reported)
Based on initial model : 7B9F

This is a wwPDB EM Validation Summary 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) : 2.31.3

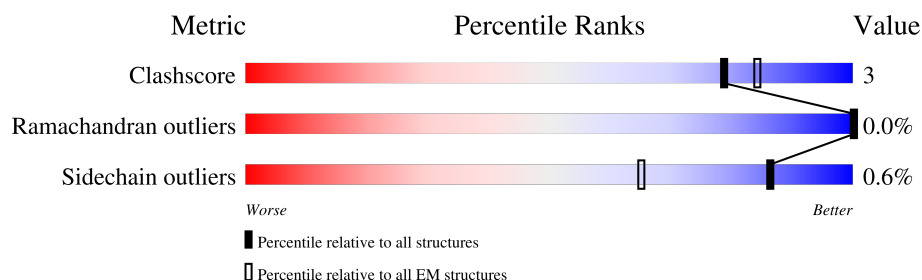
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.




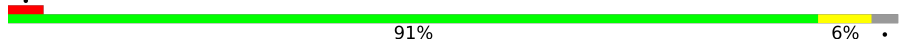

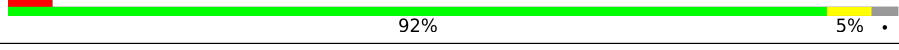

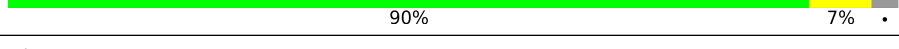
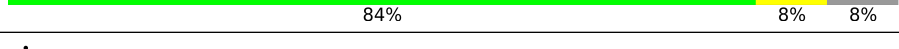
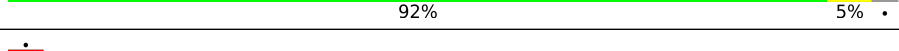
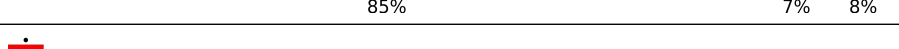
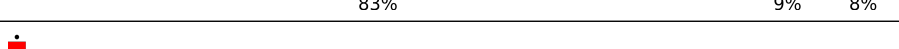












Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	4	400	<div> <div>12%</div> <div>38%</div> <div>59%</div> </div>
1	E	400	<div> <div>12%</div> <div>38%</div> <div>59%</div> </div>
1	H	400	<div> <div>12%</div> <div>38%</div> <div>59%</div> </div>
1	M	400	<div> <div>12%</div> <div>38%</div> <div>59%</div> </div>
1	R	400	<div> <div>13%</div> <div>38%</div> <div>59%</div> </div>
1	Y	400	<div> <div>13%</div> <div>38%</div> <div>59%</div> </div>
2	3	502	<div> <div>90%</div> <div>6%</div> </div>
2	5	502	<div> <div>84%</div> <div>8%</div> <div>8%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	502	 90%7%
2	G	502	 91%6%
2	I	502	 86%6%8%
2	L	502	 5%92%5%
2	N	502	 87%5%8%
2	Q	502	 90%7%
2	S	502	 84%8%8%
2	W	502	 92%5%
2	X	502	 85%7%8%
2	Z	502	 83%9%8%
3	2	1392	 25%72%
3	C	1392	 25%72%
3	F	1392	 25%72%
3	K	1392	 25%72%
3	P	1392	 25%72%
3	V	1392	 25%72%
4	1	506	 11%88%
4	A	506	 12%88%
4	B	506	 11%88%
4	J	506	 12%88%
4	O	506	 12%88%
4	T	506	 12%88%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 72030 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 EccE5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	165	Total	C	N	O	S	0	0
			1305	814	249	240	2		
1	H	165	Total	C	N	O	S	0	0
			1305	814	249	240	2		
1	M	165	Total	C	N	O	S	0	0
			1305	814	249	240	2		
1	R	165	Total	C	N	O	S	0	0
			1305	814	249	240	2		
1	Y	165	Total	C	N	O	S	0	0
			1305	814	249	240	2		
1	4	165	Total	C	N	O	S	0	0
			1305	814	249	240	2		

- Molecule 2 is a protein called EccD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	462	Total	C	N	O	S	0	0
			3469	2272	598	581	18		
2	D	485	Total	C	N	O	S	0	0
			3644	2382	628	616	18		
2	I	462	Total	C	N	O	S	0	0
			3469	2272	598	581	18		
2	G	485	Total	C	N	O	S	0	0
			3644	2382	628	616	18		
2	N	462	Total	C	N	O	S	0	0
			3469	2272	598	581	18		
2	L	485	Total	C	N	O	S	0	0
			3644	2382	628	616	18		
2	S	462	Total	C	N	O	S	0	0
			3469	2272	598	581	18		
2	Q	485	Total	C	N	O	S	0	0
			3644	2382	628	616	18		
2	Z	462	Total	C	N	O	S	0	0
			3469	2272	598	581	18		

Continued on next page...

Continued from previous page...

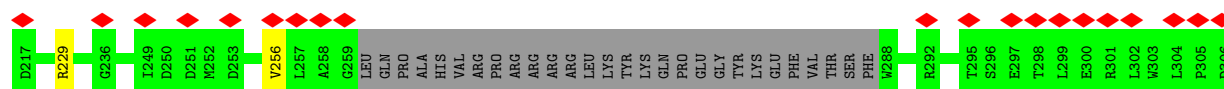
Mol	Chain	Residues	Atoms					AltConf	Trace
2	W	485	Total	C	N	O	S	0	0
			3644	2382	628	616	18		
2	5	462	Total	C	N	O	S	0	0
			3469	2272	598	581	18		
2	3	485	Total	C	N	O	S	0	0
			3644	2382	628	616	18		

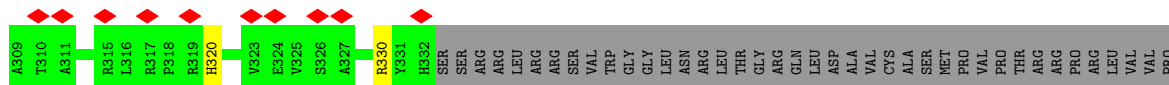
- Molecule 3 is a protein called EccC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	396	Total	C	N	O	S	0	0
			3107	1990	533	562	22		
3	F	396	Total	C	N	O	S	0	0
			3107	1990	533	562	22		
3	K	396	Total	C	N	O	S	0	0
			3107	1990	533	562	22		
3	P	396	Total	C	N	O	S	0	0
			3107	1990	533	562	22		
3	V	396	Total	C	N	O	S	0	0
			3107	1990	533	562	22		
3	2	396	Total	C	N	O	S	0	0
			3107	1990	533	562	22		

- Molecule 4 is a protein called EccB5.


Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	63	Total	C	N	O	S	0	0
			480	304	92	81	3		
4	A	63	Total	C	N	O	S	0	0
			480	304	92	81	3		
4	J	63	Total	C	N	O	S	0	0
			480	304	92	81	3		
4	O	63	Total	C	N	O	S	0	0
			480	304	92	81	3		
4	T	63	Total	C	N	O	S	0	0
			480	304	92	81	3		
4	1	63	Total	C	N	O	S	0	0
			480	304	92	81	3		

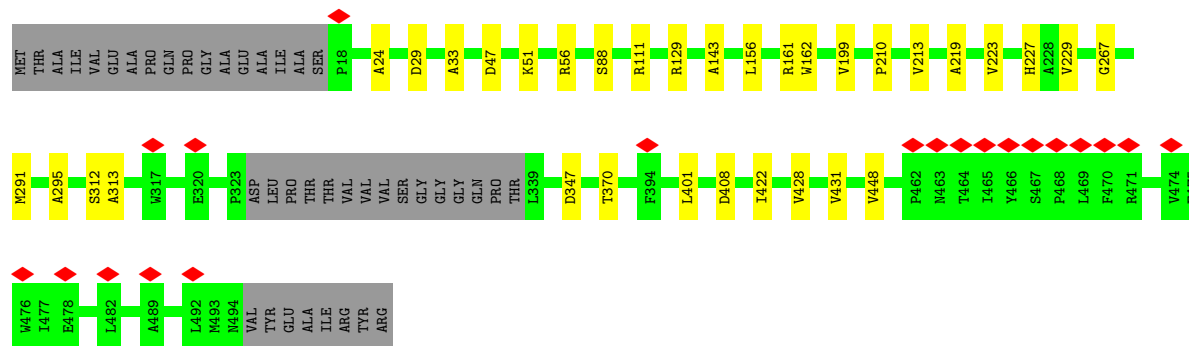




ALA
ARG
GLU
LEU
ILE
HIS
ASP
GLY
GLU
GLU
LEU
VAL
ALA
VAL
LEU
VAL
GLY
GLN
ALA
ALA
PRO
PRO
SER
PRO
SER
PRO
PRO
ALA
ALA
ALA
ARG

