



Full wwPDB EM Validation Report ⓘ

Apr 20, 2025 – 12:19 AM JST

PDB ID : 9LW8 / pdb_00009lw8
EMDB ID : EMD-63434
Title : Bottom cap of bacteriophage Mycofy1 mature head (C5 symmetry)
Authors : Li, X.; Shao, Q.; Li, L.; Xie, L.; Ruan, Z.; Fang, Q.
Deposited on : 2025-02-13
Resolution : 3.53 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

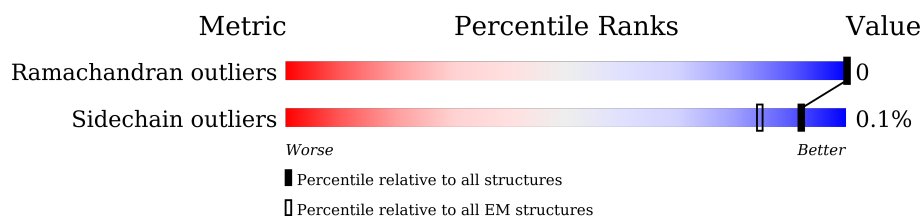
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



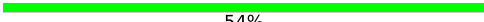
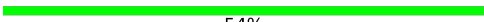













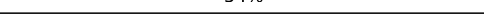
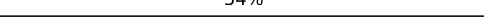
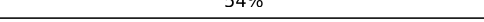
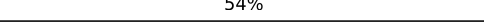
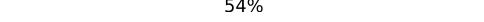
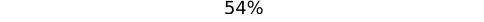
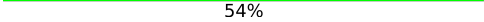
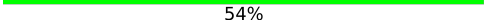
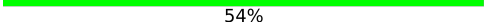
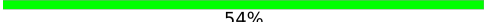
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain	
1	1	543	53%	47%
1	2	543	53%	47%
1	3	543	53%	47%
1	4	543	53%	47%
1	5	543	53%	47%
1	A	543	54%	46%
1	B	543	46%	54%
1	C	543	54%	46%
1	D	543	54%	46%
1	E	543	54%	46%

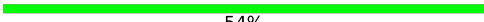
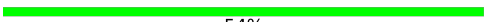










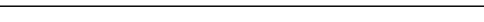


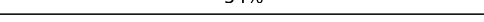
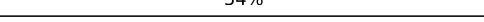
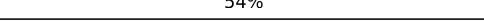
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Mol	Chain	Length	Quality of chain	
1	F	543		46%
1	G	543		46%
1	H	543		46%
1	I	543		46%
1	J	543		46%
1	K	543		46%
1	L	543		46%
1	M	543		46%
1	N	543		46%
1	O	543		46%
1	P	543		46%
1	Q	543		46%
1	R	543		46%
1	S	543		46%
1	T	543		46%
1	U	543		46%
1	V	543		46%
1	W	543		46%
1	X	543		46%
1	Y	543		46%
1	Z	543		46%
1	a	543		46%
1	b	543		46%
1	c	543		46%
1	d	543		46%

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Mol	Chain	Length	Quality of chain	
1	e	543	 54%	46%
1	f	543	 54%	46%
1	g	543	 54%	46%
1	h	543	 54%	46%
1	i	543	 54%	46%
1	j	543	 54%	46%
1	k	543	 54%	46%
1	l	543	 54%	46%
1	m	543	 54%	46%
1	n	543	 54%	46%
1	o	543	 54%	46%
1	p	543	 54%	46%
1	q	543	 54%	46%
1	r	543	 54%	46%
1	s	543	 54%	46%
1	t	543	 54%	46%
1	u	543	 54%	46%
1	v	543	 54%	46%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 118260 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 Phage capsid-like C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	288	Total	C	N	O	S	0	0
			2208	1397	379	428	4		
1	2	288	Total	C	N	O	S	0	0
			2208	1397	379	428	4		
1	3	288	Total	C	N	O	S	0	0
			2208	1397	379	428	4		
1	4	288	Total	C	N	O	S	0	0
			2208	1397	379	428	4		
1	5	288	Total	C	N	O	S	0	0
			2208	1397	379	428	4		
1	A	292	Total	C	N	O	S	0	0
			2235	1413	384	434	4		
1	B	249	Total	C	N	O	S	0	0
			1905	1207	324	371	3		
1	C	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	D	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	E	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	F	292	Total	C	N	O	S	0	0
			2235	1413	384	434	4		
1	G	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	H	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	I	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	J	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	K	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	L	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	N	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	O	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	P	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	Q	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	R	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	S	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	T	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	U	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	V	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	W	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	X	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	Y	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	Z	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	a	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	b	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	c	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	d	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	e	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	f	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	g	293	Total 2241	C 1416	N 385	O 436	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	h	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	i	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	j	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	k	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	l	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	m	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	n	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	o	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	p	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	q	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	r	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	s	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	t	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	u	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	v	293	Total 2241	C 1416	N 385	O 436	S 4	0	0

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	197	HIS	LYS	conflict	UNP Q854Z2
2	197	HIS	LYS	conflict	UNP Q854Z2
3	197	HIS	LYS	conflict	UNP Q854Z2
4	197	HIS	LYS	conflict	UNP Q854Z2
5	197	HIS	LYS	conflict	UNP Q854Z2
A	197	HIS	LYS	conflict	UNP Q854Z2
B	197	HIS	LYS	conflict	UNP Q854Z2
C	197	HIS	LYS	conflict	UNP Q854Z2
D	197	HIS	LYS	conflict	UNP Q854Z2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	197	HIS	LYS	conflict	UNP Q854Z2
F	197	HIS	LYS	conflict	UNP Q854Z2
G	197	HIS	LYS	conflict	UNP Q854Z2
H	197	HIS	LYS	conflict	UNP Q854Z2
I	197	HIS	LYS	conflict	UNP Q854Z2
J	197	HIS	LYS	conflict	UNP Q854Z2
K	197	HIS	LYS	conflict	UNP Q854Z2
L	197	HIS	LYS	conflict	UNP Q854Z2
M	197	HIS	LYS	conflict	UNP Q854Z2
N	197	HIS	LYS	conflict	UNP Q854Z2
O	197	HIS	LYS	conflict	UNP Q854Z2
P	197	HIS	LYS	conflict	UNP Q854Z2
Q	197	HIS	LYS	conflict	UNP Q854Z2
R	197	HIS	LYS	conflict	UNP Q854Z2
S	197	HIS	LYS	conflict	UNP Q854Z2
T	197	HIS	LYS	conflict	UNP Q854Z2
U	197	HIS	LYS	conflict	UNP Q854Z2
V	197	HIS	LYS	conflict	UNP Q854Z2
W	197	HIS	LYS	conflict	UNP Q854Z2
X	197	HIS	LYS	conflict	UNP Q854Z2
Y	197	HIS	LYS	conflict	UNP Q854Z2
Z	197	HIS	LYS	conflict	UNP Q854Z2
a	197	HIS	LYS	conflict	UNP Q854Z2
b	197	HIS	LYS	conflict	UNP Q854Z2
c	197	HIS	LYS	conflict	UNP Q854Z2
d	197	HIS	LYS	conflict	UNP Q854Z2
e	197	HIS	LYS	conflict	UNP Q854Z2
f	197	HIS	LYS	conflict	UNP Q854Z2
g	197	HIS	LYS	conflict	UNP Q854Z2
h	197	HIS	LYS	conflict	UNP Q854Z2
i	197	HIS	LYS	conflict	UNP Q854Z2
j	197	HIS	LYS	conflict	UNP Q854Z2
k	197	HIS	LYS	conflict	UNP Q854Z2
l	197	HIS	LYS	conflict	UNP Q854Z2
m	197	HIS	LYS	conflict	UNP Q854Z2
n	197	HIS	LYS	conflict	UNP Q854Z2
o	197	HIS	LYS	conflict	UNP Q854Z2
p	197	HIS	LYS	conflict	UNP Q854Z2
q	197	HIS	LYS	conflict	UNP Q854Z2
r	197	HIS	LYS	conflict	UNP Q854Z2
s	197	HIS	LYS	conflict	UNP Q854Z2
t	197	HIS	LYS	conflict	UNP Q854Z2

