



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 04:14 AM UTC

PDB ID : 6UOV / pdb_00006uov
EMDB ID : EMD-20833
Title : Cryo-EM reconstruction of the PrgHK periplasmic ring from Salmonella's needle complex assembled in the absence of the export apparatus
Authors : Butan, C.; Galan, J.
Deposited on : 2019-10-15
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:

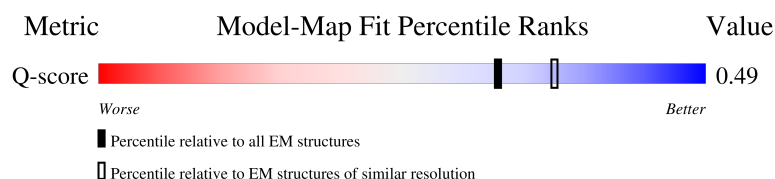
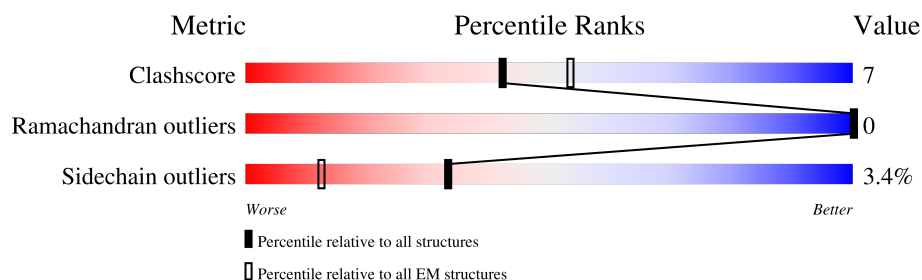
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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	A	252	5% 58% 15% 27%
1	C	252	. 58% 13% 27%
1	E	252	. 60% 12% 27%
1	G	252	5% 60% 12% 27%

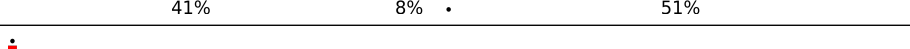
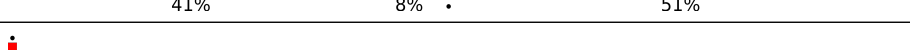
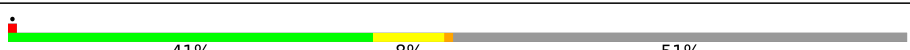
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	252	
1	K	252	
1	M	252	
1	O	252	
1	Q	252	
1	S	252	
1	U	252	
1	W	252	
1	Y	252	
1	a	252	
1	c	252	
1	e	252	
1	g	252	
1	i	252	
1	k	252	
1	m	252	
1	o	252	
1	q	252	
1	s	252	
2	B	392	
2	D	392	
2	F	392	
2	H	392	
2	J	392	
2	L	392	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	N	392	
2	P	392	
2	R	392	
2	T	392	
2	V	392	
2	X	392	
2	Z	392	
2	b	392	
2	d	392	
2	f	392	
2	h	392	
2	j	392	
2	l	392	
2	n	392	
2	p	392	
2	r	392	
2	t	392	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 69851 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	A	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	C	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	E	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	G	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	I	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	K	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	M	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	O	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	Q	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	S	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	U	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	W	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	Y	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	a	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	c	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	e	184	Total 1437	C 905	N 250	O 279	S 3	0	0
1	g	184	Total 1437	C 905	N 250	O 279	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	k	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	m	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	o	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	q	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	s	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		

- Molecule 2 is a protein called Protein PrgH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	D	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	F	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	H	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	J	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	L	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	N	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	P	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	R	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	T	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	V	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	X	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	Z	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		

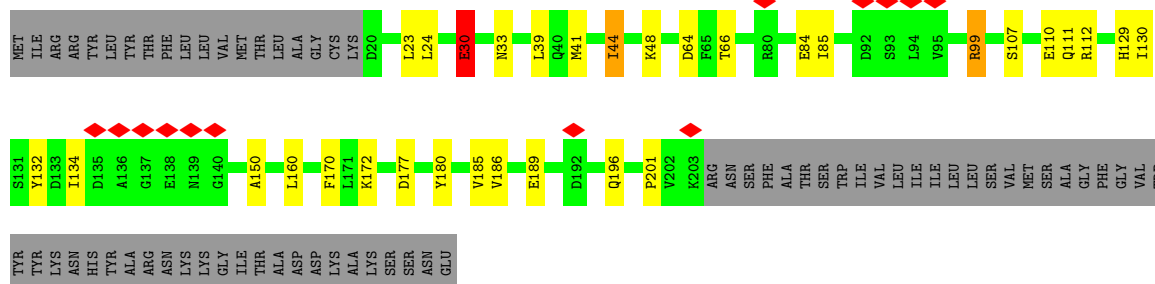
Continued on next page...

Continued from previous page...

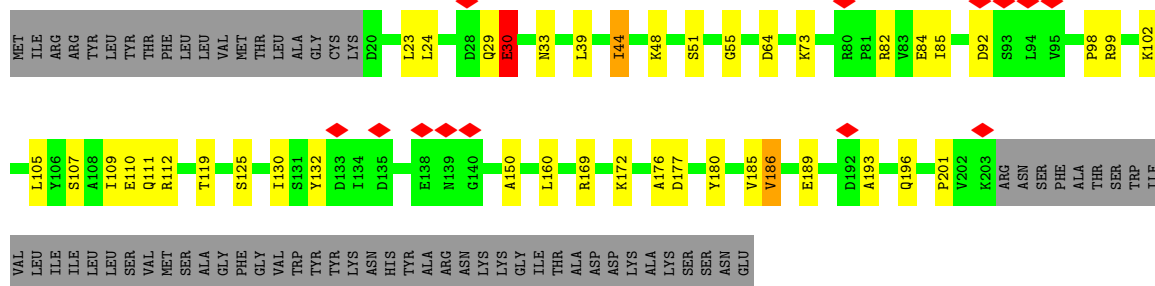
Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	d	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	f	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	h	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	j	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	l	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	n	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	p	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	r	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	t	194	Total 1600	C 1011	N 288	O 297	S 4	0	0

