



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 09:05 PM UTC

PDB ID : 6PEM / pdb_00006pem
EMDB ID : EMD-20316
Title : Focussed refinement of InvGN0N1:SpaPQR:PrgHK from Salmonella SPI-1
injectisome NC-base
Authors : Hu, J.; Worrall, L.J.; Strynadka, N.C.J.
Deposited on : 2019-06-20
Resolution : 3.50 Å(reported)

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:

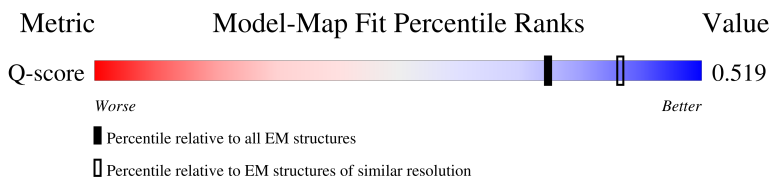
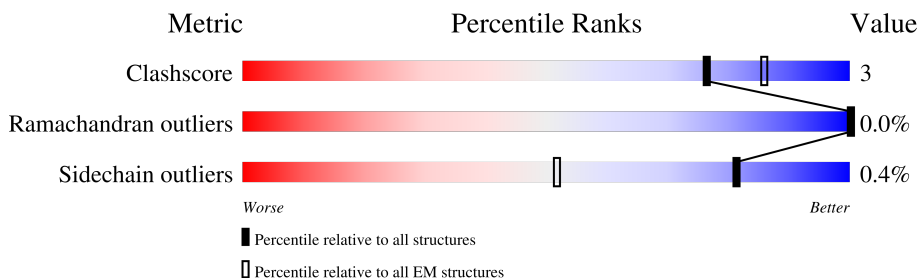
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	AA	252	
1	AB	252	
1	AC	252	
1	AD	252	

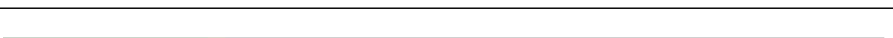
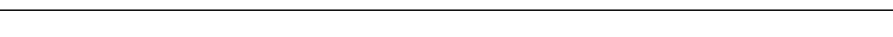
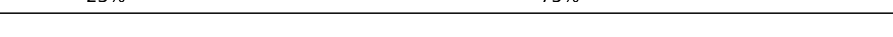
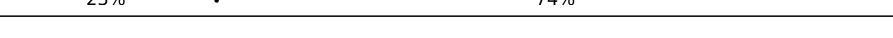
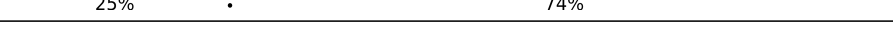
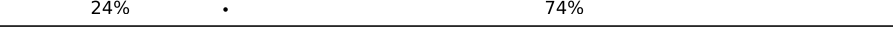
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AE	252	
1	AF	252	
1	AG	252	
1	AH	252	
1	AI	252	
1	AJ	252	
1	AK	252	
1	AL	252	
1	o	252	
1	p	252	
1	q	252	
1	r	252	
1	s	252	
1	t	252	
1	u	252	
1	v	252	
1	w	252	
1	x	252	
1	y	252	
1	z	252	
2	0	224	
2	1	224	
2	2	224	
2	3	224	
2	4	224	

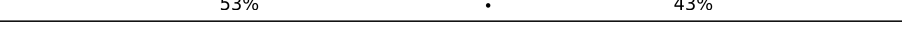
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	5	263	
4	6	86	
4	7	86	
4	8	86	
4	9	86	
5	A	562	
5	B	562	
5	C	562	
5	D	562	
5	F	562	
5	G	562	
5	H	562	
5	I	562	
5	J	562	
5	K	562	
5	L	562	
5	M	562	
5	N	562	
5	O	562	
5	P	562	
5	Q	562	
6	E	392	
6	R	392	
6	S	392	
6	T	392	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	U	392	 51%6%44%
6	V	392	 53%.43%
6	W	392	 53%.43%
6	X	392	 50%7%44%
6	Y	392	 50%7%43%
6	Z	392	 53%.43%
6	a	392	 52%.44%
6	b	392	 53%.43%
6	c	392	 49%7%43%
6	d	392	 51%6%44%
6	e	392	 54%.43%
6	f	392	 53%.43%
6	g	392	 52%.44%
6	h	392	 53%.43%
6	i	392	 54%.43%
6	j	392	 52%.44%
6	k	392	 53%.43%
6	l	392	 51%6%43%
6	m	392	 53%.44%
6	n	392	 51%5%43%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 108033 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 Lipoprotein PrgK.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AB	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AC	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AD	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AE	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AF	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AG	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AH	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AI	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AL	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	o	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	p	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	q	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	r	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	s	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	t	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	u	184	Total 1431	C 901	N 250	O 277	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	v	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	w	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	x	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	y	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	z	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AJ	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AK	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		

- Molecule 2 is a protein called Surface presentation of antigens protein SpaP.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	189	Total	C	N	O	S	0	0
			1468	982	219	256	11		
2	1	189	Total	C	N	O	S	0	0
			1475	988	220	256	11		
2	2	187	Total	C	N	O	S	0	0
			1464	981	219	253	11		
2	3	194	Total	C	N	O	S	0	0
			1520	1016	227	266	11		
2	4	211	Total	C	N	O	S	1	0
			1672	1108	255	298	11		

- Molecule 3 is a protein called Surface presentation of antigens protein SpaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	228	Total	C	N	O	S	0	0
			1718	1136	276	293	13		

- Molecule 4 is a protein called Surface presentation of antigens protein SpaQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	53	Total	C	N	O	S	0	0
			405	276	61	67	1		
4	7	84	Total	C	N	O	S	0	0
			644	436	97	109	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	84	Total	C	N	O	S	0	0
			644	436	97	109	2		
4	9	84	Total	C	N	O	S	0	0
			647	438	97	109	3		

- Molecule 5 is a protein called Protein InvG.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
5	B	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
5	C	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
5	D	144	Total	C	N	O	S	0	0
			1146	736	195	209	6		
5	F	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
5	G	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
5	H	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
5	I	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
5	J	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
5	K	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
5	L	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
5	M	144	Total	C	N	O	S	0	0
			1146	736	195	209	6		
5	N	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
5	O	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
5	P	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
5	Q	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		

- Molecule 6 is a protein called Protein PrgH.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
6	R	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
6	S	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
6	T	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
6	U	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
6	V	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
6	W	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
6	X	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
6	Y	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
6	Z	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
6	a	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
6	b	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
6	c	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
6	d	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
6	e	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
6	f	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
6	g	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
6	h	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
6	i	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
6	j	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
6	k	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
6	l	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		

Continued on next page...

Continued from previous page...

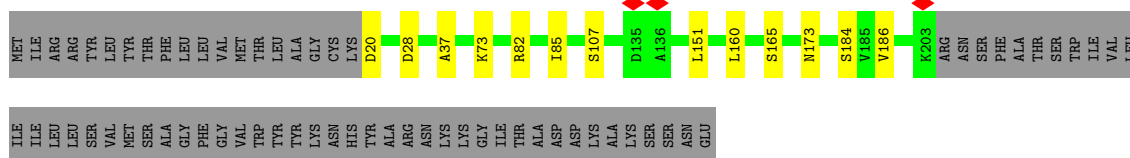
Mol	Chain	Residues	Atoms					AltConf	Trace
6	m	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
6	n	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		

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.

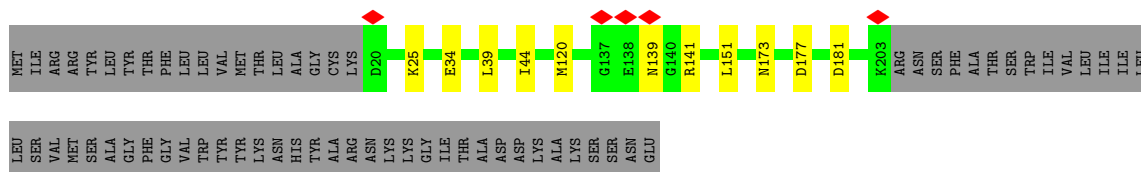
- Molecule 1: Lipoprotein PrgK

Chain AA: 



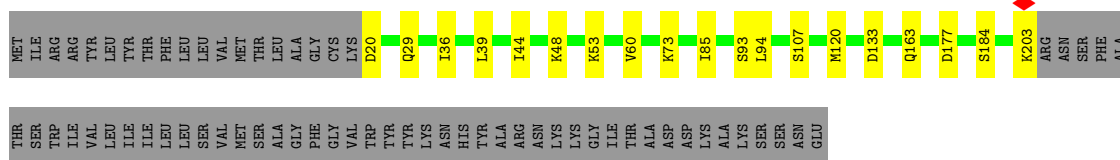
- Molecule 1: Lipoprotein PrgK

Chain AB: 



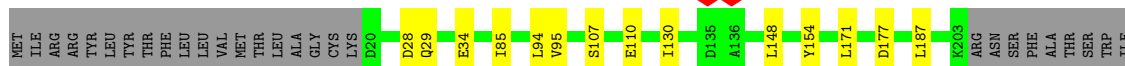
- Molecule 1: Lipoprotein PrgK

Chain AC: 



- Molecule 1: Lipoprotein PrgK

Chain AD: 



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

• Molecule 1: Lipoprotein PrgK

Chain AE:



MET
ILE
ARG
ALA
TYR
LEU
TYR
THR
PHE
LEU
LEU
VAL
MET
THR
ALA
ALA
GLY
CYS
LYS
D20
A37
S107
E110
Q111
I130
G137
L160
K168
N173
Y180
S184
K203
ARG
ASN
PHE
ALA
THR
SER
TRP
ILE
VAL
LEU
ILE
LEU
SER
VAL

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

• Molecule 1: Lipoprotein PrgK

Chain AF:



MET
ILE
ARG
ALA
TYR
LEU
TYR
THR
PHE
LEU
LEU
VAL
MET
THR
ALA
ALA
GLY
CYS
LYS
D20
E34
V35
I36
K48
V69
P78
P79
R112
N173
S174
S184
D192
K203
ARG
ASN
PHE
ALA
THR
SER
TRP
ILE
VAL
LEU
ILE
LEU
SER
VAL
MET

SER
ALA
GLY
PHE
GLY
VAL
TRP
TYR
TYR
LYS
ASN
HIS
TYR
ALA
ALA
ARG
ASN
LYS
GLY
ILE
THR
ASP
ASP
LYS
LYS
SER
SER
ASN
GLU

• Molecule 1: Lipoprotein PrgK

Chain AG:



MET
ILE
ARG
ALA
TYR
LEU
TYR
THR
PHE
LEU
LEU
VAL
MET
THR
ALA
ALA
GLY
CYS
LYS
D20
D28
E34
S51
I85
S93
L94
V95
R99
S107
I134
I164
N173
D177
S184
V185
K203
ARG
ASN
PHE
ALA
THR
SER
TRP
ILE
VAL
LEU
ILE
ILE

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

• Molecule 1: Lipoprotein PrgK

Chain AH:



MET
ILE
ARG
ALA
TYR
LEU
TYR
THR
PHE
LEU
LEU
VAL
MET
THR
ALA
ALA
GLY
CYS
LYS
D20
D28
Q29
E34
A37
V38
L39
I44
I85
D92
S93
L94
S107
V123
D135
A136
Y154
N173
D177
S184
P201
V202
K203
ARG
ASN
PHE

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

• Molecule 1: Lipoprotein PrgK

Chain AI:



MET
ILE
ARG
ALA
TYR
LEU
TYR
THR
PHE
LEU
LEU
VAL
MET
THR
ALA
ALA
GLY
CYS
LYS
D20
E34
L39
I44
V60
V69
K73
P78
P79
I85
R99
S107
D133
I134
D135
A136
G137
E138
H147
R169
D177
Y180
S184
K203

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

• Molecule 1: Lipoprotein PrgK

Chain s:  68% 5% 27%

MET
ILE
ARG
VAL
MET
LEU
TYR
THR
PHE
GLY
VAL
LEU
SER
MET
VAL
THR
LYS
ALA
GLY
HIS
TYR
CYS
LYS
D20
K21
L39
I44
V60
A61
E62
V69
P78
P79
A135
G137
N173
D177
S184
A197
K203
ARG
ASN
SER
PHE
ALA
THR
SER
TRP
ILE
VAL
LEU
ILE
ILE

