

wwPDB EM Validation Summary Report (i)

Nov 6, 2023 – 03:43 pm GMT

PDB ID	:	8PHR
EMDB ID	:	EMD-17672
Title	:	Middle part of the Borrelia bacteriophage BB1 procapsid, tenfold-symmetrized
		outer shell
Authors	:	Rumnieks, J.; Fuzik, T.; Tars, K.
Deposited on	:	2023-06-20
Resolution	:	2.65 Å(reported)
Based on initial model	:	

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 (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 2.65 Å.

Ramachandran outliers

Sidechain outliers

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	Percentile Ranks	Value
Ramachandran outliers		0
Sidechain outliers		0
Worse	Better	
Percentile relati	ive to all structures	
Percentile relation	ive to all EM structures	
Motric	Whole archive	EM structures
wiethc	(# Entries)	(# Entries)

154571

154315

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

4023

3826

Mol	Chain	Length	Quality of chain
1	А	319	98% •
1	В	319	98% •
1	С	319	98% •
1	J	319	98% •
1	Κ	319	98% •
1	L	319	98% •
1	S	319	98% •
1	Т	319	98% •
1	U	319	98%
1	b	319	98%



Mol	Chain	Length	Quality of chain	
1	с	319	98%	•
1	d	319	98%	•
1	k	319	98%	
1	m	319	98%	•
1	О	319	98%	
2	D	185	83%	17%
2	Е	185	85%	15%
2	Ν	185	82%	18%
2	Ο	185	83%	17%
2	V	185	83%	17%
2	W	185	85%	15%
2	f	185	82%	18%
2	g	185	83%	17%
3	F	190	90%	10%
3	М	190	90%	10%
3	Х	190	90%	10%
3	е	190	90%	10%
4	G	230	17% 83%	
4	Н	230	16% 84%	
4	Ι	230	16% 84%	
4	Р	230	17% 83%	
4	Q	230	16% 84%	
4	R	230	16% 84%	
4	Y	230	17% 83%	
4	Z	230	16% 84%	
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Mol	Chain	Length	Quality of chain
4	a	230	16% 84%
4	h	230	17% 83%
4	i	230	16% 84%
4	j	230	16% 84%
4	1	230	16% 84%
4	n	230	17% 83%
4	р	230	16% 84%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 57317 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Δ	919	Total	С	Ν	0	S	0	0
1	A	313	2510	1616	404	481	9	0	0
1	D	919	Total	С	Ν	0	S	0	0
1	D	313	2510	1616	404	481	9	0	0
1	С	212	Total	С	Ν	0	S	0	0
1	U	515	2510	1616	404	481	9	0	0
1	Т	313	Total	С	Ν	Ο	\mathbf{S}	0	Ο
1	0	515	2510	1616	404	481	9	0	0
1	K	313	Total	С	Ν	Ο	\mathbf{S}	0	0
		515	2510	1616	404	481	9	0	0
1	T.	313	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
		515	2510	1616	404	481	9	0	0
1	S	313	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
	5	515	2510	1616	404	481	9	0	0
1	Т	313	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
		515	2510	1616	404	481	9	0	0
1	U	313	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
-	0	515	2510	1616	404	481	9	0	0
1	h	313	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
-		515	2510	1616	404	481	9	0	0
1	C	313	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
-	C	515	2510	1616	404	481	9	0	0
1	d	313	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
1	u	515	2510	1616	404	481	9	0	0
1	k	313	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
1	К	515	2510	1616	404	481	9	0	0
1	m	313	Total	C	N	Ō	S	0	0
	111	515	2510	1616	404	481	9		0
1	0	313	Total	C	Ν	0	S	0	0
	0	515	2510	1616	404	481	9		0

• Molecule 1 is a protein called Major capsid protein.

• Molecule 2 is a protein called Decorator protein P03.



Mol	Chain	Residues		At	oms			AltConf	Trace					
2	а	152	Total	С	Ν	0	S	0	0					
	D	155	1161	730	194	233	4	0	0					
2	F	159	Total	С	Ν	0	S	0	0					
		156	1198	750	202	242	4	0	0					
2	N	151	Total	С	Ν	0	S	0	0					
	IN	151	1148	721	192	231	4	0						
2	0	0	0	0	0	0	154	Total	С	Ν	0	S	0	0
	0	104	1173	739	196	234	4	0	0					
2	V	153	Total	С	Ν	0	S	Ο	0					
	v		1161	730	194	233	4	0	0					
2	W	158	Total	С	Ν	0	\mathbf{S}	0	0					
	vv	156	1198	750	202	242	4	0	0					
2	f	151	Total	С	Ν	0	\mathbf{S}	0	0					
		101	1148	721	192	231	4							
2	ď	154	Total	С	Ν	0	S	0	0					
	g	104	1173	739	196	234	4							

• Molecule 3 is a protein called Decorator protein P05.

Mol	Chain	Residues	Atoms				AltConf	Trace		
2 F	171	Total	С	Ν	0	S	0	0		
0	Г	1/1	1358	865	231	260	2	0	0	
3	М	м	171	Total	С	Ν	0	S	0	0
3 M	1/1	1358	865	231	260	2	0	0		
2	v	171	Total	С	Ν	0	S	0	0	
	1/1	1358	865	231	260	2	0	0		
3	0	1.71	Total	С	Ν	0	S	0	0	
	е	1/1	1358	865	231	260	2	0	0	

• Molecule 4 is a protein called Scaffold protein.

