



Full wwPDB EM Validation Report ⓘ

Apr 20, 2025 – 12:10 AM JST

PDB ID : 9LW7 / pdb_00009lw7
EMDB ID : EMD-63433
Title : Midsection 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 : 3.52 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

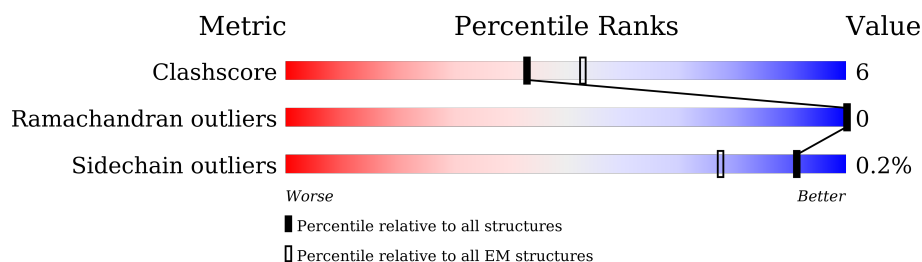
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.52 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.



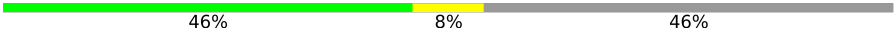
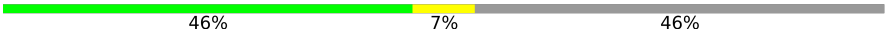
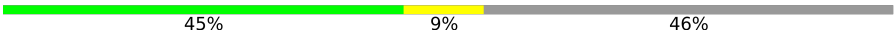
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	543	46% 8% 46%
1	B	543	46% 8% 46%
1	C	543	46% 8% 46%
1	D	543	44% 10% 46%
1	E	543	46% 8% 46%
1	F	543	44% 10% 46%
1	G	543	47% 7% 46%
1	H	543	46% 8% 46%
1	I	543	48% 6% 46%

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Mol	Chain	Length	Quality of chain
1	J	543	 46% 8% 46%
1	K	543	 46% 7% 46%
1	L	543	 45% 9% 46%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 26892 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

There are 12 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

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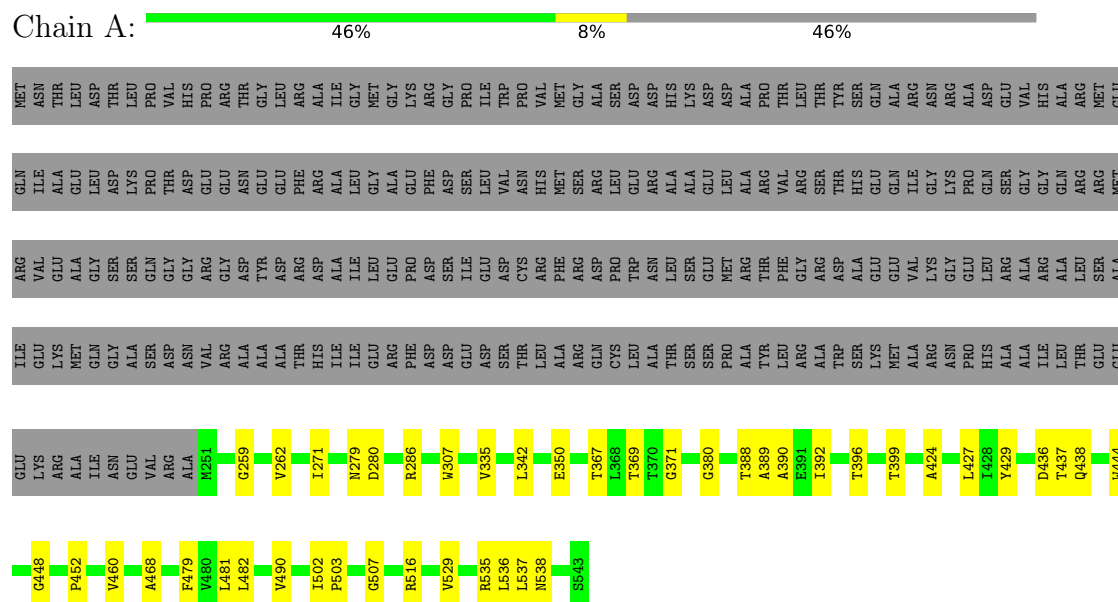
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Chain	Residue	Modelled	Actual	Comment	Reference
G	197	HIS	LYS	conflict	UNP Q854Z2
H	197	HIS	LYS	conflict	UNP Q854Z2
I	197	HIS	LYS	conflict	UNP Q854Z2
J	197	HIS	LYS	conflict	UNP Q854Z2
K	197	HIS	LYS	conflict	UNP Q854Z2
L	197	HIS	LYS	conflict	UNP Q854Z2