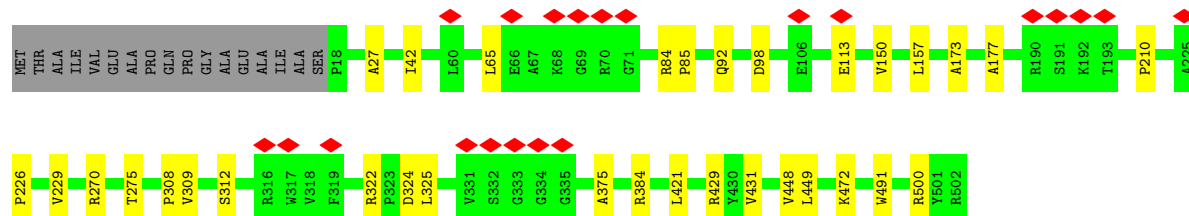
• Molecule 2: EccD5

Chain X:  85% 7% 8%




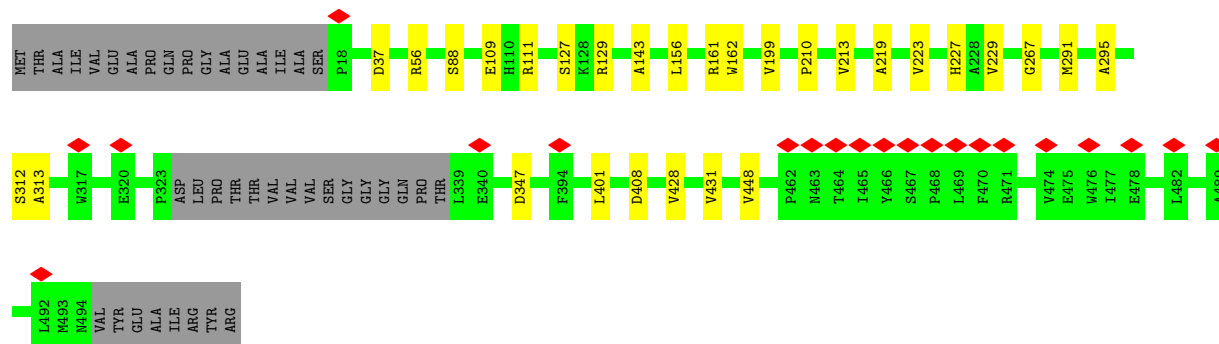
• Molecule 2: EccD5

Chain D:  90% 7% 3%

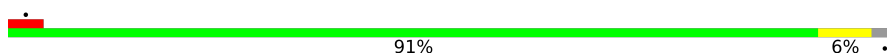


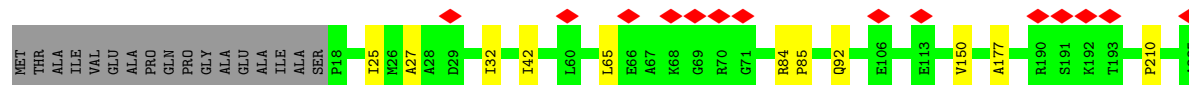
• Molecule 2: EccD5

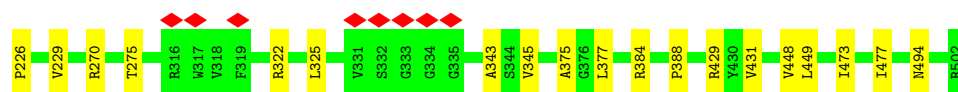
Chain I:  86% 6% 8%



• Molecule 2: EccD5

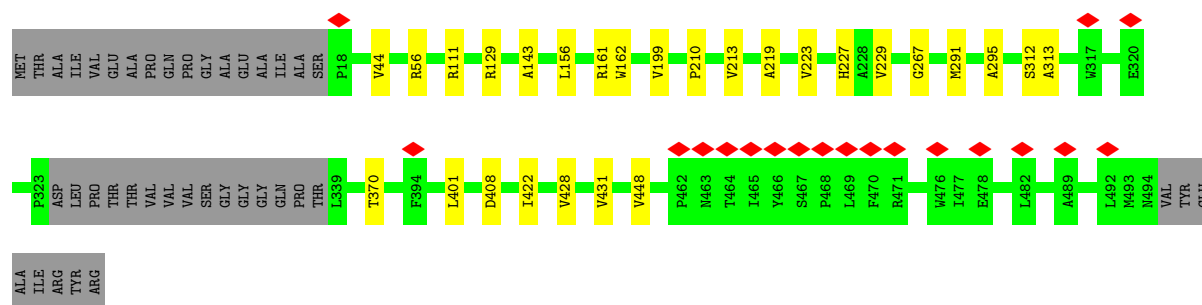
Chain G:  91% 6% 3%





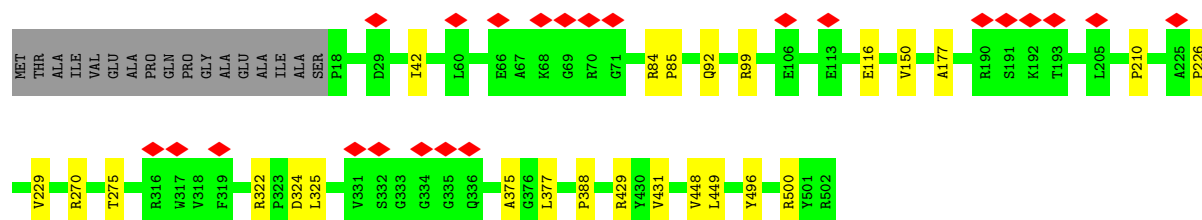
- Molecule 2: EccD5

Chain N: 87% 5% 8%



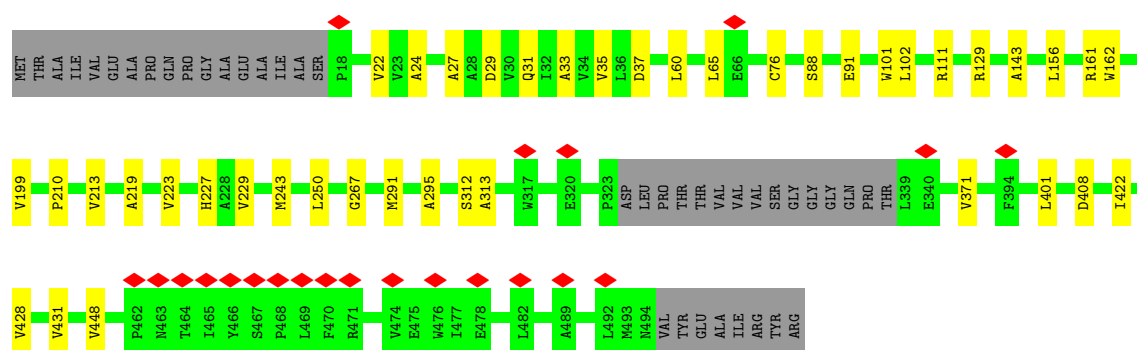
- Molecule 2: EccD5

Chain L: 5% 92% 5%



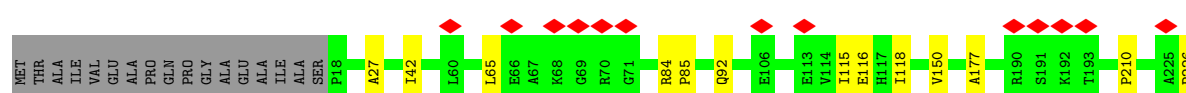
- Molecule 2: EccD5

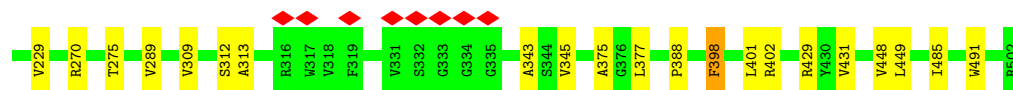
Chain S: 84% 8% 8%



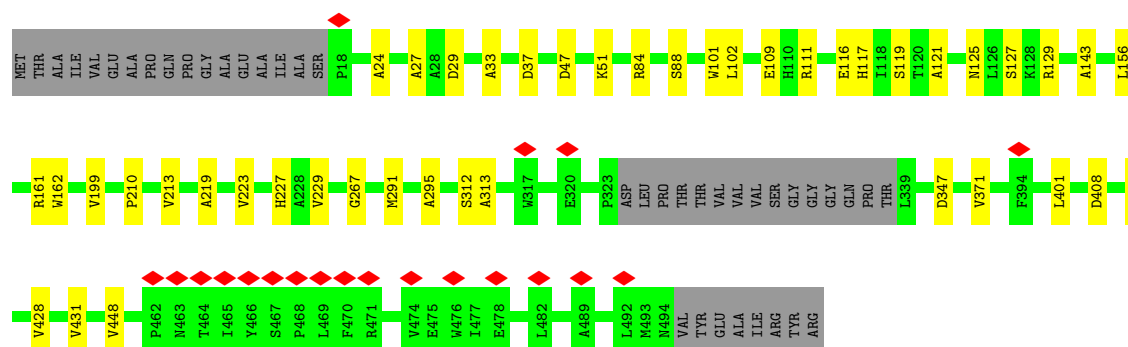
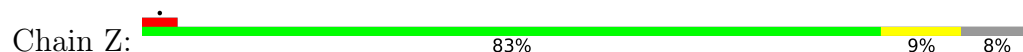
- Molecule 2: EccD5

Chain Q: 90% 7% 3%

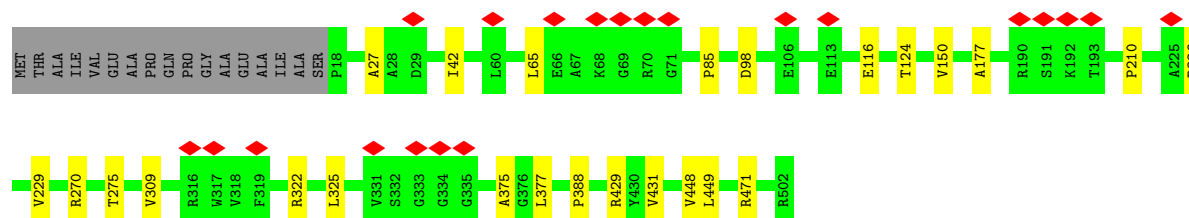




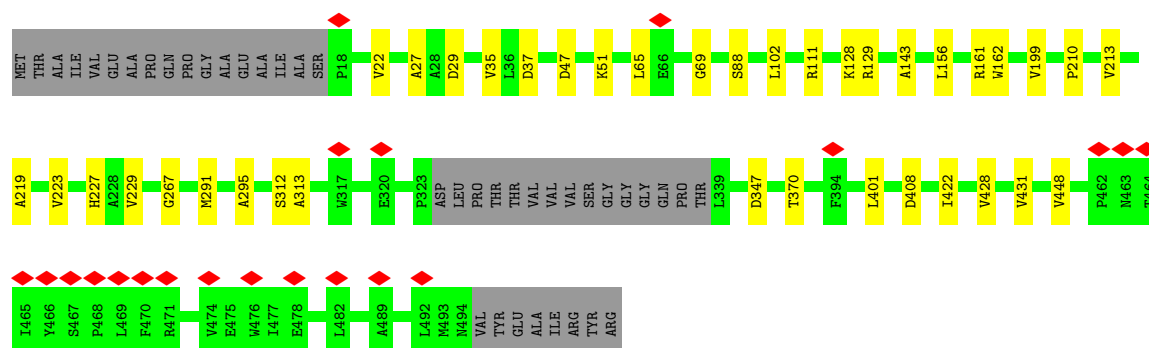
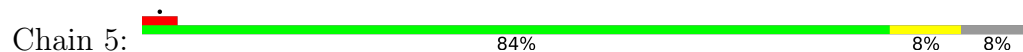
• Molecule 2: EccD5