Mol	Chain	Residues		Aton	ns		AltConf	Trace
4	C	40	Total	С	Ν	0	0	0
4	G	40	345	221	64	60	0	0
4	н	37	Total	С	Ν	0	0	0
4	11	57	315	203	55	57	0	0
4	T	37	Total	С	Ν	0	0	0
4	I		315	203	55	57	0	0
4	D	40	Total	С	Ν	0	0	0
4	1	40	345	221	64	60	0	0
4	0	37	Total	С	Ν	0	0	0
4	4 Q	51	315	203	55	57	0	0
4	В	37	Total	C	N	0	0	0
	37	315	203	55	57	0	U	



Mol	Chain	Residues	Atoms				AltConf	Trace	
4	V	40	Total	С	Ν	0	0	0	
4	I	40	345	221	64	60	0	0	
4	7	27	Total	С	Ν	0	0	0	
4	Z	51	315	203	55	57	0	0	
4	0	27	Total	С	Ν	0	0	0	
4	a	51	315	203	55	57	0	0	
4	4 h	40	Total	С	Ν	0	0	0	
4		40	345	221	64	60	0	0	
4	;	;	; 37	Total	С	Ν	0	0	0
4	1	51	315	203	55	57	0	0	
4	;	27	Total	С	Ν	0	0	0	
4	J	51	315	203	55	57	0	0	
4	1	37	Total	С	Ν	0	0	0	
4	1	51	315	203	55	57	0	0	
4	n	40	Total	С	Ν	0	0	0	
4 II	40	345	221	64	60	0	0		
4	n	37	Total	С	Ν	0	0	0	
4	р	37	315	203	55	57	U	U	

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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. 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. 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: Major capsid protein

Chain A:	98% •
MET GLU L3 ALA ALA ALA GLY GLY S319 S319	
• Molecule 1: Major capsid protein	
Chain B:	98% •
MET GLU L3 L3 A1A A1A A1A A1A A1A A218 GLY GLY S319	
• Molecule 1: Major capsid protein	
Chain C:	98% •
MET GLU L3 A218 A1A A1A A1A A12 GLN GLN GLN 3319	
• Molecule 1: Major capsid protein	
Chain J:	98% •
MET GLU L3 A1A A1A A1A A1A A1A A23 GLN GLN GLN S319	
• Molecule 1: Major capsid protein	
Chain K:	98% •
MET GLU L3 A12 A12 A12 A12 GLN GLN GLN S319 S319	
• Molecule 1: Major capsid protein	
Chain L:	98% .





• Molecule 1: Major capsid protein

Chain S:	98% •
MET GLU LU LA A218 A13 CLN A223 A223 19	
• Molecule 1: Major capsid protein	
Chain T:	98% .
MET GIU L3 ALA ALA GLY GLY S319 S319	
• Molecule 1: Major capsid protein	
Chain U:	98% .
MET GLU 134 ALA ALA ALA ALA ALA AL2 S319 S319	
• Molecule 1: Major capsid protein	
Chain b:	98%
MET GLU L3 A1218 A1218 A124 CLN A223 A223 19	
• Molecule 1: Major capsid protein	
Chain c:	98% .
MET GLU L3 ALA ALA ALA ALA GLY S319 S319	
• Molecule 1: Major capsid protein	
Chain d:	98% •
MET GJU L3 A218 A1A A1A A1A A23 A23 S319	
• Molecule 1: Major capsid protein	
Chain k:	98% •





• Molecule 1: Major capsid protein

Chain m:	98%	·
MET GLU L3 A218 ALA ALA ALA	GLY A223 Sale	
• Molecule	e 1: Major capsid protein	
Chain o:	98%	
MET GLU L3 A218 ALA ALA ALA	GLY A223 S319 S319	
• Molecule	e 2: Decorator protein P03	
Chain D:	83%	17%
MET SER ASP ASP ILE LYS ILE	CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	
• Molecule	e 2: Decorator protein P03	
Chain E:	85%	15%
MET SER ASP ASP ILE LYS ILE	GLU CIU VIS VIS VIS VIS CIU CIU CIU CIU CIU CIU CIU CIU CIU CIU	
• Molecule	e 2: Decorator protein P03	
Chain N:	82%	18%
MET SER ASP ILE LYS ILE	CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	
• Molecule	e 2: Decorator protein P03	
Chain O:	83%	17%
MET SER ASP ASP ILE LYS ILE	CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	
• Molecule	e 2: Decorator protein P03	
Chain V:	83%	17%