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

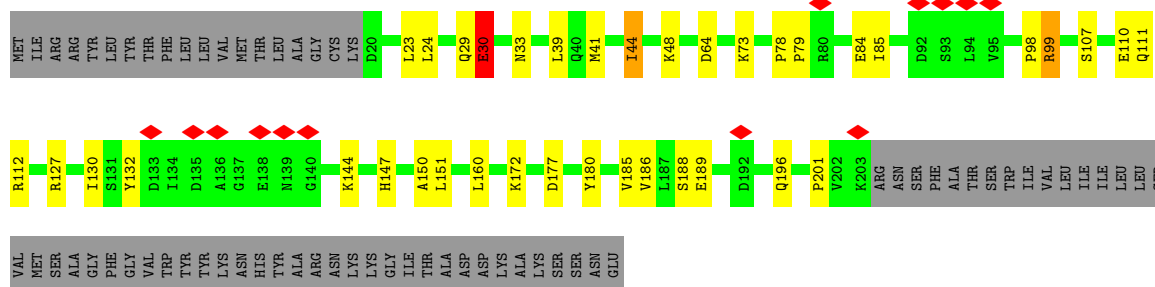
• Molecule 1: Lipoprotein PrgK



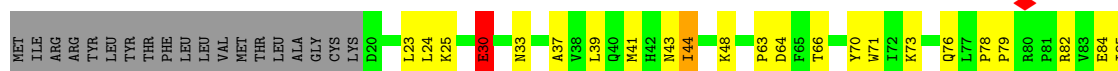
• Molecule 1: Lipoprotein PrgK



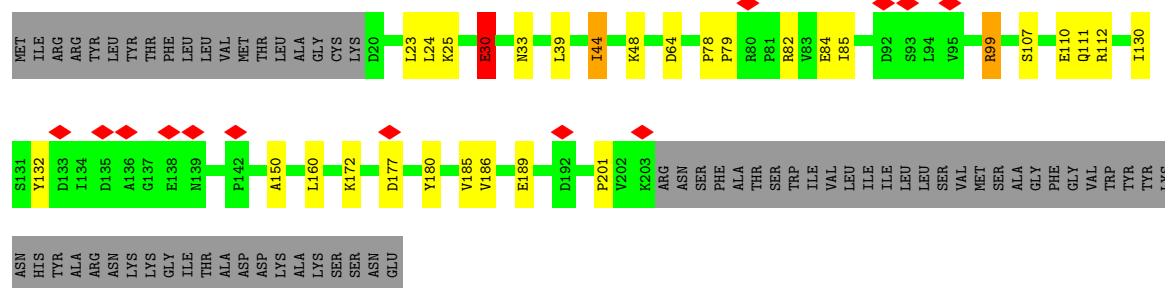
• Molecule 1: Lipoprotein PrgK



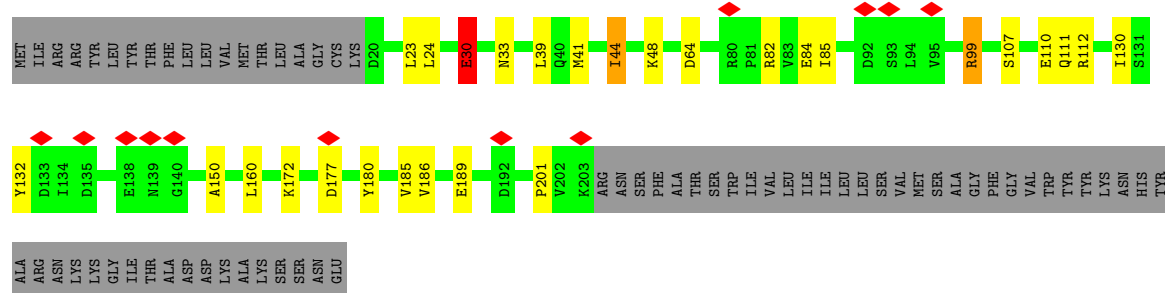
• Molecule 1: Lipoprotein PrgK



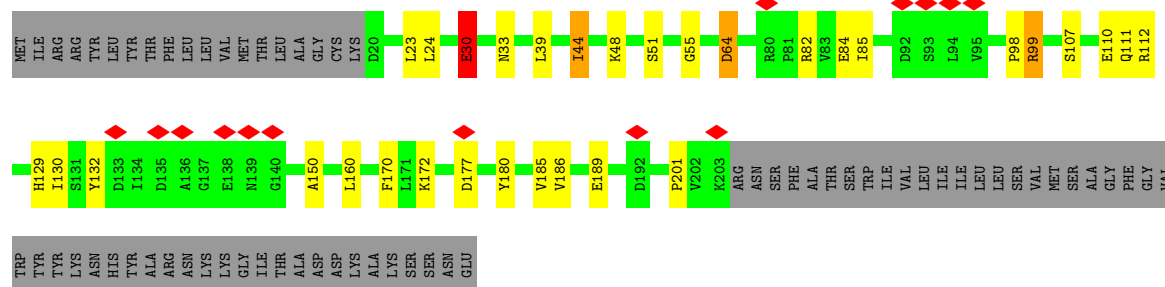
- Molecule 1: Lipoprotein PrgK



- Molecule 1: Lipoprotein PrgK

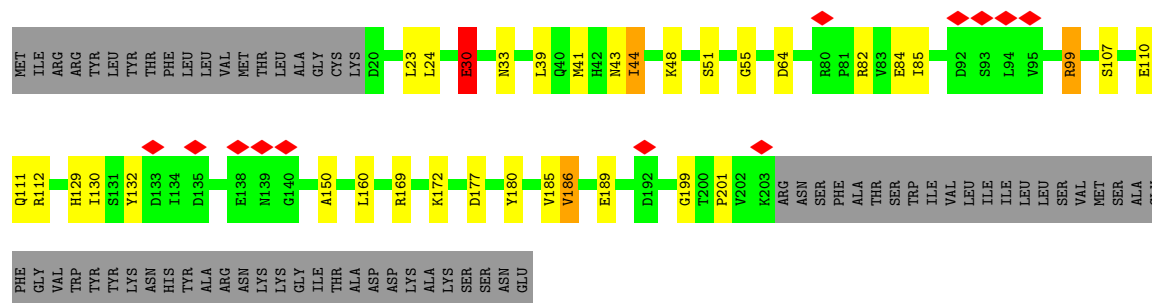


- Molecule 1: Lipoprotein PrgK

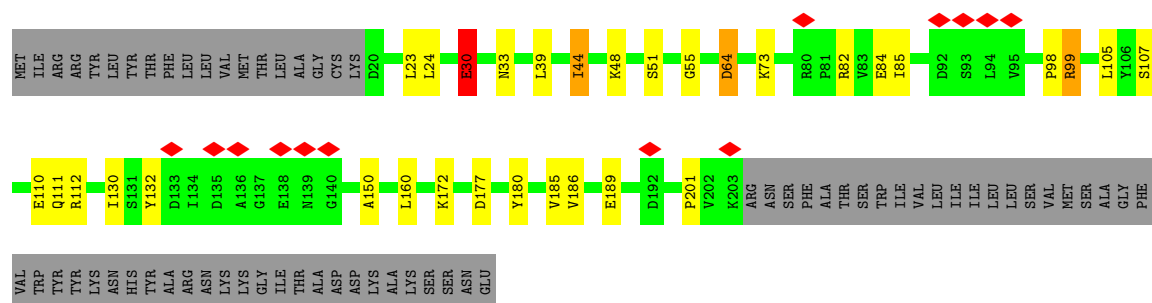


- Molecule 1: Lipoprotein PrgK

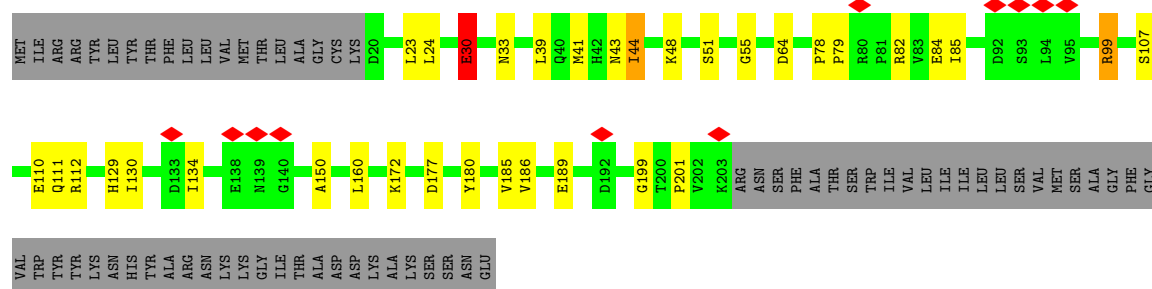




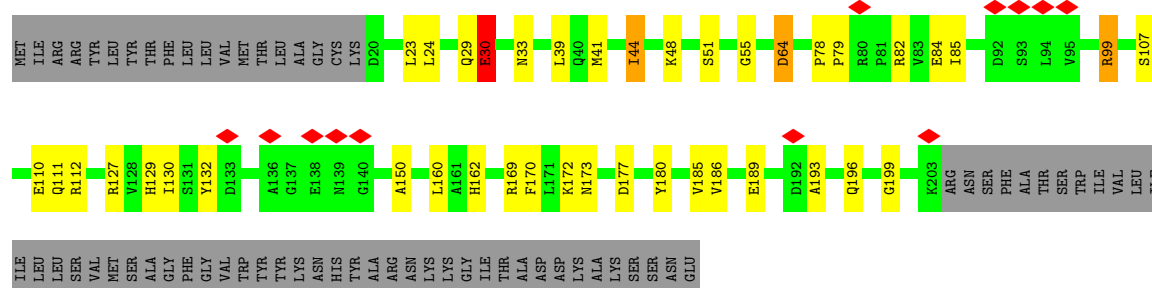
• Molecule 1: Lipoprotein PrgK



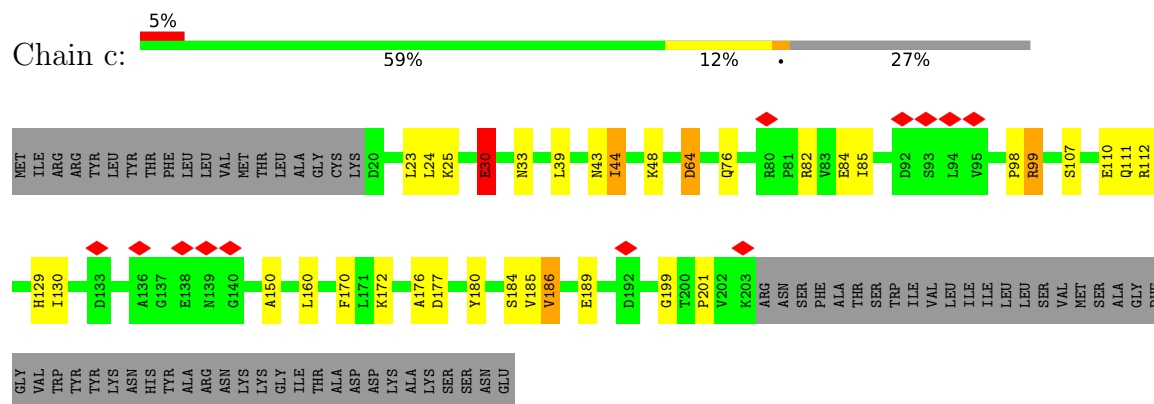
• Molecule 1: Lipoprotein PrgK



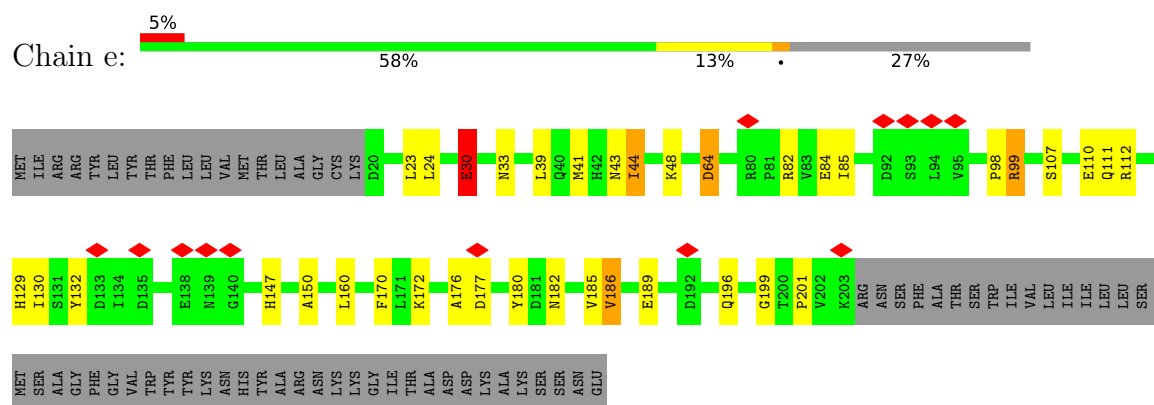
• Molecule 1: Lipoprotein PrgK



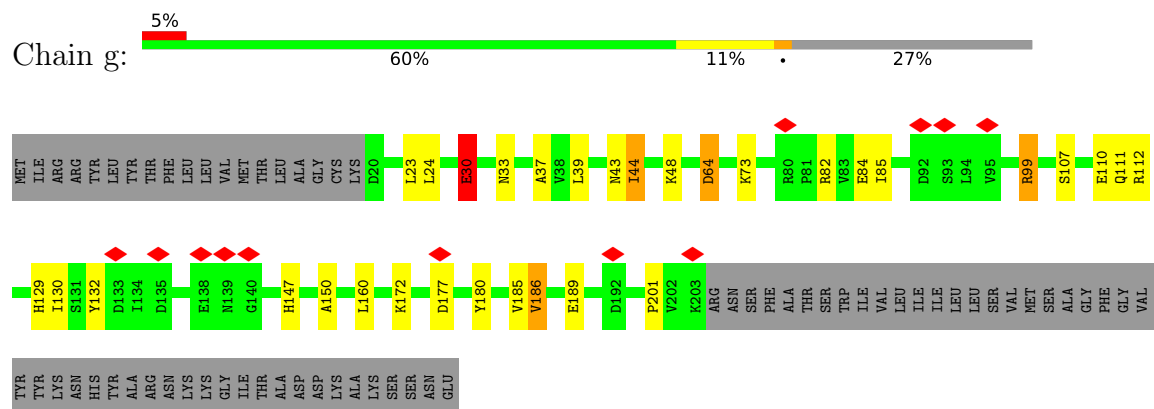
• Molecule 1: Lipoprotein PrgK



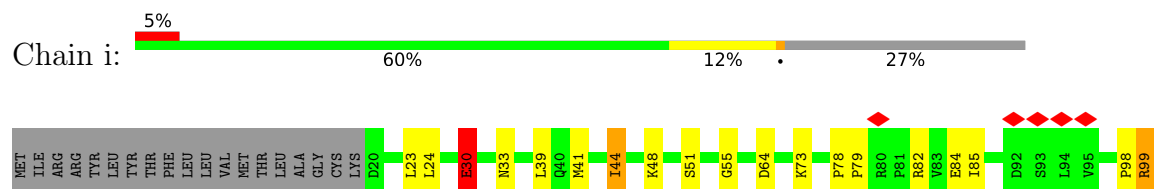
• Molecule 1: Lipoprotein PrgK

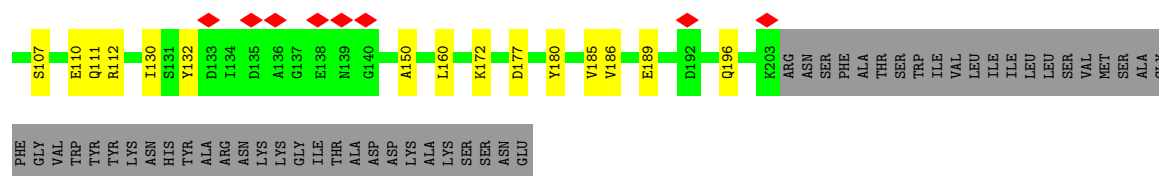


• Molecule 1: Lipoprotein PrgK

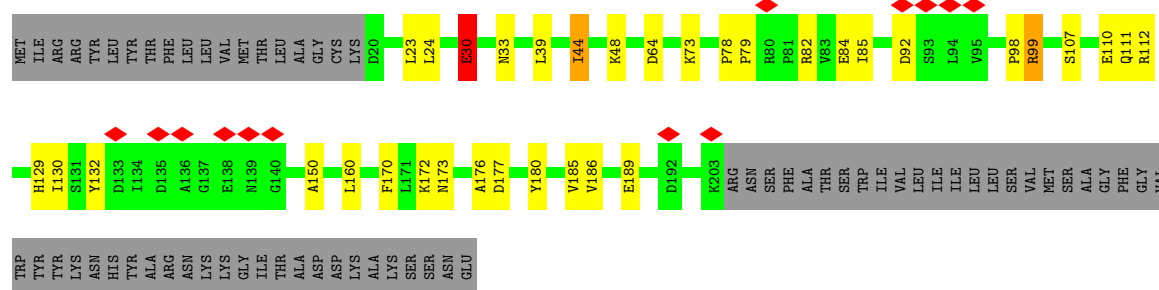


• Molecule 1: Lipoprotein PrgK

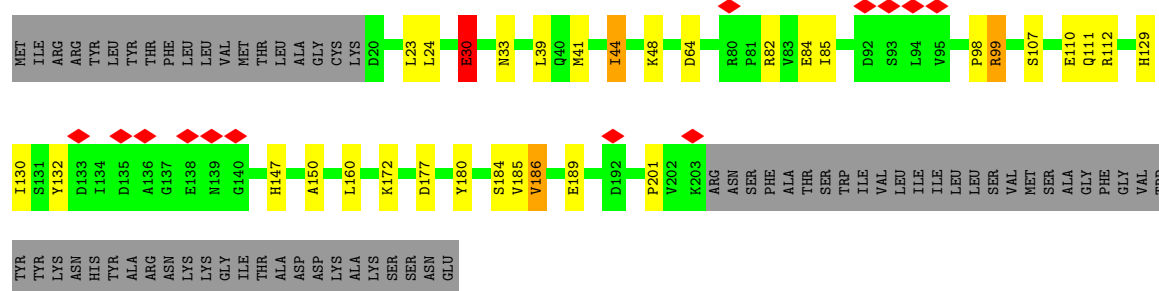




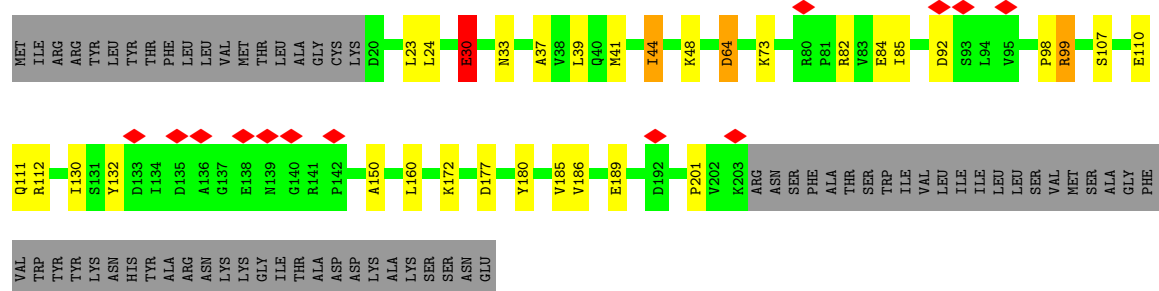
• Molecule 1: Lipoprotein PrgK



• Molecule 1: Lipoprotein PrgK



• Molecule 1: Lipoprotein PrgK



