



wwPDB EM Validation Summary Report ⓘ

Apr 20, 2025 – 12:18 AM JST

PDB ID : 9LW6 / pdb_00009lw6
EMDB ID : EMD-63432
Title : Top 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 : 3.42 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 : **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

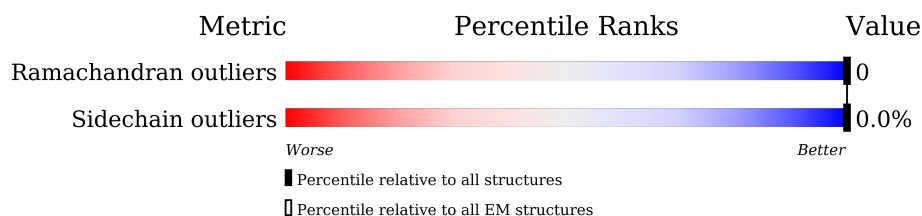
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY











The reported resolution of this entry is 3.42 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.



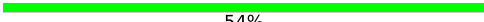
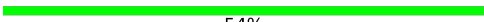













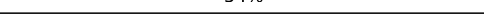
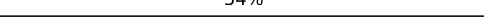
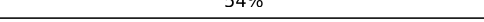
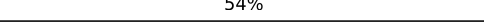
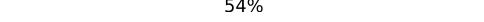
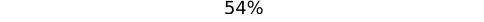
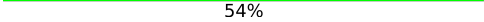
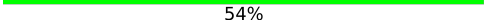
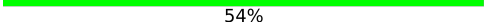
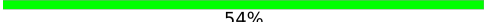
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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		
1	2	543		
1	3	543		
1	4	543		
1	5	543		
1	A	543		
1	B	543		
1	C	543		
1	D	543		
1	E	543		




















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Mol	Chain	Length	Quality of chain	
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%
1	W	543	 54%	46%
1	X	543	 54%	46%
1	Y	543	 54%	46%
1	Z	543	 54%	46%
1	a	543	 54%	46%
1	b	543	 54%	46%
1	c	543	 54%	46%
1	d	543	 54%	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%
1	w	543		53% 47%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 120816 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	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
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

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Mol	Chain	Residues	Atoms					AltConf	Trace
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
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

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	n	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	o	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	p	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	q	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	r	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	s	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	t	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	u	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	v	293	Total	C	N	O	S	0	0
			2241	1416	385	436	4		
1	w	288	Total	C	N	O	S	0	0
			2208	1397	379	428	4		
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		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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

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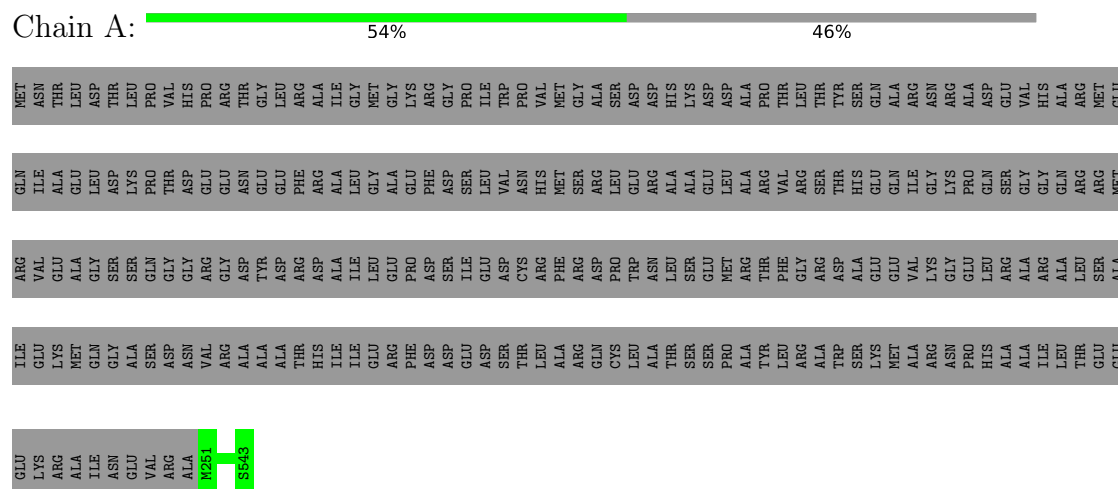
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Chain	Residue	Modelled	Actual	Comment	Reference
1	197	HIS	LYS	conflict	UNP Q854Z2
2	197	HIS	LYS	conflict	UNP Q854Z2
3	197	HIS	LYS	conflict	UNP Q854Z2
4	197	HIS	LYS	conflict	UNP Q854Z2
5	197	HIS	LYS	conflict	UNP Q854Z2