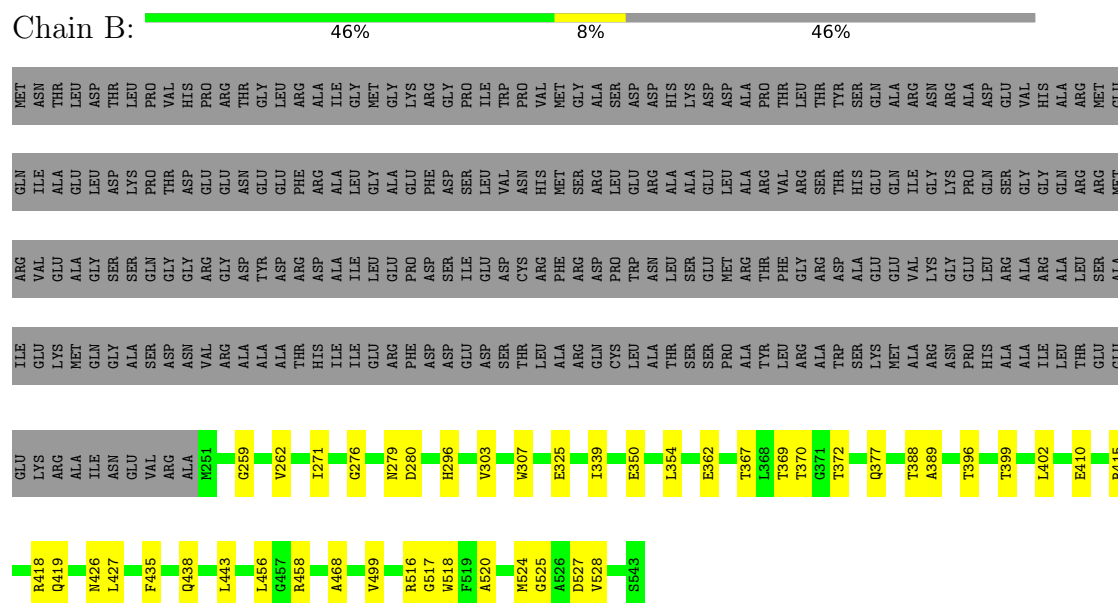
3 Residue-property plots

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.

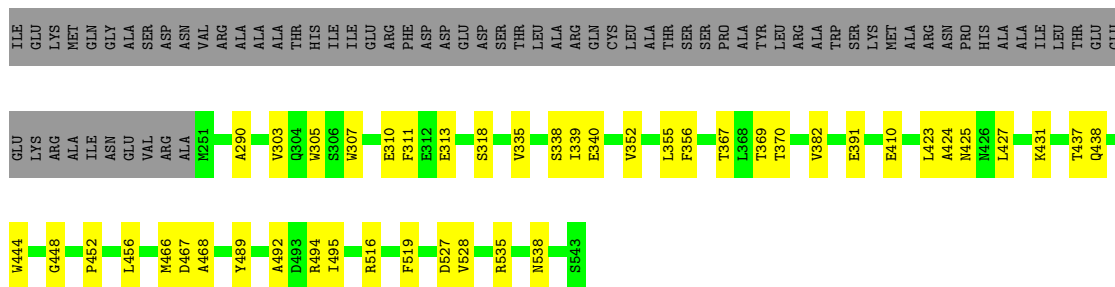
- Molecule 1: Phage capsid-like C-terminal domain-containing protein



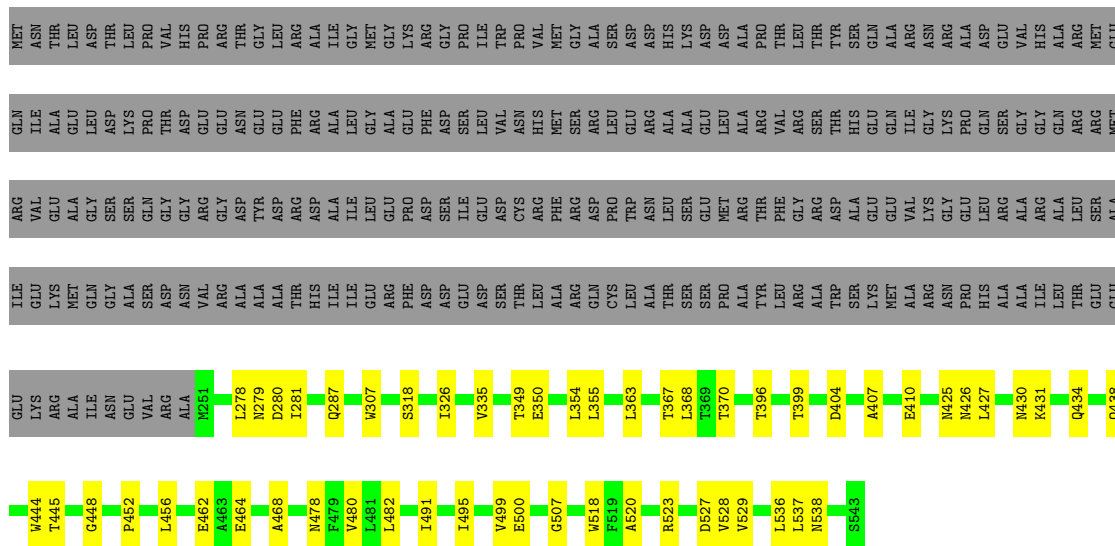
- Molecule 1: Phage capsid-like C-terminal domain-containing protein