• Molecule 2: EccD5



• Molecule 2: EccD5

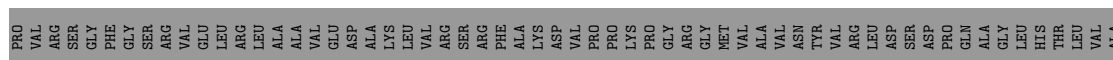
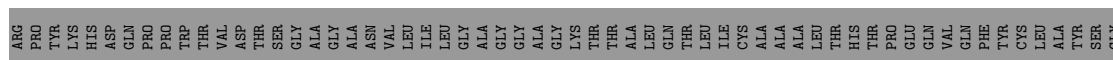
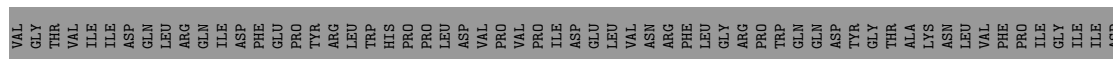
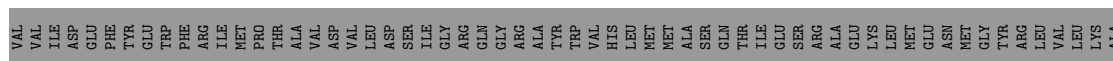
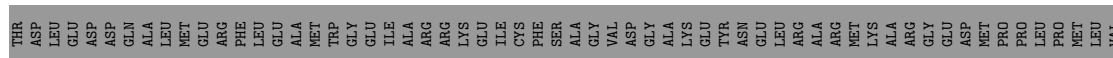
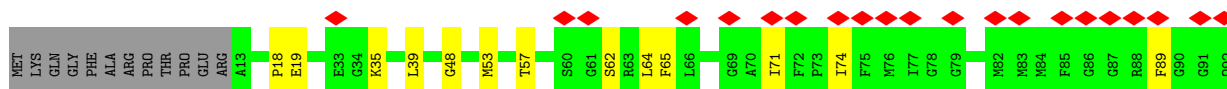


• Molecule 2: EccD5





- Molecule 3: EccC5



TLE	ARG	LEU	ALA	ALA	HIS	LEU	GLN	ASN	ALA	VAL	MET	ASP	ALA	ASP	PRO	PRO	GLU	GLY	PHE	TLE	ARG	GLY	LYS	LYS	GLY	GLY	PRO	LEU	LEU	MET	MET	ALA	ALA	GLU	ASP	THR	GLY	VAL	PHE	VAL	GLN	VAL	ALA	ALA	THR	ASP	LEU	ARG	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 3: EccC5

[illegible]

Category	Count
Q92	30
Q93	30
Q94	30
Q95	30
D123	30
D126	30
R130	30
H133	30
Q152	30
P153	30
D154	30
G155	30
K156	30
F160	30
R164	30
E173	30
V174	30
L215	30
L216	30
V217	30
L231	30
R235	30
H245	30
D248	30
V254	30
S257	30
W257	30
H270	30
F271	30
R291	30
L300	30
F301	30
R304	30
G305	30
S306	30
F307	30
T308	30
PRO	30
ARG	30
HTS	30

ALA	SER	SER	SER	ALA	GLU	T318	H223	I326	S327	D328	I329	E330	Y336	S339	S340	V343	V346	L351	D380	I387	D388	D389	A409	H414	LA14	LA17	ALA	GLU	ALA	TYR	GLU	GLU	GLU	ILE	ILE	GLN	SER	GLY	ARG	VAL	GLN	VAL	GLN	LEU	GLY	ALA	ALA	ARG	ASP	ILE	ILE	LEU	SER	SER	TYR
-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Tyr	Gly	Ile	Asp	Ala	Gly	Glu	Ile	Asp	Phe	Thr	Leu	Ser	Gly	Ser	Gly	Arg	Arg	Asp	Leu	Ser	Arg	Ser	Ser	Arg	Leu	Arg	Arg	Ala	Asp	Asn	Gly	Gly	Leu	Leu	Phe	Leu	Asp	Met	Lys	Ser	Leu	Asp	Glu	Gly	Gly	Asp	Gly	Pro	His	Gly	Val
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

MET SER GLY THR THR GLY SER GLY LYS LYS SER SER LEU VAL VAL THR THR VAL ILE ALA ALA SER LEU LEU LEU LEU HIS PRO PRO GLU GLU LEU LEU ASP LEU LEU LYS GLY GLY SER SER ASP ASP GLY VAL PRO PRO HIS VAL SER SER ARG ILE ILE THR THR ASP ASP LEU LEU GLU ASP

ASP	GLN	ALA	ALA	LEU	MET	GLU	ARG	PHE	LEU	GLU	ALA	MET	TRP	GLY	ILE	GLU	CYS	PHE	SER	ALA	GLY	VAL	ASP	GLY	ALA	LYS	GLU	TYR	ASN	LEU	LEU	ARG	ALA	ALA	GLY	GLU	ASP	MET	LYS	ALA	ARG	VAL	VAL	VAL	ILE	ASP	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PHE TYR GLU TRP PHE ARG ILE MET MET PRO THR ALA VAL ASP VAL LEU ASP SER ILE GLY ARG GLN GLY ARG ALA TYR TRP VAL VAL HIS LEU LEU MET MET SER SER GLN THR THR ILE GLU SER ARG ARG ALA ALA GLU LYS LEU LEU MET MET GLN ASN MET MET GLY TYR ARG LEU LEU VAL VAL LYS ALA GLN ALN THR THR GLY ALA ALA GLY

ALA	GLN	ALA	ALA	GLY	VAL	PRO	ASN	ALA	VAL	ASN	LEU	PRO	SER	GLN	ALA	ALA	GLY	GLY	TYR	PHE	ARG	ARG	LYS	SER	GLY	ASP	GLU	ILE	ILE	ARG	ARG	GLN	ALA	ALA	GLU	GLU	TYR	LEU	TRP	ARG	ASP	ASP	TYR	TYR	TYR	ASP	GLY	GLU	GLN	GLN	ALA	ALA	PRO	PRO	LEU	THR	HIS	SER	SER	VAL	ASP	TYR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ILE	ARG	PRO	GLN	LEU	PHE	THR	THR	ALA	ALA	PRO	ALA	PRO	LEU	GLU	VAL	VAL	SER	SER	GLY	PRO	PRO	ASP	GLY	GLN	SER	ALA	ALA	LEU	PRO	GLN	VAL	GLN	VAL	VAL	ASP	GLY	GLY	GLU	GLU	GLY	GLY	GLY	ASP	ASP	VAL	ASP	ASP	GLU	GLU	GLU	GLU	GLU	ALA	LEU	LEU	ALA	ARG	THR	THR	PRO	LYS	VAL	VAL	GLY	GLY	THR	THR	VAL	VAL	ILE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