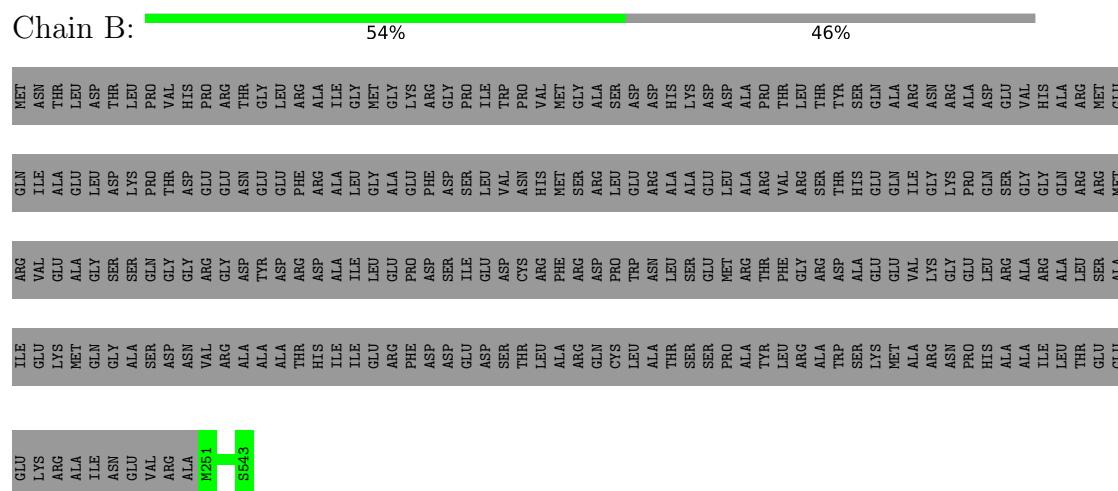
3 Residue-property plots

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.

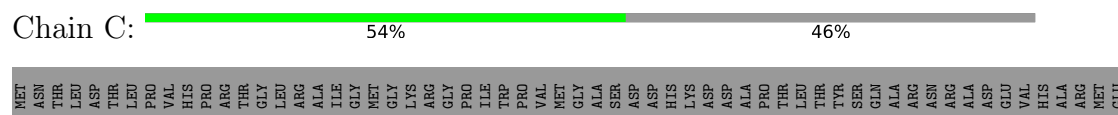
- Molecule 1: Phage capsid-like C-terminal domain-containing protein



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



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



[illegible]

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

Chain M:  54% 46%

[illegible]

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

Chain N:  54% 46%

[illegible]

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

Chain 0:  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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[illegible]

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

Chain P:  54% 46%

[illegible]

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

Chain Q:  54% 46%

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

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

Chain R:  54% 46%

MET	ASN	THR	LEU	ASP	THR	LEU	PRO	PRO	HIS	ARG	THR	GLY	GLY	ALA	ILE	GLY	MET	MET	GLY	LYS	ARG	GLY	PRO	ILE	TRP	PRO	VAL	VAL	MET	GLY	ALA	ALA	SER	ASP	ASP	HIS	LYS	ASP	ASP	ALA	ALA	PRO	THR	LEU	THR	TYR	SER	SER	GLN	ALA	ALA	ARG	ASN	ARG	ARG	ALA	ALA	ARG	ALA	MET	THR
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Chain 2: 53% 47%

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

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

Chain 3:  53% 47%

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

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

Chain 4: 53% 47%

[illegible]

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

Chain 5: 53% 47%

[illegible]