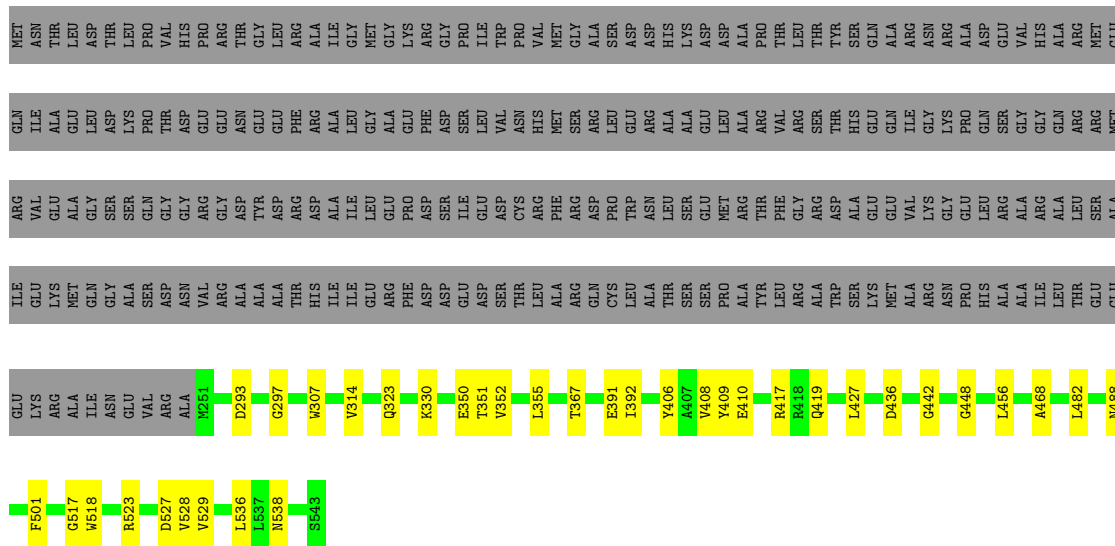
- [illegible]



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



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

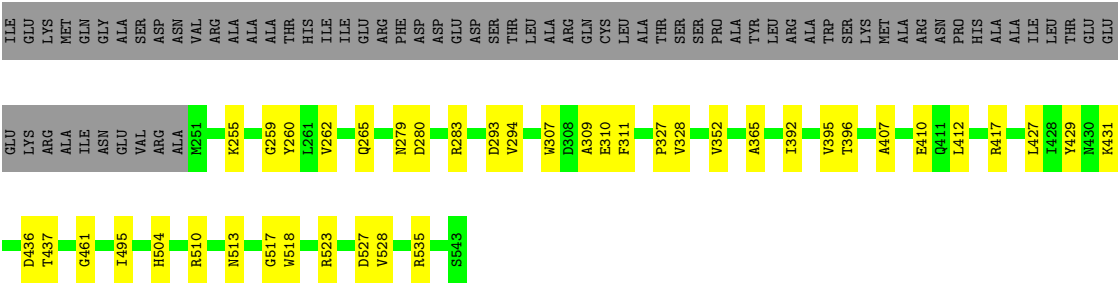


- Molecule 1: Phage capsid-like C-terminal domain-containing protein

G448	G452	L456	G461	A467	A468	M469	T472	M478	F479	L482	R494	I495	G496	M497	F519	R535	L536	L543																																	
GLU	LYS	ARG	ALA	ILE	ASN	GLU	VAL	ARG	ALA	M251	K255	G259	D308	E313	V314	Q332	T351	L354	L355	F356	A357	E358	T367	T372	G373	Q374	T379	A384	L385	Y406	A407	E410	G411	L412	N425	Y429	I432	F435	W444												
ILE	GLU	LYS	GLY	ALA	SER	ASN	ASP	ASP	VAL	ARG	ALA	ALA	THR	ILE	ILE	ARG	PHE	ASP	ASP	GLU	ASP	ILE	GLU	ASP	LYS	THR	THR	ALA	ALA	TYR	LEU	ARG	TRP	LYS	MET	ALA	ARG	PRO	HIS	ALA	ILE	LEU	THR	GLU							
ARG	VAL	ALA	GLY	SER	GLN	SER	GLN	GLY	ARG	GLY	ASP	TYR	ARG	ASP	ILE	ILE	LEU	PRO	ASP	SER	ILE	GLU	ASP	TRP	ALA	LEU	SER	SER	MET	ARG	THR	PHE	GLY	ASP	ALA	GLY	HIS	GLN	ILE	GLY	VAL	ARG	ALA								
MET	ASN	THR	LEU	PRO	THR	PRO	THR	GLY	ASN	THR	THR	GLY	ARG	ALA	ILE	GLY	ALA	PHE	ARG	GLY	PRO	ILE	GLU	VAL	ASN	ARG	ALA	LYS	ASP	ALA	ARG	THR	THR	THR	THR	GLN	ALA	ARG	ASN	LYS	PRO	ALA	GLN	SER	GLU	VAL	HIS	ARG	GLN	ARG	MET