• Molecule 1: Lipoprotein PrgK



Chain J:

40% 9% 51%

Met

Phe
Glu
Thr
Ser
Ser
Lys
Glu
Lys
Thr
Thr
Ile
Thr
Ser
Ser
Pro
Gly
Gly
Pro
Tyr

Phe
Ile
Pro
Pro
Leu
Asp
His
Gly
Gly
Val
Val
Asn
Phe
Glu
Tle
Gln
Val
Val
His
Glu
Leu
Lys
Glu
Gly
Asn
Gly
Ser
Arg
Thr
Val
Val
Gln
Gln
Val
Gly
Glu
Leu
Ile
Ile
Tle
Arg
Pro
Glu
Ser
Glu
Pro
Trp
Val

Pro
Glu
Gln
Pro
Glu
Glu
Lys
Leu
Thr
Thr
Ser
Ser
Ala
Ala
Leu
Ile
Ile
Val
Ala
Ala
Leu
Ala
Gly
Phe
Phe
Ile
Leu
Gly
Ile
Gly
Thr
Gly
Val
Gly
Thr
Leu
Leu
Trp
Ile
Leu
Asn
Ser
Pro
Gln
Arg
Gln
Ala

A171
E172

E180
L187
R190
D191
K192

Y196
V196
R202
L205
W206
R213
G214
D215
Y216
D217
N224
E225
N229
Q242
Y246
R247
F250
R254
L260
S261
R262
N265
R280
P284
Y285
A286
I291
L292
L293
D296
E304
L307
R316
V326
I327
L331
D332
F335

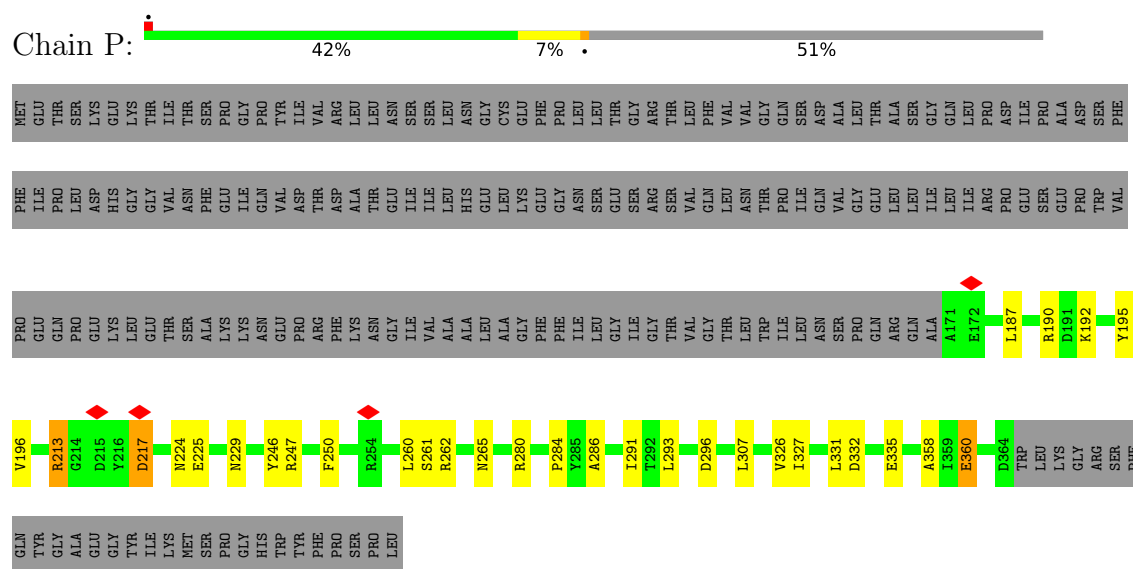
A358
I359
E360
L364
Trp
Leu
Lys
Gly
Arg
Ser
Phe
Gln
Tyr
Gly
Ala
Glu
Gly
Tyr
Ile
Lys
Met
Ser
Ser
Pro
Gly
His
Trp
Tyr
Phe
Pro
Ser
Pro
Leu

[illegible]

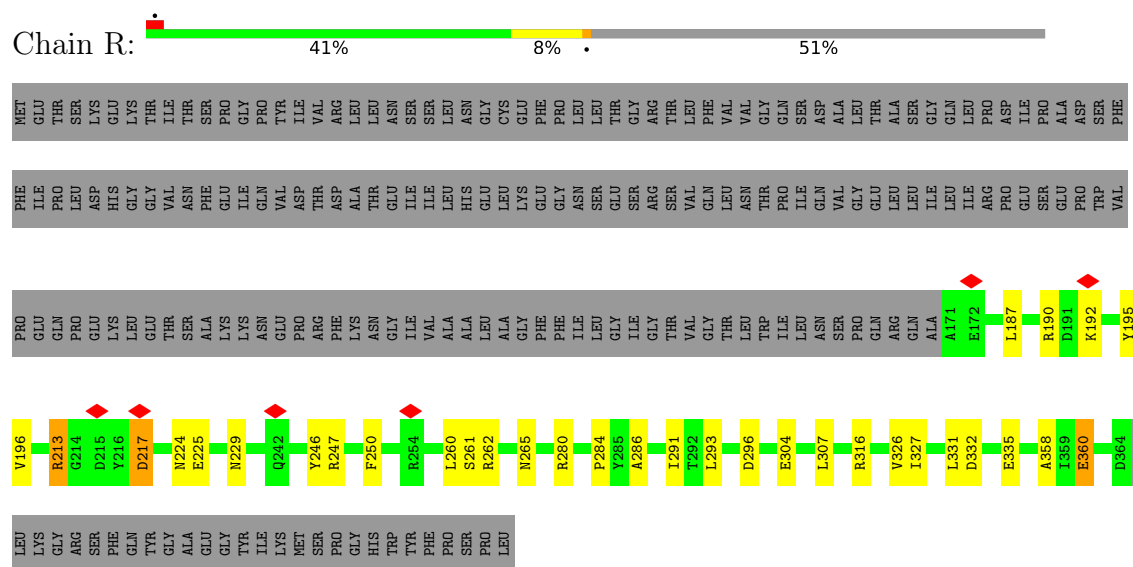
Chain N:

Amino Acid	Percentage
MET	1%
GLU	41%
THR	8%
SER	51%
LYS	1%
THR	1%
LYS	1%
THR	1%
SER	1%
PRO	1%
GLY	1%
PRO	1%
TYR	1%
ILE	1%
VAL	1%
ARG	1%
LEU	1%
LEU	1%
ASN	1%
CYS	1%
GLU	1%
PHE	1%
PRO	1%
LEU	1%
LEU	1%
THR	1%
GLY	1%
THR	1%
ARG	1%
THR	1%
LEU	1%
PHE	1%
VAL	1%
VAL	1%
GLY	1%
GLN	1%
ASP	1%
ALA	1%
LEU	1%
THR	1%
ALA	1%
SER	1%
GLY	1%
LEU	1%
LEU	1%
ARG	1%
PRO	1%
THR	1%
PHE	1%