• Molecule 1: Lipoprotein PrgK

Chain t:  67% 6% 27%

MET
ILE
ARG
VAL
TYR
TYR
PHE
THR
PHE
GLY
VAL
LEU
SER
MET
VAL
THR
LYS
ALA
GLY
HIS
CYS
LYS
D20
L24
K25
G26
L27
A37
K53
L94
V95
L117
D135
A150
R156
Q163
N173
D177
S184
V185
R190
K203
ARG
ASN
SER
PHE
ALA
THR
SER

• Molecule 1: Lipoprotein PrgK

Chain u:  63% 10% 27%

MET
ILE
ARG
VAL
TYR
TYR
PHE
THR
PHE
GLY
VAL
LEU
SER
MET
VAL
THR
LYS
ALA
GLY
HIS
CYS
LYS
D20
Q29
N33
M41
K48
I85
L94
V95
R99
S107
E110
I130
S131
Y132
D133
I134
D135
A136
N139
G140
R141
L148
Q163
I164
S165
K168
R169
E170
L171
K172
M173
D177
K203
ARG
ASN
SER
PHE
ALA
THR
SER
TRP
ILE
VAL
LEU
SER
MET
VAL
THR
LYS
ALA
GLY
HIS
TYR
CYS
LYS
D20
Q29
N33
M41
K48
I85
L94
V95
R99
S107
E110
I130
S131
Y132
D133
I134
D135
A136
N139
G140
R141
L148
Q163
I164
S165
K168
R169

• Molecule 1: Lipoprotein PrgK

Chain v:  67% 6% 27%

MET
ILE
ARG
VAL
TYR
TYR
PHE
THR
PHE
GLY
VAL
LEU
SER
MET
VAL
THR
LYS
ALA
GLY
HIS
CYS
LYS
D20
K21
D22
K25
I36
N43
K48
V60
T66
R99
I134
G137
E138
N139
G140
R141
V146
D177
V178
S184
K203
ARG
ASN
SER
PHE
ALA
THR
SER

• Molecule 1: Lipoprotein PrgK

Chain w:  68% 5% 27%

MET
ILE
ARG
VAL
TYR
TYR
PHE
THR
PHE
GLY
VAL
LEU
SER
MET
VAL
THR
LYS
ALA
GLY
HIS
CYS
LYS
D20
K25
D28
Q31
D50
S51
S52
K53
L54
G55
K73
D135
L160
Q163
I164
S165
D166
M173
D177
S184
A197
K203
ARG
ASN
SER
PHE
ALA
THR

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

• Molecule 1: Lipoprotein PrgK

Chain x:



MET ILE ARG ARG VAL TYR TRP THR PHE LEU LEU VAL MET MET THR ALA GLY PHE LEU LEU VAL MET MET THR TYR TYR LYS ALA GLY ASN CYS TYR LYS D20 D20 Q31 Q31 E34 E34 P78 P78 P79 P79 L117 L117 V123 V123 A136 A136 V146 V146 L151 L151 R169 R169 N173 N173 D177 D177 V178 V178 D179 D179 Y180 Y180 K203 K203 ARG ASN SER PHE THR THR SER TRP ILE VAL ILE

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

• Molecule 1: Lipoprotein PrgK

Chain y:



MET ILE ARG ARG TYR TRP THR PHE LEU LEU VAL MET MET THR ALA GLY PHE LEU LEU VAL MET MET THR TYR TYR LYS ALA TYR CYS TYR LYS D20 D20 K21 K21 D22 D22 L23 L23 M43 M43 E62 E62 A68 A68 P78 P78 P79 P79 M120 M120 D135 D135 E138 E138 M139 M139 R141 R141 K172 K172 V178 V178 D179 D179 S184 S184 K203 K203 ARG ASN SER PHE THR THR SER TRP TRP ILE VAL

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

• Molecule 1: Lipoprotein PrgK

Chain z:



MET ILE ARG ARG TYR TRP THR PHE LEU LEU VAL MET MET THR ALA GLY PHE LEU LEU VAL MET MET THR TYR TYR LYS ALA TYR CYS TYR LYS D20 D20 K21 K21 L39 L39 I44 I44 E62 E62 V69 V69 N173 N173 S174 S174 D177 D177 Y180 Y180 S184 S184 K203 K203 ARG ASN SER PHE ALA THR THR TRP TRP ILE VAL LEU ILE ILE LEU LEU LEU SER LEU VAL MET MET ALA

GLY PHE GLY VAL TYR TRP TYR LYS ASN HIS LEU LEU VAL MET MET THR ALA GLY PHE LEU LEU VAL MET MET THR TYR TYR LYS ALA TYR CYS TYR LYS D20 D20 K21 K21 L39 L39 I44 I44 E62 E62 V69 V69 N173 N173 S174 S174 D177 D177 Y180 Y180 S184 S184 K203 K203 ARG ASN SER PHE ALA THR THR TRP TRP ILE VAL LEU ILE ILE LEU LEU LEU SER LEU VAL MET MET ALA

• Molecule 1: Lipoprotein PrgK

Chain AJ:



MET ILE ARG ARG TYR TRP THR PHE LEU LEU VAL MET MET THR ALA GLY PHE LEU LEU VAL MET MET THR TYR TYR LYS ALA TYR CYS TYR LYS D20 D20 I36 I36 A37 A37 V38 V38 L39 L39 I44 I44 K48 K48 I49 I49 D50 D50 S51 S51 K73 K73 R99 R99 K102 K102 E110 E110 Q111 Q111 R112 R112 I134 I134 G137 G137 E138 E138 Q163 Q163 I164 I164 S165 S165 N173 N173 D177 D177 S184 S184 V185 V185 K203 K203

ARG ASN SER PHE ALA TYR TRP THR PHE LEU LEU VAL MET MET THR ALA GLY PHE LEU LEU VAL MET MET THR TYR TYR LYS ALA TYR CYS TYR LYS D20 D20 I36 I36 A37 A37 V38 V38 L39 L39 I44 I44 K48 K48 I49 I49 D50 D50 S51 S51 K73 K73 R99 R99 K102 K102 E110 E110 Q111 Q111 R112 R112 I134 I134 G137 G137 E138 E138 Q163 Q163 I164 I164 S165 S165 N173 N173 D177 D177 S184 S184 V185 V185 K203 K203

• Molecule 1: Lipoprotein PrgK

Chain AK:

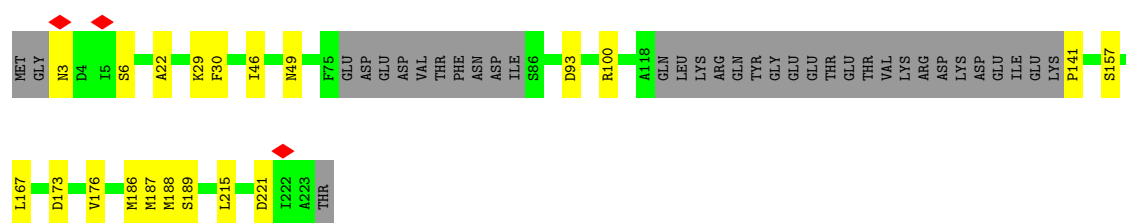


MET ILE ARG ARG TYR TRP THR PHE LEU LEU VAL MET MET THR ALA GLY PHE LEU LEU VAL MET MET THR TYR TYR LYS ALA TYR CYS TYR LYS D20 D20 M43 M43 V69 V69 E110 E110 I130 I130 D135 D135 A136 A136 L150 L150 N173 N173 S184 S184 L187 L187 K203 K203 ARG ASN SER PHE THR THR SER TRP TRP ILE VAL LEU LEU ILE ILE LEU LEU SER SER VAL MET MET SER

ALA
GLY
PHE
GLY
VAL
TRP
TYR
LYS
ASN
HIS
TYR
VAL
ARG
ASN
LYS
LYS
GLY
ILE
THR
ALA
ASP
ASP
LYS
ALA
LYS
SER
SER
ASN
GLU

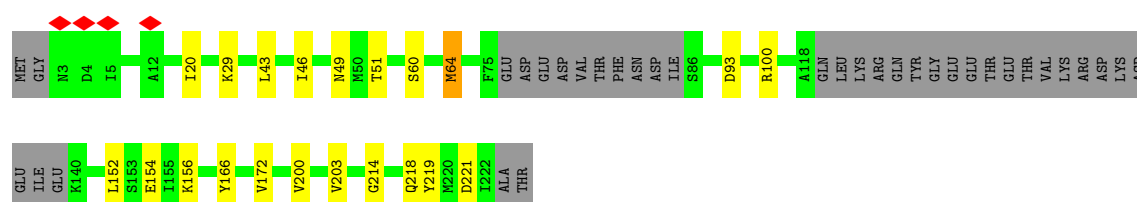
• Molecule 2: Surface presentation of antigens protein SpaP

Chain 0: 



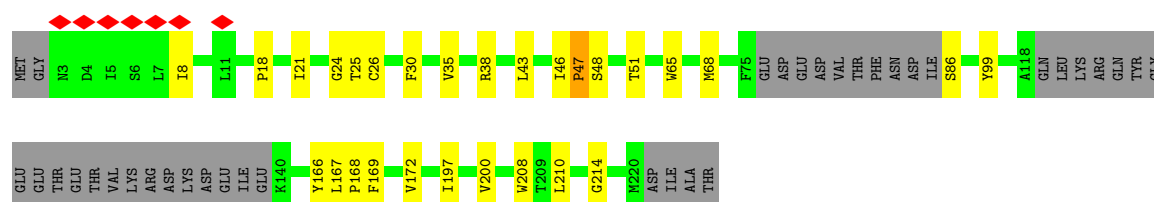
• Molecule 2: Surface presentation of antigens protein SpaP

Chain 1: 



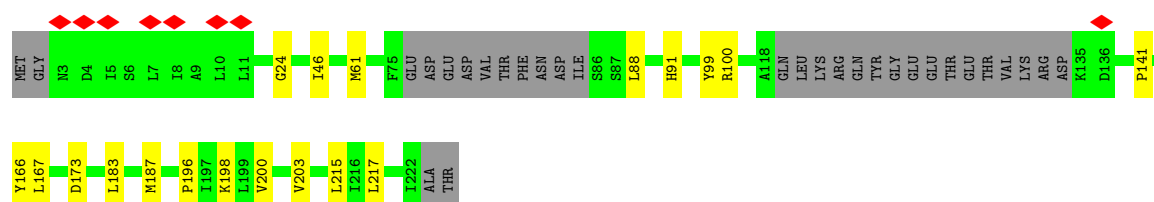
• Molecule 2: Surface presentation of antigens protein SpaP

Chain 2: 



• Molecule 2: Surface presentation of antigens protein SpaP

Chain 3: 

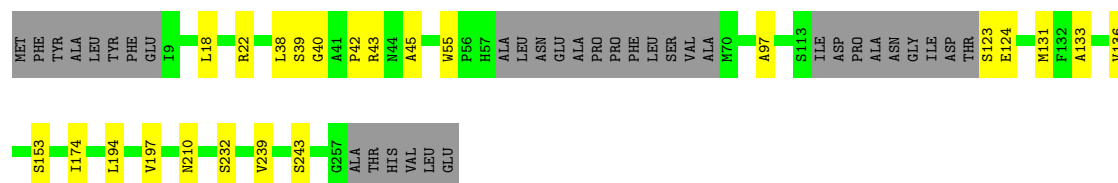
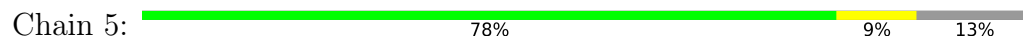


• Molecule 2: Surface presentation of antigens protein SpaP

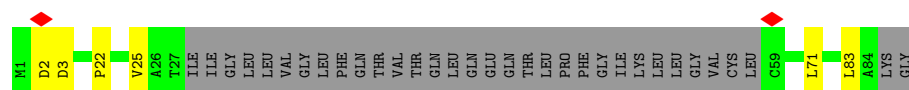
Chain 4: 



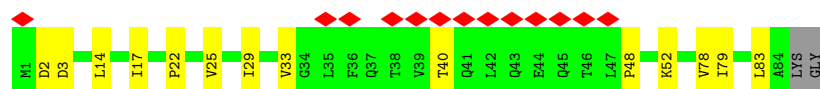
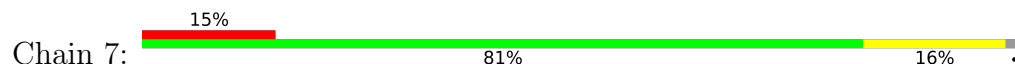
- Molecule 3: Surface presentation of antigens protein SpaR