MET SER TLSP TLSP TLS TLS TLS CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	V131 V148 THR ALA ALA ALA ALA ALA CLY CLYS GLY GLY	
• Molecule 2: Decorator protein P03		
Chain W:	85%	15%
MET SER SER TLE TLE TLE TLY CVS CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	K163 A B LTRS CLY CLY	
• Molecule 2: Decorator protein P03		
Chain f: 829	%	18%
MET MET ASP THR ASP LYS LYS CLU GLU CLY CLYS CLY ASP ALA ALA ALA ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	ASN GLY V131 THR THR GLN GLN CLN CLN CLN CLN CLN GLN CLN GLN GLN	
• Molecule 2: Decorator protein P03		
Chain g:	3%	17%
MET SER SER SER SER THR THR THR CVS CLVS CLVS CLVS CLVS CLVS CLV CLVS CLV CLVS CLV CLS CLV CLS CLV CLS CLV CLS CLV CLS CLS CLS CLS CLS CLS CLS CLS CLS CLS	CLY V131 V148 THR CLY ALA ALA ALA ALA ALA ALA CLY CLY CLY CLY CLY CLY CLY	
• Molecule 3: Decorator protein P05		
Chain F:	90%	10%
MET ASP ASP ASP ASP Q78 Q78 Q18 ALU ALU ALU ALA ASP ALA ASP ASP ASP ASP ASP ASP ASP ASS ASP ASP	ASN	
• Molecule 3: Decorator protein P05		
Chain M:	90%	10%
MET ASP ASP ASP Q78 Q78 Q18 ALU ALU ALU ALA ASP ASP ASP ASP ASP ASP ASP ASS ASP ASS ASP ASS ASP ASS ASP ASS ASP ASS ASP ASS ASP ASS ASP ASP	ASN	
• Molecule 3: Decorator protein P05		
Chain X:	90%	10%
MET MET ASP ASP ASP Q78 Q78 Q178 Q178 ASS ASS ASS ASS ASS ASS ALA ASS ALA ASS ASS	ASN	
• Molecule 3: Decorator protein P05		
Chain e:	90%	10%



Chain G:

83%



• Molecule 4: Scaffold protein

17%

LLEU VALL PHE PTHE PTHE GGLU GGLU GGLU GGLU TILLE CLYS SGLN AALA AALA AASN CLUYS SCRR LLEU CLUYS SCRR LLEU CLUYS SCRR LLEU CLUYS SCRR LLEU AASSCR LLEU CLUYS SCRR LLEU AASSCR LLEU VALL CLUSS SCRR SCRR AASSCR CLUYS SCRR AASSCR AASSCR CLUYS SCRR AASSCR CLUYS SCRR AASSCR CLUYS SCRR AASSCR CLUYS SCRR AASSCR AASSCR CLUYS SCRR AASSCR A ILE LYS SER GLU GLU GLU THR SER ILE ALA • Molecule 4: Scaffold protein Chain H: 16% 84% ILE LYS SER SER GLU GLU GLU HIS LYS ARG ARG SER SER ILE • Molecule 4: Scaffold protein Chain I: 16% 84% LIYS addition of the second of ILE LYS SER GLU GLU ARC ARC ARC SEF SEF AL/

• Molecule 4: Scaffold protein

Chain P: 17%

83%



MET THE CLVS CLVS CLVS CLVS CLVS CLVS CLVS CLVS
LYS LEVE ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
LEU LAN LAN LYS LYS LYS LYS LYS LYS LAN TLE CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
LICE SER ALB7 THR THR SER ALA
• Molecule 4: Scaffold protein
Chain Q: 16% 84%
MRT MRT CLUU CLUU CLUU CLUU CLUU CLUU CLUU CLU
LYS LYS ALA ALA ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
LEU VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL
ILE SER SER ARG AI87 AI87 AI87 AIA ALA ALA
• Molecule 4: Scaffold protein
Chain R: 16% 84%
MET MET MET CVS GLU GLU GLU GLU GLU GLU GLU CLNS CLNS CLNS CLNS CLNS CLNS CLNS CLNS
LYS LYS VAL VAL VAL VAL CLU VAL CLU CLU CLU CLU CLU CLU CLU CLU CLU CL
LEU LAN LAN LYS LYS LYS LYS LYS LYS LYS LUS CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN
ILE LVS SER ALB7 ALB7 ALB7 ALB7 ALA ALA ALA ALA
• Molecule 4: Scaffold protein
Chain Y: 17% 83%
MRT MRT CLUU CLUU CLUU CLUU CLUU CLUU CLUU CLU
LYS LYS ALA ALA VAL CULU VAL CULU ARG ARG ARG ARG ALA ARG CLU CLU ARD ARG CLU CLU ALA ALA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS
LLEU ARG ARG CGLN ARG CGLN ARG GLN GGLN CGLN CGLN CGLN CGLN CGLN CGLN