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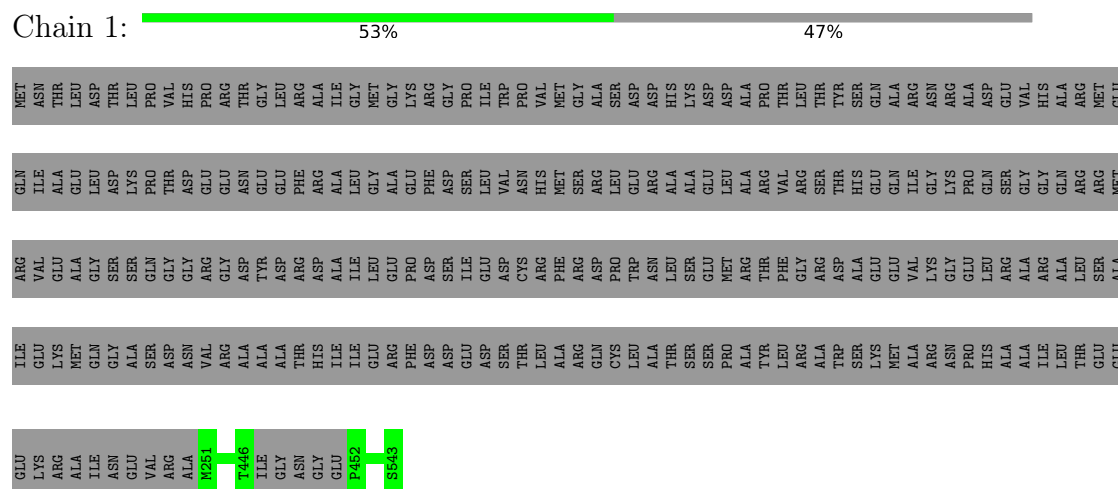
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Chain	Residue	Modelled	Actual	Comment	Reference
u	197	HIS	LYS	conflict	UNP Q854Z2
v	197	HIS	LYS	conflict	UNP Q854Z2

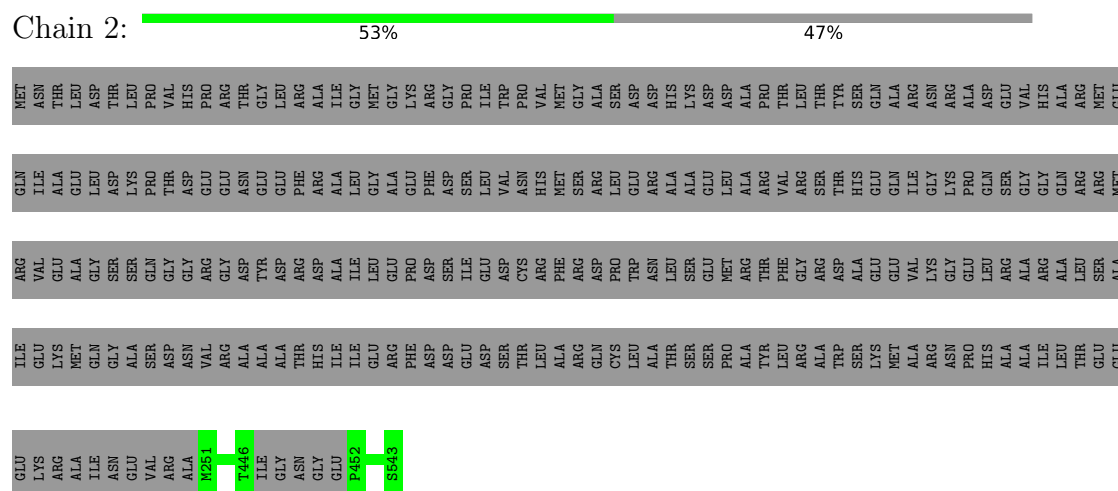
3 Residue-property plots

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.

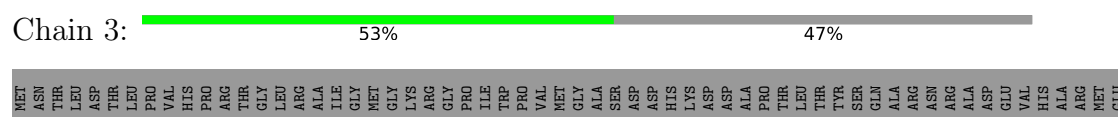
- Molecule 1: Phage capsid-like C-terminal domain-containing protein