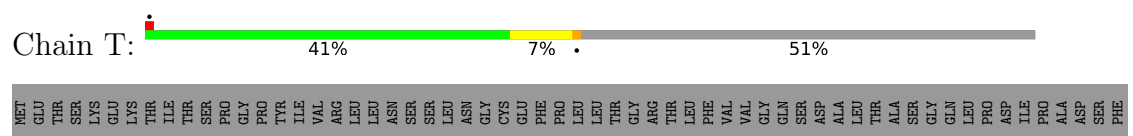
- Molecule 2: Protein PrgH

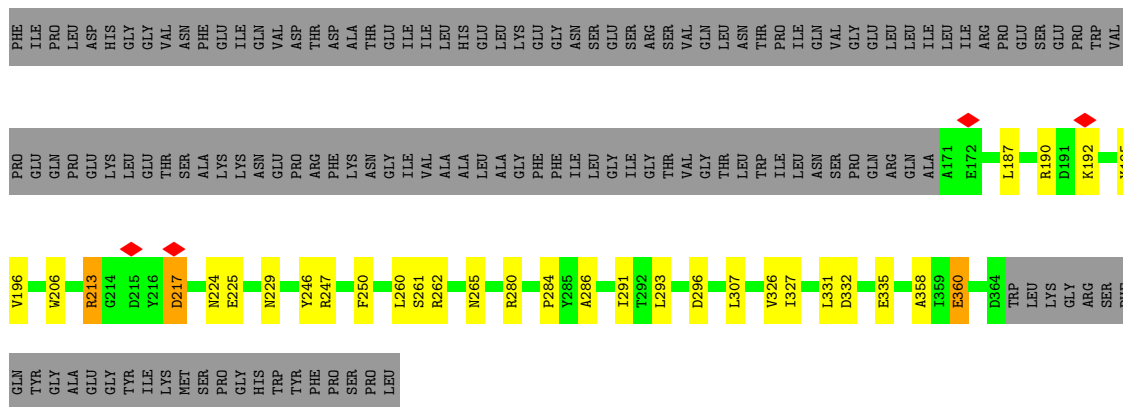


- Molecule 2: Protein PrgH

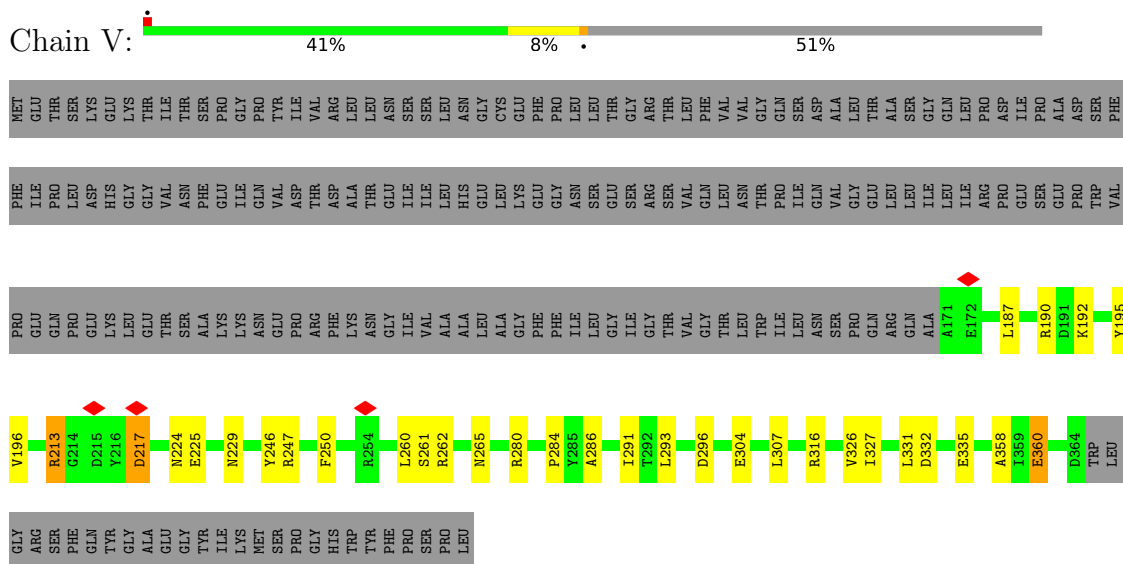


- Molecule 2: Protein PrgH

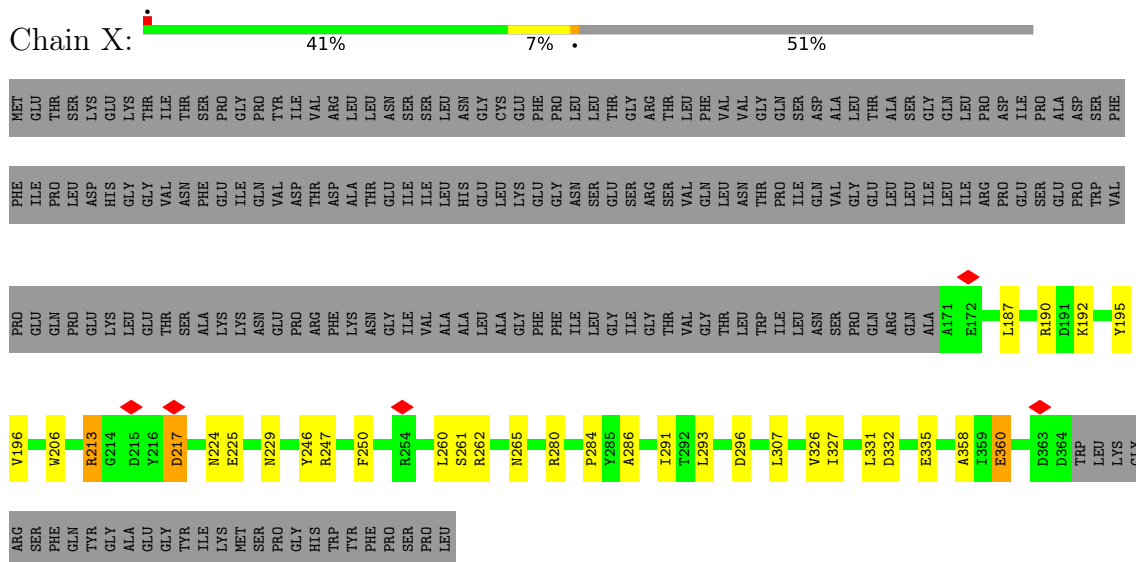




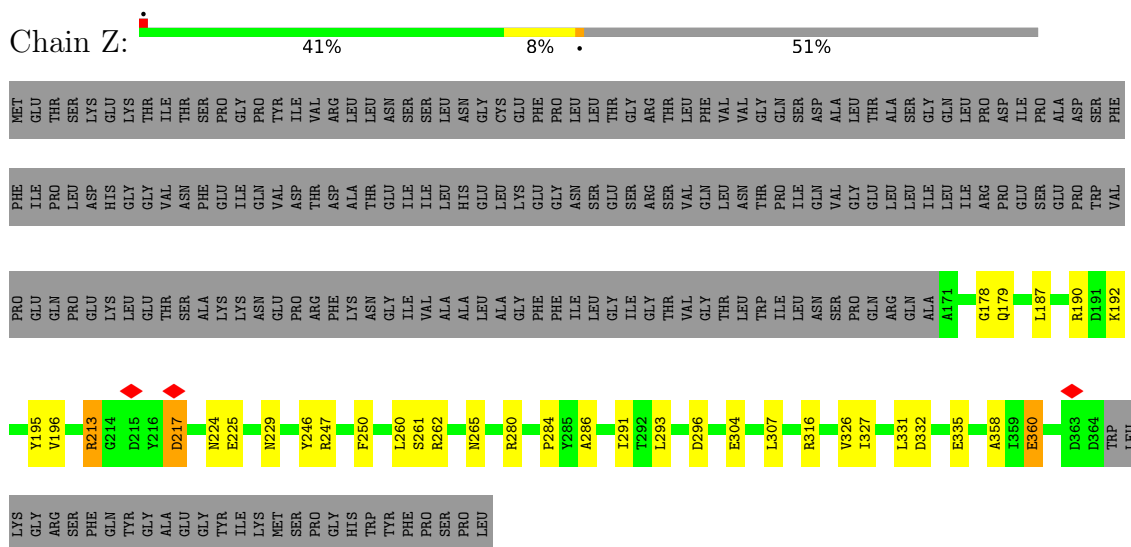
- Molecule 2: Protein PrgH



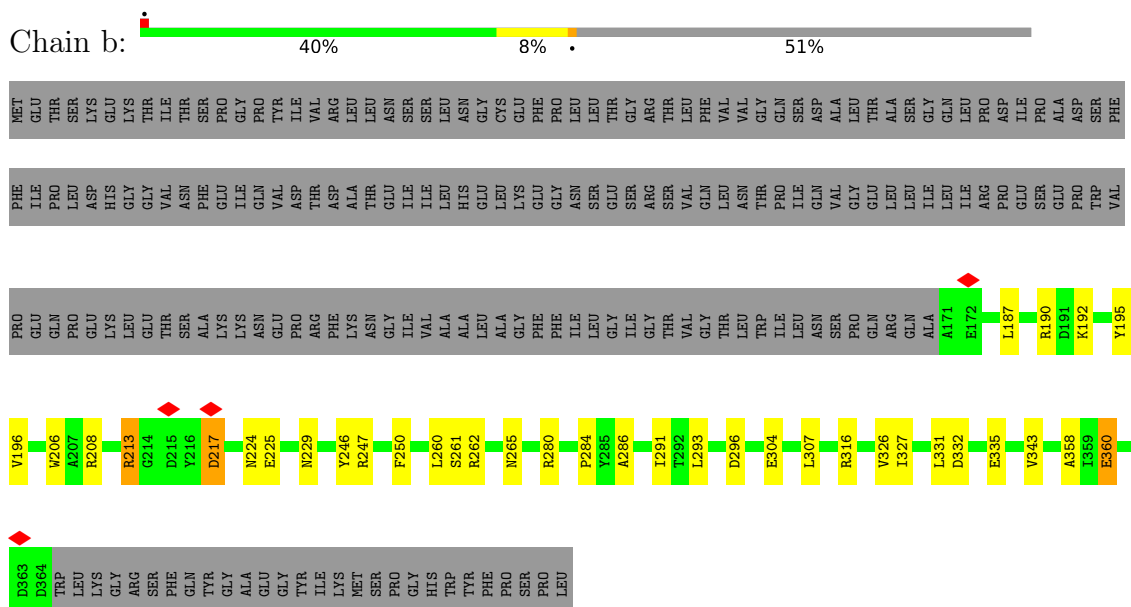
- Molecule 2: Protein PrgH



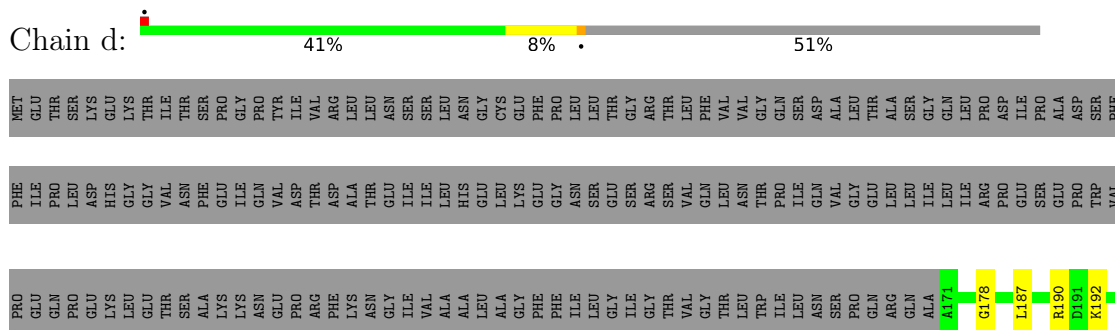
- Molecule 2: Protein PrgH

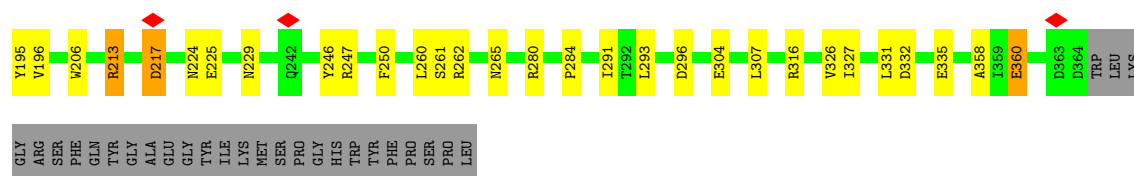


- Molecule 2: Protein PrgH

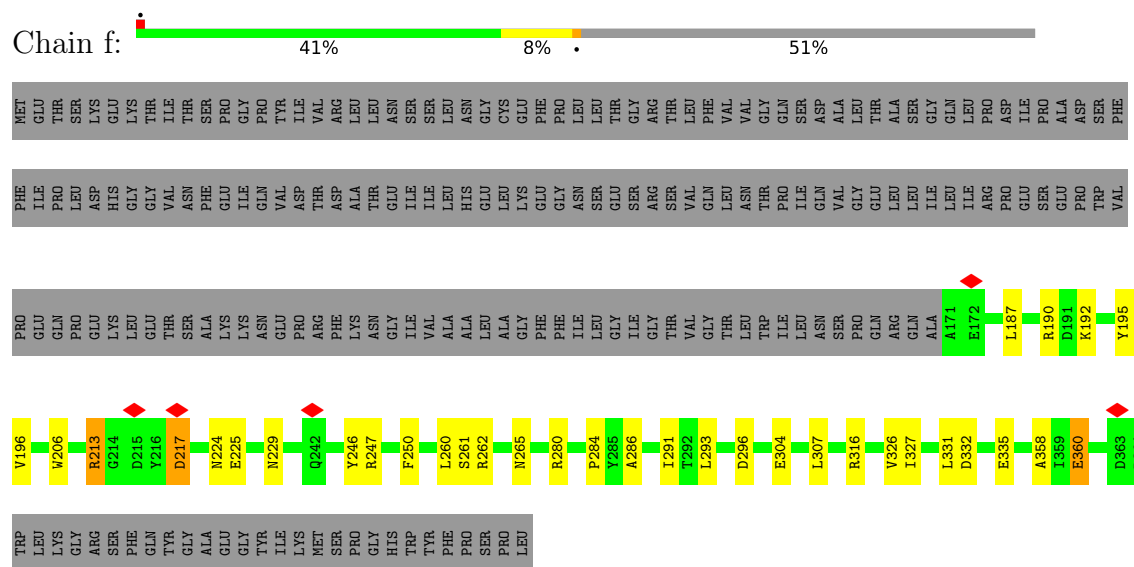


- Molecule 2: Protein PrgH

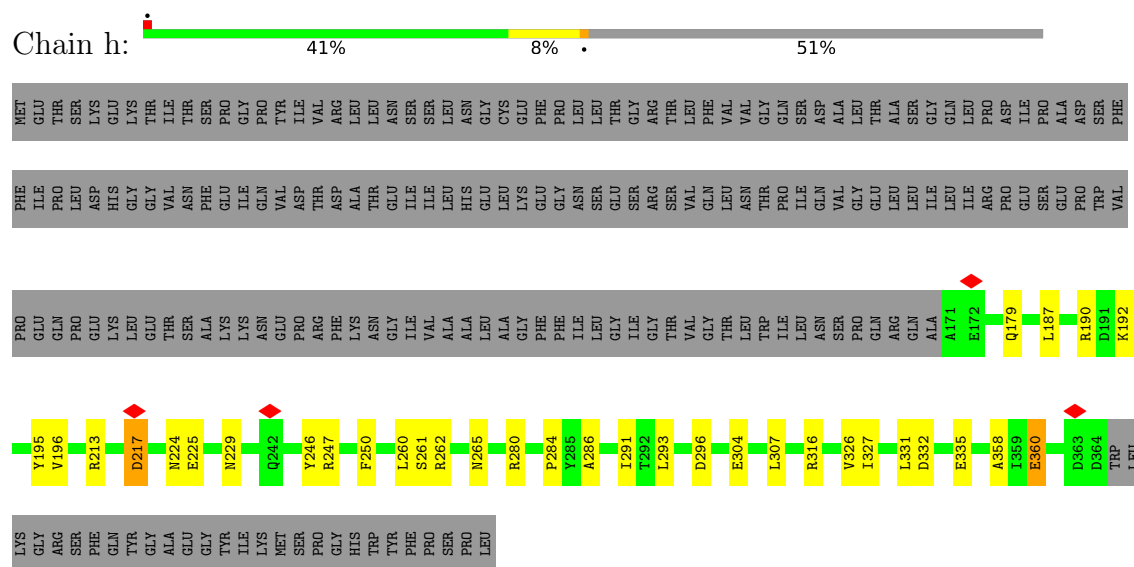




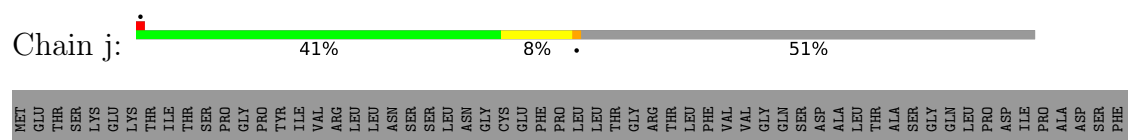
• Molecule 2: Protein PrgH

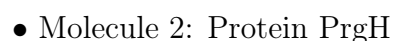


• Molecule 2: Protein PrgH



• Molecule 2: Protein PrgH





LEU
LYS
GLY
ARG
SER
PHE
GLN
TYR
GLY
ALA
GLU
GLY
TYR
ILE
LYS
MET
SER
PRO
GLY
HIS
TRP
TYR
PHE
PRO
SER
PRO
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C23	Depositor
Number of particles used	10674	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	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.287	Depositor
Minimum map value	-0.190	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.038	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/1465	0.63	2/1989 (0.1%)
1	C	0.46	0/1465	0.63	2/1989 (0.1%)
1	E	0.46	0/1465	0.63	2/1989 (0.1%)
1	G	0.46	0/1465	0.63	2/1989 (0.1%)
1	I	0.46	0/1465	0.63	2/1989 (0.1%)
1	K	0.46	0/1465	0.63	2/1989 (0.1%)
1	M	0.46	0/1465	0.63	2/1989 (0.1%)
1	O	0.46	0/1465	0.63	2/1989 (0.1%)
1	Q	0.46	0/1465	0.63	2/1989 (0.1%)
1	S	0.46	0/1465	0.63	2/1989 (0.1%)
1	U	0.46	0/1465	0.63	2/1989 (0.1%)
1	W	0.46	0/1465	0.63	2/1989 (0.1%)
1	Y	0.46	0/1465	0.63	2/1989 (0.1%)
1	a	0.46	0/1465	0.63	2/1989 (0.1%)
1	c	0.46	0/1465	0.63	2/1989 (0.1%)
1	e	0.46	0/1465	0.63	2/1989 (0.1%)
1	g	0.46	0/1465	0.63	2/1989 (0.1%)
1	i	0.46	0/1465	0.63	2/1989 (0.1%)
1	k	0.46	0/1465	0.63	2/1989 (0.1%)
1	m	0.46	0/1465	0.63	2/1989 (0.1%)
1	o	0.46	0/1465	0.63	2/1989 (0.1%)
1	q	0.46	0/1465	0.63	2/1989 (0.1%)
1	s	0.46	0/1465	0.63	2/1989 (0.1%)
2	B	0.34	0/1632	0.64	2/2204 (0.1%)
2	D	0.34	0/1632	0.64	2/2204 (0.1%)
2	F	0.34	0/1632	0.64	2/2204 (0.1%)
2	H	0.34	0/1632	0.64	2/2204 (0.1%)
2	J	0.34	0/1632	0.64	2/2204 (0.1%)
2	L	0.34	0/1632	0.64	2/2204 (0.1%)
2	N	0.34	0/1632	0.64	2/2204 (0.1%)
2	P	0.34	0/1632	0.64	2/2204 (0.1%)
2	R	0.34	0/1632	0.64	2/2204 (0.1%)
2	T	0.34	0/1632	0.64	2/2204 (0.1%)
2	V	0.34	0/1632	0.64	2/2204 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	X	0.34	0/1632	0.64	2/2204 (0.1%)
2	Z	0.34	0/1632	0.64	2/2204 (0.1%)
2	b	0.34	0/1632	0.64	2/2204 (0.1%)
2	d	0.34	0/1632	0.64	2/2204 (0.1%)
2	f	0.34	0/1632	0.64	2/2204 (0.1%)
2	h	0.34	0/1632	0.64	2/2204 (0.1%)
2	j	0.34	0/1632	0.64	2/2204 (0.1%)
2	l	0.34	0/1632	0.64	2/2204 (0.1%)
2	n	0.34	0/1632	0.64	2/2204 (0.1%)
2	p	0.34	0/1632	0.64	2/2204 (0.1%)
2	r	0.34	0/1632	0.64	2/2204 (0.1%)
2	t	0.34	0/1632	0.64	2/2204 (0.1%)
All	All	0.40	0/71231	0.64	92/96439 (0.1%)

There are no bond length outliers.

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	360	GLU	CA-CB-CG	7.61	129.32	114.10
2	H	360	GLU	CA-CB-CG	7.61	129.31	114.10
2	p	360	GLU	CA-CB-CG	7.61	129.31	114.10
2	V	360	GLU	CA-CB-CG	7.60	129.30	114.10
2	f	360	GLU	CA-CB-CG	7.60	129.30	114.10

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	A	1437	0	1434	34	0
1	C	1437	0	1434	31	0
1	E	1437	0	1434	26	0
1	G	1437	0	1434	26	0
1	I	1437	0	1434	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1437	0	1434	32	0
1	M	1437	0	1434	50	0
1	O	1437	0	1434	21	0
1	Q	1437	0	1434	19	0
1	S	1437	0	1434	23	0
1	U	1437	0	1434	26	0
1	W	1437	0	1434	24	0
1	Y	1437	0	1434	25	0
1	a	1437	0	1434	34	0
1	c	1437	0	1434	30	0
1	e	1437	0	1434	31	0
1	g	1437	0	1434	26	0
1	i	1437	0	1434	25	0
1	k	1437	0	1434	26	0
1	m	1437	0	1434	24	0
1	o	1437	0	1434	26	0
1	q	1437	0	1434	27	0
1	s	1437	0	1434	28	0
2	B	1600	0	1580	23	0
2	D	1600	0	1580	27	0
2	F	1600	0	1580	24	0
2	H	1600	0	1580	19	0
2	J	1600	0	1580	27	0
2	L	1600	0	1580	18	0
2	N	1600	0	1580	19	0
2	P	1600	0	1580	17	0
2	R	1600	0	1580	18	0
2	T	1600	0	1580	19	0
2	V	1600	0	1580	18	0
2	X	1600	0	1580	20	0
2	Z	1600	0	1580	21	0
2	b	1600	0	1580	23	0
2	d	1600	0	1580	20	0
2	f	1600	0	1580	19	0
2	h	1600	0	1580	18	0
2	j	1600	0	1580	17	0
2	l	1600	0	1580	18	0
2	n	1600	0	1580	18	0
2	p	1600	0	1580	20	0
2	r	1600	0	1580	18	0
2	t	1600	0	1580	21	0
All	All	69851	0	69322	936	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 7.

The worst 5 of 936 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:J:213:ARG:HE	1:M:201:PRO:HB3	1.49	0.76
1:a:112:ARG:HG3	1:c:82:ARG:HH22	1.54	0.71
1:I:98:PRO:HB3	1:M:99:ARG:NH2	2.04	0.71
1:K:127:ARG:HH21	1:M:119:THR:HG21	1.56	0.69
1:K:112:ARG:HG3	1:O:82:ARG:HH22	1.57	0.69