• Molecule 4: Scaffold protein

Chain Z:	16%	84%
MET THR GLU GLU GLU GLU ASP LEU LEU	GLN ALA GLN GLN ASP ASP GLU GLU CLN GLU THR THR THR THR THR THR THR CLU CLU SER VIL SER VIL CLU CLU	CLU TTR MET MET MET MET ARG CLU CLV CLV CLV CLV CLV CLV CLV SER ARG CLV CLV SER ARG CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV
LYS GLU GLU ALA GLU GLU GLU GLU GLU	ARG GLU GLU GLU GLN ILEU ILEU ILEU GLU GLU GLU ALA ARG ALA ARG ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	LEU LEU AISN PHE AISN PHE AISN AISN AISN CLYS CLYS CLYS THR THR THR THR THR THR AISA AISA AISA AISA AISA AISA AISA AIS
LEU VAL ARG LYS PHE PHE VAL PRO TLE GLU GLU	TILE LYS ALA LYS LYS ALA LYS SER SER SER SER SER SER CUV CUV CUV CUV CUV SER SER SER SER SER SER SER SER SER SER	LEU LATS VAL LATS VAL LASU LEU LEU LEU LAS ALS SER SER SER SER SER SER SER SER SER SE
ILE LYS SER GLU GLU GLU ARG A187 A187 A1223 HIS	LTE ARG THR SER ILE ALA	
• Molecule 4:	Scaffold protein	
Chain a:	16%	84%
MET THR GLU CYS GLU GLU GLU ASP LEU	dLA dLA dLA dSP dSP dSP dLU dLU dLA dLA dSP dLU SER SER SER SER SER SER SER SER SER SER	GLU MET MET MET MET MET MET ARG GLU GLU GLU GLU GLU ASR ASR ASR ASR ASR ASR ASR ASR ASR ASR
LYS GLU GLU ALA GLU GLU GLU GLU GLU	ARG CLU CLV CLV CLV CLN CLN CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	LEU SER ASN HIS ASN ASN ASN ASN ASN CUV VAL LEU VAL LEU VAL LEU CLY STAR ASP ASN ASP ASN ASN ALA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS
LEU VAL ARG LYS PHE PHE PRO TLE GLU GLN	11.1. LYS LYS LYS LYS SER SER SER SER SER SER SER CUY CUN CUN SER SER SER SER SER SER SER SER SER SER	LEU LYS VAL LYS VAL LYS LLEU LLEU LLEU LLEU LLEU ASN SER SER SER SER SER SER SER SER SER SER
ILE LYS SER GLU GLU GLU A187 A187 H1223 H12	LYS ARG TARG SER SER ILE ALA	
• Molecule 4:	Scaffold protein	
Chain h:	17%	83%
MET THR GLU CYS GLU GLU GLU ASP LEU	GLN GLN ASP ASP CLU CLN GLU GLU THR THR THR THR THR THR THR CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	GLU MET MET MET MET MET MET ARG ALN ALN ALN ALN CLU CLU SER ARG CLU CLU SER ARG CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
LYS GLU GLU ALA GLU GLU GLU GLU GLU	ARG CLU CLV CLV CLV CLN CLN CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	LEU SER ASN HIS ASN ASN ASN ASN ASN CUV VAL LEU VAL LEU VAL LEU CLY STAR ASP ASN ASP ASN ASN ALA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS
LEU VAL ARG LYS PHE PHE PRO TLE GLU GLU	LILE ALA ALA ALA ALA ALA LYS SER VAL ASP ASP ASP ASP ASP ASP ASP ASP ASP CLV GLV GLV GLV VAL	LEU LEU VAL VAL VAL ITE ILYS ARR ARR ARR SER SER SER SER SER SER SER SER SER S
ILE LYS SER GLU GLU GLU ARG A187 A187 THR	SER TLE ALA	