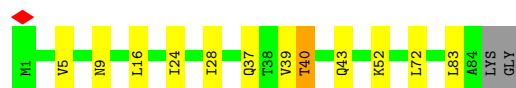
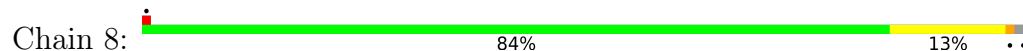
- Molecule 4: Surface presentation of antigens protein SpaQ



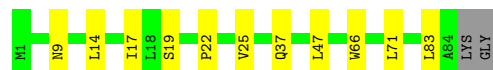
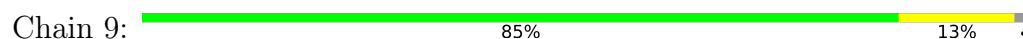
- Molecule 4: Surface presentation of antigens protein SpaQ



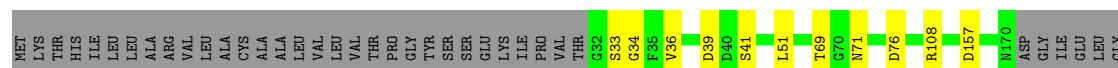
- Molecule 4: Surface presentation of antigens protein SpaQ



- Molecule 4: Surface presentation of antigens protein SpaQ



- Molecule 5: Protein InvG



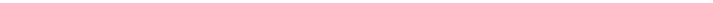
[illegible]

- Molecule 5: Protein InvG

Chain B: 23% 1% 74%

[illegible]

- Molecule 5: Protein InvG

Chain C:  23% . 75%

[illegible]

- Molecule 5: Protein InvG

[illegible]

- Molecule 5: Protein InvG

[illegible]

[illegible]

- Molecule 5: Protein InvG

[illegible]

- Molecule 5: Protein InvG

[illegible]

[illegible]

- Molecule 5: Protein InvG

[illegible]

- Molecule 5: Protein InvG

[illegible]

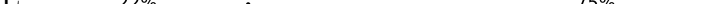
[illegible]

- Molecule 5: Protein InvG

Chain K: 23% . 74%

[illegible]

- Molecule 5: Protein InvG

Chain L:  22% 1% 75%

[illegible]



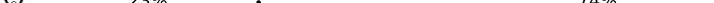
- Molecule 5: Protein InvG

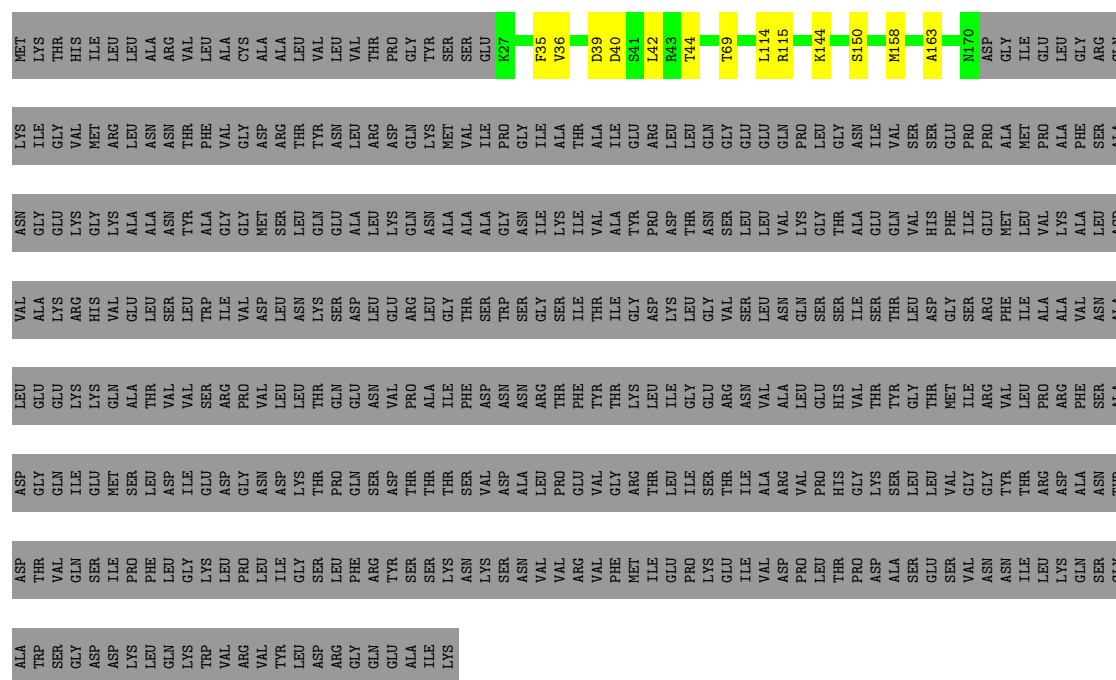
[illegible]

- Molecule 5: Protein InvG

[illegible]

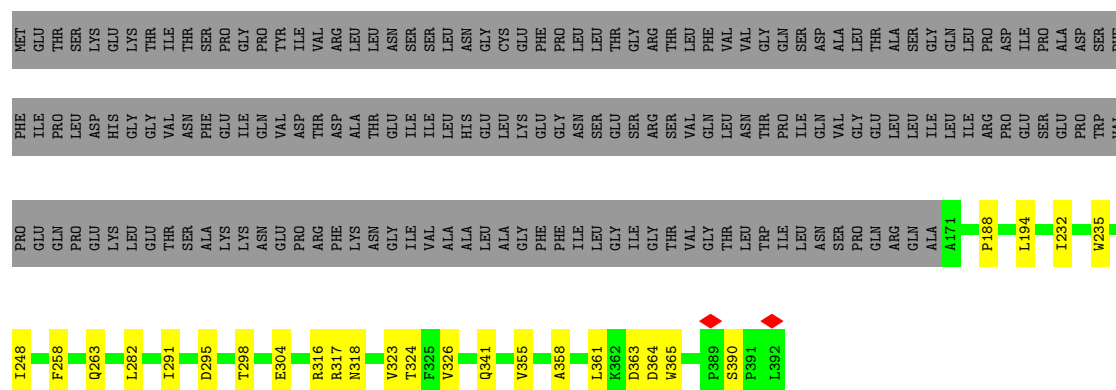
- Molecule 5: Protein InvG

Chain Q:  23% . 74%

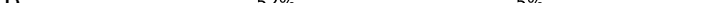


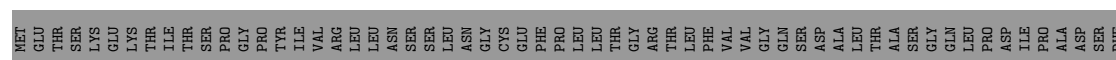
- Molecule 6: Protein PrgH

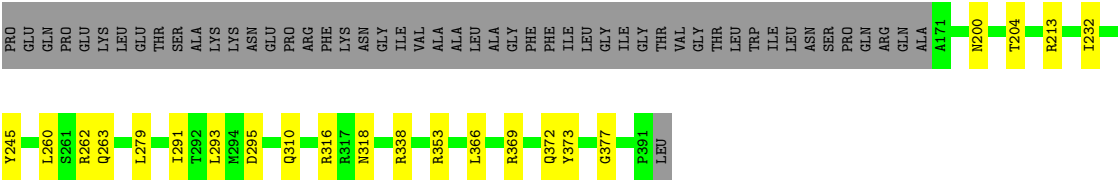
Chain E: 50% 7% 43%



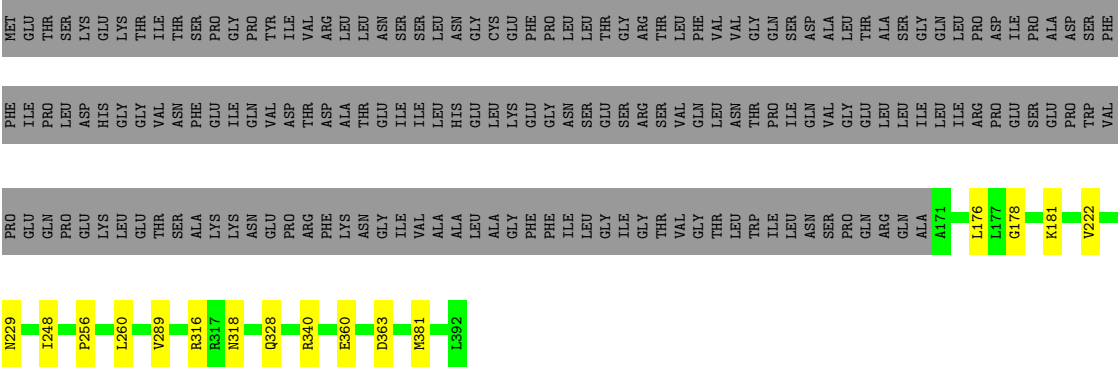
- Molecule 6: Protein PrgH

Chain R:  52% 5% 44%

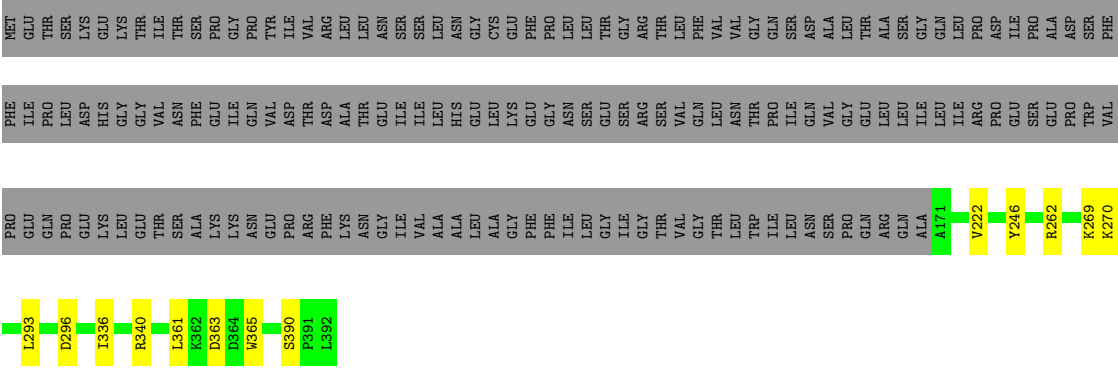




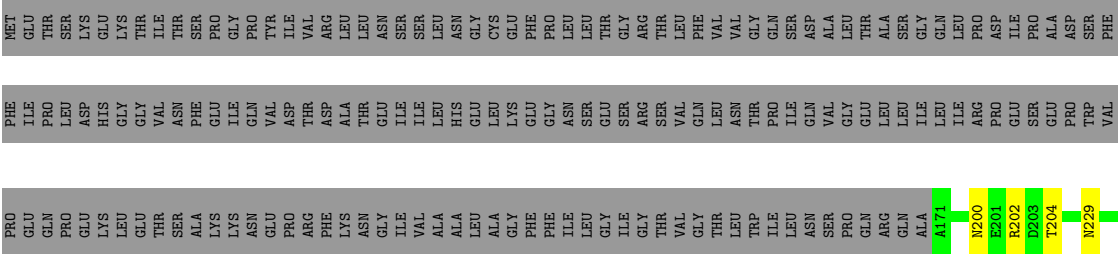
• Molecule 6: Protein PrgH



• Molecule 6: Protein PrgH

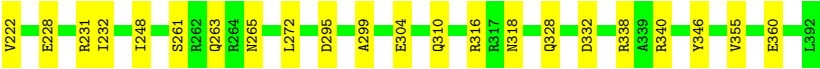
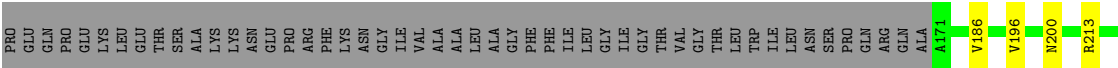
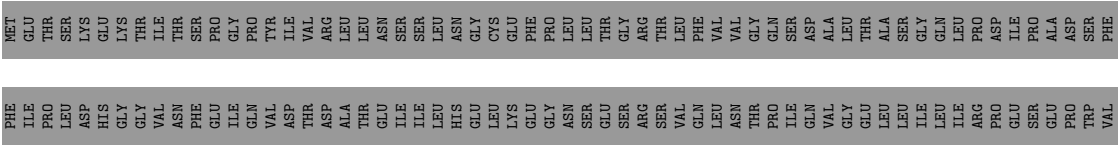