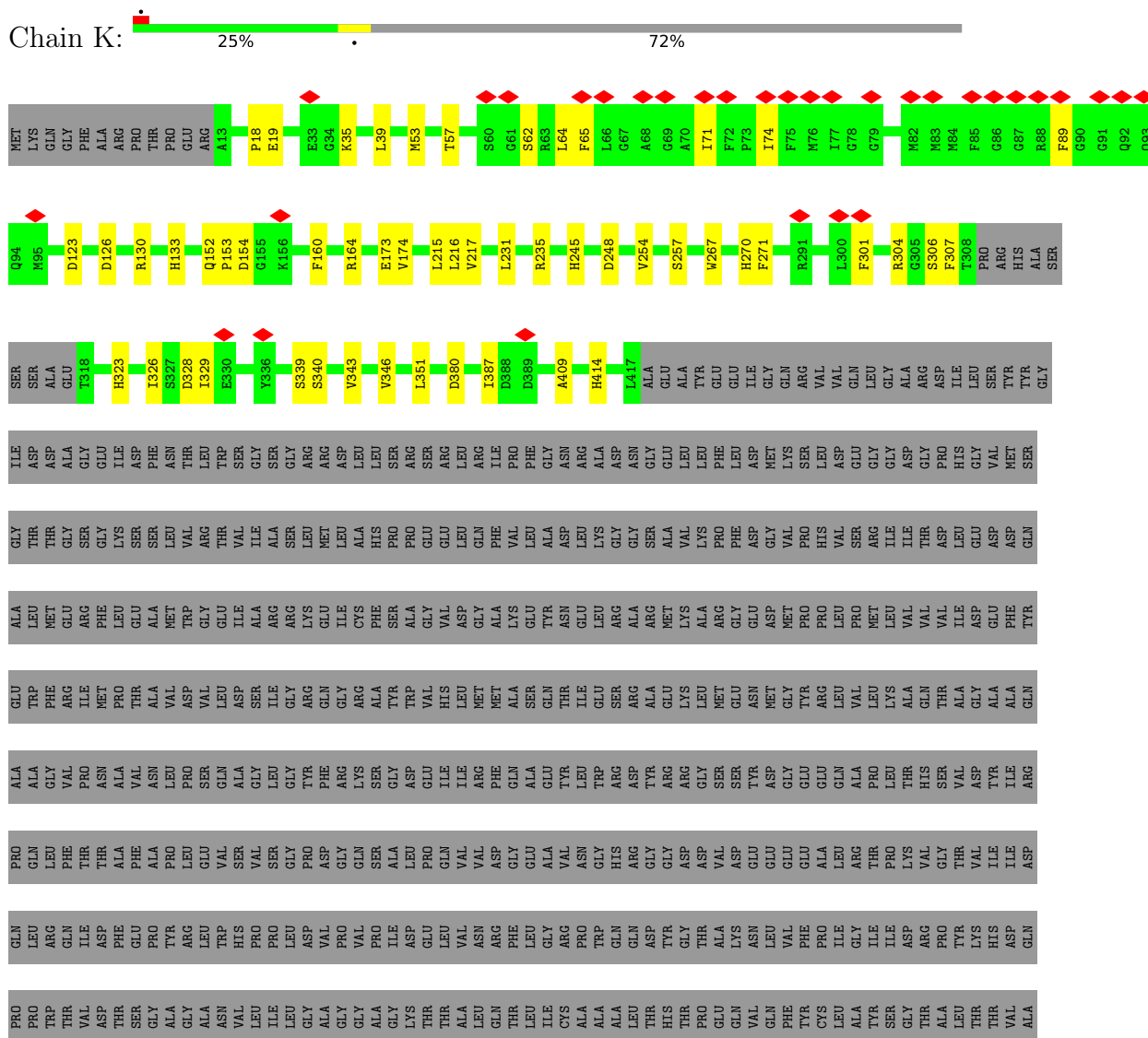
TLE	GLN	ASP	GLN	ARG	ILE	ASP	PHE	GLU	PRO	TYR	ARG	LEU	TRP	HIS	PRO	PRO	LEU	ASP	VAL	VAL	PRO	ILE	ASP	GLU	LEU	VAL	ASN	ARG	PHE	LEU	GLY	GLY	TYR	ASP	GLN	GLN	TRP	PRO	ARG	PRO	THR	ALA	LYS	ASN	LEU	VAL	PHE	PRO	ILE	GLY	ILE	ILE	ASP	ARG	PRO	TYR	LYS	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASP	GLN	PRO	PRO	TRP	THR	VAL	ASP	SER	THR	GLY	ALA	GLY	ASN	VAL	LEU	ILE	LEU	GLY	ALA	GLY	ALA	GLN	LEU	THR	THR	ALA	ALA	GLN	LEU	CYS	ILE	ILE	ALA	ALA	LEU	LEU	HIS	THR	PRO	GLU	GLN	VAL	GLN	PHE	TYR	CYS	LEU	ALA	TYR	SER	GLY	THR	LEU	ALA	THR	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

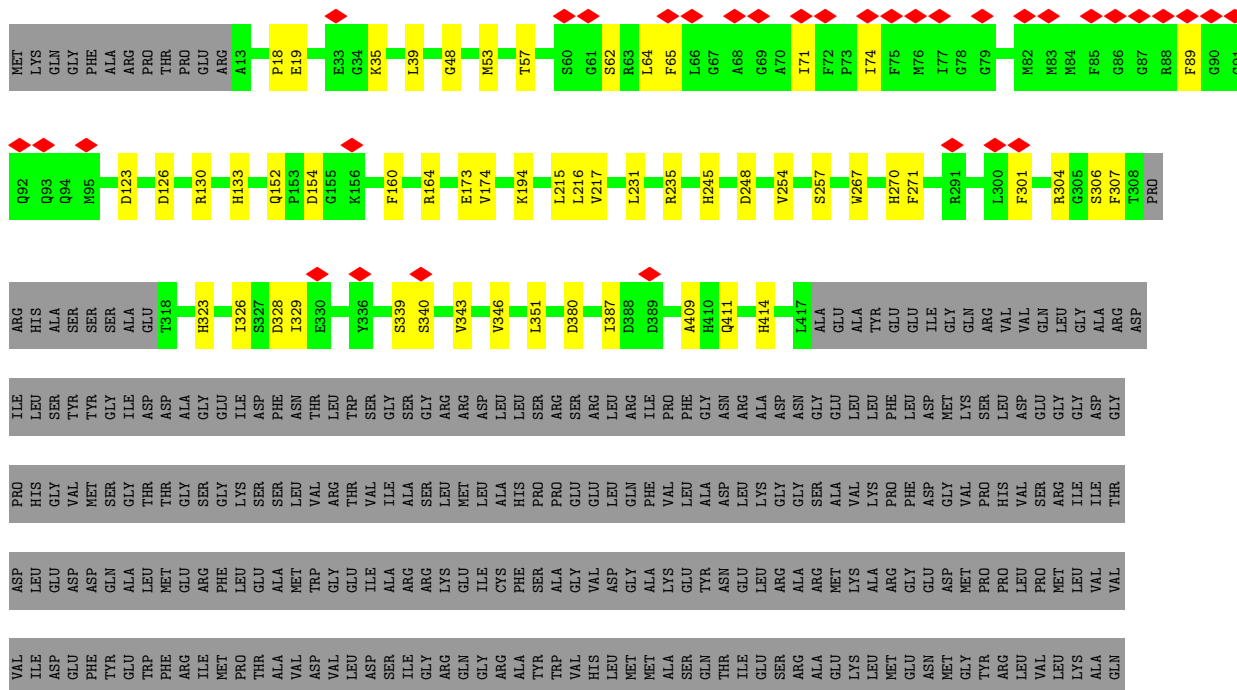
VAL	ALA	ASN	LEU	PRO	HIS	VAL	GLY	GLY	VAL	SER	GLY	PRO	THR	ASP	PRO	GLY	VAL	ARG	ARG	THR	VAL	ALA	GLU	VAL	LEU	GLY	LEU	VAL	ARG	ASP	ARG	LYS	ARG	SER	PHE	LEU	GLU	TYR	ASP	VAL	PRO	SER	MET	GLU	VAL	PHE	ARG	ARG	LYS	PHE	GLY	GLY	GLU	PRO	GLY	GLY	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PRO	ASP	ASP	ASP	GLY	PHE	GLY	ASP	VAL	TYR	LEU	VAL	ILE	ASP	ASN	TYR	ARG	ALA	LEU	ALA	GLU	GLU	ASN	GLN	VAL	VAL	GLU	ILE	ILE	ILE	ASN	GLN	GLY	PRO	SER	PHE	GLY	GLY	VAL	HIS	VAL	VAL	ALA	THR	THR	ALA	ALA	ASP	ASP	ARG	GLU	GLU	SER	SER	GLU	LEU	ARG	PRO	PRO	VAL	VAL	ARG	ARG	SER	TYR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 3: EccC5



- Molecule 3: EccC5





[illegible]

- Molecule 4: EccB5

Chain O:  12% . 88%

[illegible]