- Molecule 1: Phage capsid-like C-terminal domain-containing protein



- Molecule 1: Phage capsid-like C-terminal domain-containing protein



GLU	LYS	ILE	GLU	ILE	ARG	GLN
ARG	ARG	GLY	GLU	VAL	VAL	ILE
ALA	ALA	MET	ALA	ALA	ALA	GLU
ILE	ILE	GLN	GLY	GLY	GLY	LEU
ASN	ASN	GLY	GLY	SER	SER	ASP
GLU	GLU	ALA	ALA	SER	LYS	LYS
VAL	VAL	SER	SER	GLN	PHO	PHO
ARG	ARG	ASP	GLY	GLY	THR	THR
ALA	ALA	ASN	ASN	ASP	ASP	ASP
M251	M251	VAL	ARG	ARG	GLU	GLU
T446	T446	ALA	ARG	GLY	ASN	ASN
ILE	ILE	ALA	ALA	TYR	GLU	GLU
GLY	GLY	ALA	ASP	ASP	GLU	GLU
ASN	ASN	THR	THR	ARG	PHE	PHE
GLY	GLY	HIS	ILE	ALA	ARG	ALA
P462	P462	ILE	ILE	ILE	LEU	LEU
S643	S643	GLU	GLU	LEU	GLY	GLY
		PHO	PHO	ALA	ALA	ALA
		PHE	PHE	LEU	LEU	LEU
		ASP	ASP	ASP	ASP	ASP
		ASP	ASP	ILE	SER	SER
		GLU	GLU	GLU	VAL	VAL
		SER	SER	ASP	ASN	ASN
		THR	THR	CYS	HIS	HIS
		LEU	LEU	ARG	MET	MET
		ALA	ALA	PHE	ARG	ARG
		GLN	GLN	ASP	SER	SER
		CYS	CYS	PRO	LEU	LEU
		LEU	LEU	TRP	GLU	GLU
		ALA	ALA	ASN	ARG	ARG
		THR	THR	LEU	ALA	ALA
		SER	SER	SER	ALA	ALA
		SER	SER	ALA	HIS	HIS
		LYS	LYS	GLU	GLU	GLN
		MET	MET	VAL	ILE	ILE
		ALA	ALA	VAL	GLY	GLY
		ARG	ARG	GLY	LYS	LYS
		ASN	ASN	GLU	PRO	PRO
		PRO	PRO	LEU	GLN	GLN
		HIS	HIS	LEU	SER	SER
		ALA	ALA	ARG	GLY	GLY
		ILE	ILE	ALA	ARG	ARG
		LEU	LEU	ALA	GLN	GLN
		THR	THR	LEU	ARG	ARG
		GLU	GLU	SER	ARG	MET

- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain 4:  53% 47%

GLU	LYS	GLU	ILE	ARG	GLN	MET
ARG	ARG	GLU	LYS	VAL	ILE	ASN
ALA	ALA	GLU	GLY	ALA	GLU	THR
ILE	ILE	MET	GLN	GLY	LEU	LEU
ASN	ASN	GLY	GLY	SER	ASP	THR
GLU	GLU	ALA	ALA	SER	LYS	LEU
VAL	VAL	SER	SER	GLN	PRO	PRO
ARG	ARG	ASP	GLY	GLY	THR	VAL
ALA	ALA	ASN	ASN	ARG	ASP	HIS
M251	+	VAL	VAL	ARG	GLU	PRO
		ARG	ARG	GLY	GLU	ARG
T446	+	ALA	ALA	ASP	ASN	THR
ILE	ILE	ALA	ALA	TYR	GLU	GLY
GLY	GLY	ALA	ASP	ARG	LEU	GLY
ASN	ASN	THR	THR	ARG	PHE	ARG
GLY	GLY	HIS	HIS	ASP	ARG	ALA
		ILE	ILE	ALA	ALA	ILE
P462	+	ILE	ILE	ILE	LEU	GLY
		GLU	GLU	LEU	GLY	MET
S543	+	ARG	ARG	GLU	ALA	GLY
		ASP	PHE	PRO	ALA	LYS
		ASP	ASP	ASP	PHE	ARG
		GLU	GLU	ILE	SER	GLY
		ASP	ASP	SER	PRO	PRO
		ASP	ASP	GLU	LEU	ILE
		SER	SER	GLU	VAL	TRP
		THR	THR	CYS	ASN	TRP
		ARG	ARG	ARG	ASN	PRO
		ALA	ALA	PHE	HIS	VAL
		ALA	ALA	ARG	MET	MET
		GLN	GLN	ASP	ARG	GLY
		THR	THR	ASP	LEU	ALA
		THR	THR	PRO	SER	SER
		ALA	ALA	TRP	GLU	ASP
		THR	THR	ALA	ASP	ALA
		LYS	LYS	GLY	ARG	PRO
		MET	MET	GLU	VAL	THR
		ALA	ALA	VAL	ILE	ALA
		ARG	ARG	GLY	GLN	ARG
		ASN	ASN	LYS	ASN	ASN
		PRO	PRO	GLU	PRO	ALA
		HIS	HIS	LEU	GLN	ASP
		ALA	ALA	ARG	SER	GLU
		ILE	ILE	ALA	GLY	VAL
		LEU	LEU	ALA	GLN	HIS
		THR	THR	LEU	ARG	ARG
		GLU	GLU	SER	MET	GLY
		THR	THR	ALA	THR	THR

- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain 5:  53% 47%

[illegible]

- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain A: 54% 46%

MET	ASN	THR	LEU	ASP	THR	LEU	PRO	PRO	HIS	ARG	THR	GLY	LEU	ARG	ALA	ILE	GLY	MET	LYS	GLY	ARG	GLY	PRO	PRO	ILE	TRP	PRO	VAL	MET	GLY	ALA	SER	ASP	ASP	HIS	LYS	ASP	ALA	ALA	THR	THR	LEU	THR	TYR	SER	SER	GLN	ALA	ALA	ARG	ASN	ARG	ALA	ALA	ARG	ALA	ASP	GLU	VAL	HIS	ALA	ARG	MET	THR
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GLU	LYS	GLU	TLE	ARG	GLN
ARG	ARG	GLY	GLU	VAL	TLE
ALA	ALA	MET	ALA	GLU	ALA
TLE	TLE	GLN	GLY	GLY	LEU
ASN	ASN	GLY	SER	SER	ASP
GLU	GLU	ALA	ALA	GLN	LYS
VAL	VAL	SER	SER	GLN	PRO
ARG	ARG	ASP	GLY	GLY	THR
ALA	ALA	ASN	GLY	ASP	THR
M25-1	VAL	VAL	ARG	GLY	GLU
ALA	ALA	ALA	ASP	ASP	ASN
15-2	ALA	ALA	TTR	GLU	GLU
SER	SER	THR	THR	ASP	ASP
	HIS	TLE	TLE	ALA	ALA
	TLE	TLE	LEU	LEU	GLY
	GLU	ARG	GLU	GLU	ALA
	ARG	PHE	PRO	PRO	GLU
	ASP	ASP	ASP	SER	PHE
	GLU	TLE	TLE	SER	ASP
	ASP	ASP	GLU	GLU	SER
	THR	THR	CYS	ASP	VAL
	LEU	LEU	ARG	ASN	LEU
	ALA	ALA	PHE	MET	MET
	ARG	ARG	ARG	SER	SER
	GLN	GLN	ARG	ARG	ARG
	CYS	LEU	PRO	LEU	GLU
	LEU	THR	THR	GLU	ARG
	ALA	THR	LEU	ALA	ALA
	SER	SER	SER	ALA	ALA
	SER	SER	ASP	ALA	GLY
	LYS	MET	GLU	GLY	GLN
	ALA	ALA	VAL	TLE	TLE
	ASN	ARG	GLY	LYS	GLY
	PRO	PRO	GLU	GLU	LYS
	HIS	ALA	LEU	GLN	GLN
	ALA	ALA	ARG	SER	SER
	TLE	TLE	ALA	GLY	GLY
	LEU	LEU	ALA	GLN	ARG
	THR	THR	LEU	LEU	GLN
	GLU	GLU	SER	ARG	ARG
	THR	THR	ALA	MET	MET

- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain B:  46% 54%

ARG	GLU	ILE	ARG	GLN	MET
G537	LYS	GLU	VAL	ILE	ASN
A542	ARG	LYS	GLU	ALA	THR
SER	ALA	MET	ALA	LEU	LEU
	ILE	GLN	GLY	LEU	ASP
	ASN	GLY	SER	ASP	THR
	GLU	ALA	SER	LYS	LEU
	VAL	SER	GLN	PRO	PRO
	ARG	ASP	GLY	THR	VAL
	ALA	ASN	GLY	ASP	HIS
	MET	VAL	ARG	GLU	PRO
	GLY	ARG	GLY	GLU	ARG
	LEU	ALA	ASP	ASN	THR
	THR	ALA	TYR	GLU	GLY
	LYS	ALA	ASP	GLU	LEU
	ALA	THR	ARG	PHE	ARG
	ASP	HIS	ASP	ARG	ALA
	GLY	ILE	ALA	ALA	ILE
	GLY	ILE	ILE	LEU	GLY
	TYR	ILE	LEU	GLY	MET
	LEU	ARG	GLU	GLU	LYS
	VAL	PHE	PRO	ALA	GLY
	PRO	ASP	ASP	PHE	ARG
	GLN	ASP	SER	SER	GLY
	LEU	GLU	ILE	SER	PRO
	ASP	ASP	GLU	ASP	PRO
	PRO	THR	CYS	ASN	THR
T269	LEU	ARG	PHE	MET	VAL
	ALA	ARG	ARG	MET	GLY
F336	ARG	GLN	ASP	SER	ALA
ILE	SER	CYS	ASP	ARG	GLY
ILE	ILE	LEU	TRP	LEU	SER
GLU	GLU	ALA	ASN	GLU	ASP
ALA	LEU	THR	LEU	ALA	ASP
LEU	LEU	SER	SER	ALA	HIS
GLN	GLN	SER	GLU	LEU	LYS
ASP	PRO	PRO	MET	GLU	ASP
GLU	GLU	ALA	ARG	ALA	ALA
ALA	ALA	TYR	THR	ARG	PRO
ASN	ASN	LEU	PHE	VAL	THR
VAL	VAL	ARG	GLY	ARG	LEU
T349	GLN	ALA	ARG	SER	THR
	TRP	SER	ASP	THR	TYR
N426	SER	SER	ALA	HIS	SER
	LYS	MET	GLU	GLN	GLN
F503	ALA	ALA	VAL	ILE	ALA
HIS	LEU	ARG	LYS	GLY	ARG
LEU	PHE	ASN	GLY	LYS	ASN
THR	GLY	PRO	LEU	PRO	ALA
THR	THR	HIS	GLU	GLN	ASP
ASN	ASN	ALA	ARG	SER	GLU
ARG	ARG	ILE	ALA	GLY	VAL
PRO	PRO	LEU	ALA	GLN	HIS
ASN	ASN	THR	LEU	ARG	ALA
GLY	GLY	THR	LEU	ARG	ARG
SER	SER	GLU	ALA	MET	MET
		THR	ALA	THR	GLU

- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain C: 54% 46%

GLU	LYS	TLE	ARG	GLN	MET
ARG	GLY	GLU	VAL	ILE	ASN
ALA	LYS	ALA	GLU	ALA	THR
ILE	MET	ALA	GLY	LEU	LEU
ASN	GLY	GLN	GLY	LEU	ASP
GLU	ALA	ALA	SER	LYS	THR
VAL	SER	SER	GLN	PRO	LEU
ALA	ASP	GLY	GLY	THR	PRO
ARG	ASN	GLY	GLY	ASP	GLY
M25-1	VAL	ARG	GLY	GLU	ARG
S54-3	ALA	ALA	ASP	ASN	THR
	ALA	ALA	TYR	GLU	GLY
	ALA	ASP	ASP	GLU	LEU
	THR	ARG	ARG	PHE	ARG
	HIS	ALA	ALA	ALA	ALA
	ILE	ILE	ILE	LEU	ILE
	ILE	GLU	LEU	GLY	GLY
	GLU	GLU	GLU	GLY	GLY
	ASP	PHE	PRO	ALA	ALA
	ASP	ASP	ASP	ASP	PHE
GLU	GLU	ILE	ILE	SER	
ASP	ASP	GLU	GLU	LEU	
SER	SER	SER	ASP	VAL	
THR	THR	THR	CYS	ASN	
LEU	LEU	ARG	ARG	HIS	
ALA	ALA	PHE	MET	MET	
ARG	ARG	ARG	ASP	GLY	
GLN	CYS	GLN	ASP	ALA	
LEU	LEU	LEU	PRO	SER	
ALA	ALA	ALA	ASN	ARG	
THR	THR	THR	LEU	ALA	
ARG	LEU	PHE	ARG	LYS	
ALA	ARG	GLY	GLY	ASP	
ALA	ALA	ARG	GLY	ASP	
PRO	PRO	ALA	GLY	GLN	
PRO	LYS	GLY	ILE	ALA	
ASN	ARG	LYS	GLY	ARG	
HIS	GLN	GLN	GLN	ALA	
ALA	THR	VAL	VAL	ARG	
ASP	GLU	GLU	LEU	ASP	
GLU	GLY	SER	ARG	GLY	
VAL	HIS	ALA	ARG	THR	
ALA	ALA	ALA	ALA	VAL	
ILE	ILE	ILE	ALA	HIS	
THR	THR	THR	ARG	GLY	
LEU	LEU	LEU	GLU	GLN	
ARG	ARG	LEU	GLY	ALA	
ASP	ASP	SER	GLY	ARG	
GLU	GLU	MET	LEU	ARG	
VAL	GLU	ALA	GLN	MET	
THR	THR	GLY	GLY	GLY	
ASP	ASP	ASP	ASP	ASP	
GLY	GLY	GLY	GLY	GLY	
PRO	PRO	PRO	PRO	PRO	
ILE	ILE	ILE	ILE	ILE	
LEU	LEU	LEU	LEU	LEU	
VAL	VAL	VAL	VAL	VAL	
ARG	ARG	ARG	ARG	ARG	
ASN	ASN	ASN	ASN	ASN	
THR	THR	THR	THR	THR	
GLY	GLY	GLY	GLY	GLY	
ASP	ASP	ASP	ASP	ASP	
PRO	PRO	PRO	PRO	PRO	
ILE	ILE	ILE	ILE	ILE	
LEU	LEU	LEU	LEU	LEU	
VAL	VAL	VAL	VAL	VAL	
ARG	ARG	ARG	ARG	ARG	
ASN	ASN	ASN	ASN	ASN	
THR	THR	THR	THR	THR	
GLY	GLY	GLY	GLY	GLY	
ASP	ASP	ASP	ASP	ASP	
PRO	PRO	PRO	PRO	PRO	
ILE	ILE	ILE	ILE	ILE	
LEU	LEU	LEU	LEU	LEU	
VAL	VAL	VAL	VAL	VAL	
ARG	ARG	ARG	ARG	ARG	
ASN	ASN	ASN	ASN	ASN	
THR	THR	THR	THR	THR	
GLY	GLY	GLY	GLY	GLY	
ASP	ASP	ASP	ASP	ASP	
PRO	PRO	PRO	PRO	PRO	
ILE	ILE	ILE	ILE	ILE	
LEU	LEU	LEU	LEU	LEU	
VAL	VAL	VAL	VAL	VAL	
ARG	ARG	ARG	ARG	ARG	
ASN	ASN	ASN	ASN	ASN	
THR	THR	THR	THR	THR	
GLY	GLY	GLY	GLY	GLY	
ASP	ASP	ASP	ASP	ASP	
PRO	PRO	PRO	PRO	PRO	
ILE	ILE	ILE	ILE	ILE	
LEU	LEU	LEU	LEU	LEU	
VAL	VAL	VAL	VAL	VAL	
ARG	ARG	ARG	ARG	ARG	
ASN	ASN	ASN	ASN	ASN	
THR	THR	THR	THR	THR	
GLY	GLY	GLY	GLY	GLY	
ASP	ASP	ASP	ASP	ASP	
PRO	PRO	PRO	PRO	PRO	
ILE	ILE	ILE	ILE	ILE	
LEU	LEU	LEU	LEU	LEU	
VAL	VAL	VAL	VAL	VAL	
ARG	ARG	ARG	ARG	ARG	
ASN	ASN	ASN	ASN	ASN	
THR	THR	THR	THR	THR	
GLY	GLY	GLY	GLY	GLY	
ASP	ASP	ASP	ASP	ASP	
PRO	PRO	PRO	PRO	PRO	
ILE	ILE	ILE	ILE	ILE	
LEU	LEU	LEU	LEU	LEU	
VAL	VAL	VAL	VAL	VAL	
ARG	ARG	ARG	ARG	ARG	
ASN	ASN	ASN	ASN	ASN	
THR	THR				

- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain D:  54% 46%

[illegible]

- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain Q:  54% 46%

[illegible]

- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain R: 54% 46%

M251 K360 S543	GLU	LYS	ARG	ALA	ILE	ASN	GLU	VAL	THR	LEU	ASP	GLY	THR	GLN	ILE	ASN	MET
	LYS	ARG	ALA	ILE	ASN	GLU	VAL	THR	LEU	ASP	GLY	THR	GLN	ILE	ASN	MET	
	ILE	ASN	GLU	VAL	THR	LEU	ASP	GLY	THR	GLN	ILE	ASN	MET	GLU	VAL	THR	
	ASN	GLU	VAL	THR	LEU	ASP	GLY	THR	GLN	ILE	ASN	MET	GLU	VAL	THR		
	GLU	VAL	THR	LEU	ASP	GLY	THR	GLN	ILE	ASN	MET	GLU	VAL	THR			
	VAL	THR	LEU	ASP	GLY	THR	GLN	ILE	ASN	MET	GLU	VAL	THR				
	ARG	ALA	ILE	ASN	GLU	VAL	THR	LEU	ASP	GLY	THR	GLN	ILE	ASN	MET		
	M251	K360	S543	GLU	VAL	THR	LEU	ASP	GLY	THR	GLN	ILE	ASN	MET	GLU	VAL	
	K360	S543	GLU	VAL	THR	LEU	ASP	GLY	THR	GLN	ILE	ASN	MET	GLU	VAL		
	S543	GLU	VAL	THR	LEU	ASP	GLY	THR	GLN	ILE	ASN	MET	GLU	VAL			
	GLU	VAL	THR	LEU	ASP	GLY	THR	GLN	ILE	ASN	MET	GLU	VAL				
	VAL	THR	LEU	ASP	GLY	THR	GLN	ILE	ASN	MET	GLU	VAL					
	THR	LEU	ASP	GLY	THR	GLN	ILE	ASN	MET	GLU	VAL						
	LEU	ASP	GLY	THR	GLN	ILE	ASN	MET	GLU	VAL							
	ASP	GLY	THR	GLN	ILE	ASN	MET	GLU	VAL								
	THR	GLN	ILE	ASN	MET	GLU	VAL										

- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain S:  54% 46%



GLU	LYS	TLE	ARG	GLN	MET
ARG	ARG	GLU	VAL	ILE	ASN
ALA	ALA	MET	GLU	ALA	THR
ILE	ILE	GLN	GLY	LEU	ASP
ASN	ASN	GLY	SER	ASP	THR
GLU	GLU	ALA	SER	LYS	LEU
VAL	SER	SER	GLN	PRO	PRO
ARG	ASP	GLY	GLY	THR	VAL
ALA	ASN	ASN	GLY	ASP	HIS
M2E1	VAL	ARG	ARG	GLU	PRO
S543	ARG	GLY	GLY	GLU	ARG
	ALA	ALA	ASP	ASN	THR
	ALA	ALA	ASP	GLU	GLY
	ALA	THR	ARG	PHE	ARG
	HIS	ASP	ALA	ARG	ALA
	ILE	ILE	ALA	LEU	TLE
	ILE	GLU	LEU	GLY	MET
	PHE	PHE	GLU	ALA	GLY
	ASP	ASP	SER	SER	ARG
	GLU	GLU	ILE	SER	PRO
	ASP	ASP	GLU	SER	GLY
	THR	THR	CYS	ASN	THR
	LEU	LEU	ARG	HIS	VAL
ALA	ALA	PHE	MET	VAL	
GLN	GLN	ARG	SER	GLY	
CYS	LYS	ASP	PRO	ALA	
LEU	THR	TRP	LEU	SER	
ALA	ALA	ASN	ARG	ASP	
THR	THR	LEU	ALA	HIS	
SER	SER	SER	ALA	LYS	
SER	SER	GLU	GLU	ASP	
PRO	PRO	ALA	ALA	ALA	
THR	THR	THR	ARG	PRO	
ARG	ARG	PHE	VAL	THR	
ALA	ALA	GLY	ARG	THR	
THR	THR	ASP	SER	THR	
TYR	TYR	HIS	THR	TYR	
SER	SER	ALA	ALA	SER	
GLN	GLN	GLU	GLU	GLN	
ALA	ALA	TLE	TLE	ALA	
ASN	ASN	LYS	LYS	ASN	
ASP	ASP	PRO	GLU	ASP	
GLU	GLU	HIS	LEU	ASP	
VAL	VAL	ALA	ARG	GLU	
THR	THR	TLE	ALA	VAL	
ARG	ARG	GLY	GLY	THR	
ALA	ALA	GLN	GLN	ALA	
THR	THR	ARG	ARG	ARG	
GLY	GLY	THR	THR	ARG	
ASN	ASN	LEU	LEU	ASN	
THR	THR	ASP	ASP	THR	
GLU	GLU	MET	ALA	GLU	

- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain f:  54% 46%

GLU	LYS	TLE	ARG	GLN	MET
ARG	ARG	GLU	VAL	ILE	ASN
ALA	ALA	GLN	ALA	GLU	THR
ILE	ILE	GLN	GLY	LEU	LEU
ASN	ASN	GLY	SER	ASP	THR
GLU	ALA	ALA	SER	LYS	LEU
VAL	SER	SER	GLN	PRO	PRO
ARG	ASP	ASP	GLY	THR	GLY
ALA	ASN	ASN	GLY	ASP	HIS
M2E1	VAL	VAL	ARG	GLU	PRO
S543	ARG	ARG	GLY	GLU	ARG
	ALA	ALA	ASP	ASN	THR
	ALA	ALA	TYR	GLU	GLY
	ALA	ALA	ASP	LEU	GLY
	THR	THR	ARG	PHE	ARG
	HIS	HIS	ASP	ARG	ALA
	ILE	ILE	ILE	ALA	TLE
	ILE	ILE	ILE	LEU	GLY
	GLU	ARG	GLU	GLY	MET
	ARG	PHE	PRO	GLU	LYS
	ASP	ASP	SER	ASP	GLY
	GLU	ILE	ILE	SER	PRO
	ASP	GLU	GLU	LEU	ILE
	SER	SER	GLU	VAL	TRP
	THR	THR	CYS	ASN	ASN
	LEU	LEU	ARG	HIS	VAL
	ALA	ALA	PHE	MET	MET
	GLN	GLN	ARG	SER	GLY
	CYS	CYS	ASP	ARG	ALA
	LEU	LEU	PRO	LEU	SER
	ALA	ALA	TRP	GLU	ASP
	THR	THR	ASN	ARG	ASP
	SER	SER	LEU	ALA	HIS
	SER	SER	SER	ALA	LYS
	PRO	PRO	GLU	GLU	ASP
	THR	THR	THR	ARG	PRO
	LEU	LEU	PHE	VAL	THR
	ARG	ARG	GLY	ARG	THR
	ALA	ALA	ARG	SER	THR
	TRP	TRP	ASP	THR	TYR
	SER	SER	ALA	HIS	SER
	LYS	LYS	GLU	GLN	GLN
	MET	MET	GLU	TLE	ALA
	ALA	ALA	VAL	ILE	ARG
	ASN	ASN	GLY	LYS	ASN
	PRO	PRO	GLU	PRO	ALA
	HIS	HIS	LEU	GLN	ASP
	ALA	ALA	ARG	SER	GLU
	ILE	ILE	ALA	GLY	VAL
	LEU	LEU	ALA	GLN	HIS
	THR	THR	LEU	ARG	ARG
	GLU	GLU	SER	MET	ARG
	GLU	GLU	ALA	MET	GLN

- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain g:  54% 46%

GLU	LYS	ILE	ARG	VAL	GLN	MET
ARG	GLY	GLU	VAL	VAL	ILE	ASN
ALA	MET	GLU	ALA	ALA	ALA	THR
ILE	GLN	LEU	GLY	GLY	LEU	ASP
ASN	GLY	SER	SER	SER	ASP	THR
GLU	ALA	SER	GLN	LYS	LYS	LEU
VAL	SER	GLN	GLN	PRO	PRO	PRO
ARG	ASP	GLY	GLY	VAL	THR	HIS
ALA	ALA	ASN	ARG	ASP	ASP	ARG
M251	VAL	VAL	ARG	GLY	GLU	PRO
5543	ARG	ALA	ASP	ASN	ASN	ARG
	ALA	ALA	TYR	GLY	GLY	THR
	THR	THR	ARG	PHE	ARG	ARG
	HIS	ALA	ALA	ALA	ALA	ALA
	ILE	ILE	ILE	LEU	LEU	ILE
	ILE	GLU	GLU	GLY	GLY	GLY
	PHE	PHE	PRO	GLU	ALA	GLY
	ASP	ASP	SER	PHE	ASP	ARG
	GLU	GLU	ILE	SER	SER	GLY
	ASP	ASP	GLU	LEU	LEU	PRO
	SER	SER	ASP	VAL	ILE	THR
	THR	THR	CYS	ASN	ASN	PRO
	LEU	LEU	ARG	HIS	VAL	VAL
	ALA	ALA	PHE	MET	MET	MET
	ARG	GLN	ARG	SER	GLY	GLY
	CYS	CYS	PRO	LEU	SER	ALA
	LEU	LEU	TRP	GLU	ASP	ASP
	ALA	ALA	ASN	ARG	ASP	ASP
	THR	THR	LEU	ALA	ALA	HIS
	SER	SER	SER	ALA	LYS	LYS
	SER	SER	GLU	THR	GLU	GLN
	LYS	MET	GLU	GLN	ALA	ALA
	ALA	ALA	VAL	ILE	ARG	ARG
	ARG	ARG	LYS	GLY	ASN	ASN
	ASN	ASN	GLU	PRO	ALA	ARG
	PRO	PRO	LEU	GLN	ASP	ASP
	HIS	HIS	ARG	SER	GLU	GLU
	ALA	ALA	ALA	GLY	VAL	VAL
	ILE	ILE	ARG	GLY	HIS	HIS
	THR	THR	LEU	ALA	GLN	ALA
	THR	THR	LEU	LEU	ARG	ARG
	GLU	GLU	SER	MET	ARG	MET
	GLU	ALA	ALA	ALA	THR	THR

- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain h: 54% 46%



GLU	LYS	TLE	ARG	GLN	MET
ARG	ARG	GLU	VAL	TLE	ASN
ALA	ALA	MET	GLU	ALA	THR
ILE	ILE	GLN	GLY	LEU	ASP
ASN	ASN	GLY	SER	ASP	THR
GLU	GLU	ALA	SER	LYS	LEU
VAL	SER	SER	GLN	PRO	PRO
ARG	ASP	GLY	GLY	THR	VAL
ALA	ASN	ASN	GLY	ASP	HIS
M2E1	VAL	ARG	ARG	GLU	PRO
S543	ARG	GLY	GLY	GLU	ARG
	ALA	ALA	ASP	ASN	THR
	ALA	ALA	ASP	GLU	GLY
	ALA	THR	ARG	PHE	ARG
	HIS	ASP	ALA	ARG	ALA
	ILE	ILE	ALA	LEU	TLE
	ILE	GLU	LEU	GLY	MET
	PHE	PHE	GLU	ALA	GLY
	ASP	ASP	SER	PHE	LYS
	GLU	GLU	ILE	SER	PRO
THR	SER	ASP	CYS	ASN	
LEU	LEU	ARG	HIS	VAL	
ALA	ALA	PHE	MET	MET	
GLN	GLN	ARG	SER	GLY	
CYS	LYS	PRO	LEU	ALA	
LEU	THR	TRP	GLU	SER	
ALA	ALA	ASN	ARG	ASP	
THR	THR	LEU	ALA	HIS	
SER	SER	SER	SER	LYS	
PRO	PRO	GLU	GLU	ASP	
ALA	ALA	THR	ARG	ALA	
THR	THR	PHE	VAL	PRO	
LEU	ARG	GLY	ARG	THR	
ALA	ALA	ARG	SER	LEU	
TRP	TRP	ASP	SER	THR	
LYS	LYS	GLU	HIS	TYR	
MET	MET	GLU	THR	SER	
ALA	ALA	TLE	GLN	GLN	
ASN	ASN	TLE	ALA	ALA	
GLY	GLY	LYS	GLY	ARG	
PRO	PRO	GLU	PRO	ASN	
ALA	ALA	LEU	GLN	ASP	
HIS	HIS	ARG	SER	GLU	
VAL	VAL	GLY	ALA	VAL	
GLU	GLU	ARG	LEU	ARG	
MET	MET	ALA	ARG	ARG	
THR	THR	ALA	SER	THR	
GLN	GLN	GLU	THR	GLU	
ASN	ASN	ALA	ALA	GLN	
THR	THR	ILE	ARG	GLY	
GLY	GLY	THR	THR	HIS	
ARG	ARG	LEU	LEU	ARG	
ALA	ALA	GLU	ASP	ALA	
THR	THR	GLU	GLU	THR	
ASN	ASN	VAL	VAL	GLY	
GLY	GLY	THR	THR	VAL	
ARG	ARG	ILE	ILE	THR	
PRO	PRO	GLN	GLN	ASP	
ASP	ASP	GLU	GLU	GLU	
THR	THR	ALA	ALA	ALA	
LEU	LEU	THR	THR	THR	
GLU	GLU	GLY	GLY	GLY	
ASN	ASN	ILE	ILE	ILE	
THR	THR	ALA	ALA	ALA	
ARG	ARG	ASP	ASP	ASP	
ALA	ALA	GLY	GLY	GLY	
PRO	PRO	LEU	LEU	LEU	
GLY	GLY	ALA	ALA	ALA	
THR	THR	ASN	ASN	ASN	
ASP	ASP	THR	THR	THR	
ARG	ARG	GLU	GLU	GLU	
ALA	ALA	ILE	ILE	ILE	
PRO	PRO	GLN	GLN	GLN	
GLY	GLY	VAL	VAL	VAL	
THR	THR	ARG	ARG	ARG	
ASN	ASN	THR	THR	THR	
GLU	GLU	GLY	GLY	GLY	
VAL	VAL	ALA	ALA	ALA	
ARG	ARG	THR	THR	THR	
ALA	ALA	GLU	GLU	GLU	
PRO	PRO	ILE	ILE	ILE	
GLY	GLY	ALA	ALA	ALA	
THR	THR	ASN	ASN	ASN	
ASP	ASP	THR	THR	THR	
ARG	ARG	GLU	GLU	GLU	
ALA	ALA	VAL	VAL	VAL	
PRO	PRO	ARG	ARG	ARG	
GLY	GLY	THR	THR	THR	
THR	THR	ALA	ALA	ALA	
ASN	ASN	THR	THR	THR	
GLU	GLU	GLY	GLY	GLY	
VAL	VAL	ILE	ILE	ILE	
ARG	ARG	ALA	ALA	ALA	
ALA	ALA	ASP	ASP	ASP	
PRO	PRO	GLU	GLU	GLU	
GLY	GLY	THR	THR	THR	
THR	THR	ASN	ASN	ASN	
ASP	ASP	THR	THR	THR	
ARG	ARG	GLU	GLU	GLU	
ALA	ALA	ILE	ILE	ILE	
PRO	PRO	ALA	ALA	ALA	
GLY	GLY	ASP	ASP	ASP	
THR	THR	LEU	LEU	LEU	
ASN	ASN	SER	SER	SER	
GLU	GLU	ILE	ILE	ILE	
VAL	VAL	ALA	ALA	ALA	
ARG	ARG	THR	THR	THR	
ALA	ALA	GLU	GLU	GLU	
PRO	PRO	VAL	VAL	VAL	
GLY	GLY	ARG	ARG	ARG	
THR	THR	THR	THR	THR	
ASN	ASN	GLN	GLN	GLN	
GLU	GLU	TLE	TLE	TLE	
VAL	VAL	ALA</			

- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain r:  54% 46%

[illegible]

- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain s:  54% 46%

[illegible]

- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain t:  54% 46%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	19700	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	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	1	0.26	0/2258	0.48	0/3081
1	2	0.26	0/2258	0.48	0/3081
1	3	0.26	0/2258	0.48	0/3081
1	4	0.27	0/2258	0.48	0/3081
1	5	0.26	0/2258	0.49	0/3081
1	A	0.27	0/2286	0.49	0/3121
1	B	0.27	0/1947	0.48	0/2658
1	C	0.27	0/2292	0.48	0/3129
1	D	0.27	0/2292	0.49	0/3129
1	E	0.27	0/2292	0.49	0/3129
1	F	0.28	0/2286	0.48	0/3121
1	G	0.27	0/2292	0.49	0/3129
1	H	0.28	0/2292	0.49	0/3129
1	I	0.27	0/2292	0.48	0/3129
1	J	0.27	0/2292	0.49	0/3129
1	K	0.27	0/2292	0.49	0/3129
1	L	0.28	0/2292	0.49	0/3129
1	M	0.27	0/2292	0.48	0/3129
1	N	0.26	0/2292	0.47	0/3129
1	O	0.27	0/2292	0.49	0/3129
1	P	0.28	0/2292	0.48	0/3129
1	Q	0.27	0/2292	0.49	0/3129
1	R	0.26	0/2292	0.48	0/3129
1	S	0.26	0/2292	0.48	0/3129
1	T	0.26	0/2292	0.48	0/3129
1	U	0.26	0/2292	0.48	0/3129
1	V	0.27	0/2292	0.48	0/3129
1	W	0.27	0/2292	0.49	0/3129
1	X	0.27	0/2292	0.48	0/3129
1	Y	0.27	0/2292	0.49	0/3129
1	Z	0.26	0/2292	0.49	0/3129
1	a	0.27	0/2292	0.49	0/3129
1	b	0.26	0/2292	0.47	0/3129
1	c	0.27	0/2292	0.49	0/3129