• Molecule 6: Protein PrgH

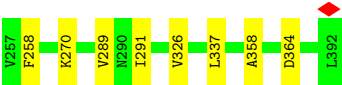
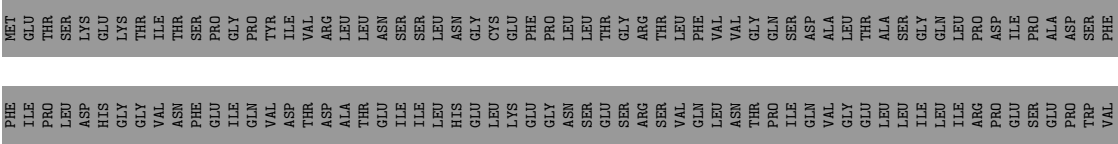




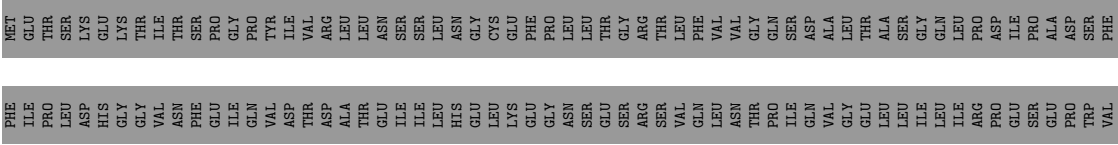
• Molecule 6: Protein PrgH



• Molecule 6: Protein PrgH



• Molecule 6: Protein PrgH



• Molecule 6: Protein PrgH

43%

F258 V274 K278 I291 R317 T324 V355 D363 L366 R369 K380 L392

43%

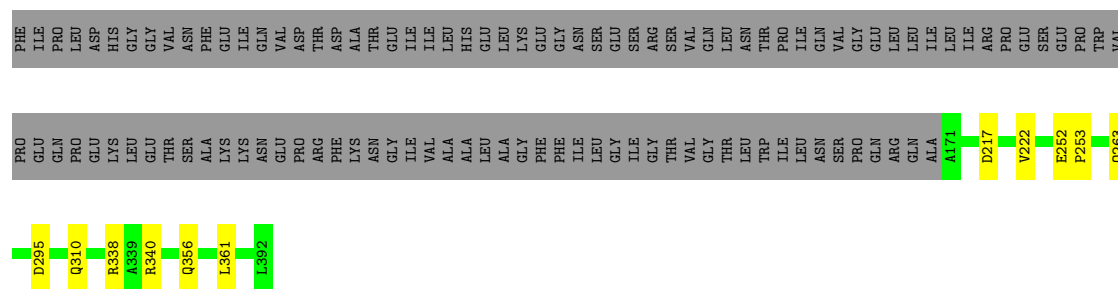
E227	E228	R231	L236	P256	V257	F258	R262	V274	K278	Y285	A286	V289	A290	I291	D295	A299	E304	R316	Y346	L361	K362	D363	D364	W365	A375	S390	F391	L392
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

44%

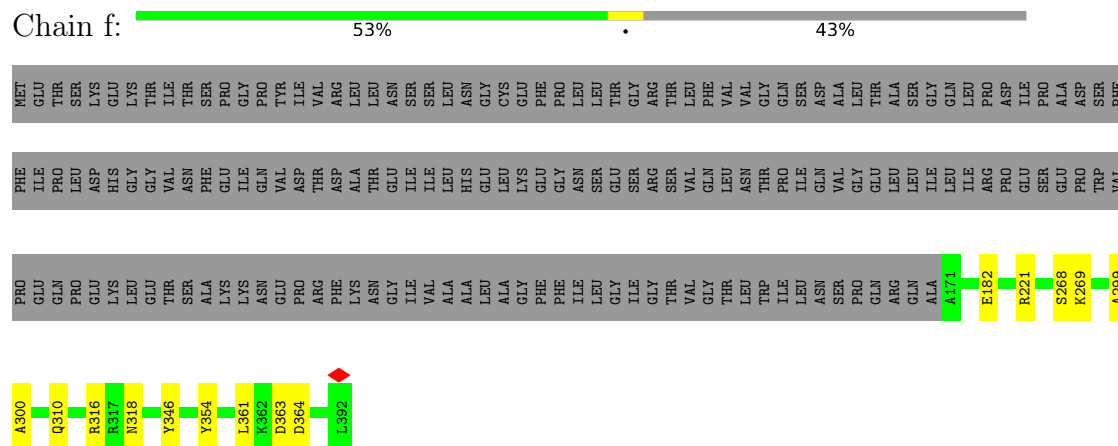
R247	S261	L282	V297	E304	R316	L337	Y346	D363	L366	K380	P391
R262	Q263		T298		R317		Y347	D364			LEU
			A299		N318		R348	W365			

43%

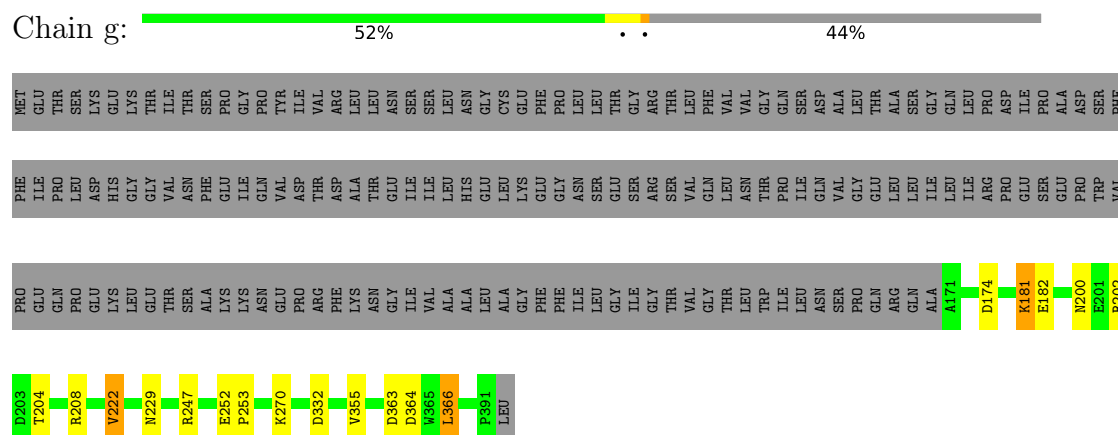
MET	GLU	THR	SER	LYS	GLU	LYS	THR	ILE	THR	PRO	SER	PRO	GLY	TYR	VAL	ARG	LEU	LEU	ASN	CYS	PHE	PRO	LEU	LEU	THR	GLY	THR	ARG	LEU	PHE	VAL	VAL	GLN	ASP	ASP	ALA	LEU	LEU	THR	ALA	SER	GLY	GLN	LEU	LEU	ASP	PRO	ALA	ASP	SER	...
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----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



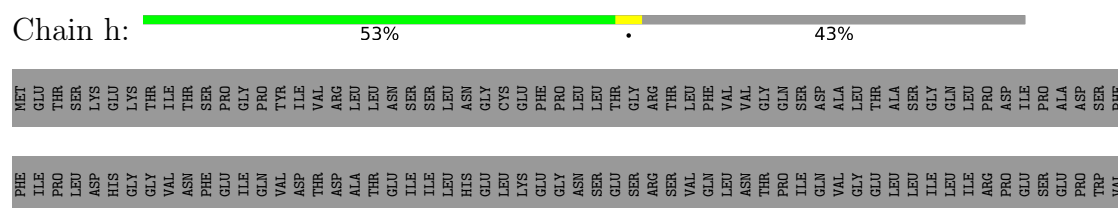
- Molecule 6: Protein PrgH

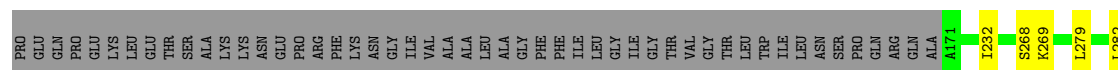


- Molecule 6: Protein PrgH



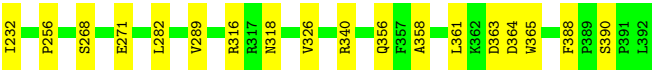
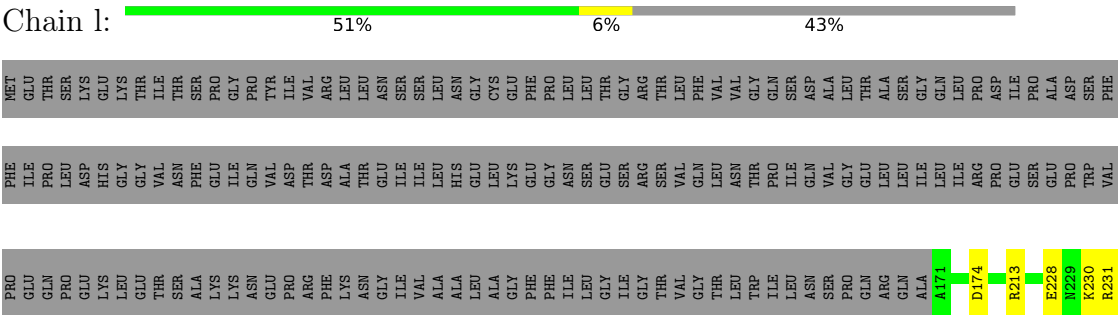
- Molecule 6: Protein PrgH



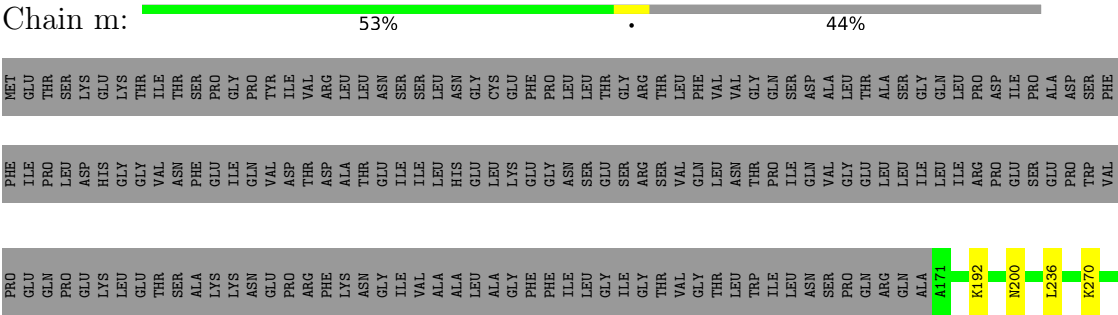




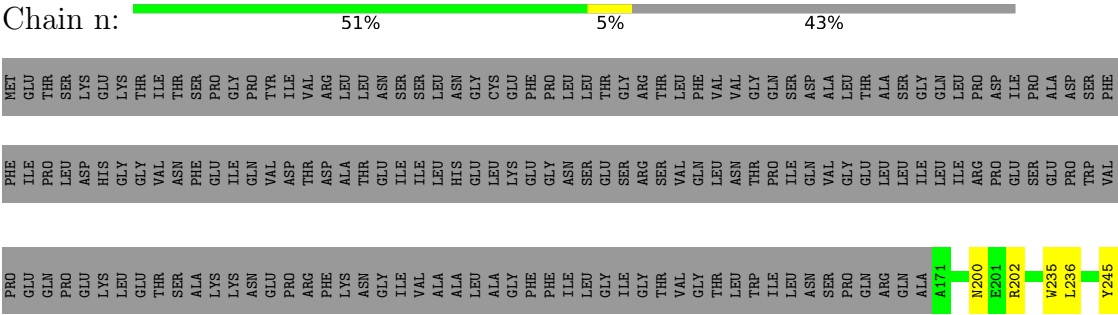
• Molecule 6: Protein PrgH



• Molecule 6: Protein PrgH



• Molecule 6: Protein PrgH



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	144097	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 ($e^-/\text{\AA}^2$)	51.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.267	Depositor
Minimum map value	-0.159	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	427.5, 427.5, 427.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.71, 1.71, 1.71	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.33	0/1458	0.52	0/1979
1	AB	0.34	0/1458	0.53	0/1979
1	AC	0.32	0/1458	0.52	0/1979
1	AD	0.33	0/1458	0.56	0/1979
1	AE	0.33	0/1458	0.54	0/1979
1	AF	0.34	0/1458	0.52	0/1979
1	AG	0.33	0/1458	0.51	0/1979
1	AH	0.32	0/1458	0.52	0/1979
1	AI	0.33	0/1458	0.54	0/1979
1	AJ	0.33	0/1458	0.53	0/1979
1	AK	0.33	0/1458	0.54	0/1979
1	AL	0.33	0/1458	0.54	0/1979
1	o	0.32	0/1458	0.53	0/1979
1	p	0.31	0/1458	0.50	0/1979
1	q	0.32	0/1458	0.50	0/1979
1	r	0.32	0/1458	0.54	0/1979
1	s	0.33	0/1458	0.53	0/1979
1	t	0.32	0/1458	0.56	0/1979
1	u	0.32	0/1458	0.55	0/1979
1	v	0.34	0/1458	0.55	0/1979
1	w	0.32	0/1458	0.52	0/1979
1	x	0.33	0/1458	0.52	0/1979
1	y	0.33	0/1458	0.52	0/1979
1	z	0.33	0/1458	0.55	0/1979
2	0	0.30	0/1501	0.70	0/2040
2	1	0.32	0/1508	0.69	0/2049
2	2	0.29	0/1497	0.69	1/2032 (0.0%)
2	3	0.27	0/1553	0.62	0/2107
2	4	0.30	0/1710	0.65	0/2318
3	5	0.31	0/1758	0.65	0/2402
4	6	0.22	0/414	0.60	0/565
4	7	0.29	0/657	0.75	1/897 (0.1%)
4	8	0.28	0/657	0.73	0/897
4	9	0.28	0/660	0.62	0/900