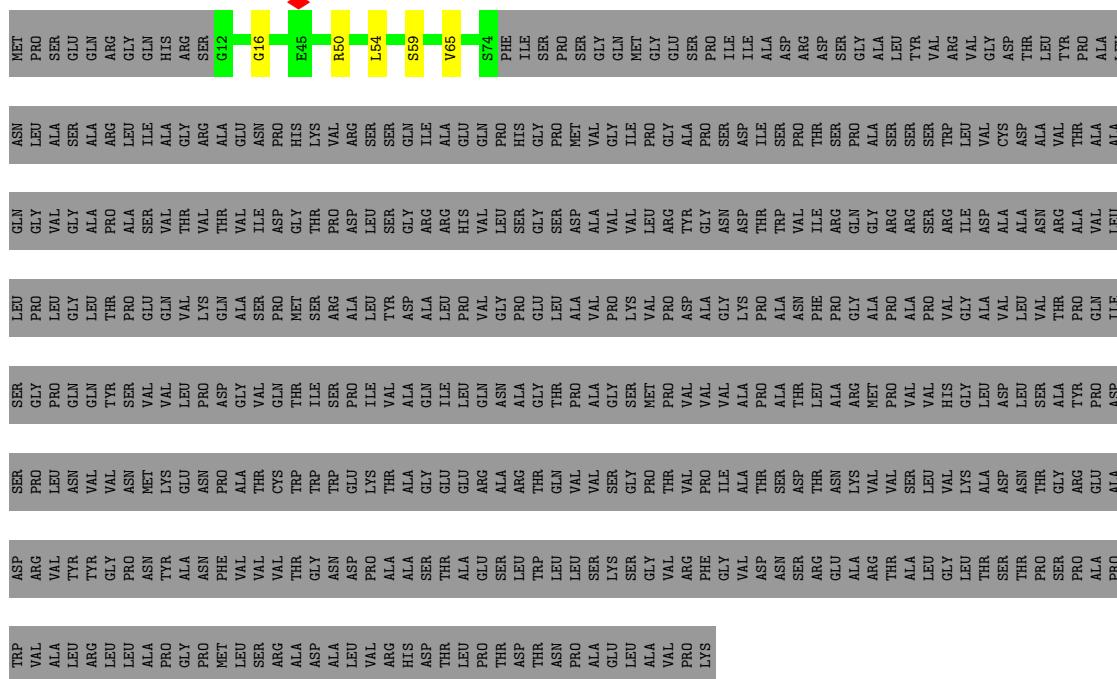
- Molecule 4: EccB5

Chain T: 12% . 88%

ASN	SER	PRO	ALA	LEU	MET
ASN	VAL	GLN	SER	ILE	PRO
MET	VAL	GLN	VAL	ALA	SER
GLU	LEU	VAL	THR	GLY	GLU
PRO	PRO	LYS	VAL	ARG	GLN
ALA	ASP	GLN	THR	ALA	ARG
GLY	ALA	ALA	VAL	GLU	GLY
THR	VAL	SER	ILE	ASN	GLN
GLN	GLN	PRO	ASP	PRO	HIS
CYS	THR	MET	GLY	HIS	ARG
TRP	TRP	SER	THR	LYS	SER
TRP	SER	ARG	PRO	VAL	SER
GLU	PRO	ALA	ASP	ARG	G12
GLU	ILE	LEU	LEU	SER	
THR	VAL	TYR	SER	SER	W40
ALA	ALA	ASP	GLY	GLN	R50
GLY	GLN	ALA	ARG	ILE	
GLU	ILE	LEU	ARG	ALA	L54
GLU	LEU	PRO	HIS	GLU	
ARG	GLN	VAL	VAL	GLN	S74
ALA	ASN	GLY	LEU	PRO	PHE
ALA	ALA	PRO	SER	HIS	ILE
ARG	GLY	GLU	GLY	GLY	SER
THR	THR	LEU	SER	PRO	PRO
VAL	PRO	ALA	ASP	MET	SER
VAL	ALA	VAL	VAL	VAL	GLY
SER	GLY	PRO	VAL	GLN	GLU
GLY	LYS	VAL	VAL	ILE	SER
PRO	MET	VAL	LEU	PRO	PRO
THR	THR	PRO	ARG	GLY	GLU
VAL	VAL	ASP	TTR	ALA	SER
PRO	VAL	ALA	GLY	PRO	PRO
ILE	GLY	LYS	ASN	ILE	ILE
ALA	ALA	LYS	ASP	ASP	ILE
THR	PRO	PRO	THR	ILE	ALA
SER	ALA	ALA	TTP	SER	ASP
ASP	THR	ASN	VAL	PRO	ARG
THR	LEU	PHE	ILE	THR	SER
ASN	ASN	PRO	ARG	SER	SER
LYS	ARG	GLY	GLN	PRO	GLY
VAL	MET	ALA	GLY	ALA	ALA
VAL	PRO	ALA	ARG	SER	LEU
SER	VAL	ALA	ARG	SER	THR
LEU	VAL	PRO	ARG	SER	VAL
VAL	VAL	PRO	ARG	TRP	ARG
LYS	HIS	GLY	ILE	VAL	VAL
GLY	LYS	VAL	ASP	VAL	GLY
LEU	ALA	ALA	ALA	CYS	ASP
ASP	ASP	VAL	ALA	ASP	THR
ASN	LEU	LEU	ALA	VAL	LEU
THR	SER	THR	ASN	ALA	LEU
GLY	ALA	VAL	ARG	VAL	TYR
ARG	TYR	PRO	ALA	THR	PRO
GLU	PRO	GLN	VAL	ALA	ALA
ALA	ASP	ILE	LEU	ALA	LEU
ASP	SER	SER	LEU	GLN	LEU
ARG	PRO	GLY	PRO	VAL	SER
VAL	LEU	LEU	GLY	VAL	GLY
TYR	ASN	GLN	GLY	GLY	GLY
TYR	VAL	GLN	LEU	THR	ALA
TYR	VAL	THR	THR	PRO	ASP

LEU
ALA
PRO
GLY
PRO
MET
LEU
SER
ARG
ALA
ASP
ALA
LEU
VAL
ARG
HIS
ASP
THR
LEU
PRO
THR
ASP
THR
ASN
PRO
ALA
GLU
LEU
ALA
VAL
PRO
LYS

Chain 1: 11% 88%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121974	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.34	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.687	Depositor
Minimum map value	-0.260	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	580.5, 580.5, 580.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.29, 1.29, 1.29	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	4	0.26	0/1330	0.58	0/1814
1	E	0.26	0/1330	0.58	0/1814
1	H	0.26	0/1330	0.58	0/1814
1	M	0.26	0/1330	0.58	0/1814
1	R	0.26	0/1330	0.58	0/1814
1	Y	0.26	0/1330	0.58	0/1814
2	3	0.38	0/3727	0.58	1/5110 (0.0%)
2	5	0.34	0/3547	0.61	5/4862 (0.1%)
2	D	0.37	0/3727	0.58	1/5110 (0.0%)
2	G	0.38	0/3727	0.60	1/5110 (0.0%)
2	I	0.33	0/3547	0.61	4/4862 (0.1%)
2	L	0.39	0/3727	0.61	1/5110 (0.0%)
2	N	0.33	0/3547	0.60	2/4862 (0.0%)
2	Q	0.38	0/3727	0.59	0/5110
2	S	0.33	0/3547	0.60	4/4862 (0.1%)
2	W	0.39	0/3727	0.60	1/5110 (0.0%)
2	X	0.33	0/3547	0.61	4/4862 (0.1%)
2	Z	0.34	0/3547	0.62	5/4862 (0.1%)
3	2	0.33	0/3196	0.56	0/4355
3	C	0.33	0/3196	0.56	0/4355
3	F	0.33	0/3196	0.56	0/4355
3	K	0.33	0/3196	0.56	0/4355
3	P	0.33	0/3196	0.56	0/4355
3	V	0.33	0/3196	0.56	0/4355
4	1	0.45	0/487	0.63	0/659
4	A	0.45	0/487	0.63	0/659
4	B	0.45	0/487	0.63	0/659
4	J	0.45	0/487	0.63	0/659
4	O	0.45	0/487	0.63	0/659
4	T	0.45	0/487	0.63	0/659
All	All	0.35	0/73722	0.59	29/100800 (0.0%)

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	347	ASP	CB-CG-OD1	7.29	124.86	118.30
2	5	347	ASP	CB-CG-OD1	7.25	124.82	118.30
2	I	347	ASP	CB-CG-OD1	7.22	124.80	118.30
2	X	347	ASP	CB-CG-OD1	7.22	124.80	118.30
2	Z	29	ASP	CB-CG-OD1	6.38	124.04	118.30

There are no chirality outliers.

There are no planarity outliers.

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	4	1305	0	1283	5	0
1	E	1305	0	1283	8	0
1	H	1305	0	1283	8	0
1	M	1305	0	1283	8	0
1	R	1305	0	1283	9	0
1	Y	1305	0	1283	8	0
2	3	3644	0	3854	18	0
2	5	3469	0	3679	18	0
2	D	3644	0	3854	20	0
2	G	3644	0	3854	15	0
2	I	3469	0	3679	13	0
2	L	3644	0	3854	14	0
2	N	3469	0	3679	14	0
2	Q	3644	0	3854	22	0
2	S	3469	0	3679	22	0
2	W	3644	0	3854	15	0
2	X	3469	0	3679	17	0
2	Z	3469	0	3679	22	0
3	2	3107	0	3031	30	0
3	C	3107	0	3031	36	0
3	F	3107	0	3031	34	0
3	K	3107	0	3031	31	0
3	P	3107	0	3031	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	V	3107	0	3031	33	0
4	1	480	0	503	4	0
4	A	480	0	503	3	0
4	B	480	0	503	6	0
4	J	480	0	503	2	0
4	O	480	0	503	3	0
4	T	480	0	503	3	0
All	All	72030	0	74100	415	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 3.

The worst 5 of 415 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)
2:Q:375:ALA:O	2:Q:429:ARG:NH1	2.27	0.68
2:W:375:ALA:O	2:W:429:ARG:NH1	2.29	0.66
2:G:375:ALA:O	2:G:429:ARG:NH1	2.28	0.66
4:J:43:ARG:NH1	2:Q:313:ALA:O	2.28	0.66
2:L:375:ALA:O	2:L:429:ARG:NH1	2.28	0.66

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	4	157/400 (39%)	145 (92%)	12 (8%)	0	100	100
1	E	157/400 (39%)	145 (92%)	12 (8%)	0	100	100
1	H	157/400 (39%)	145 (92%)	12 (8%)	0	100	100
1	M	157/400 (39%)	146 (93%)	11 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	157/400 (39%)	146 (93%)	11 (7%)	0	100	100
1	Y	157/400 (39%)	145 (92%)	12 (8%)	0	100	100
2	3	483/502 (96%)	466 (96%)	17 (4%)	0	100	100
2	5	458/502 (91%)	447 (98%)	10 (2%)	1 (0%)	47	78
2	D	483/502 (96%)	466 (96%)	17 (4%)	0	100	100
2	G	483/502 (96%)	465 (96%)	18 (4%)	0	100	100
2	I	458/502 (91%)	448 (98%)	10 (2%)	0	100	100
2	L	483/502 (96%)	468 (97%)	15 (3%)	0	100	100
2	N	458/502 (91%)	449 (98%)	9 (2%)	0	100	100
2	Q	483/502 (96%)	463 (96%)	20 (4%)	0	100	100
2	S	458/502 (91%)	447 (98%)	11 (2%)	0	100	100
2	W	483/502 (96%)	464 (96%)	19 (4%)	0	100	100
2	X	458/502 (91%)	447 (98%)	11 (2%)	0	100	100
2	Z	458/502 (91%)	448 (98%)	10 (2%)	0	100	100
3	2	392/1392 (28%)	374 (95%)	18 (5%)	0	100	100
3	C	392/1392 (28%)	374 (95%)	18 (5%)	0	100	100
3	F	392/1392 (28%)	374 (95%)	18 (5%)	0	100	100
3	K	392/1392 (28%)	374 (95%)	18 (5%)	0	100	100
3	P	392/1392 (28%)	374 (95%)	18 (5%)	0	100	100
3	V	392/1392 (28%)	374 (95%)	18 (5%)	0	100	100
4	1	61/506 (12%)	60 (98%)	1 (2%)	0	100	100
4	A	61/506 (12%)	60 (98%)	1 (2%)	0	100	100
4	B	61/506 (12%)	60 (98%)	1 (2%)	0	100	100
4	J	61/506 (12%)	60 (98%)	1 (2%)	0	100	100
4	O	61/506 (12%)	60 (98%)	1 (2%)	0	100	100
4	T	61/506 (12%)	60 (98%)	1 (2%)	0	100	100
All	All	9306/19812 (47%)	8954 (96%)	351 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	5	69	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4	136/328 (42%)	135 (99%)	1 (1%)	84	92
1	E	136/328 (42%)	135 (99%)	1 (1%)	84	92
1	H	136/328 (42%)	135 (99%)	1 (1%)	84	92
1	M	136/328 (42%)	135 (99%)	1 (1%)	84	92
1	R	136/328 (42%)	135 (99%)	1 (1%)	84	92
1	Y	136/328 (42%)	135 (99%)	1 (1%)	84	92
2	3	381/392 (97%)	379 (100%)	2 (0%)	88	94
2	5	362/392 (92%)	358 (99%)	4 (1%)	73	86
2	D	381/392 (97%)	379 (100%)	2 (0%)	88	94
2	G	381/392 (97%)	380 (100%)	1 (0%)	92	97
2	I	362/392 (92%)	357 (99%)	5 (1%)	67	83
2	L	381/392 (97%)	380 (100%)	1 (0%)	92	97
2	N	362/392 (92%)	359 (99%)	3 (1%)	81	91
2	Q	381/392 (97%)	379 (100%)	2 (0%)	88	94
2	S	362/392 (92%)	360 (99%)	2 (1%)	86	94
2	W	381/392 (97%)	380 (100%)	1 (0%)	92	97
2	X	362/392 (92%)	359 (99%)	3 (1%)	81	91
2	Z	362/392 (92%)	356 (98%)	6 (2%)	60	80
3	2	330/1127 (29%)	329 (100%)	1 (0%)	92	97
3	C	330/1127 (29%)	329 (100%)	1 (0%)	92	97
3	F	330/1127 (29%)	329 (100%)	1 (0%)	92	97
3	K	330/1127 (29%)	329 (100%)	1 (0%)	92	97
3	P	330/1127 (29%)	329 (100%)	1 (0%)	92	97
3	V	330/1127 (29%)	329 (100%)	1 (0%)	92	97
4	1	48/402 (12%)	48 (100%)	0	100	100
4	A	48/402 (12%)	48 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	48/402 (12%)	48 (100%)	0	100	100
4	J	48/402 (12%)	48 (100%)	0	100	100
4	O	48/402 (12%)	48 (100%)	0	100	100
4	T	48/402 (12%)	48 (100%)	0	100	100
All	All	7542/15846 (48%)	7498 (99%)	44 (1%)	86	94