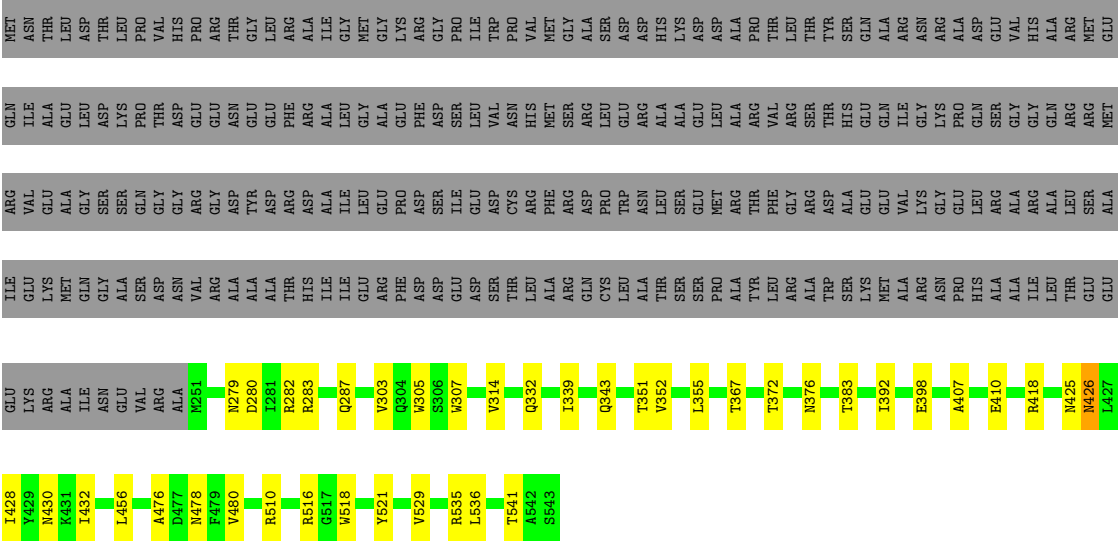
R536	GLU	ILE	ARG	GLN	MET
L536	LYS	GLU	VAL	ILE	ASN
V539	ARG	LYS	GLU	ALA	THR
E540	ALA	MET	ALA	GLU	LEU
T541	ILE	GLN	GLY	LEU	ASP
A542	ASN	GLY	SER	ASP	THR
S543	GLU	ALA	SER	LYS	LEU
	VAL	SER	GLN	PRO	PRO
	ARG	ASP	GLY	THR	VAL
	ALA	ASN	GLY	ASP	HIS
	M2E1	VAL	ARG	GLU	PRO
		ARG	GLY	GLU	ARG
	R286	ALA	ASP	ASN	THR
		ALA	TYR	GLU	GLY
	T291	ALA	ASP	GLU	LEU
		THR	ARG	PHE	ARG
	G297	HIS	ASP	ALA	ALA
		ILE	ALA	ILE	ILE
	Q323	ILE	LEU	LEU	GLY
		GLU	LEU	GLY	MET
	Q332	ARG	GLU	ALA	GLY
		PHE	PRO	GLU	LYS
	T369	ASP	ASP	PHE	ARG
	T370	ASP	SER	ASP	ARG
		GLU	ILE	ASP	GLY
		ASP	GLU	SER	PRO
	T392	SER	GLU	LEU	PRO
		ASP	ASP	VAL	TRP
	A424	THR	CYS	ASN	TRP
	N425	LEU	ARG	HIS	VAL
	N426	ALA	PHE	MET	VAL
	L427	ARG	ARG	SER	MET
		GLN	ASP	GLY	GLY
	N430	CYS	ASP	LEU	ALA
		LEU	TRP	GLU	ASP
		ALA	ASN	ARG	ASP
	R433	THR	LEU	ALA	HIS
	Q434	SER	SER	ALA	LYS
		SER	GLU	GLU	ASP
	G448	PRO	MET	LEU	ASP
		ALA	ARG	ALA	ALA
	E451	TYR	THR	ARG	PRO
		LEU	PHE	VAL	THR
	M466	ARG	GLY	LEU	THR
	D467	ARG	ARG	SER	SER
	A468	TRP	ASP	THR	THR
	N469	SER	ALA	HIS	SER
	W470	LYS	GLU	GLN	GLN
		MET	GLU	ILE	ALA
	D477	ALA	VAL	ARG	ARG
	N478	ARG	LYS	GLY	ASN
	F479	ASN	GLY	LYS	ASN
		PRO	LEU	PRO	ALA
	L482	HIS	LEU	GLN	ASP
		ALA	ARG	SER	GLU
	Y489	ILE	ALA	GLY	VAL
	V490	ILE	ARG	GLY	HIS
		LEU	ALA	GLN	ALA
	F519	THR	LEU	ARG	ARG
		GLU	ALA	MET	ARG
	V528	GLU	SER	THR	GLN
		THR	ALA	ARG	THR