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	A	0.30	0/1131	0.53	0/1525
5	B	0.31	0/1181	0.53	0/1593
5	C	0.31	0/1131	0.54	0/1525
5	D	0.30	0/1170	0.53	0/1579
5	F	0.31	0/1131	0.54	0/1525
5	G	0.31	0/1181	0.57	0/1593
5	H	0.30	0/1131	0.52	0/1525
5	I	0.30	0/1181	0.54	0/1593
5	J	0.30	0/1131	0.55	0/1525
5	K	0.31	0/1181	0.58	0/1593
5	L	0.32	0/1131	0.58	0/1525
5	M	0.30	0/1170	0.52	0/1579
5	N	0.31	0/1131	0.53	0/1525
5	O	0.31	0/1181	0.56	0/1593
5	P	0.31	0/1131	0.53	0/1525
5	Q	0.31	0/1181	0.57	0/1593
6	E	0.30	0/1881	0.53	0/2541
6	R	0.30	0/1872	0.54	0/2530
6	S	0.31	0/1876	0.56	0/2536
6	T	0.31	0/1881	0.54	0/2541
6	U	0.30	0/1872	0.54	0/2530
6	V	0.30	0/1876	0.52	0/2536
6	W	0.29	0/1881	0.52	0/2541
6	X	0.29	0/1872	0.51	0/2530
6	Y	0.31	0/1876	0.56	0/2536
6	Z	0.30	0/1881	0.52	0/2541
6	a	0.30	0/1872	0.51	0/2530
6	b	0.32	0/1876	0.56	0/2536
6	c	0.31	0/1881	0.54	0/2541
6	d	0.30	0/1872	0.50	0/2530
6	e	0.31	0/1876	0.55	0/2536
6	f	0.31	0/1881	0.52	0/2541
6	g	0.30	0/1872	0.54	0/2530
6	h	0.31	0/1876	0.56	0/2536
6	i	0.30	0/1881	0.52	0/2541
6	j	0.30	0/1872	0.55	0/2530
6	k	0.31	0/1876	0.54	0/2536
6	l	0.31	0/1881	0.52	0/2541
6	m	0.30	0/1872	0.50	0/2530
6	n	0.31	0/1876	0.54	0/2536
All	All	0.31	0/110413	0.55	2/149475 (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
4	8	0	2
6	b	0	1
6	k	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	167	LEU	N-CA-C	5.23	121.38	109.81
4	7	40	THR	CA-CB-CG2	5.04	119.06	110.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	8	16	LEU	Mainchain
4	8	40	THR	Peptide
6	b	366	LEU	Peptide
6	k	366	LEU	Peptide

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	AA	1431	0	1424	12	0
1	AB	1431	0	1424	9	0
1	AC	1431	0	1424	14	0
1	AD	1431	0	1424	9	0
1	AE	1431	0	1424	8	0
1	AF	1431	0	1424	9	0
1	AG	1431	0	1424	10	0
1	AH	1431	0	1424	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AI	1431	0	1424	12	0
1	AJ	1431	0	1424	17	0
1	AK	1431	0	1424	7	0
1	AL	1431	0	1424	12	0
1	o	1431	0	1424	11	0
1	p	1431	0	1424	10	0
1	q	1431	0	1424	5	0
1	r	1431	0	1424	11	0
1	s	1431	0	1424	9	0
1	t	1431	0	1424	12	0
1	u	1431	0	1424	16	0
1	v	1431	0	1424	11	0
1	w	1431	0	1424	10	0
1	x	1431	0	1424	10	0
1	y	1431	0	1424	9	0
1	z	1431	0	1424	9	0
2	0	1468	0	1509	12	0
2	1	1475	0	1525	13	0
2	2	1464	0	1524	19	0
2	3	1520	0	1577	11	0
2	4	1672	0	1734	10	0
3	5	1718	0	1767	14	0
4	6	405	0	418	5	0
4	7	644	0	685	9	0
4	8	644	0	685	6	0
4	9	647	0	692	8	0
5	A	1108	0	1103	7	0
5	B	1154	0	1163	10	0
5	C	1108	0	1103	8	0
5	D	1146	0	1150	8	0
5	F	1108	0	1103	9	0
5	G	1154	0	1163	6	0
5	H	1108	0	1103	9	0
5	I	1154	0	1163	10	0
5	J	1108	0	1103	5	0
5	K	1154	0	1163	10	0
5	L	1108	0	1103	11	0
5	M	1146	0	1150	4	0
5	N	1108	0	1103	10	0
5	O	1154	0	1163	9	0
5	P	1108	0	1103	9	0
5	Q	1154	0	1163	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1836	0	1800	16	0
6	R	1827	0	1789	10	0
6	S	1831	0	1788	13	0
6	T	1836	0	1800	19	0
6	U	1827	0	1789	13	0
6	V	1831	0	1788	10	0
6	W	1836	0	1800	9	0
6	X	1827	0	1789	17	0
6	Y	1831	0	1788	16	0
6	Z	1836	0	1800	10	0
6	a	1827	0	1789	8	0
6	b	1831	0	1788	12	0
6	c	1836	0	1800	18	0
6	d	1827	0	1789	14	0
6	e	1831	0	1788	6	0
6	f	1836	0	1800	10	0
6	g	1827	0	1789	13	0
6	h	1831	0	1788	10	0
6	i	1836	0	1800	6	0
6	j	1827	0	1789	13	0
6	k	1831	0	1788	8	0
6	l	1836	0	1800	17	0
6	m	1827	0	1789	11	0
6	n	1831	0	1788	11	0
All	All	108033	0	107410	655	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 655 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)
5:A:39:ASP:H	5:A:69:THR:HG22	1.51	0.75
5:Q:39:ASP:H	5:Q:69:THR:HG22	1.52	0.74
5:P:39:ASP:H	5:P:69:THR:HG22	1.61	0.66
6:E:361:LEU:HD13	1:O:165:SER:HB2	1.77	0.66
2:O:187:MET:HE1	3:5:210:ASN:HA	1.77	0.65

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
1	AB	182/252 (72%)	178 (98%)	4 (2%)	0	100	100
1	AC	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	AD	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	AE	182/252 (72%)	177 (97%)	5 (3%)	0	100	100
1	AF	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	AG	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	AH	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	AI	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	AJ	182/252 (72%)	178 (98%)	4 (2%)	0	100	100
1	AK	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	AL	182/252 (72%)	177 (97%)	5 (3%)	0	100	100
1	o	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	p	182/252 (72%)	172 (94%)	10 (6%)	0	100	100
1	q	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	r	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
1	s	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	t	182/252 (72%)	179 (98%)	3 (2%)	0	100	100
1	u	182/252 (72%)	178 (98%)	4 (2%)	0	100	100
1	v	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	w	182/252 (72%)	177 (97%)	5 (3%)	0	100	100
1	x	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	y	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	z	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
2	0	183/224 (82%)	178 (97%)	4 (2%)	1 (0%)	24	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	183/224 (82%)	176 (96%)	6 (3%)	1 (0%)	24	57
2	2	181/224 (81%)	174 (96%)	6 (3%)	1 (1%)	21	54
2	3	188/224 (84%)	185 (98%)	3 (2%)	0	100	100
2	4	208/224 (93%)	199 (96%)	9 (4%)	0	100	100
3	5	222/263 (84%)	216 (97%)	6 (3%)	0	100	100
4	6	49/86 (57%)	48 (98%)	1 (2%)	0	100	100
4	7	82/86 (95%)	80 (98%)	2 (2%)	0	100	100
4	8	82/86 (95%)	79 (96%)	3 (4%)	0	100	100
4	9	82/86 (95%)	81 (99%)	1 (1%)	0	100	100
5	A	137/562 (24%)	136 (99%)	1 (1%)	0	100	100
5	B	143/562 (25%)	139 (97%)	4 (3%)	0	100	100
5	C	137/562 (24%)	134 (98%)	3 (2%)	0	100	100
5	D	142/562 (25%)	138 (97%)	4 (3%)	0	100	100
5	F	137/562 (24%)	135 (98%)	2 (2%)	0	100	100
5	G	143/562 (25%)	137 (96%)	6 (4%)	0	100	100
5	H	137/562 (24%)	134 (98%)	3 (2%)	0	100	100
5	I	143/562 (25%)	141 (99%)	2 (1%)	0	100	100
5	J	137/562 (24%)	135 (98%)	2 (2%)	0	100	100
5	K	143/562 (25%)	139 (97%)	4 (3%)	0	100	100
5	L	137/562 (24%)	135 (98%)	2 (2%)	0	100	100
5	M	142/562 (25%)	137 (96%)	5 (4%)	0	100	100
5	N	137/562 (24%)	134 (98%)	3 (2%)	0	100	100
5	O	143/562 (25%)	140 (98%)	3 (2%)	0	100	100
5	P	137/562 (24%)	136 (99%)	1 (1%)	0	100	100
5	Q	143/562 (25%)	139 (97%)	4 (3%)	0	100	100
6	E	220/392 (56%)	213 (97%)	7 (3%)	0	100	100
6	R	219/392 (56%)	213 (97%)	6 (3%)	0	100	100
6	S	220/392 (56%)	208 (94%)	12 (6%)	0	100	100
6	T	220/392 (56%)	210 (96%)	10 (4%)	0	100	100
6	U	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
6	V	220/392 (56%)	207 (94%)	13 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	W	220/392 (56%)	212 (96%)	8 (4%)	0	100	100
6	X	219/392 (56%)	213 (97%)	6 (3%)	0	100	100
6	Y	220/392 (56%)	205 (93%)	15 (7%)	0	100	100
6	Z	220/392 (56%)	210 (96%)	10 (4%)	0	100	100
6	a	219/392 (56%)	213 (97%)	6 (3%)	0	100	100
6	b	220/392 (56%)	206 (94%)	14 (6%)	0	100	100
6	c	220/392 (56%)	211 (96%)	9 (4%)	0	100	100
6	d	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
6	e	220/392 (56%)	208 (94%)	12 (6%)	0	100	100
6	f	220/392 (56%)	209 (95%)	11 (5%)	0	100	100
6	g	219/392 (56%)	210 (96%)	9 (4%)	0	100	100
6	h	220/392 (56%)	207 (94%)	13 (6%)	0	100	100
6	i	220/392 (56%)	212 (96%)	8 (4%)	0	100	100
6	j	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
6	k	220/392 (56%)	205 (93%)	15 (7%)	0	100	100
6	l	220/392 (56%)	210 (96%)	10 (4%)	0	100	100
6	m	219/392 (56%)	214 (98%)	5 (2%)	0	100	100
6	n	220/392 (56%)	207 (94%)	13 (6%)	0	100	100
All	All	13338/26175 (51%)	12863 (96%)	472 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	0	49	ASN
2	2	47	PRO
2	1	49	ASN