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Z	84	ARG
2	W	322	ARG
2	Z	88	SER
2	Z	129	ARG
2	5	88	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

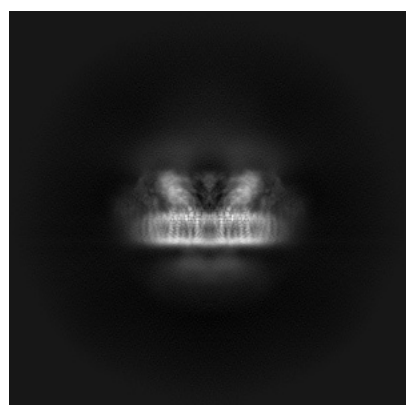
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12105. These allow visual inspection of the internal detail of the map and identification of artifacts.

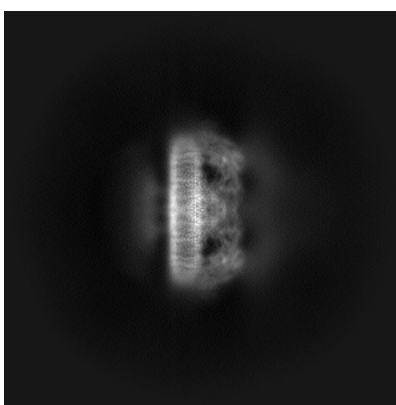
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

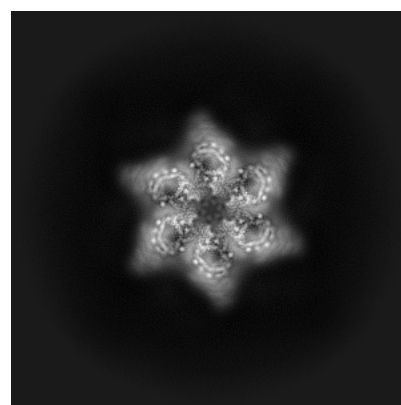
6.1.1 Primary map



X



Y

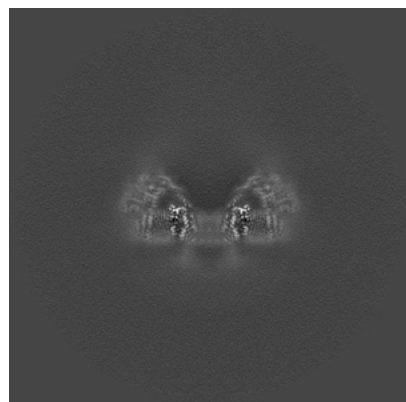


Z

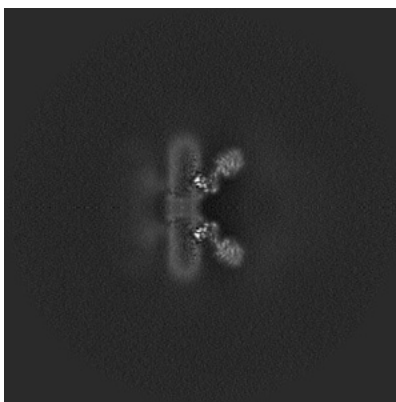
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

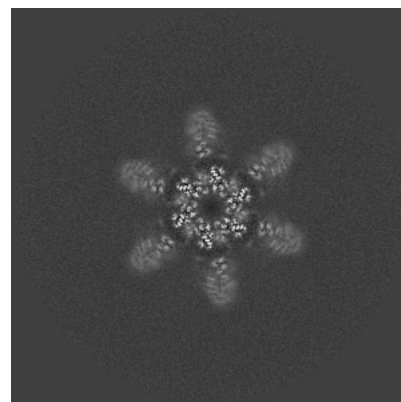
6.2.1 Primary map



X Index: 225



Y Index: 225

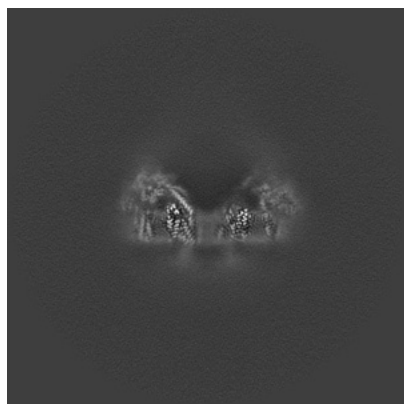


Z Index: 225

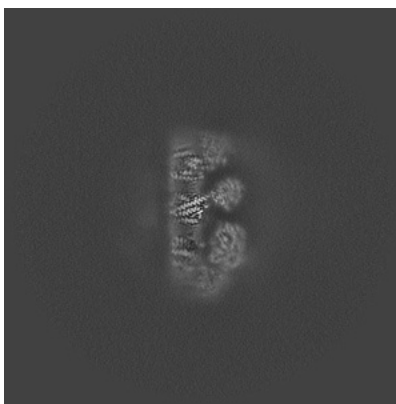
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

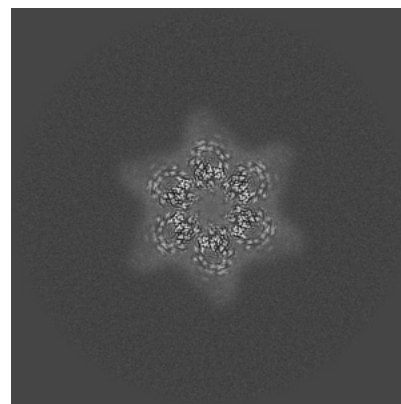
6.3.1 Primary map



X Index: 222



Y Index: 267



Z Index: 215

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 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