• Molecule 4: Scaffold protein

Chain i: 16%



MET THR GLU GLU GLU GLU GLU	LYS GLU ASP	LEU GLN GLN GLN	ASP LYS GLU	GLN GLN ILE	LYS ALA ASP	THR LYS VAI	ILE SER	VAL GLN GLU	PHE GLU	GLU TYR MET	ARG PHE	GLU GLU	ALA ASN	SER	SER LYS	GLU	ARG	ASP LEU	ILE ASN	GLU ARG	THR
LYS GLU LEU ALA GLU VAL	GLU GLU ARG	GLU ARG ILE GLU	LYS GLN LEU	LEU GLU ALA	GLU ARG ILE	ASN GLU TI F	ASP THR	LEU ALA LYS	ALA HIS	LEU SER ASN	HIS PHE	ASN LYS GLU	VAL LEU	LEU ALA	CLY CLY	THR	LEU	ASP ILE	GLN	GLN ARG	ARG GLU
LEU VAL ARG LYS PHE VAL	PRO ILE GLU	GLN ILE LYS ALA	ILE ALA LYS VAT	VAL SER ASP ILE	SER HIS ILE	ASP GLY CI II	TLEU	GLU GLN LEU	VAL SER	LEU ALA LYS	VAL ASN	LYS LYS	ARG LYS	ASN ALA	SER	SER	SER SER	ASP	I VS	GLY ASN	ILE ALA
ILE LYS SER GLU ARG	A187 R223	HIS LYS ARG THR	SER ILE ALA																		
• Molec	ule 4	: Sca	ffold	prot	ein																
Chain j:		16%	_			-	-	-	-	84%	-	-	-			-	-	-	_		
MET THR GLU LYS GLU GLU	LYS GLU ASP	LEU GLN GLN GLN	ASP GLU GLU	GLN GLN ILE	LYS ALA ASP	THR LYS VAI	TLE SER	VAL GLN GLU	PHE GLU	GLU TYR MET	ARG PHE	GLU GLN	ALA ASN	SER LYS	SER LYS	GLU	SER ARG	ASP LEU	ILE ASN	GLU ARG	THR
LYS GLU LEU ALA GLU VAL	GLU GLU ARG	GLU ARG ILE GLU	L EU L EU L EU	LEU GLU ALA	GLU ARG ILE	ASN GLU TIF	ASP THR	LEU ALA LYS	ALA HIS	LEU SER ASN	HIS PHE	LYS GLU	VAL LEU	LEU ALA	CLY GLY	THR	LEU	ASP ILE	GLN	GLN ARG	ARG GLU
LEU VAL ARG LYS PHE VAL	PRO ILE GLU	GLN ILE LYS ALA	ILE ALA LYS VAT	VAL SER ASP ILE	SER HIS ILE	GLY GLY	TLEU	GLU GLN LEU	VAL SER	LEU ALA LYS	VAL ASN	LEU	ARG LYS	ASN ALA	SER	SER	SER SER	ASP	JLE IVS	GLY ASN	ILE ALA
LLE LYS SER 3LU ARG	A187 1223	HIS LYS ARG THR	SER TLE ALA																		
• Molec	ule 4	: Sca	ffold	prot	ein																
• Molec Chain l:	ule 4	: Sca 16%	ffold	prot	ein					84%									_		
• Molec Chain l:	ule 4	: Sca 16%	ffold		ein ^{ALA} ASP	THR LYS VAI	ILE SER	VAL GLN GLU	PHE GLU	84% BTD WEL	ARG PHE	GLN GLU STN	ALA ASN	SER LYS	SER LYS	GLU THR	SER ARG	ASP LEU	SER ILE ASN	GLU ABG	ILE THR
Molec Chain l:	ule 4	: Sca 16% NY VIV 100 NY VIV 100 NY VIV 100 NY VIV	Hold CIN ASP CIN ASP C		GLU LYS ARG ALA ILE ASP	ASN THR GLU LYS TTE VAT	ASP ILE THR SER	LEU VAL ALA GLN LYS GLU	ALA PHE HIS GLU	LEU GLU 84% SER TYR ASN MET ASN	HIS ARG PHE PHE	ASN LYS LYS GLU GLU GLN	VAL ALA LEU ASN	LEU SER ALA LYS	LYS SER GLY LYS	TYR GLU THR THR	LEU SER LYS ARG	ASP ASP ILE LEU	MEI SEK GLN ILE AIA ASN	ALA ACH GLU ARG ABG	ARG ILE GLU THR
Molecc Chain 1: Law SATI 010 ATT 100	ule 4	: Sca	TLE LYS ASP ALA GLN LYS ASP LFU GLU VII CIII CIII	Protection of the second secon	HIS CLU LYS ARG ALA ALA ASP ASP ASP ASP ASP ASP ASP ASP ASP AS	ASP ASN THR GLY GLU LYS CTII TIF VAI	LEU THR SER	GLU LEU VAL GLN ALA GLN LEU LYS GLU	VAL ALA PHE SER HIS GLU	LEU LEU GLU 8 ALA SER TYR 8 LYS ASN MET	VAL HIS ARG ASN PHE PHE	LLE ASN LYS LYS LYS GLU LEU GLU GLN	ARG VAL ALA LYS LEU ASN	ASN LEU SER ALA ALA LYS	SER LYS SER SER GLY LYS	SER TYR GLU SER THR THR	SER LEU SER SER LYS ARG	VAL ASP ASP ASP LEU AND UND AND AND AND AND AND AND AND AND AND A	SEK MEI SEK ILE GLN ILE TLE GLN ASN	GLY GLN GLU ASIN ARG ARG	ILE ARG ILE ALA GLU THR
Molecc Chain 1: In 1:	187 PR0 GLU LYS 223 GLU ARG ASF	ISCA	LE LYS ASP LE LYS ASP LE LEU LYS ASP LEU LYS LEU LYN LYN LUN LYN LYN LYN L	AND LEG CLN ASP CLU CLN ASP CLU CLN ALL CLN CLN	ER GLU LYS HIS ARC ALA ILE ASP ASP	ASP ASN THR GLY GLU LYS CTT TTF VAL	TLE ASP TLE LEU THR SER	GLU LEU VAL GLN ALA GLN LEU LYS GLU	VAL ALA PHE SER HIS GLU	LEO LEO GLU 88 ALA SER TYR LYS ASN MET	VAL HIS ARC ASN PHE PHE	LLE ASN LYS LYS LYS GLU LEU GLU GLU	ARG VAL ALA LYS LEU ASN	ASN LEU SER ALA ALA LYS	SER LYS SER SER GLY LYS	SER TYR GLU SER THR THR THR THR	SER LEU SER SER LYS ARG	VAL ASP ASP ASP LEU ASP ASP	SEK MEI SEK ILE GLN ILE IVS ATA ASN	GLY GLN GLU ASN ARG ARG	ILE ARG ILE ALA GLU THR