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	AA	155/215 (72%)	155 (100%)	0	100	100
1	AB	155/215 (72%)	155 (100%)	0	100	100
1	AC	155/215 (72%)	155 (100%)	0	100	100
1	AD	155/215 (72%)	155 (100%)	0	100	100
1	AE	155/215 (72%)	155 (100%)	0	100	100
1	AF	155/215 (72%)	155 (100%)	0	100	100
1	AG	155/215 (72%)	155 (100%)	0	100	100
1	AH	155/215 (72%)	155 (100%)	0	100	100
1	AI	155/215 (72%)	153 (99%)	2 (1%)	61	72
1	AJ	155/215 (72%)	155 (100%)	0	100	100
1	AK	155/215 (72%)	155 (100%)	0	100	100
1	AL	155/215 (72%)	155 (100%)	0	100	100
1	o	155/215 (72%)	154 (99%)	1 (1%)	78	79
1	p	155/215 (72%)	155 (100%)	0	100	100
1	q	155/215 (72%)	155 (100%)	0	100	100
1	r	155/215 (72%)	155 (100%)	0	100	100
1	s	155/215 (72%)	154 (99%)	1 (1%)	78	79
1	t	155/215 (72%)	155 (100%)	0	100	100
1	u	155/215 (72%)	154 (99%)	1 (1%)	78	79
1	v	155/215 (72%)	155 (100%)	0	100	100
1	w	155/215 (72%)	155 (100%)	0	100	100
1	x	155/215 (72%)	155 (100%)	0	100	100
1	y	155/215 (72%)	155 (100%)	0	100	100
1	z	155/215 (72%)	155 (100%)	0	100	100
2	0	162/199 (81%)	161 (99%)	1 (1%)	78	79
2	1	164/199 (82%)	161 (98%)	3 (2%)	51	69
2	2	164/199 (82%)	164 (100%)	0	100	100
2	3	170/199 (85%)	167 (98%)	3 (2%)	51	69
2	4	187/199 (94%)	187 (100%)	0	100	100
3	5	187/219 (85%)	186 (100%)	1 (0%)	81	80
4	6	41/71 (58%)	41 (100%)	0	100	100
4	7	69/71 (97%)	69 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	8	69/71 (97%)	68 (99%)	1 (1%)	59	71
4	9	70/71 (99%)	70 (100%)	0	100	100
5	A	119/477 (25%)	119 (100%)	0	100	100
5	B	125/477 (26%)	125 (100%)	0	100	100
5	C	119/477 (25%)	119 (100%)	0	100	100
5	D	124/477 (26%)	124 (100%)	0	100	100
5	F	119/477 (25%)	118 (99%)	1 (1%)	73	77
5	G	125/477 (26%)	125 (100%)	0	100	100
5	H	119/477 (25%)	119 (100%)	0	100	100
5	I	125/477 (26%)	125 (100%)	0	100	100
5	J	119/477 (25%)	119 (100%)	0	100	100
5	K	125/477 (26%)	125 (100%)	0	100	100
5	L	119/477 (25%)	119 (100%)	0	100	100
5	M	124/477 (26%)	124 (100%)	0	100	100
5	N	119/477 (25%)	118 (99%)	1 (1%)	73	77
5	O	125/477 (26%)	125 (100%)	0	100	100
5	P	119/477 (25%)	118 (99%)	1 (1%)	73	77
5	Q	125/477 (26%)	125 (100%)	0	100	100
6	E	190/337 (56%)	190 (100%)	0	100	100
6	R	189/337 (56%)	187 (99%)	2 (1%)	65	74
6	S	188/337 (56%)	187 (100%)	1 (0%)	81	80
6	T	190/337 (56%)	188 (99%)	2 (1%)	65	74
6	U	189/337 (56%)	188 (100%)	1 (0%)	81	80
6	V	188/337 (56%)	186 (99%)	2 (1%)	65	74
6	W	190/337 (56%)	189 (100%)	1 (0%)	81	80
6	X	189/337 (56%)	188 (100%)	1 (0%)	81	80
6	Y	188/337 (56%)	187 (100%)	1 (0%)	81	80
6	Z	190/337 (56%)	190 (100%)	0	100	100
6	a	189/337 (56%)	187 (99%)	2 (1%)	65	74
6	b	188/337 (56%)	187 (100%)	1 (0%)	81	80
6	c	190/337 (56%)	190 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	d	189/337 (56%)	188 (100%)	1 (0%)	81	80
6	e	188/337 (56%)	186 (99%)	2 (1%)	65	74
6	f	190/337 (56%)	189 (100%)	1 (0%)	81	80
6	g	189/337 (56%)	185 (98%)	4 (2%)	47	66
6	h	188/337 (56%)	188 (100%)	0	100	100
6	i	190/337 (56%)	189 (100%)	1 (0%)	81	80
6	j	189/337 (56%)	188 (100%)	1 (0%)	81	80
6	k	188/337 (56%)	187 (100%)	1 (0%)	81	80
6	l	190/337 (56%)	190 (100%)	0	100	100
6	m	189/337 (56%)	187 (99%)	2 (1%)	65	74
6	n	188/337 (56%)	186 (99%)	2 (1%)	65	74
All	All	11489/22378 (51%)	11443 (100%)	46 (0%)	81	81

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	d	366	LEU
6	g	366	LEU
6	e	222	VAL
6	g	181	LYS
6	j	355	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
6	k	319	HIS
1	AJ	163	GLN
1	o	115	GLN
1	t	173	ASN
5	M	123	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

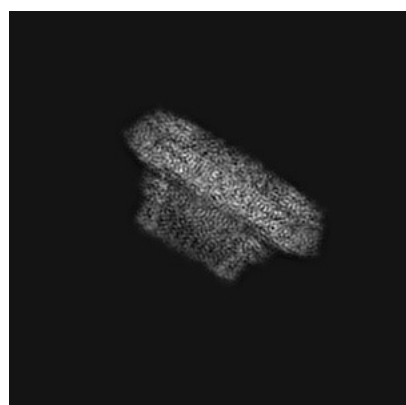
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20316. These allow visual inspection of the internal detail of the map and identification of artifacts.

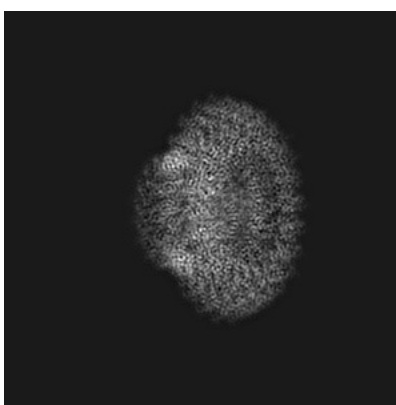
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

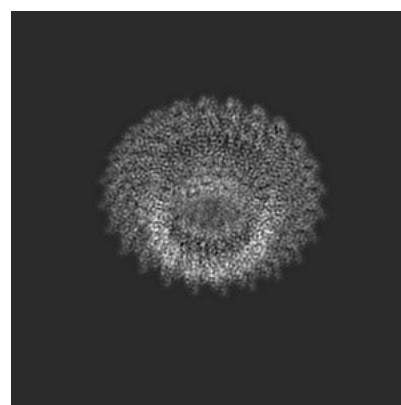
6.1.1 Primary map



X



Y

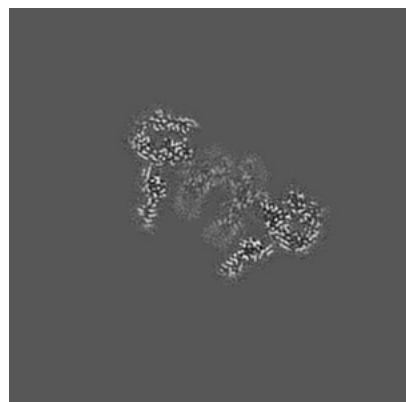


Z

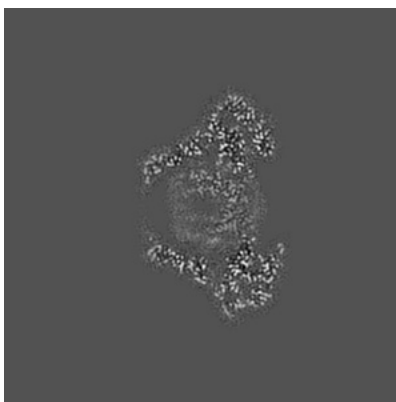
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

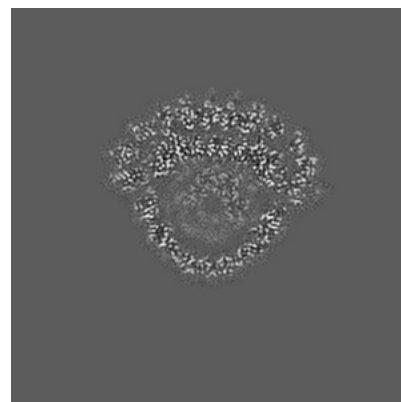
6.2.1 Primary map



X Index: 125



Y Index: 125

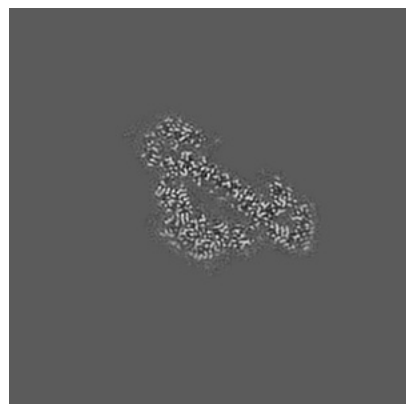


Z Index: 125

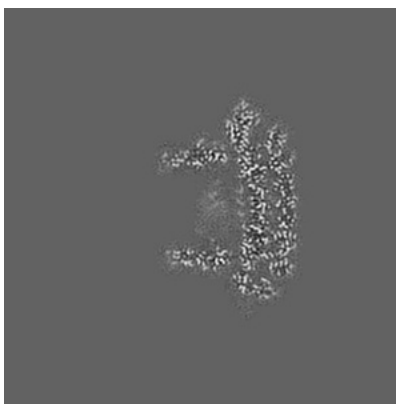
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

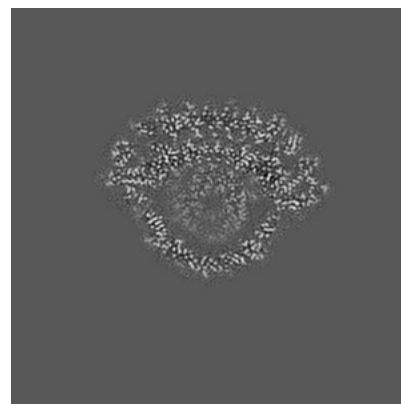
6.3.1 Primary map



X Index: 155



Y Index: 107

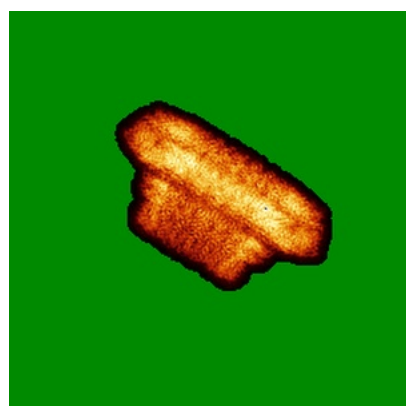


Z Index: 129

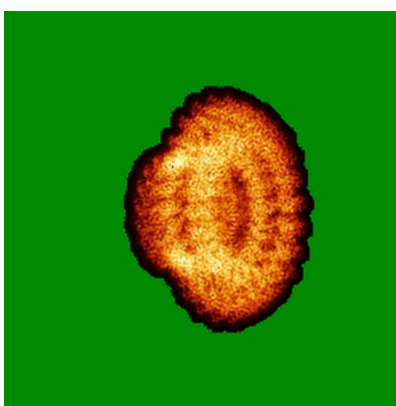
The images above show the largest variance slices of the map in three orthogonal directions.