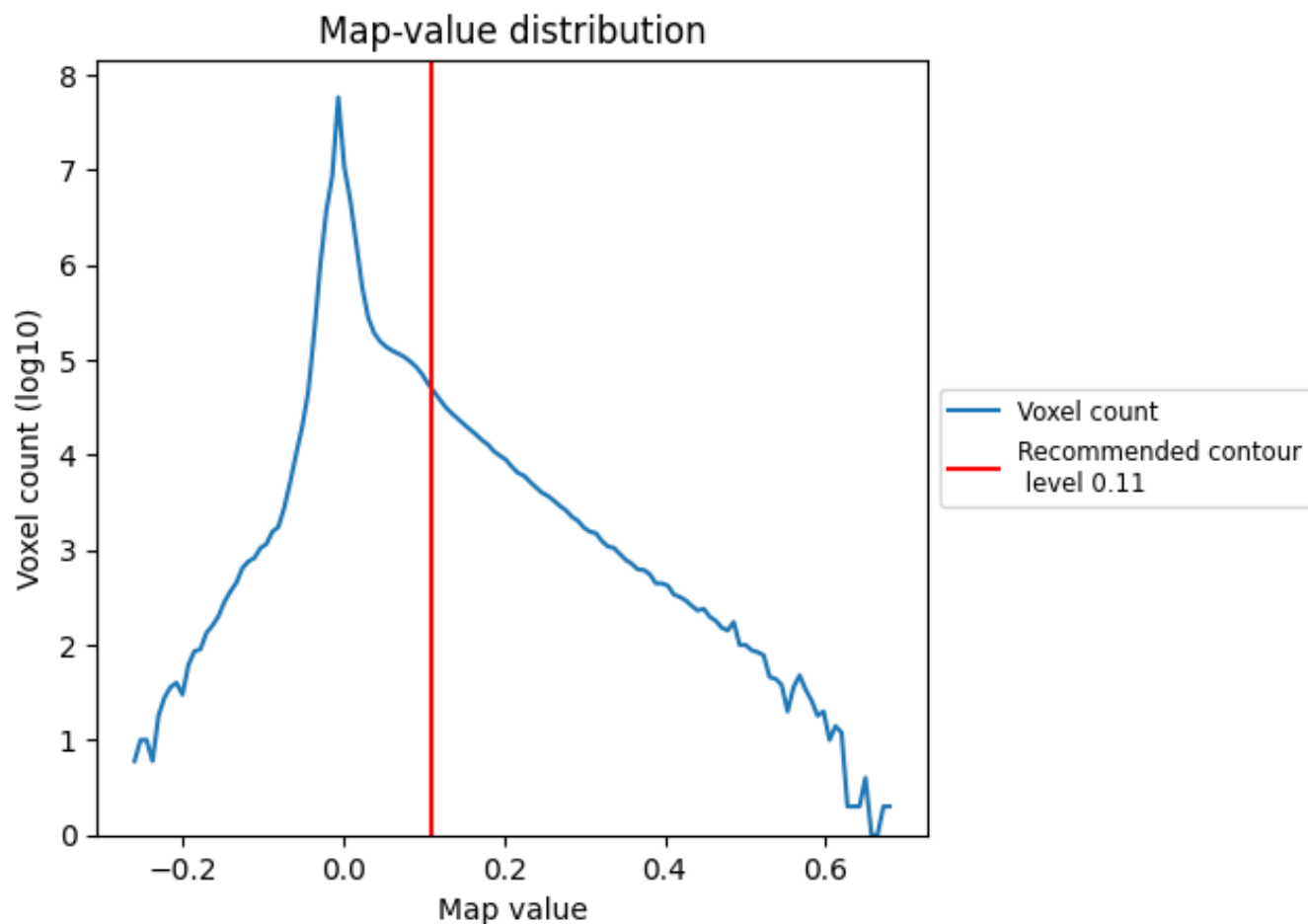
6.5 Mask visualisation

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

7 Map analysis [i](#)

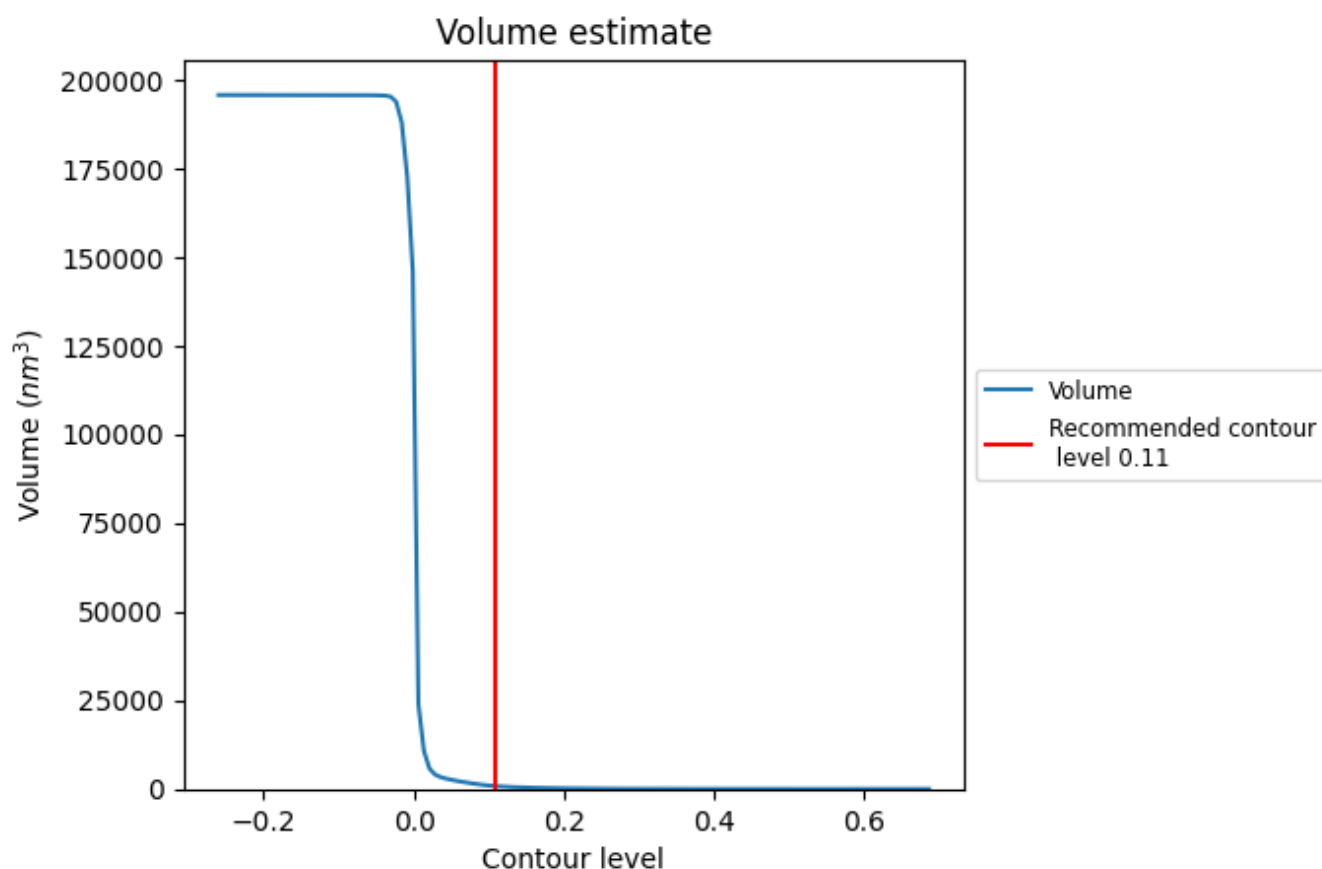
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

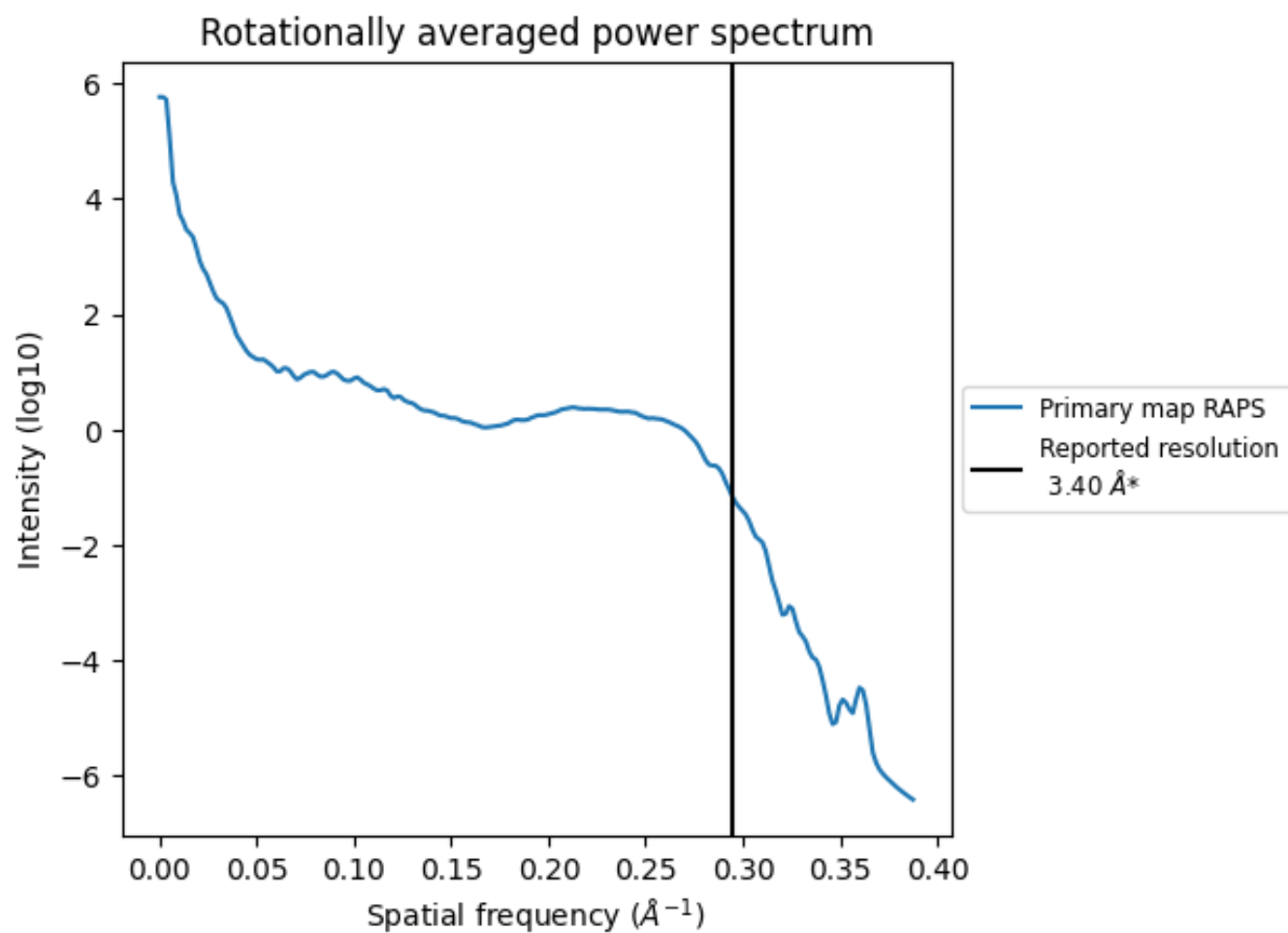
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 786 nm^3 ; this corresponds to an approximate mass of 710 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

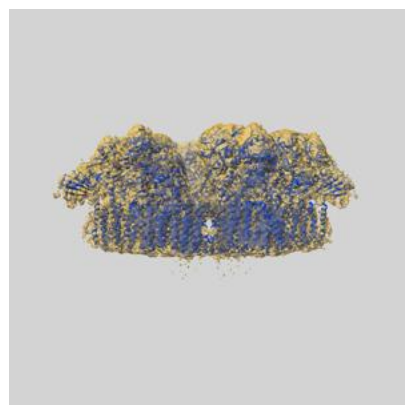
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