Molec Chain l: Law End Street None None Molec	ule 4 august 1 august 1 augus	: Sca 16% 16% 178 178 178 178 178 178 178 178	ffold		ein HIS CU LYS HIS ARC ALA ILE ASP ein	ASP ASN THR GLY CLU LYS CTI TTE VAL	LLEU THR SER	GLU LEU VAL GLA ALA GLA LEU LYS GLU	VAL ALA PHE SER HIS GLU	88 010 021 021 84 UAL WSK VIA	VAL HIS ARC ASN PHE PHE	LLE ASN LYS LYS LYS GLU LEV GLU GEN	ARG VAL ALA LYS LEU ASN	ASN LEU SER ALA ALA LYS	SER LYS SER SER GLY LYS	SER TYR GLU SER THR THR THR	SER LEU SER SER LYS ARC	VAL ASP ASP ASP ILE LEU Ann unter ann	SER MEI SER ILE GLN TLE IVS AIA ASN	GLY GLM GLU ASN ARG ARG	ILE ARG ILE ALA GLU THR
Molec Chain 1: Multiple of the second se	ule 4	: Sca 16% NTD NTD NTD NTD NTD NTD NTD NTD NTD NTD	ffold are rise are r		ein BER GUU LVS HIS ARG ALA ILE ASP ein	ASP ASN THR GLY GLU LYS CUI TTF VAT	ILE ASP ILE LEU THR SER	GLU LEU VAL GLN ALA GLN LEU LEU LY GLU	VAL ALA PHE SER HIS CLU	84% JAW NSY SATI	VAL HIS ARG ASN PHE PHE	LLE ASN LVS LLE ASN LVS LEU GLU GLU	ARG VAL ALA LYS LEU ASN	ASN LEU SER ALA ALA LYS	SER LYS SER SER GLY LYS	SER TYR GLU SER THR THR THR	SER LEU SER SER LYS ARG	VAL ASP ASP ASP ILE LEU	SEK MEI SEK ILE GLN ILE IVS AIA ASN	CLU CLU CLV CLU ASIV ARG ARG	ILE ARG ILE ALA GLU THR
Molec Chain l:	ule 4	: Sca 16% NTP 211 NTP 211 NTP 211 STR 211	ffold are rate for rate are rate for rate for rate are rate for		ein REA CLU LYS HIS ARC ALA ILE ASP ein	RR ASP ASV THR (S CLY CLU LYS C CLY CLU LYS	THE ASP TLE	AL GLU LEU VAL LA GLU ALA GLA U LEU LYS GLU	HE VAL ALA PHE DU SER HIS GLU	84% JAN AND AND AND AND AND AND AND AND AND A	AG C VAL HIS ARG	TS LLE ASN LTS LU LLE ASN LTS L V CLU LEU CLU CLU	LA ARG VAL ALA SN LYS LEU ASN	ER ASN LEU SER (5 ALA ALA LYS	ER SER LYS SER (S SER GLY LYS	LU SER TYR GLU IR SER THR THR THR	ER LEU SER LEU SER LU SER LEU SER LEU SER LEU SER LEU SER L'YS ARG	NAL ASP ASP ALL ASP ASP AND ILE LEU AND AND AND AND AND AND AND AND AND AND	LE DE CAN DE SEK MEI SEK LE GLM ILE NY IVY ANN ANN	CU CLY CLN CLU CLY CLN CLU C ASN ARG ARG	LE ANG ILE ANG ILE ALA GLU THR
 Molec Chain l: Chain l: Chain l: Chain l: Chain l: N N	ule 4	: Sca 16% MID 019 NID 019	Here and the set of th		LYS LYS SER GLU LYS ARG ALA ASP US AS	THR ASP ASN THR LYS GLY GLU LYS VAT	THE ASP TIE ASP TIE SER	VAL GLU LEU VAL GLN GLN GLN GLN GLN GLU LEU LY GLU	PHE VAL ALA PHE CLU SER HIS CLU	84% AND THE TATE OF THE AND TH	ARC O VAL HIS ARC PHE ON VAL HIS ARC	LYS LYS LYS LYS LUS CLU	ALA ARG VAL ALA ASN LYS LEU ASN	SER ASN LEU SER LYS ALA ALA LYS	SER LYS SER LYS SER LYS LYS LYS SER CLY LYS	GLU SER TYR GLU THR SER THR THR THR THR THR THR	SER LEU SER LEU SER	ASP ASP VAL ASP ASP ILE LEU ADD ADD ASP ASP	ILE ILE CLA ILE CLA ILE ANA ASU ASU	ALLA ALLA ALLA ALLA ALLA ALLA ALLA ALL	ILE ARG ILE THR ALA GUU THR
Molec Chain l: Million Sillion for Million Sillion for Million Sillion for Molec Chain n Molec Chain n Million for Molec Chain n Million for Million for	ule 4 add draw argue ar	: Sca 16% 16% 10% 10% 10% 10% 10% 10% 10% 10	LYS ASP TIE LYS AS		ciu LYS SER CIU LYS ARC ALA ILE ASP UE ASP U	ASV THR ASP ASV THR GLU LYS GLU LYS TIE VAN CUI IIP VAN	ASP ILE ILE ILE ASP ILE THR SER LEU THR SER	LEU VAL GLU LEU VAL ALA GLN GLN ALA GLN LYS GLU LEU LYS GLU	ALA PHE VAL ALA PHE HIS 0LU SER HIS 0LU	84 UAL WAS VIT 833 AT WAS SALE AND CALL WAS SALE	HIS ARG OVAL HIS ARG PHE PHE ASIN PHE PHE ASIN PHE PHE ASIN PHE AS	ASN LTS LLE ASN LTS LYS GLU LYS CLU GLU GLU LEV GLU GLU	VAL ALA ARG VAL ALA LEU ASN LY LEU ASN	LEU SER ASN LEU SER ALA LYS ALA ALA LYS	LYS SER SER LYS SER LYS SER CLY LYS SER GLY LYS	TYR GLU SER TYR GLU THR THR SER THR THR THR THR THR THR	LEU SER SER SER LEU SER LEU SER	ASP ASP ASP VAL ASP	MEI SEK MEI SEK MEI SEK GLN ILE ILE GLN ILE AT A SEN TYS ASN	CLV GLU GLU GLU GLU ARG	ARG TLE ILE ARG TLE ARG TLE GLU THR GLU THR