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	C	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	E	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	G	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	I	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	K	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	M	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	O	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	Q	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	S	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	U	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	W	182/252 (72%)	171 (94%)	11 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	a	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	c	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	e	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	g	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	i	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	k	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	m	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	o	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	q	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
1	s	182/252 (72%)	171 (94%)	11 (6%)	0	100	100
2	B	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	D	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	F	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	H	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	J	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	L	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	N	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	P	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	R	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	T	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	V	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	X	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	Z	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	b	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	d	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	f	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	h	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	j	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	l	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	n	192/392 (49%)	179 (93%)	13 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	p	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	r	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
2	t	192/392 (49%)	179 (93%)	13 (7%)	0	100	100
All	All	8602/14812 (58%)	8050 (94%)	552 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	A	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	C	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	E	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	G	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	I	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	K	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	M	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	O	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	Q	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	S	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	U	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	W	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	Y	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	a	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	c	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	e	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	g	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	i	157/215 (73%)	152 (97%)	5 (3%)	34	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	k	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	m	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	o	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	q	157/215 (73%)	152 (97%)	5 (3%)	34	59
1	s	157/215 (73%)	152 (97%)	5 (3%)	34	59
2	B	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	D	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	F	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	H	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	J	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	L	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	N	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	P	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	R	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	T	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	V	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	X	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	Z	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	b	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	d	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	f	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	h	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	j	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	l	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	n	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	p	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	r	167/337 (50%)	161 (96%)	6 (4%)	31	57
2	t	167/337 (50%)	161 (96%)	6 (4%)	31	57
All	All	7452/12696 (59%)	7199 (97%)	253 (3%)	33	57

5 of 253 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	V	192	LYS
1	o	44	ILE
1	a	30	GLU
2	n	360	GLU
2	r	192	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	k	76	GLN
2	t	224	ASN
2	l	224	ASN
1	q	76	GLN
2	L	224	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

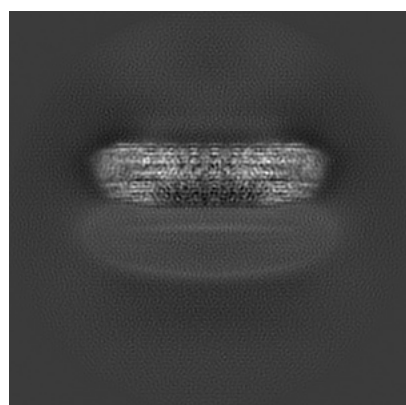
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20833. These allow visual inspection of the internal detail of the map and identification of artifacts.