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

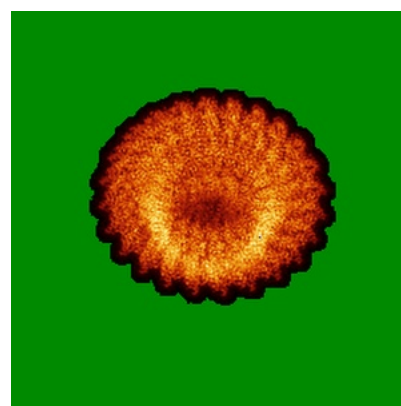
6.4.1 Primary map



X



Y

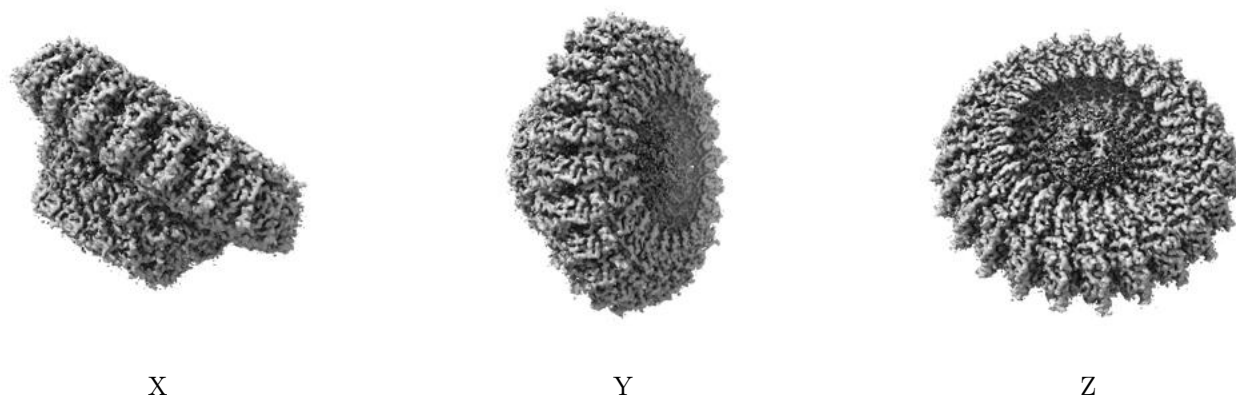


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

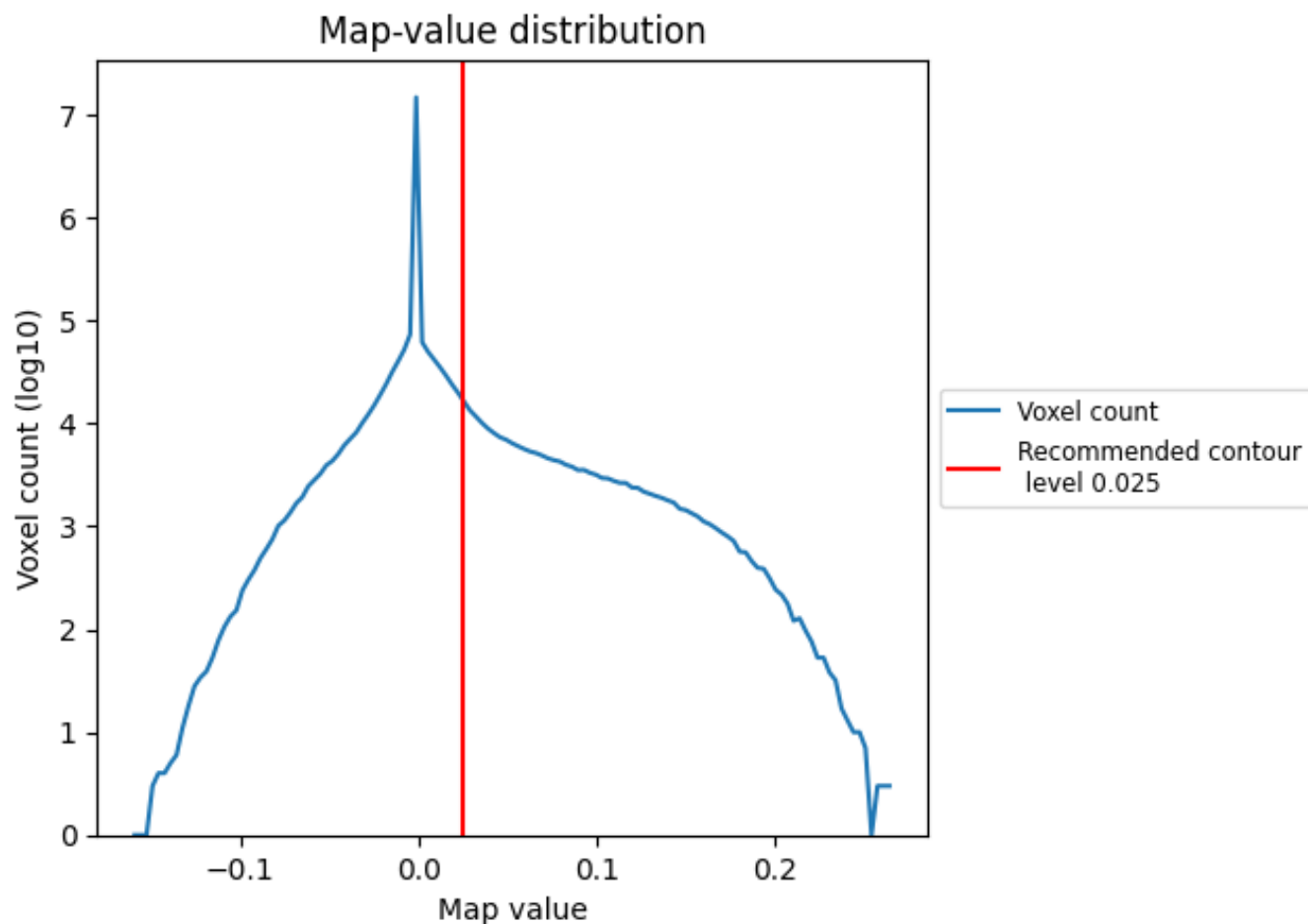
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

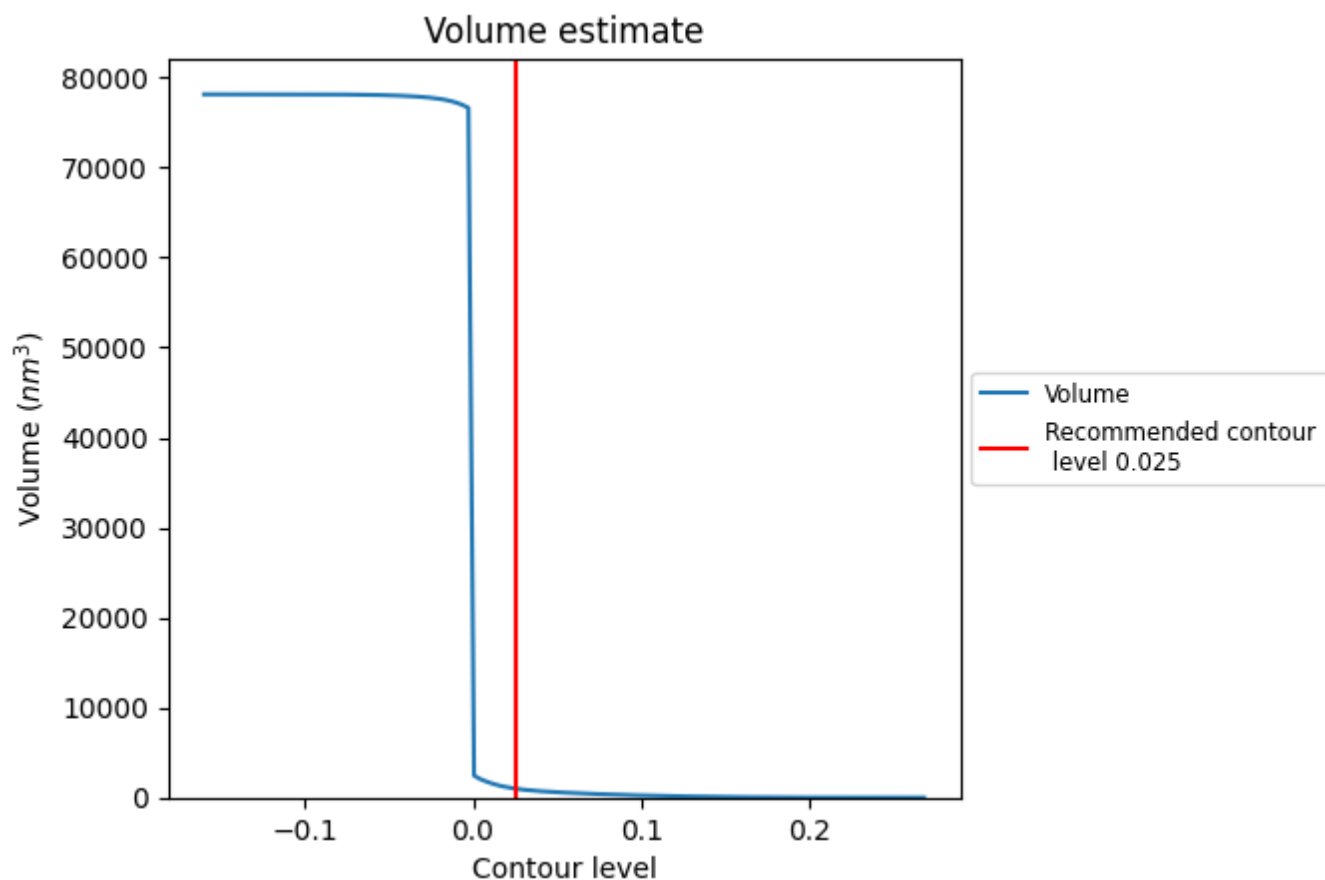
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

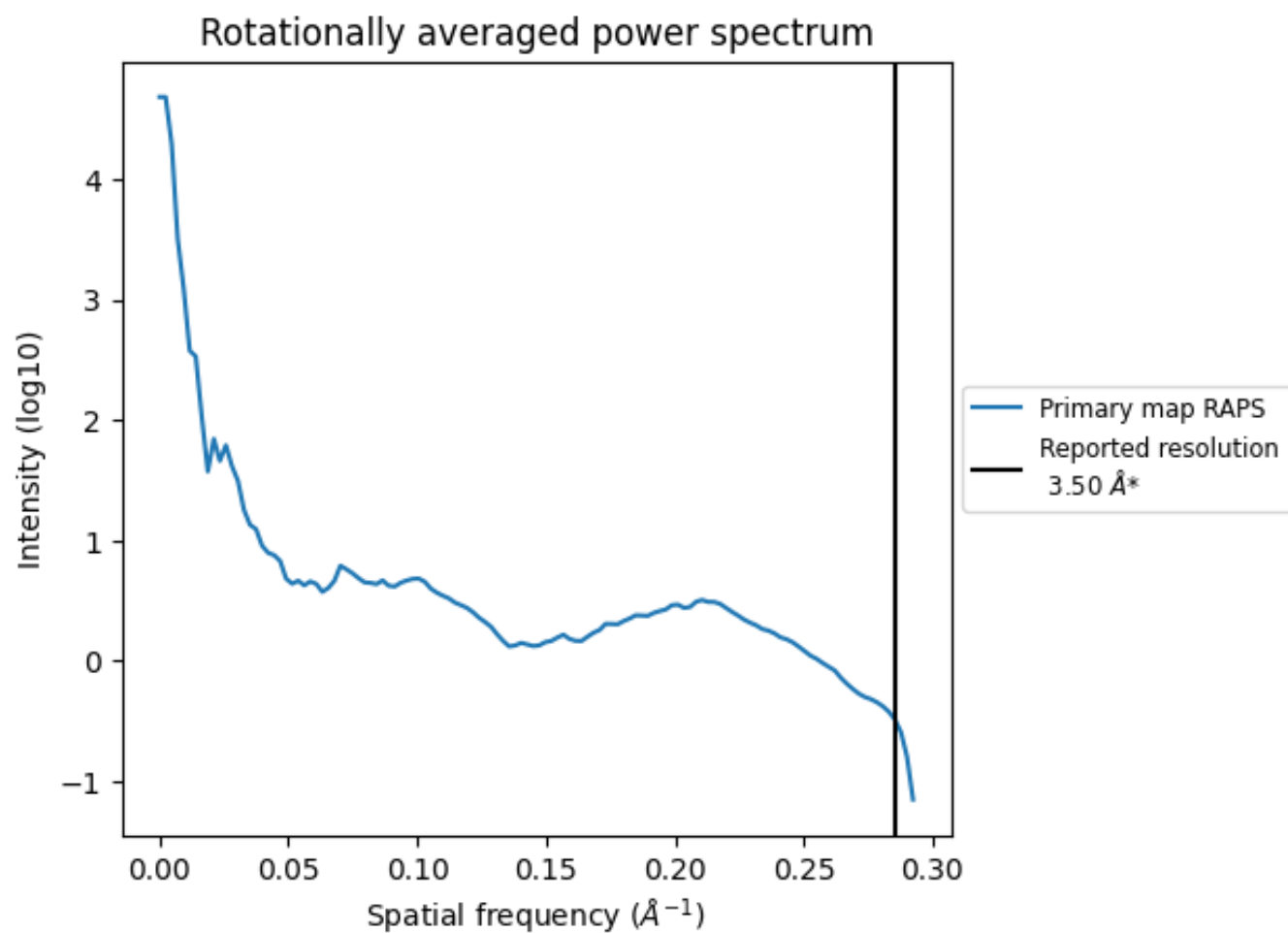
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 996 nm³; this corresponds to an approximate mass of 899 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 0.286 Å⁻¹