• Molecule 4: Scaffold protein

 Chain p:
 16%
 84%

 Image: State of the sta





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D5	Depositor
Number of particles used	29011	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	44	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 (6k x 4k)	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).

Mal	Chain	Bond	lengths	Bond angles			
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	А	0.24	0/2558	0.42	0/3458		
1	В	0.24	0/2558	0.43	0/3458		
1	С	0.24	0/2558	0.42	0/3458		
1	J	0.24	0/2558	0.43	0/3458		
1	Κ	0.24	0/2558	0.42	0/3458		
1	L	0.24	0/2558	0.43	0/3458		
1	S	0.24	0/2558	0.42	0/3458		
1	Т	0.24	0/2558	0.43	0/3458		
1	U	0.24	0/2558	0.42	0/3458		
1	b	0.24	0/2558	0.42	0/3458		
1	с	0.24	0/2558	0.42	0/3458		
1	d	0.24	0/2558	0.43	0/3458		
1	k	0.24	0/2558	0.43	0/3458		
1	m	0.24	0/2558	0.42	0/3458		
1	0	0.24	0/2558	0.42	0/3458		
2	D	0.24	0/1178	0.45	0/1586		
2	Е	0.24	0/1216	0.44	0/1637		
2	N	0.24	0/1165	0.43	0/1568		
2	0	0.24	0/1190	0.44	0/1601		
2	V	0.24	0/1178	0.45	0/1586		
2	W	0.24	0/1216	0.44	0/1637		
2	f	0.24	0/1165	0.44	0/1568		
2	g	0.24	0/1190	0.44	0/1601		
3	F	0.24	0/1381	0.45	0/1855		
3	М	0.24	0/1381	0.45	0/1855		
3	Х	0.24	0/1381	0.45	0/1855		
3	е	0.24	0/1381	0.45	0/1855		
4	G	0.24	0/352	0.46	0/472		
4	Н	0.25	0/321	0.43	0/432		
4	Ι	0.25	0/321	0.42	0/432		
4	Р	0.24	0/352	0.45	0/472		
4	Q	0.25	0/321	0.43	0/432		
4	R	0.25	0/321	0.43	0/432		
4	Y	0.24	0/352	0.46	0/472		



Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ # Z > 5		RMSZ	# Z > 5	
4	Ζ	0.25	0/321	0.43	0/432	
4	a	0.25	0/321	0.42	0/432	
4	h	0.24	0/352	0.45	0/472	
4	i	0.25	0/321	0.43	0/432	
4	j	0.25	0/321	0.43	0/432	
4	l	0.25	0/321	0.43	0/432	
4	n	0.25	0/352	0.46	0/472	
4	р	0.25	0/321	0.42	0/432	
All	All	0.24	0/58362	0.43	0/78754	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	309/319~(97%)	305~(99%)	4 (1%)	0	100 100
1	В	309/319~(97%)	306~(99%)	3 (1%)	0	100 100
1	С	309/319~(97%)	306~(99%)	3 (1%)	0	100 100
1	J	309/319~(97%)	302~(98%)	7 (2%)	0	100 100
1	К	309/319~(97%)	307~(99%)	2 (1%)	0	100 100
1	L	309/319~(97%)	305~(99%)	4 (1%)	0	100 100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	S	309/319~(97%)	305~(99%)	4 (1%)	0	100	100
1	Т	309/319~(97%)	307~(99%)	2(1%)	0	100	100
1	U	309/319~(97%)	305~(99%)	4 (1%)	0	100	100
1	b	309/319~(97%)	301 (97%)	8 (3%)	0	100	100
1	с	309/319~(97%)	305~(99%)	4 (1%)	0	100	100
1	d	309/319~(97%)	305 (99%)	4 (1%)	0	100	100
1	k	309/319~(97%)	307~(99%)	2 (1%)	0	100	100
1	m	309/319~(97%)	305 (99%)	4 (1%)	0	100	100
1	О	309/319~(97%)	305 (99%)	4 (1%)	0	100	100
2	D	147/185~(80%)	145 (99%)	2 (1%)	0	100	100
2	Е	154/185~(83%)	153 (99%)	1 (1%)	0	100	100
2	Ν	145/185~(78%)	144 (99%)	1 (1%)	0	100	100
2	Ο	148/185~(80%)	146 (99%)	2 (1%)	0	100	100
2	V	147/185~(80%)	146 (99%)	1 (1%)	0	100	100
2	W	154/185~(83%)	152 (99%)	2 (1%)	0	100	100
2	f	145/185~(78%)	145 (100%)	0	0	100	100
2	g	148/185~(80%)	147 (99%)	1 (1%)	0	100	100
3	F	165/190~(87%)	164 (99%)	1 (1%)	0	100	100
3	М	165/190~(87%)	163 (99%)	2 (1%)	0	100	100
3	Х	165/190~(87%)	163 (99%)	2 (1%)	0	100	100
3	е	165/190~(87%)	162 (98%)	3 (2%)	0	100	100
4	G	38/230~(16%)	38 (100%)	0	0	100	100
4	Н	35/230~(15%)	35 (100%)	0	0	100	100
4	Ι	35/230~(15%)	35 (100%)	0	0	100	100
4	Р	38/230~(16%)	38 (100%)	0	0	100	100
4	Q	35/230~(15%)	35 (100%)	0	0	100	100
4	R	35/230~(15%)	35 (100%)	0	0	100	100
4	Y	38/230~(16%)	38 (100%)	0	0	100	100
4	Z	35/230~(15%)	35 (100%)	0	0	100	100
4	a	35/230~(15%)	35 (100%)	0	0	100	100
4	h	38/230~(16%)	38 (100%)	0	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
4	i	35/230~(15%)	35~(100%)	0	0	100	100
4	j	35/230~(15%)	35~(100%)	0	0	100	100
4	1	35/230~(15%)	35~(100%)	0	0	100	100
4	n	38/230~(16%)	38 (100%)	0	0	100	100
4	р	35/230~(15%)	35 (100%)	0	0	100	100
All	All	7023/10475~(67%)	6946 (99%)	77 (1%)	0	100	100