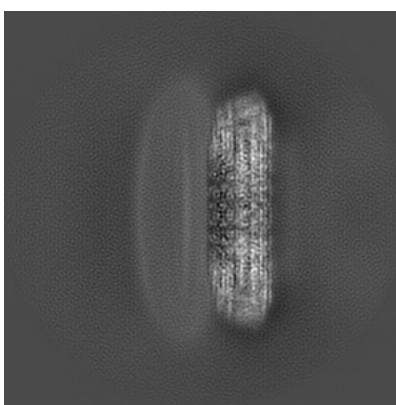
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

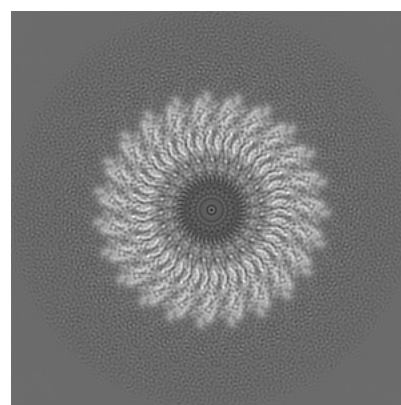
6.1.1 Primary map



X



Y

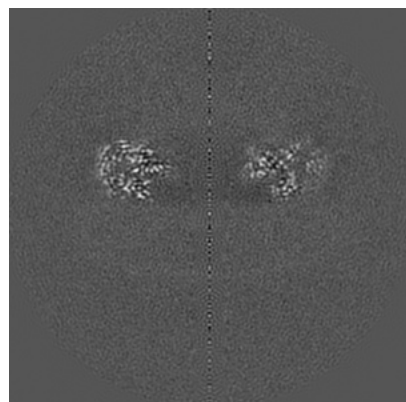


Z

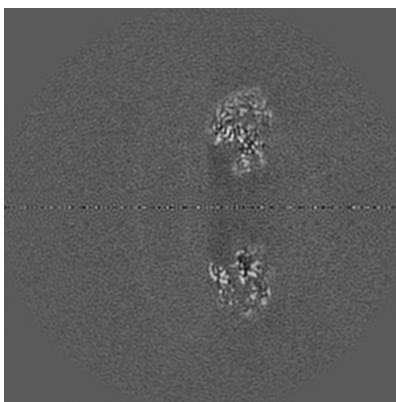
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

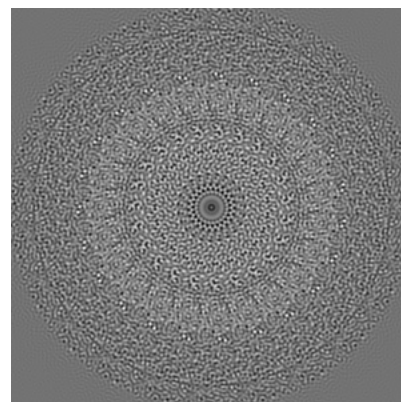
6.2.1 Primary map



X Index: 180



Y Index: 180

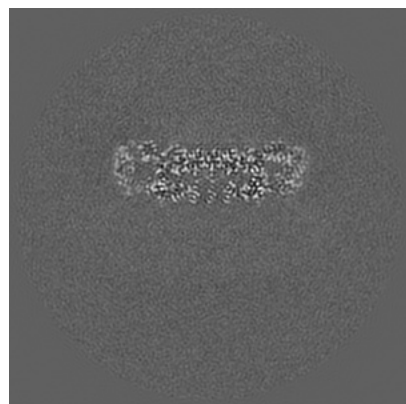


Z Index: 180

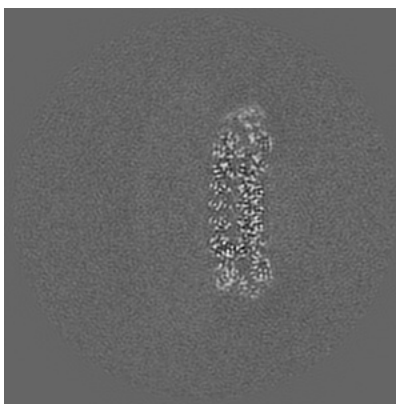
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

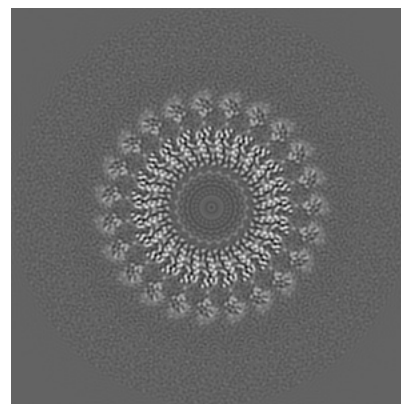
6.3.1 Primary map



X Index: 126



Y Index: 125

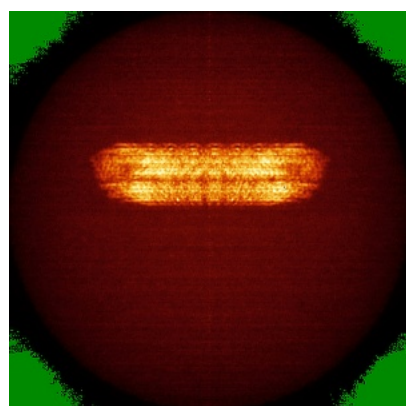


Z Index: 214

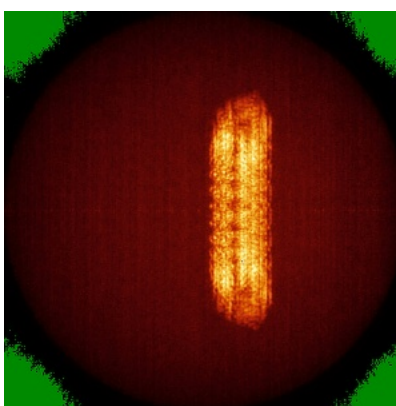
The images above show the largest variance slices of the map in three orthogonal directions.

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

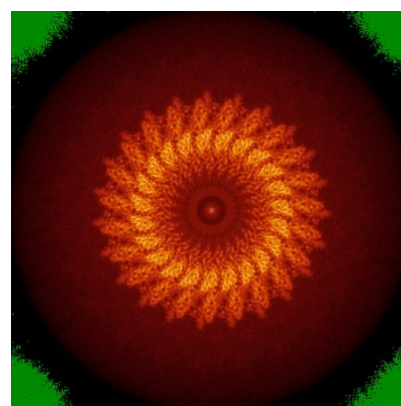
6.4.1 Primary map



X



Y

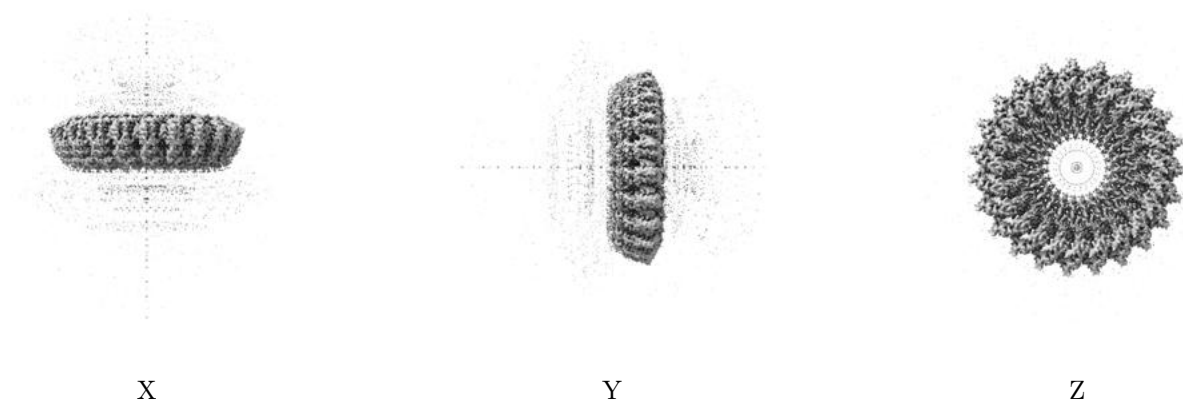


Z

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

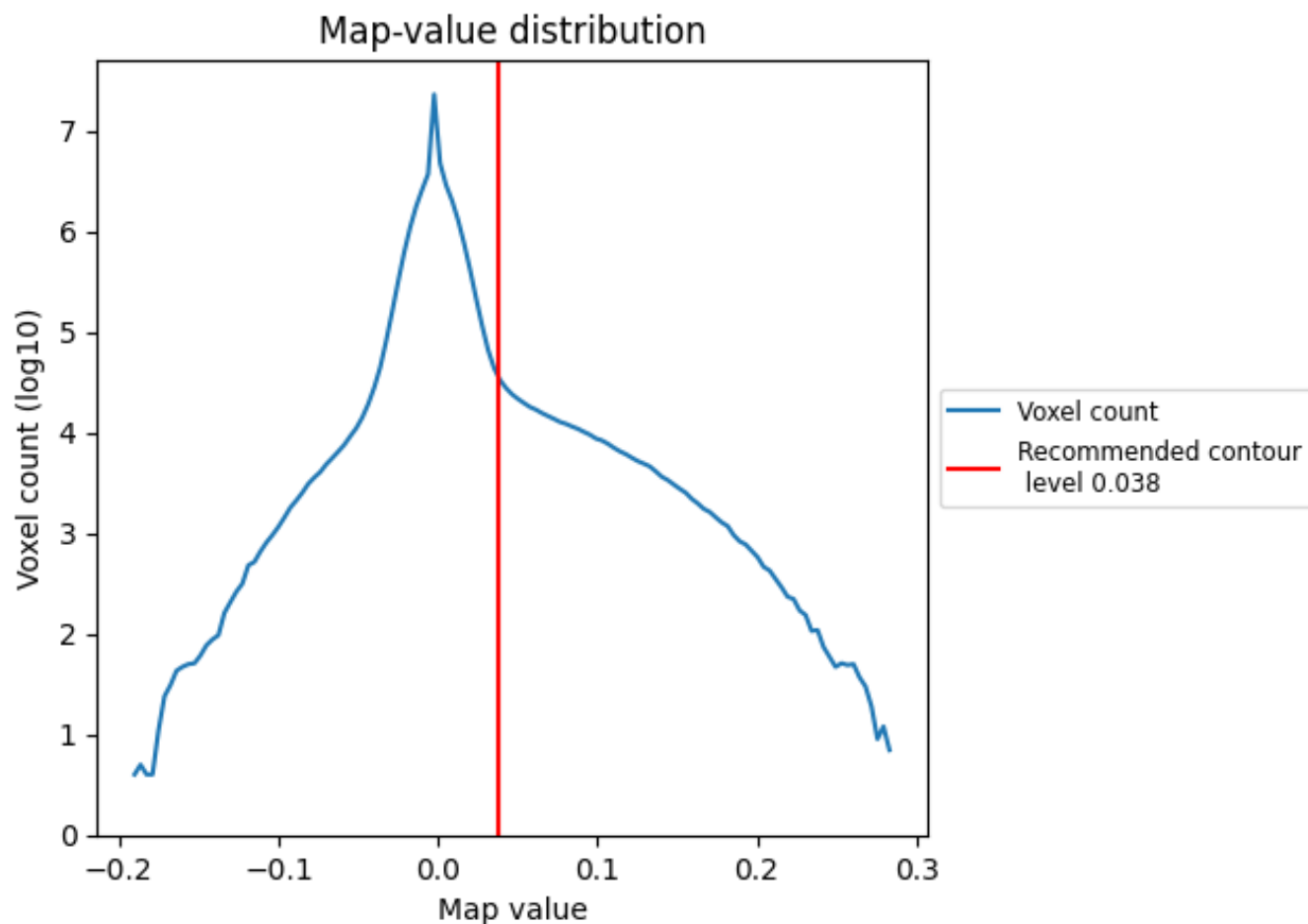
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