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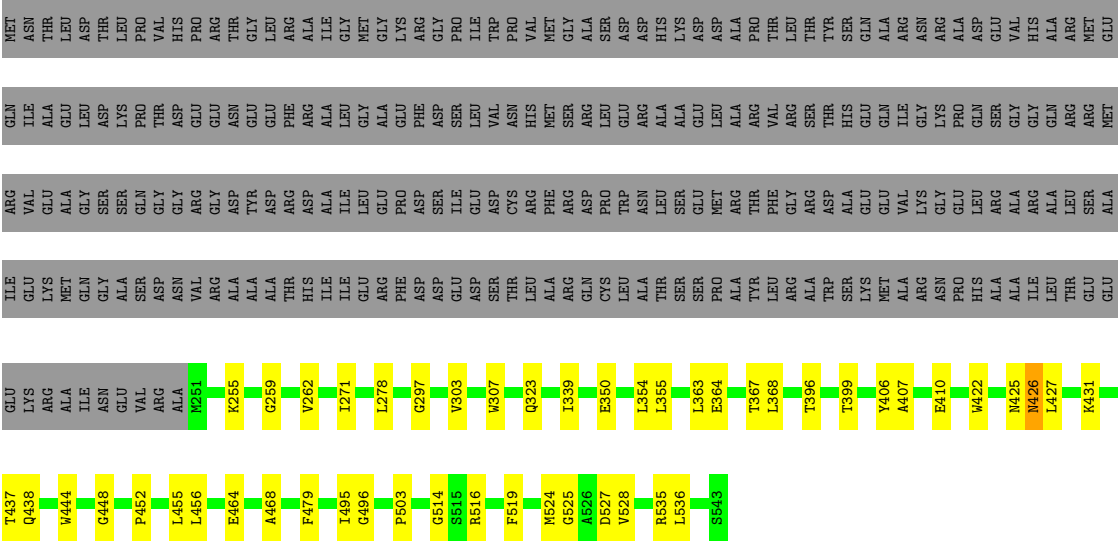
● Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain K: 46% 7% 46%



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

Chain L: 45% 9% 46%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	19761	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 [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	A	0.37	0/2292	0.52	0/3129
1	B	0.37	0/2292	0.52	0/3129
1	C	0.37	0/2292	0.51	0/3129
1	D	0.37	0/2292	0.51	0/3129
1	E	0.37	0/2292	0.51	0/3129
1	F	0.36	0/2292	0.52	0/3129
1	G	0.36	0/2292	0.53	0/3129
1	H	0.39	0/2292	0.51	0/3129
1	I	0.36	0/2292	0.50	0/3129
1	J	0.37	0/2292	0.52	0/3129
1	K	0.37	0/2292	0.53	0/3129
1	L	0.36	0/2292	0.50	0/3129
All	All	0.37	0/27504	0.52	0/37548