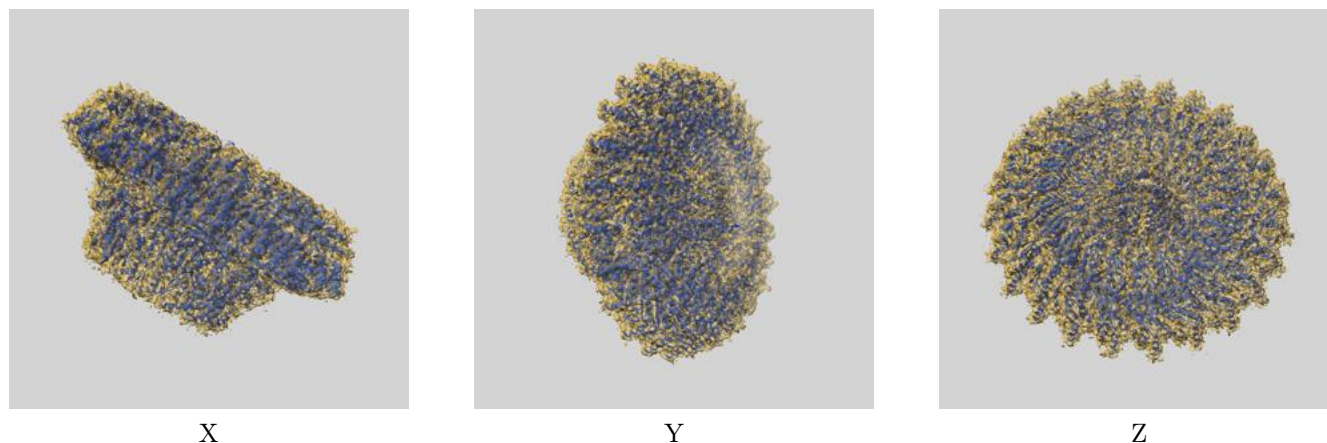
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

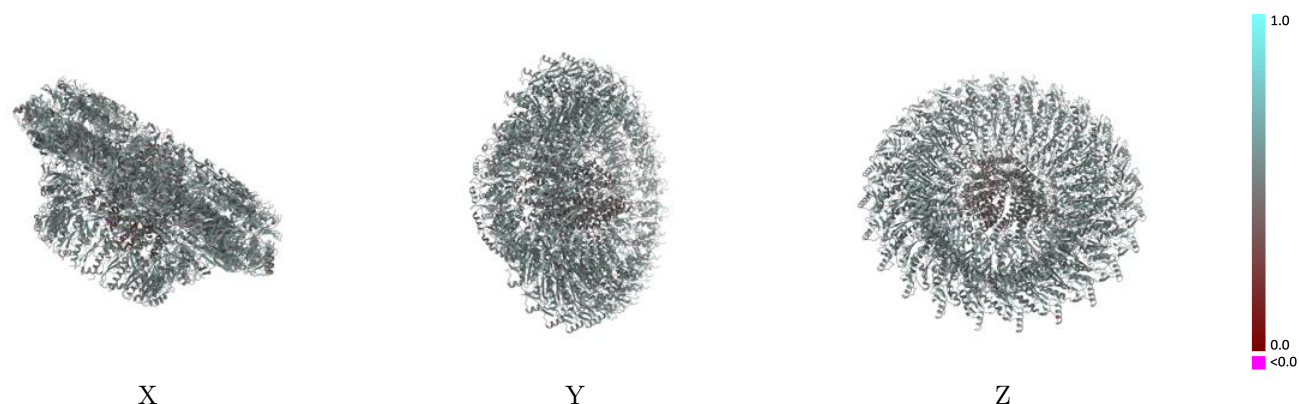
This section contains information regarding the fit between EMDB map EMD-20316 and PDB model 6PEM. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



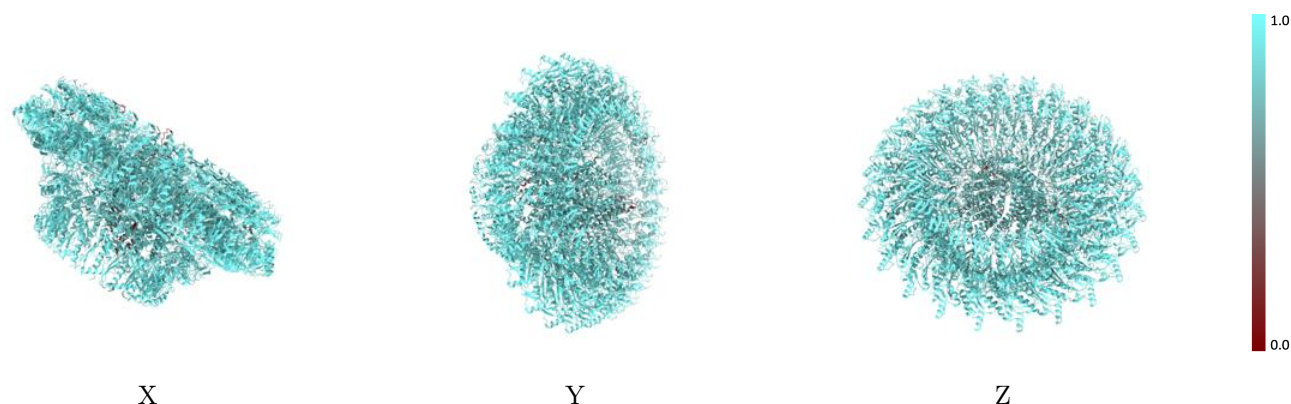
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



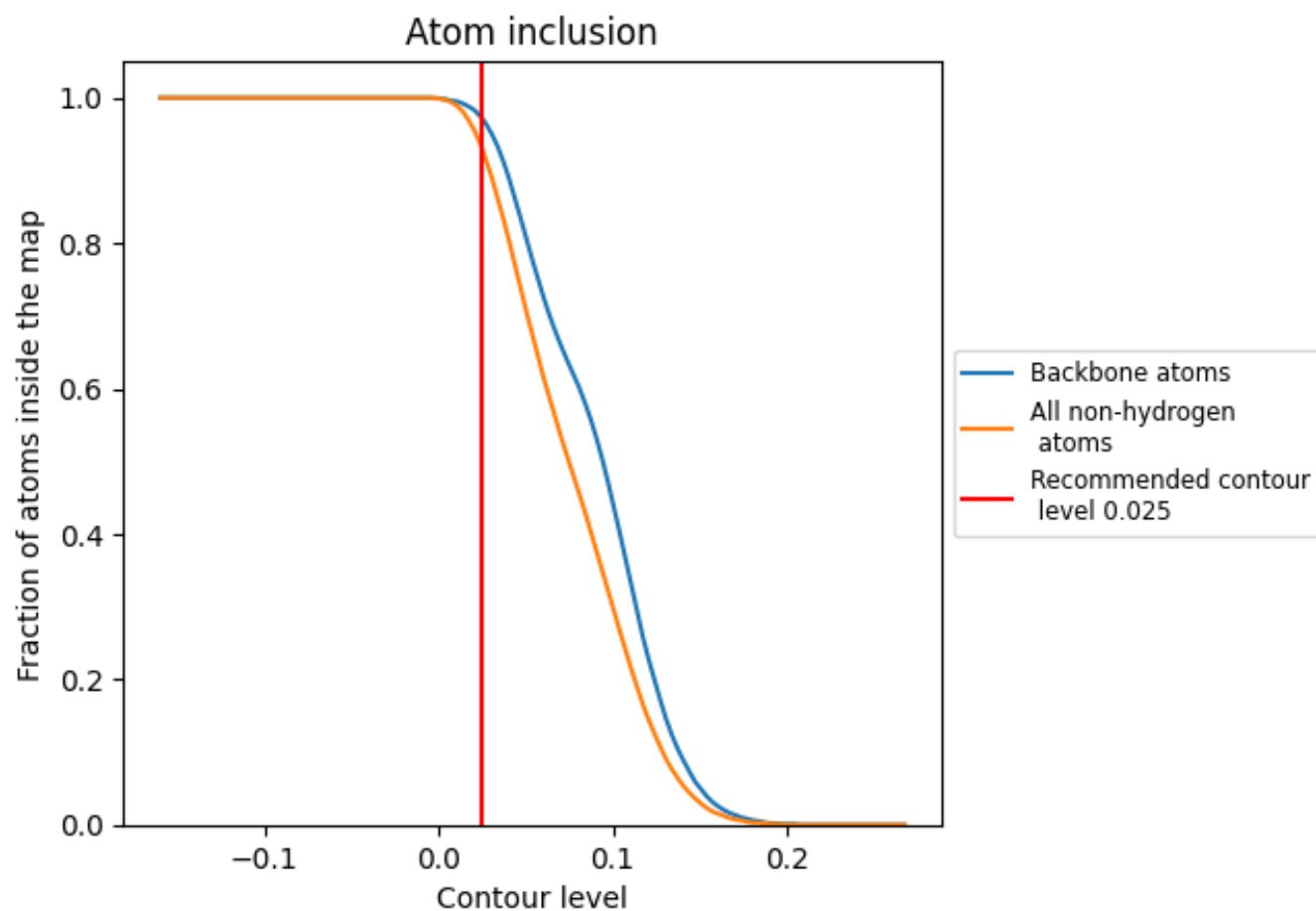
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9310	 0.5190
0	 0.8550	 0.4650
1	 0.8200	 0.4340
2	 0.8220	 0.4470
3	 0.8440	 0.4590
4	 0.8250	 0.4700
5	 0.9110	 0.4980
6	 0.7410	 0.4600
7	 0.6970	 0.4290
8	 0.8400	 0.4590
9	 0.8700	 0.4900
A	 0.9700	 0.5310
AA	 0.9280	 0.5260
AB	 0.9270	 0.5270
AC	 0.9360	 0.5310
AD	 0.9360	 0.5250
AE	 0.9250	 0.5260
AF	 0.9370	 0.5270
AG	 0.9270	 0.5230
AH	 0.9300	 0.5290
AI	 0.9320	 0.5290
AJ	 0.9280	 0.5240
AK	 0.9170	 0.5210
AL	 0.9360	 0.5240
B	 0.9570	 0.5170
C	 0.9600	 0.5260
D	 0.9570	 0.5150
E	 0.9370	 0.5250
F	 0.9310	 0.5210
G	 0.9310	 0.5180
H	 0.9550	 0.5220
I	 0.9520	 0.5130
J	 0.9670	 0.5260
K	 0.9470	 0.5040
L	 0.9450	 0.5240



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
M	 0.9560	 0.5170
N	 0.9590	 0.5220
O	 0.9410	 0.5110
P	 0.9480	 0.5230
Q	 0.9620	 0.5170
R	 0.9570	 0.5330
S	 0.9520	 0.5330
T	 0.9420	 0.5260
U	 0.9550	 0.5280
V	 0.9550	 0.5290
W	 0.9450	 0.5310
X	 0.9500	 0.5280
Y	 0.9490	 0.5280
Z	 0.9510	 0.5250
a	 0.9550	 0.5290
b	 0.9500	 0.5320
c	 0.9440	 0.5290
d	 0.9590	 0.5320
e	 0.9500	 0.5220
f	 0.9410	 0.5280
g	 0.9510	 0.5260
h	 0.9510	 0.5290
i	 0.9390	 0.5310
j	 0.9580	 0.5330
k	 0.9530	 0.5360
l	 0.9450	 0.5310
m	 0.9530	 0.5310
n	 0.9480	 0.5260
o	 0.9320	 0.5320
p	 0.9220	 0.5290
q	 0.9340	 0.5250
r	 0.9280	 0.5270
s	 0.9220	 0.5190
t	 0.9280	 0.5260
u	 0.9270	 0.5220
v	 0.9310	 0.5210
w	 0.9020	 0.5160
x	 0.9190	 0.5200
y	 0.9240	 0.5310
z	 0.9370	 0.5310