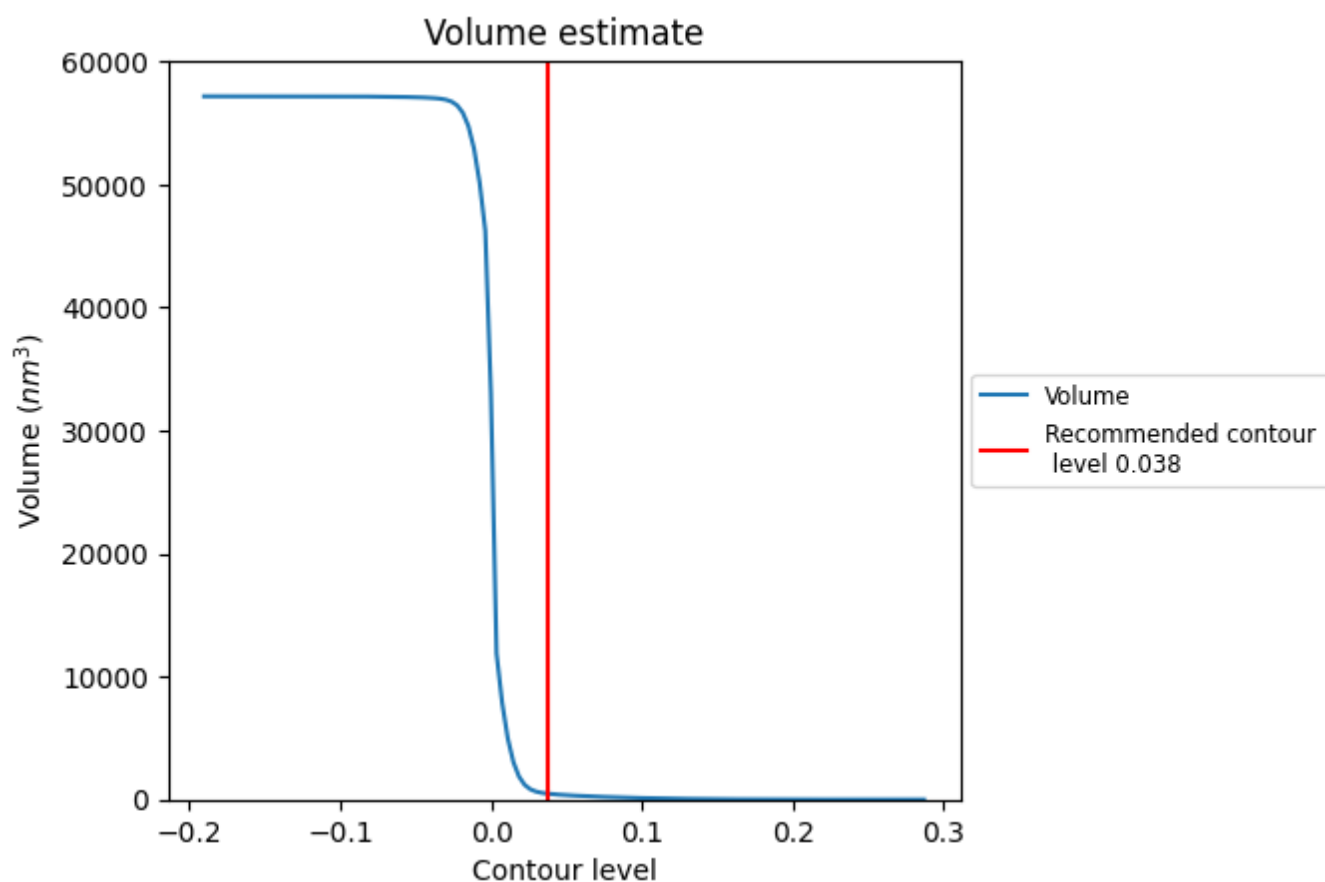
This section contains the results of statistical analysis of the map.

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.

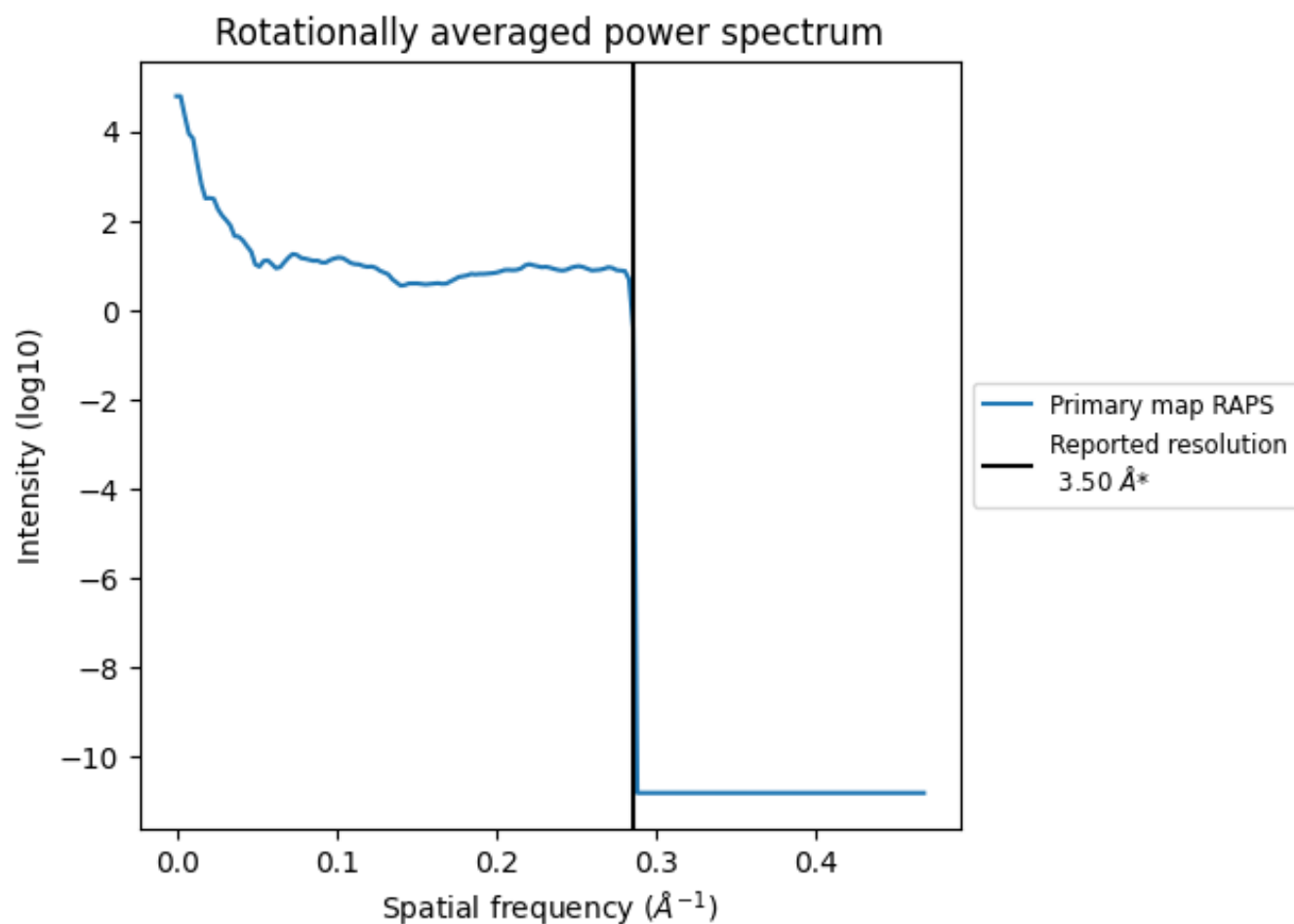
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 474 nm³; this corresponds to an approximate mass of 428 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 ⓘ