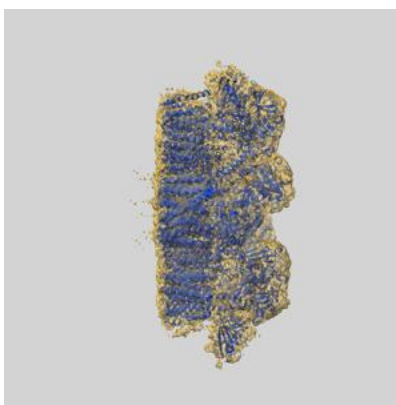
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12105 and PDB model 7B9S. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

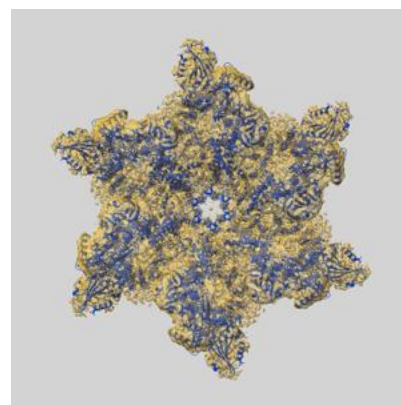
9.1 Map-model overlay [i](#)



X



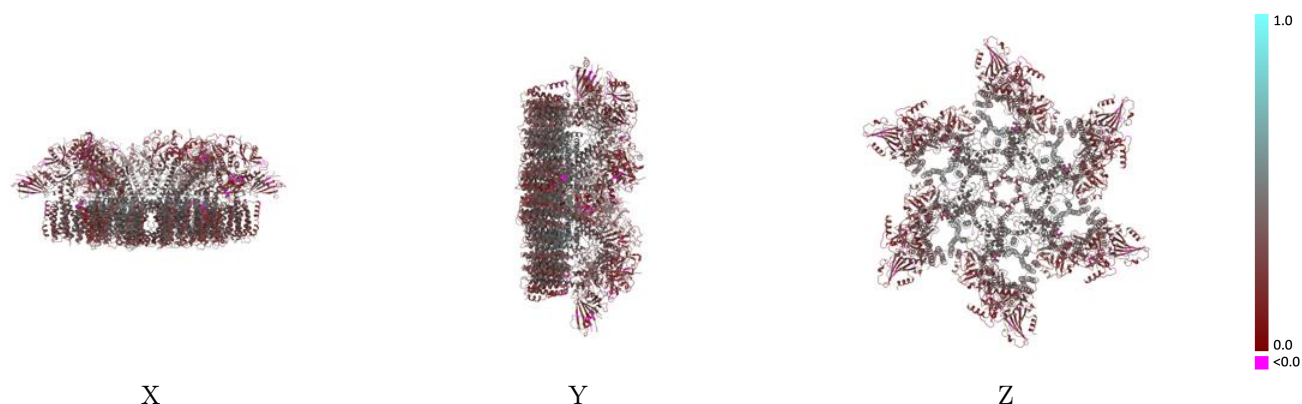
Y



Z

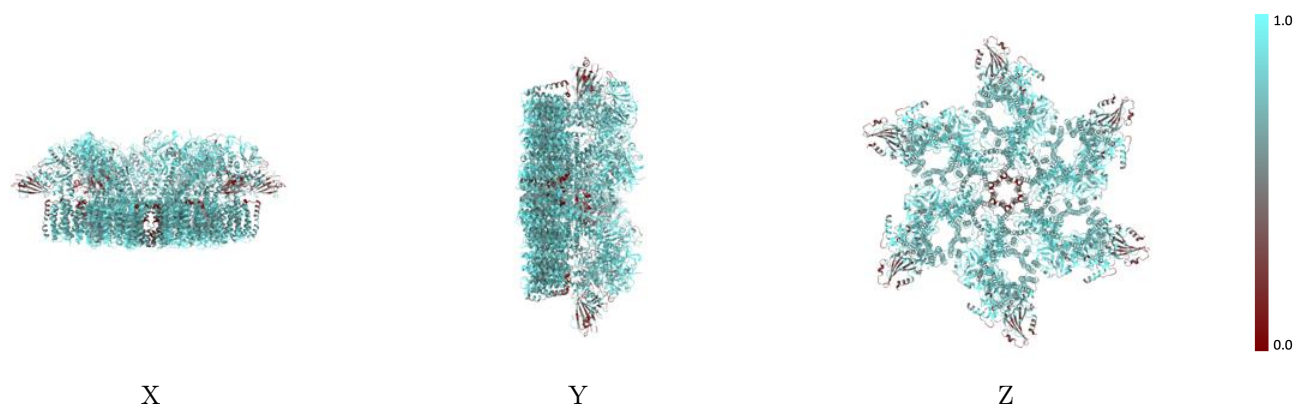
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



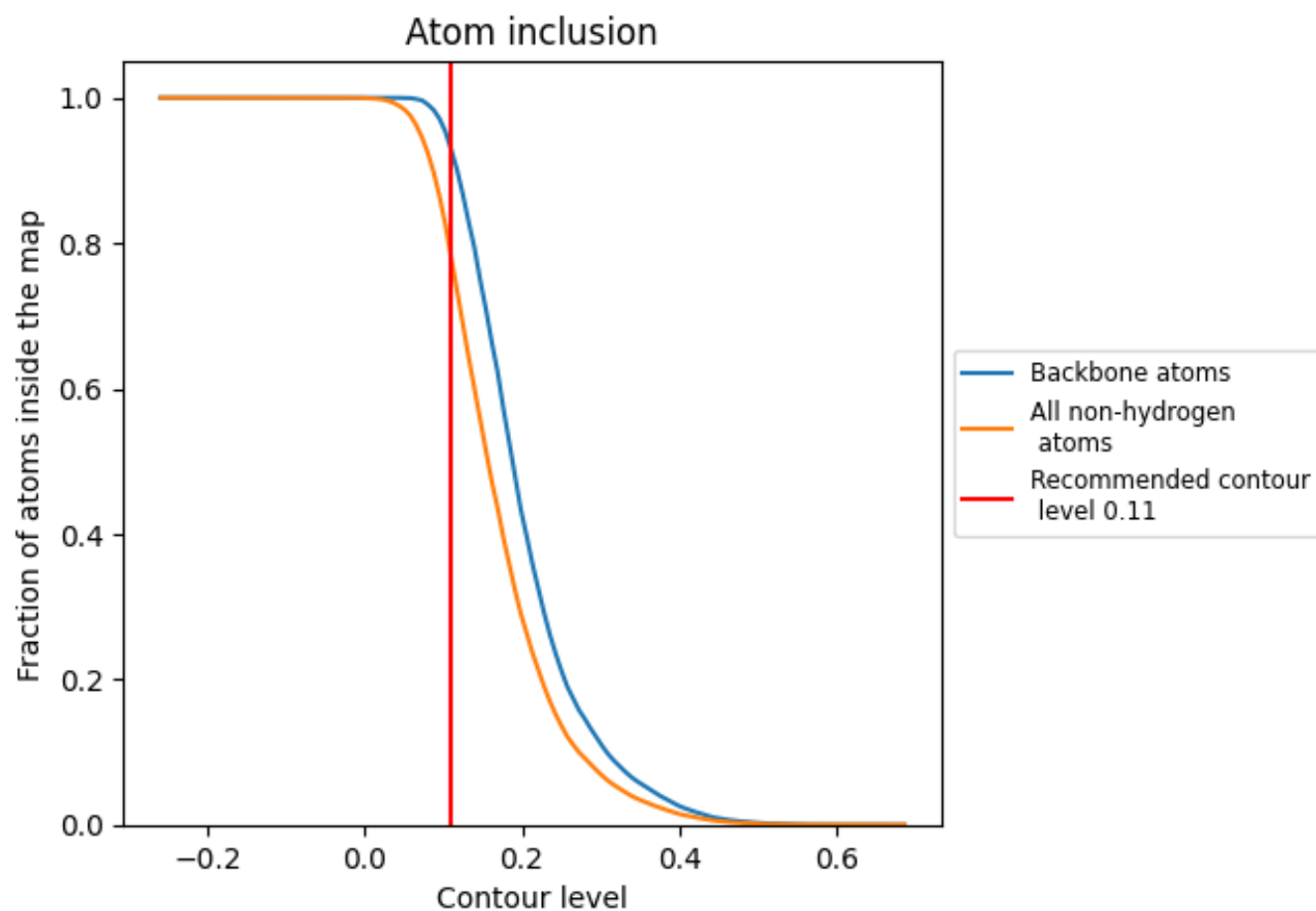
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.11).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 78% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7800	 0.3320
1	 0.8848	 0.4460
2	 0.8080	 0.3130
3	 0.8246	 0.3550
4	 0.5695	 0.2620
5	 0.7751	 0.3340
A	 0.9000	 0.4490
B	 0.8696	 0.4440
C	 0.8074	 0.3130
D	 0.8240	 0.3570
E	 0.5663	 0.2660
F	 0.8057	 0.3140
G	 0.8249	 0.3550
H	 0.5655	 0.2630
I	 0.7783	 0.3340
J	 0.8783	 0.4300
K	 0.8067	 0.3140
L	 0.8218	 0.3540
M	 0.5624	 0.2630
N	 0.7772	 0.3350
O	 0.8870	 0.4410
P	 0.8074	 0.3150
Q	 0.8240	 0.3590
R	 0.5655	 0.2640
S	 0.7727	 0.3350
T	 0.8739	 0.4340
V	 0.8041	 0.3140
W	 0.8226	 0.3550
X	 0.7733	 0.3340
Y	 0.5671	 0.2630
Z	 0.7789	 0.3350