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	d	0.28	0/2292	0.51	0/3129
1	e	0.27	0/2292	0.48	0/3129
1	f	0.27	0/2292	0.49	0/3129
1	g	0.27	0/2292	0.49	0/3129
1	h	0.27	0/2292	0.49	0/3129
1	i	0.26	0/2292	0.49	0/3129
1	j	0.27	0/2292	0.48	0/3129
1	k	0.27	0/2292	0.48	0/3129
1	l	0.26	0/2292	0.49	0/3129
1	m	0.27	0/2292	0.48	0/3129
1	n	0.26	0/2292	0.48	0/3129
1	o	0.26	0/2292	0.48	0/3129
1	p	0.27	0/2292	0.49	0/3129
1	q	0.27	0/2292	0.51	0/3129
1	r	0.26	0/2292	0.48	0/3129
1	s	0.26	0/2292	0.48	0/3129
1	t	0.27	0/2292	0.48	0/3129
1	u	0.26	0/2292	0.49	0/3129
1	v	0.27	0/2292	0.49	0/3129
All	All	0.27	0/120949	0.49	0/165110

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	1	284/543 (52%)	280 (99%)	4 (1%)	0	100	100
1	2	284/543 (52%)	281 (99%)	3 (1%)	0	100	100
1	3	284/543 (52%)	280 (99%)	4 (1%)	0	100	100
1	4	284/543 (52%)	279 (98%)	5 (2%)	0	100	100
1	5	284/543 (52%)	281 (99%)	3 (1%)	0	100	100
1	A	290/543 (53%)	284 (98%)	6 (2%)	0	100	100
1	B	243/543 (45%)	240 (99%)	3 (1%)	0	100	100
1	C	291/543 (54%)	285 (98%)	6 (2%)	0	100	100
1	D	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	E	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	F	290/543 (53%)	285 (98%)	5 (2%)	0	100	100
1	G	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	H	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	I	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	J	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	K	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	L	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	M	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	N	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	O	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	P	291/543 (54%)	290 (100%)	1 (0%)	0	100	100
1	Q	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	R	291/543 (54%)	283 (97%)	8 (3%)	0	100	100
1	S	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	T	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	U	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	V	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	W	291/543 (54%)	285 (98%)	6 (2%)	0	100	100
1	X	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	Y	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	Z	291/543 (54%)	283 (97%)	8 (3%)	0	100	100
1	a	291/543 (54%)	291 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	c	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	d	291/543 (54%)	280 (96%)	11 (4%)	0	100	100
1	e	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	f	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	g	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	h	291/543 (54%)	285 (98%)	6 (2%)	0	100	100
1	i	291/543 (54%)	280 (96%)	11 (4%)	0	100	100
1	j	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	k	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	l	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	m	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	n	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	o	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	p	291/543 (54%)	285 (98%)	6 (2%)	0	100	100
1	q	291/543 (54%)	284 (98%)	7 (2%)	0	100	100
1	r	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	s	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	t	291/543 (54%)	291 (100%)	0	0	100	100
1	u	291/543 (54%)	284 (98%)	7 (2%)	0	100	100
1	v	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
All	All	15338/28779 (53%)	15110 (98%)	228 (2%)	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	1	226/432 (52%)	226 (100%)	0	100	100
1	2	226/432 (52%)	226 (100%)	0	100	100
1	3	226/432 (52%)	226 (100%)	0	100	100
1	4	226/432 (52%)	226 (100%)	0	100	100
1	5	226/432 (52%)	226 (100%)	0	100	100
1	A	228/432 (53%)	228 (100%)	0	100	100
1	B	193/432 (45%)	192 (100%)	1 (0%)	86	93
1	C	229/432 (53%)	229 (100%)	0	100	100
1	D	229/432 (53%)	229 (100%)	0	100	100
1	E	229/432 (53%)	229 (100%)	0	100	100
1	F	228/432 (53%)	228 (100%)	0	100	100
1	G	229/432 (53%)	229 (100%)	0	100	100
1	H	229/432 (53%)	229 (100%)	0	100	100
1	I	229/432 (53%)	229 (100%)	0	100	100
1	J	229/432 (53%)	228 (100%)	1 (0%)	89	95
1	K	229/432 (53%)	229 (100%)	0	100	100
1	L	229/432 (53%)	229 (100%)	0	100	100
1	M	229/432 (53%)	228 (100%)	1 (0%)	89	95
1	N	229/432 (53%)	229 (100%)	0	100	100
1	O	229/432 (53%)	229 (100%)	0	100	100
1	P	229/432 (53%)	229 (100%)	0	100	100
1	Q	229/432 (53%)	229 (100%)	0	100	100
1	R	229/432 (53%)	228 (100%)	1 (0%)	89	95
1	S	229/432 (53%)	229 (100%)	0	100	100
1	T	229/432 (53%)	229 (100%)	0	100	100
1	U	229/432 (53%)	229 (100%)	0	100	100
1	V	229/432 (53%)	229 (100%)	0	100	100
1	W	229/432 (53%)	229 (100%)	0	100	100
1	X	229/432 (53%)	229 (100%)	0	100	100
1	Y	229/432 (53%)	229 (100%)	0	100	100
1	Z	229/432 (53%)	229 (100%)	0	100	100
1	a	229/432 (53%)	229 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	229/432 (53%)	229 (100%)	0	100	100
1	c	229/432 (53%)	229 (100%)	0	100	100
1	d	229/432 (53%)	229 (100%)	0	100	100
1	e	229/432 (53%)	229 (100%)	0	100	100
1	f	229/432 (53%)	229 (100%)	0	100	100
1	g	229/432 (53%)	229 (100%)	0	100	100
1	h	229/432 (53%)	229 (100%)	0	100	100
1	i	229/432 (53%)	229 (100%)	0	100	100
1	j	229/432 (53%)	229 (100%)	0	100	100
1	k	229/432 (53%)	229 (100%)	0	100	100
1	l	229/432 (53%)	228 (100%)	1 (0%)	89	95
1	m	229/432 (53%)	229 (100%)	0	100	100
1	n	229/432 (53%)	229 (100%)	0	100	100
1	o	229/432 (53%)	229 (100%)	0	100	100
1	p	229/432 (53%)	228 (100%)	1 (0%)	89	95
1	q	229/432 (53%)	229 (100%)	0	100	100
1	r	229/432 (53%)	229 (100%)	0	100	100
1	s	229/432 (53%)	229 (100%)	0	100	100
1	t	229/432 (53%)	229 (100%)	0	100	100
1	u	229/432 (53%)	229 (100%)	0	100	100
1	v	229/432 (53%)	228 (100%)	1 (0%)	89	95
All	All	12084/22896 (53%)	12077 (100%)	7 (0%)	92	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	426	ASN
1	J	426	ASN
1	M	532	ASN
1	R	360	LYS
1	l	374	GLN
1	p	510	ARG
1	v	426	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	D	454	GLN
1	H	469	ASN
1	M	343	GLN
1	P	454	GLN
1	U	332	GLN
1	U	376	ASN
1	X	430	ASN
1	a	279	ASN
1	a	430	ASN
1	g	376	ASN
1	l	374	GLN
1	m	275	ASN
1	n	416	HIS
1	n	419	GLN
1	o	376	ASN
1	q	275	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 ⓘ

There are no chain breaks in this entry.