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

GLU

LYS

ARG

ALA

ILE

ASN

GLU

VAL

ARG

ALA

M251

T448

ILE

GLY

ASN

GLY

GLU

P452

S943

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	19765	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 ($e^-/\text{\AA}^2$)	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	0.28	0/2258	0.49	0/3081
1	2	0.28	0/2258	0.50	0/3081
1	3	0.28	0/2258	0.49	0/3081
1	4	0.28	0/2258	0.50	0/3081
1	5	0.28	0/2258	0.49	0/3081
1	A	0.29	0/2292	0.49	0/3129
1	B	0.28	0/2292	0.50	0/3129
1	C	0.29	0/2292	0.48	0/3129
1	D	0.29	0/2292	0.50	0/3129
1	E	0.29	0/2292	0.50	0/3129
1	F	0.29	0/2292	0.51	0/3129
1	G	0.28	0/2292	0.50	0/3129
1	H	0.29	0/2292	0.50	0/3129
1	I	0.29	0/2292	0.51	0/3129
1	J	0.29	0/2292	0.50	0/3129
1	K	0.28	0/2292	0.49	0/3129
1	L	0.28	0/2292	0.49	0/3129
1	M	0.29	0/2292	0.50	0/3129
1	N	0.28	0/2292	0.50	0/3129
1	O	0.28	0/2292	0.50	0/3129
1	P	0.28	0/2292	0.49	0/3129
1	Q	0.28	0/2292	0.49	0/3129
1	R	0.28	0/2292	0.49	0/3129
1	S	0.28	0/2292	0.49	0/3129
1	T	0.29	0/2292	0.51	0/3129
1	U	0.28	0/2292	0.48	0/3129
1	V	0.29	0/2292	0.50	0/3129
1	W	0.27	0/2292	0.49	0/3129
1	X	0.28	0/2292	0.50	0/3129
1	Y	0.29	0/2292	0.50	0/3129
1	Z	0.28	0/2292	0.50	0/3129
1	a	0.28	0/2292	0.50	0/3129
1	b	0.28	0/2292	0.50	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	0.27	0/2292	0.50	0/3129
1	e	0.28	0/2292	0.51	0/3129
1	f	0.28	0/2292	0.49	0/3129
1	g	0.28	0/2292	0.49	0/3129
1	h	0.28	0/2292	0.50	0/3129
1	i	0.28	0/2292	0.50	0/3129
1	j	0.28	0/2292	0.49	0/3129
1	k	0.28	0/2292	0.50	0/3129
1	l	0.28	0/2292	0.50	0/3129
1	m	0.28	0/2292	0.50	0/3129
1	n	0.27	0/2292	0.48	0/3129
1	o	0.27	0/2292	0.49	0/3129
1	p	0.28	0/2292	0.49	0/3129
1	q	0.28	0/2292	0.49	0/3129
1	r	0.27	0/2292	0.48	0/3129
1	s	0.27	0/2292	0.49	0/3129
1	t	0.27	0/2292	0.49	0/3129
1	u	0.27	0/2292	0.48	0/3129
1	v	0.27	0/2292	0.47	0/3129
1	w	0.28	0/2258	0.49	0/3081
All	All	0.28	0/123564	0.49	0/168678

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%)	278 (98%)	6 (2%)	0	100	100
1	2	284/543 (52%)	274 (96%)	10 (4%)	0	100	100
1	3	284/543 (52%)	277 (98%)	7 (2%)	0	100	100
1	4	284/543 (52%)	278 (98%)	6 (2%)	0	100	100
1	5	284/543 (52%)	278 (98%)	6 (2%)	0	100	100
1	A	291/543 (54%)	282 (97%)	9 (3%)	0	100	100
1	B	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	C	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	D	291/543 (54%)	285 (98%)	6 (2%)	0	100	100
1	E	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	F	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	G	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	H	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	I	291/543 (54%)	289 (99%)	2 (1%)	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%)	288 (99%)	3 (1%)	0	100	100
1	N	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	O	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	P	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	Q	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	R	291/543 (54%)	284 (98%)	7 (2%)	0	100	100
1	S	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	T	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	U	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	V	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	W	291/543 (54%)	284 (98%)	7 (2%)	0	100	100
1	X	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	Y	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	Z	291/543 (54%)	285 (98%)	6 (2%)	0	100	100
1	a	291/543 (54%)	289 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	291/543 (54%)	285 (98%)	6 (2%)	0	100	100
1	c	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	d	291/543 (54%)	283 (97%)	8 (3%)	0	100	100
1	e	291/543 (54%)	282 (97%)	9 (3%)	0	100	100
1	f	291/543 (54%)	290 (100%)	1 (0%)	0	100	100
1	g	291/543 (54%)	283 (97%)	8 (3%)	0	100	100
1	h	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	i	291/543 (54%)	282 (97%)	9 (3%)	0	100	100
1	j	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	k	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	l	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	m	291/543 (54%)	290 (100%)	1 (0%)	0	100	100
1	n	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	o	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	p	291/543 (54%)	284 (98%)	7 (2%)	0	100	100
1	q	291/543 (54%)	285 (98%)	6 (2%)	0	100	100
1	r	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	s	291/543 (54%)	281 (97%)	10 (3%)	0	100	100
1	t	291/543 (54%)	290 (100%)	1 (0%)	0	100	100
1	u	291/543 (54%)	281 (97%)	10 (3%)	0	100	100
1	v	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	w	284/543 (52%)	278 (98%)	6 (2%)	0	100	100
All	All	15672/29322 (53%)	15415 (98%)	257 (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	229/432 (53%)	229 (100%)	0	100	100
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%)	228 (100%)	1 (0%)	89	93
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%)	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%)	229 (100%)	0	100	100
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%)	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%)	228 (100%)	1 (0%)	89	93
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%)	229 (100%)	0	100	100
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%)	229 (100%)	0	100	100
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%)	228 (100%)	1 (0%)	89	93
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	93
1	w	226/432 (52%)	226 (100%)	0	100	100
All	All	12348/23328 (53%)	12344 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	426	ASN
1	e	426	ASN
1	s	418	ARG
1	v	426	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	t	279	ASN
1	q	275	ASN
1	U	376	ASN
1	g	376	ASN
1	U	296	HIS

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.