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](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2241	0	2151	33	0
1	B	2241	0	2151	33	0
1	C	2241	0	2151	37	0
1	D	2241	0	2151	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2241	0	2151	36	0
1	F	2241	0	2151	42	0
1	G	2241	0	2151	32	0
1	H	2241	0	2151	36	0
1	I	2241	0	2151	23	0
1	J	2241	0	2151	29	0
1	K	2241	0	2151	30	0
1	L	2241	0	2151	35	0
All	All	26892	0	25812	336	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (336) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:307:TRP:HE1	1:K:367:THR:HG21	1.29	0.96
1:E:307:TRP:HE1	1:F:367:THR:HG21	1.32	0.92
1:G:367:THR:HG21	1:L:307:TRP:HE1	1.38	0.88
1:A:367:THR:HG21	1:F:307:TRP:HE1	1.48	0.78
1:H:425:ASN:HD22	1:H:468:ALA:HB2	1.48	0.78
1:G:307:TRP:HE1	1:H:367:THR:HG21	1.50	0.77
1:A:307:TRP:HE1	1:B:367:THR:HG21	1.50	0.75
1:B:307:TRP:HE1	1:C:367:THR:HG21	1.52	0.74
1:D:527:ASP:OD1	1:D:528:VAL:N	2.20	0.74
1:C:307:TRP:HE1	1:D:367:THR:HG21	1.55	0.71
1:H:314:VAL:HG11	1:I:519:PHE:HE1	1.55	0.71
1:A:388:THR:HG22	1:A:389:ALA:H	1.58	0.69
1:D:438:GLN:HG3	1:E:438:GLN:HG2	1.76	0.68
1:D:388:THR:HG21	1:D:531:PRO:HB2	1.76	0.68
1:H:372:THR:HG22	1:H:374:GLN:H	1.58	0.67
1:H:308:ASP:OD2	1:I:332:GLN:NE2	2.27	0.67
1:C:415:ARG:NH2	1:D:274:SER:O	2.22	0.66
1:E:369:THR:HG22	1:E:370:THR:HG23	1.76	0.65
1:F:527:ASP:OD1	1:F:528:VAL:N	2.23	0.65
1:E:437:THR:HG23	1:E:438:GLN:HG3	1.77	0.65
1:B:372:THR:HG22	1:B:377:GLN:HB2	1.78	0.65
1:G:352:VAL:HG21	1:G:518:TRP:CZ3	2.32	0.65
1:I:479:PHE:HB3	1:I:536:LEU:HD11	1.80	0.64
1:G:482:LEU:HD12	1:G:536:LEU:HD13	1.79	0.63
1:J:307:TRP:NE1	1:K:367:THR:HG21	2.08	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:392:ILE:HD11	1:I:535:ARG:HD2	1.80	0.62
1:H:432:ILE:HD13	1:H:435:PHE:HE2	1.63	0.62
1:J:352:VAL:HG21	1:J:518:TRP:CZ3	2.34	0.62
1:A:286:ARG:HD3	1:A:490:VAL:HG12	1.81	0.62
1:G:427:LEU:HD22	1:G:468:ALA:HB1	1.82	0.62
1:F:425:ASN:HD22	1:F:468:ALA:HB2	1.64	0.62
1:K:282:ARG:NH1	1:K:287:GLN:OE1	2.32	0.62
1:C:282:ARG:NH1	1:C:287:GLN:OE1	2.32	0.61
1:B:524:MET:HG2	1:B:525:GLY:H	1.65	0.61
1:K:456:LEU:H	1:L:448:GLY:HA2	1.65	0.61
1:D:307:TRP:HE1	1:E:367:THR:HG21	1.66	0.61
1:B:369:THR:HG22	1:B:370:THR:HG23	1.81	0.61
1:D:503:PRO:O	1:D:504:HIS:ND1	2.34	0.61
1:B:402:LEU:HD13	1:B:435:PHE:HD2	1.65	0.61
1:G:391:GLU:OE2	1:G:538:ASN:ND2	2.25	0.61
1:A:482:LEU:HD12	1:A:536:LEU:HD13	1.81	0.60
1:G:307:TRP:NE1	1:H:367:THR:HG21	2.16	0.60
1:A:479:PHE:HB3	1:A:536:LEU:HD11	1.83	0.60
1:L:437:THR:HG23	1:L:438:GLN:HG3	1.83	0.60
1:D:330:LYS:HB3	1:D:523:ARG:HG2	1.84	0.59
1:J:412:LEU:HB3	1:J:417:ARG:HG3	1.85	0.59
1:L:255:LYS:HA	1:L:259:GLY:HA3	1.84	0.59
1:C:307:TRP:NE1	1:D:367:THR:HG21	2.18	0.58
1:D:282:ARG:HD3	1:D:287:GLN:HE21	1.68	0.58