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There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	283/286~(99%)	283 (100%)	0	100 100
1	В	283/286~(99%)	283 (100%)	0	100 100
1	С	283/286~(99%)	283 (100%)	0	100 100
1	J	283/286~(99%)	283 (100%)	0	100 100
1	Κ	283/286~(99%)	283 (100%)	0	100 100
1	L	283/286~(99%)	283 (100%)	0	100 100
1	S	283/286~(99%)	283 (100%)	0	100 100
1	Т	283/286~(99%)	283 (100%)	0	100 100
1	U	283/286~(99%)	283 (100%)	0	100 100
1	b	283/286~(99%)	283 (100%)	0	100 100
1	с	283/286~(99%)	283 (100%)	0	100 100
1	d	283/286~(99%)	283 (100%)	0	100 100
1	k	283/286~(99%)	283 (100%)	0	100 100
1	m	283/286~(99%)	283 (100%)	0	100 100
1	О	283/286~(99%)	283 (100%)	0	100 100
2	D	128/154~(83%)	128 (100%)	0	100 100



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	J	1	r J

Mol	Chain	Analysed	Rotameric	Outliers	Percentile	\mathbf{s}
2	Ε	132/154~(86%)	132~(100%)	0	100 100	
2	Ν	127/154~(82%)	127~(100%)	0	100 100	
2	Ο	130/154~(84%)	130 (100%)	0	100 100	
2	V	128/154~(83%)	128 (100%)	0	100 100	
2	W	132/154~(86%)	132 (100%)	0	100 100	
2	f	127/154~(82%)	127 (100%)	0	100 100	
2	g	130/154 (84%)	130 (100%)	0	100 100	
3	F	148/163 (91%)	148 (100%)	0	100 100	
3	М	148/163 (91%)	148 (100%)	0	100 100	
3	Х	148/163 (91%)	148 (100%)	0	100 100	
3	е	148/163~(91%)	148 (100%)	0	100 100	
4	G	38/210 (18%)	38 (100%)	0	100 100	
4	Н	35/210~(17%)	35 (100%)	0	100 100	
4	Ι	35/210~(17%)	35 (100%)	0	100 100	
4	Р	38/210 (18%)	38 (100%)	0	100 100	
4	Q	35/210~(17%)	35 (100%)	0	100 100	
4	R	35/210~(17%)	35 (100%)	0	100 100	
4	Y	38/210 (18%)	38 (100%)	0	100 100	
4	Ζ	35/210~(17%)	35 (100%)	0	100 100	
4	a	35/210~(17%)	35 (100%)	0	100 100	
4	h	38/210 (18%)	38 (100%)	0	100 100	
4	i	35/210~(17%)	35 (100%)	0	100 100	
4	j	35/210~(17%)	35 (100%)	0	100 100	
4	l	35/210~(17%)	35 (100%)	0	100 100	
4	n	38/210 (18%)	38 (100%)	0	100 100	
4	р	35/210~(17%)	35 (100%)	0	100 100	
All	All	6411/9324~(69%)	6411 (100%)	0	100 100	

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:



Mol	Chain	Res	Type
1	С	85	GLN
1	S	132	HIS
1	U	85	GLN
2	f	180	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-17672. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

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

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

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)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



8 Fourier-Shell correlation (i)

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



9 Map-model fit (i)

This section was not generated.

