



## 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](mailto: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>.

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

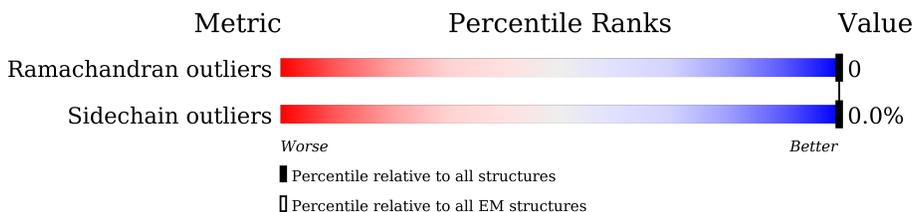
EMDB validation analysis : **FAILED**  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline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



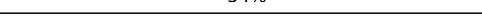
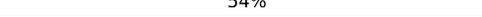
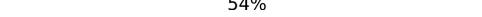
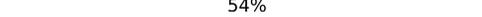
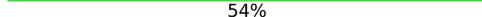
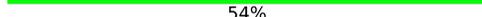
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	 54%	 46%
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	 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 [i](#)

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
			Total	C	N	O	S		
1	A	293	2241	1416	385	436	4	0	0
1	B	293	2241	1416	385	436	4	0	0
1	C	293	2241	1416	385	436	4	0	0
1	D	293	2241	1416	385	436	4	0	0
1	E	293	2241	1416	385	436	4	0	0
1	F	293	2241	1416	385	436	4	0	0
1	G	293	2241	1416	385	436	4	0	0
1	H	293	2241	1416	385	436	4	0	0
1	I	293	2241	1416	385	436	4	0	0
1	J	293	2241	1416	385	436	4	0	0
1	K	293	2241	1416	385	436	4	0	0
1	L	293	2241	1416	385	436	4	0	0
1	M	293	2241	1416	385	436	4	0	0
1	N	293	2241	1416	385	436	4	0	0
1	O	293	2241	1416	385	436	4	0	0
1	P	293	2241	1416	385	436	4	0	0
1	Q	293	2241	1416	385	436	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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<b>Chain</b>	<b>Residue</b>	<b>Modelled</b>	<b>Actual</b>	<b>Comment</b>	<b>Reference</b>
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





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

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

Chain G:  54% 46%

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

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

Chain H:  54% 46%

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

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

Chain I:  54% 46%

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































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T446  
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S543

## 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 [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	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 [i](#)

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.