1:C:308:ASP:OD2	1:D:332:GLN:NE2	2.37	0.58
1:H:407:ALA:HA	1:H:410:GLU:HG2	1.86	0.57
1:B:307:TRP:NE1	1:C:367:THR:HG21	2.19	0.57
1:C:279:ASN:OD1	1:C:280:ASP:N	2.37	0.57
1:E:338:SER:OG	1:E:340:GLU:OE2	2.23	0.57
1:A:307:TRP:NE1	1:B:367:THR:HG21	2.19	0.56
1:D:427:LEU:HD22	1:D:468:ALA:HB1	1.87	0.56
1:I:427:LEU:HD22	1:I:468:ALA:HB1	1.87	0.56
1:J:427:LEU:O	1:J:431:LYS:HG3	2.04	0.56
1:K:426:ASN:HD22	1:K:426:ASN:C	2.07	0.56
1:L:278:LEU:N	1:L:464:GLU:OE2	2.36	0.56
1:L:396:THR:HG23	1:L:399:THR:HB	1.87	0.56
1:H:494:ARG:HG3	1:H:495:ILE:HG13	1.87	0.56
1:B:350:GLU:O	1:B:354:LEU:HG	2.06	0.55
1:D:281:ILE:HD11	1:D:423:LEU:HD21	1.88	0.55
1:I:369:THR:HG22	1:I:370:THR:HG23	1.88	0.55
1:B:524:MET:HG2	1:B:525:GLY:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ASN:OD1	1:B:280:ASP:N	2.40	0.55
1:B:415:ARG:NH2	1:C:274:SER:O	2.22	0.54
1:C:425:ASN:HD22	1:C:468:ALA:HB2	1.72	0.54
1:F:404:ASP:HB3	1:F:537:LEU:HD11	1.89	0.54
1:A:271:ILE:HD13	1:F:529:VAL:HG11	1.90	0.54
1:A:429:TYR:CZ	1:A:460:VAL:HG13	2.42	0.54
1:D:307:TRP:NE1	1:E:367:THR:HG21	2.22	0.54
1:F:500:GLU:OE1	1:J:504:HIS:NE2	2.39	0.54
1:H:255:LYS:HA	1:H:259:GLY:HA3	1.90	0.54
1:K:478:ASN:O	1:K:480:VAL:HG13	2.08	0.54
1:A:335:VAL:HG23	1:F:318:SER:HA	1.90	0.53
1:E:444:TRP:CE2	1:E:452:PRO:HG2	2.44	0.53
1:A:367:THR:HG21	1:F:307:TRP:NE1	2.21	0.52
1:J:429:TYR:OH	1:J:461:GLY:O	2.23	0.52
1:H:432:ILE:HA	1:H:435:PHE:CE2	2.44	0.52
1:C:444:TRP:CE2	1:C:452:PRO:HG2	2.44	0.52
1:F:396:THR:HG23	1:F:399:THR:HB	1.91	0.52
1:G:392:ILE:HD11	1:G:408:VAL:HG22	1.92	0.52
1:G:448:GLY:HA2	1:L:456:LEU:H	1.74	0.52
1:K:339:ILE:HG22	1:K:516:ARG:HE	1.74	0.52
1:A:448:GLY:HA2	1:F:456:LEU:H	1.75	0.52
1:E:410:GLU:OE2	1:F:427:LEU:HB2	2.09	0.52
1:E:425:ASN:HD22	1:E:468:ALA:HB2	1.75	0.52
1:G:352:VAL:HG11	1:G:518:TRP:HZ3	1.74	0.52
1:J:352:VAL:HG11	1:J:518:TRP:HZ3	1.75	0.52
1:J:495:ILE:HG22	1:J:523:ARG:HB2	1.91	0.51
1:D:352:VAL:HG21	1:D:518:TRP:CZ3	2.45	0.51
1:F:478:ASN:O	1:F:480:VAL:HG13	2.10	0.51
1:G:419:GLN:O	1:G:419:GLN:HG2	2.10	0.51
1:E:313:GLU:HA	1:J:513:ASN:HA	1.91	0.51
1:F:279:ASN:OD1	1:F:281:ILE:HG13	2.11	0.51
1:K:372:THR:HA	1:K:383:THR:HG21	1.91	0.51
1:C:499:VAL:HG12	1:C:520:ALA:HB2	1.93	0.51
1:F:278:LEU:N	1:F:464:GLU:OE2	2.43	0.51
1:I:489:TYR:HD1	1:I:528:VAL:HG22	1.76	0.51
1:L:350:GLU:O	1:L:354:LEU:HG	2.10	0.51
1:C:425:ASN:OD1	1:C:426:ASN:N	2.44	0.51
1:H:356:PHE:HB3	1:H:497:MET:HE3	1.92	0.50
1:K:339:ILE:O	1:K:343:GLN:HG3	2.11	0.50
1:B:527:ASP:OD1	1:B:528:VAL:N	2.44	0.50
1:J:309:ALA:HB2	1:K:376:ASN:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:ILE:HG13	1:F:527:ASP:HB3	1.94	0.50
1:J:407:ALA:HA	1:J:410:GLU:HG2	1.94	0.50
1:A:390:ALA:HA	1:A:535:ARG:NH1	2.27	0.49
1:A:427:LEU:HG	1:A:468:ALA:HB1	1.93	0.49