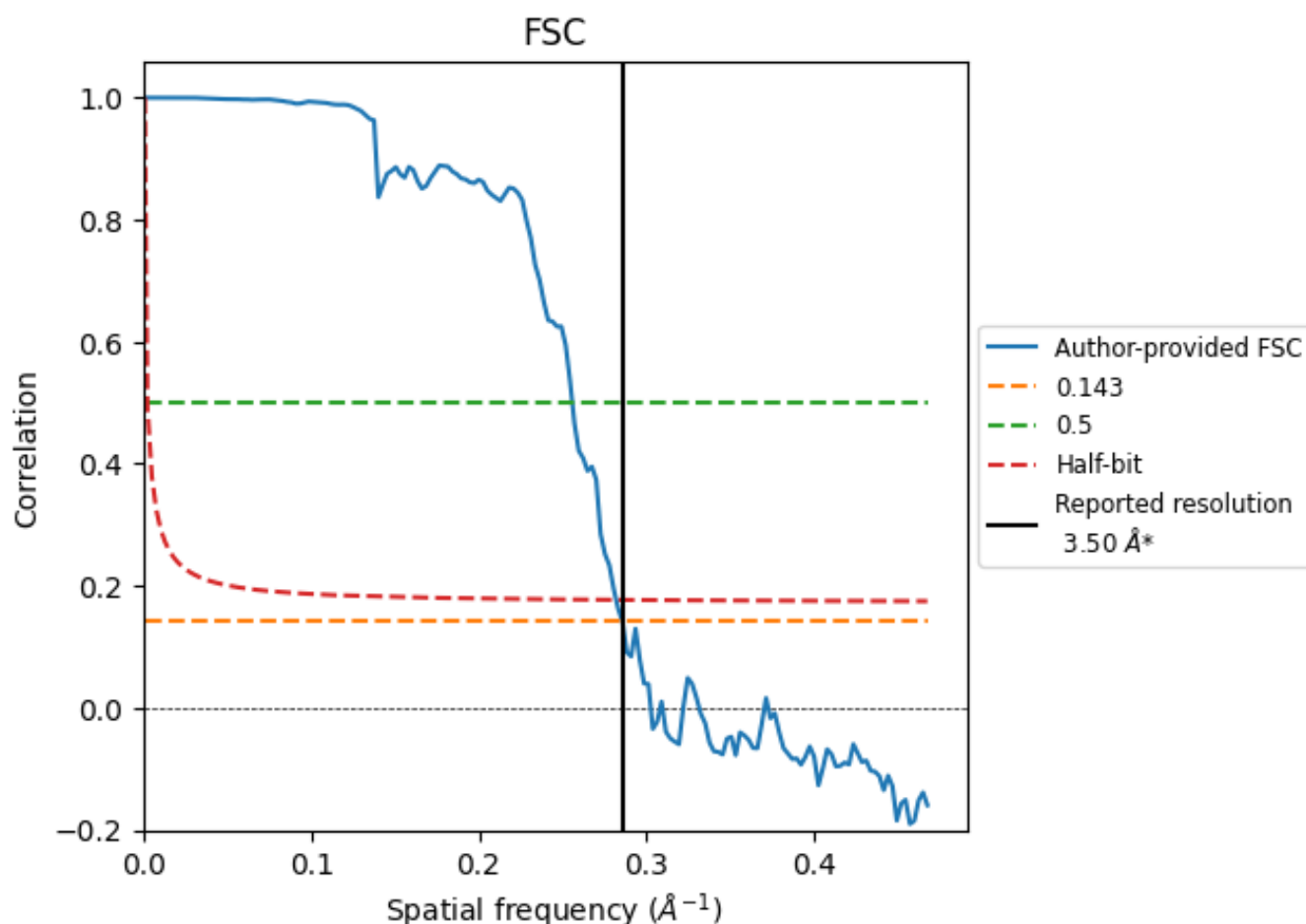


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

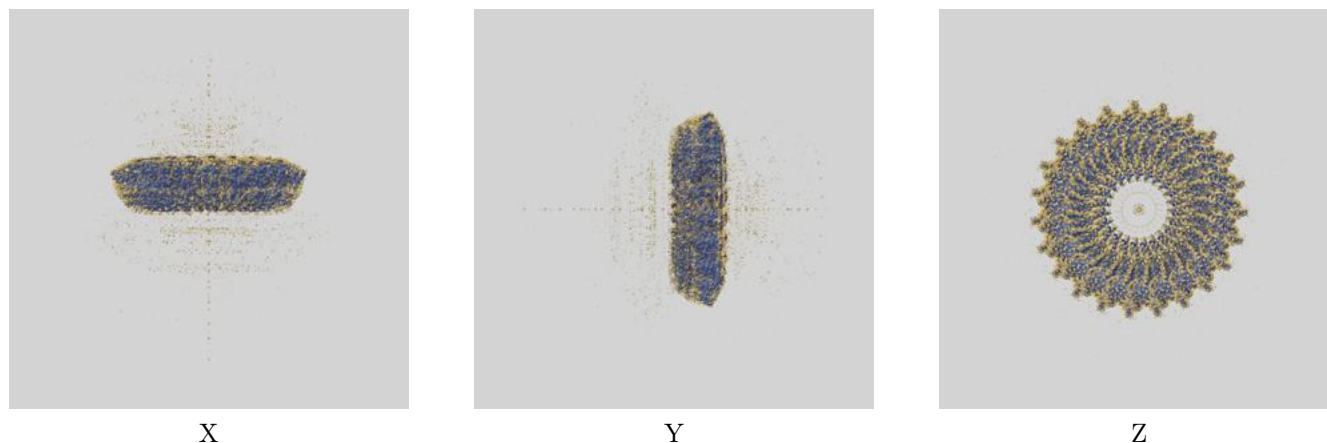
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	3.91	3.55
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

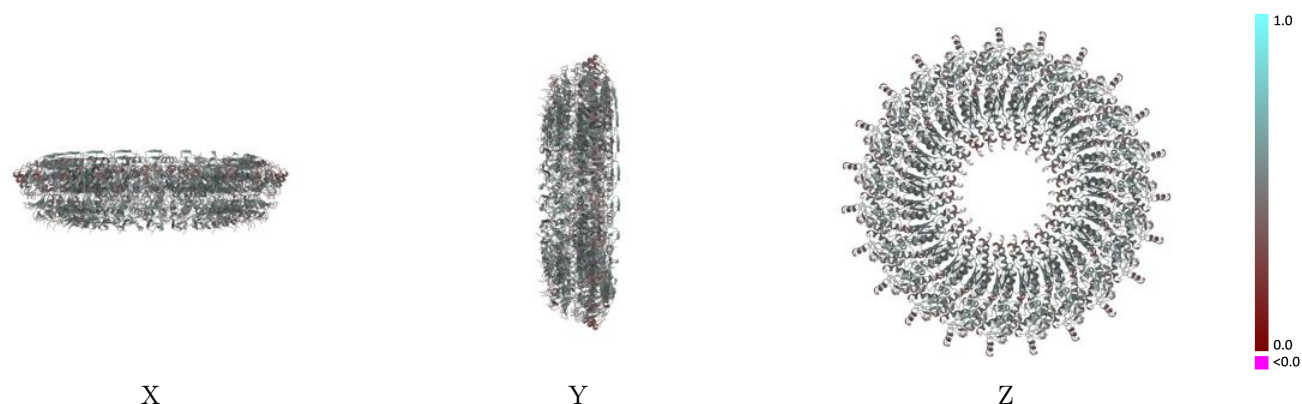
This section contains information regarding the fit between EMDB map EMD-20833 and PDB model 6UOV. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



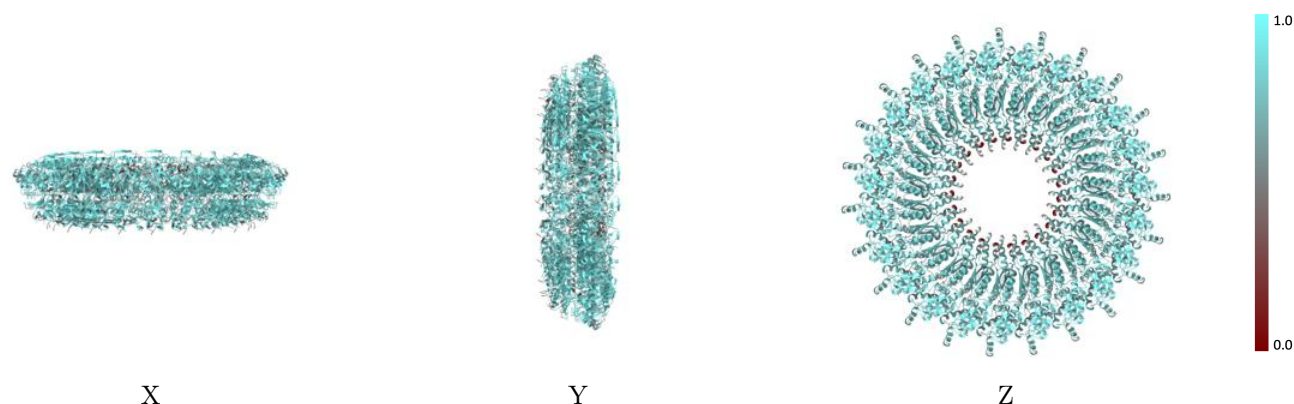
The images above show the 3D surface view of the map at the recommended contour level 0.038 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



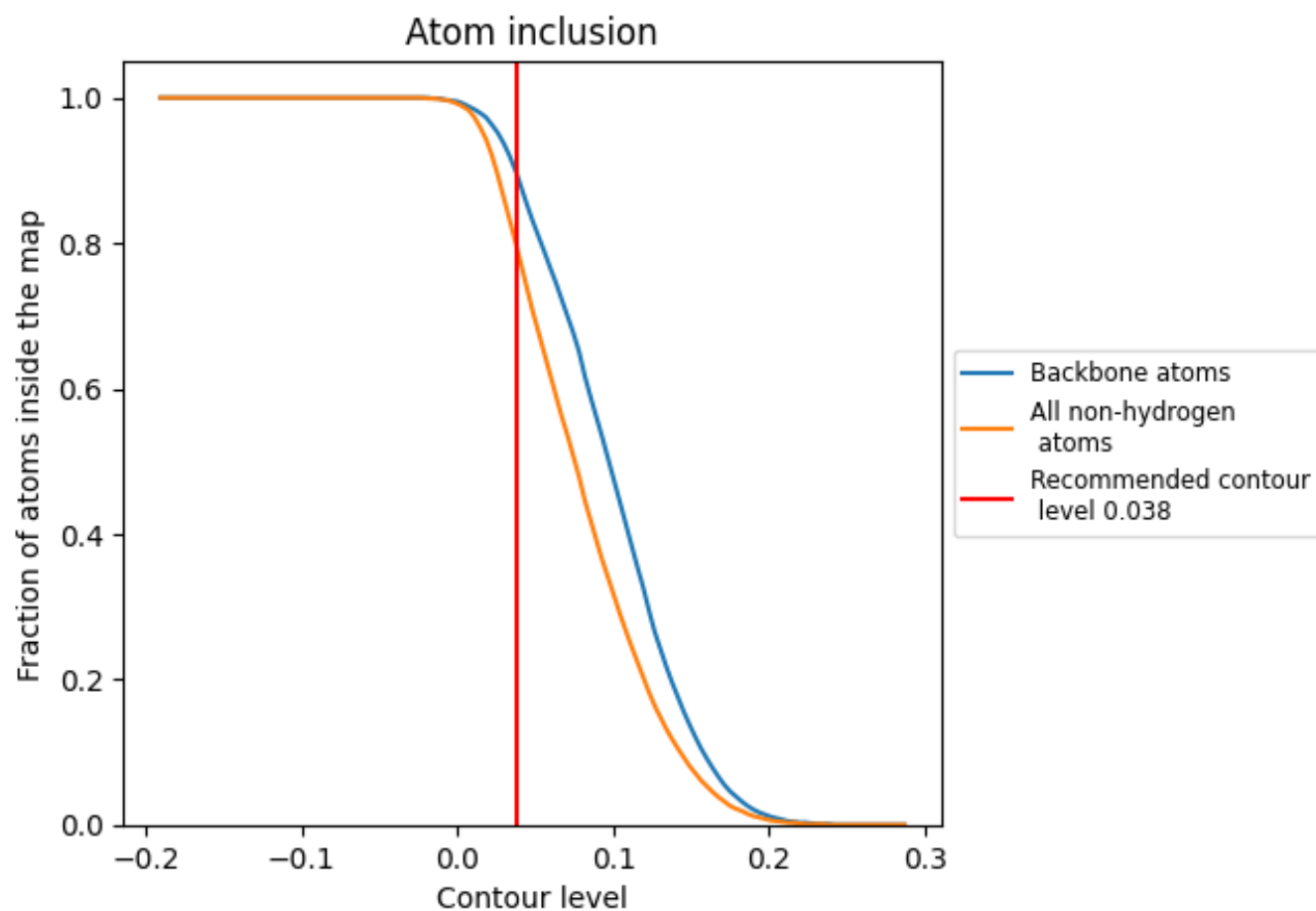
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.038).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 80% 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 (0.038) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7970	 0.4900
A	 0.7920	 0.5020
B	 0.8000	 0.4800
C	 0.7930	 0.5030
D	 0.8000	 0.4790
E	 0.7830	 0.5000
F	 0.8090	 0.4780
G	 0.7930	 0.5000
H	 0.8100	 0.4790
I	 0.7860	 0.5000
J	 0.8080	 0.4800
K	 0.7840	 0.5020
L	 0.8100	 0.4770
M	 0.7710	 0.4770
N	 0.8100	 0.4770
O	 0.7900	 0.5020
P	 0.8130	 0.4790
Q	 0.7900	 0.5040
R	 0.8050	 0.4790
S	 0.7830	 0.5040
T	 0.8110	 0.4790
U	 0.7880	 0.5030
V	 0.8050	 0.4790
W	 0.7880	 0.5030
X	 0.8120	 0.4780
Y	 0.7880	 0.5030
Z	 0.8020	 0.4810
a	 0.7880	 0.5000
b	 0.8050	 0.4820
c	 0.7910	 0.5040
d	 0.7980	 0.4810
e	 0.7880	 0.5000
f	 0.8010	 0.4810
g	 0.7890	 0.5020
h	 0.8020	 0.4820



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.7850	 0.4960
j	 0.8040	 0.4790
k	 0.7850	 0.5020
l	 0.8030	 0.4810
m	 0.7850	 0.5040
n	 0.8040	 0.4810
o	 0.7900	 0.5020
p	 0.7990	 0.4800
q	 0.7930	 0.5030
r	 0.8060	 0.4790
s	 0.7890	 0.5020
t	 0.8110	 0.4780