1:H:314:VAL:HG12	1:I:332:GLN:NE2	2.27	0.49
1:F:507:GLY:C	1:J:510:ARG:HD3	2.32	0.49
1:A:396:THR:HG23	1:A:399:THR:HB	1.95	0.49
1:C:482:LEU:HD12	1:C:536:LEU:HD13	1.93	0.49
1:G:409:TYR:CZ	1:G:417:ARG:HD2	2.48	0.49
1:I:482:LEU:HD12	1:I:536:LEU:HD13	1.94	0.49
1:K:279:ASN:OD1	1:K:280:ASP:N	2.45	0.49
1:D:303:VAL:HG23	1:E:355:LEU:HB3	1.94	0.49
1:D:427:LEU:O	1:D:431:LYS:HG2	2.13	0.49
1:E:391:GLU:OE2	1:E:538:ASN:ND2	2.44	0.49
1:H:354:LEU:O	1:H:358:GLU:HG2	2.13	0.49
1:B:276:GLY:HA2	1:B:362:GLU:OE2	2.13	0.49
1:D:388:THR:HG22	1:D:389:ALA:H	1.77	0.48
1:D:407:ALA:O	1:D:411:GLN:HG3	2.13	0.48
1:H:356:PHE:HB3	1:H:497:MET:CE	2.43	0.48
1:A:479:PHE:CD1	1:A:538:ASN:HB3	2.48	0.48
1:D:371:GLY:H	1:D:380:GLY:HA3	1.78	0.48
1:G:314:VAL:HG12	1:H:332:GLN:HG3	1.94	0.48
1:D:388:THR:HG22	1:D:389:ALA:N	2.29	0.48
1:F:279:ASN:OD1	1:F:280:ASP:N	2.47	0.48
1:F:287:GLN:HG2	1:F:491:ILE:HD11	1.94	0.48
1:L:524:MET:HG2	1:L:525:GLY:H	1.77	0.48
1:A:279:ASN:ND2	1:A:369:THR:OG1	2.47	0.48
1:B:438:GLN:HE21	1:C:438:GLN:HE21	1.62	0.48
1:F:444:TRP:CE2	1:F:452:PRO:HG2	2.49	0.48
1:C:489:TYR:HD1	1:C:528:VAL:HG22	1.79	0.48
1:E:352:VAL:HG12	1:E:356:PHE:CE2	2.49	0.48
1:H:467:ASP:OD2	1:H:478:ASN:ND2	2.36	0.48
1:C:279:ASN:ND2	1:C:369:THR:OG1	2.47	0.48
1:J:293:ASP:O	1:J:328:VAL:HG12	2.14	0.48
1:K:351:THR:O	1:K:355:LEU:HG	2.14	0.48
1:B:443:LEU:O	1:C:446:THR:OG1	2.31	0.48
1:H:410:GLU:HB3	1:I:430:ASN:ND2	2.29	0.48
1:B:339:ILE:HG22	1:B:516:ARG:HD2	1.96	0.48
1:G:314:VAL:HG11	1:H:519:PHE:HE1	1.78	0.48
1:L:427:LEU:HG	1:L:468:ALA:HB1	1.96	0.48
1:B:396:THR:HG23	1:B:399:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:294:VAL:HG12	1:J:327:PRO:HA	1.96	0.47
1:L:364:GLU:HG2	1:L:368:LEU:HD23	1.96	0.47
1:A:342:LEU:HD22	1:A:516:ARG:HD2	1.97	0.47
1:C:394:PRO:HD3	1:C:538:ASN:O	2.14	0.47
1:J:279:ASN:HD22	1:J:365:ALA:HB1	1.78	0.47
1:K:314:VAL:HG11	1:L:519:PHE:HE1	1.79	0.47
1:B:418:ARG:HH11	1:B:418:ARG:HB2	1.80	0.47
1:H:385:LEU:HD23	1:H:536:LEU:HB2	1.96	0.47
1:J:255:LYS:HG3	1:J:260:TYR:CE1	2.49	0.47
1:K:303:VAL:HG23	1:L:355:LEU:HB3	1.97	0.47
1:E:456:LEU:H	1:F:448:GLY:HA2	1.80	0.47
1:G:409:TYR:CE2	1:G:417:ARG:HD2	2.49	0.47
1:K:407:ALA:HA	1:K:410:GLU:HG2	1.97	0.47
1:K:529:VAL:HG11	1:L:271:ILE:HD13	1.96	0.47
1:D:423:LEU:HD23	1:D:482:LEU:HD23	1.97	0.47
1:G:297:GLY:O	1:G:323:GLN:HG3	2.15	0.47
1:K:418:ARG:HB2	1:K:418:ARG:NH1	2.30	0.47
1:A:424:ALA:HB2	1:A:481:LEU:HD12	1.97	0.46
1:K:392:ILE:N	1:K:536:LEU:O	2.43	0.46
1:B:418:ARG:HB2	1:B:418:ARG:NH1	2.30	0.46
1:D:297:GLY:O	1:D:324:PRO:HD2	2.16	0.46
1:H:429:TYR:OH	1:H:461:GLY:O	2.23	0.46
1:K:307:TRP:HZ2	1:L:367:THR:HG21	1.80	0.46
1:B:456:LEU:H	1:C:448:GLY:HA2	1.81	0.46
1:E:427:LEU:O	1:E:431:LYS:HG2	2.15	0.46
1:L:427:LEU:O	1:L:431:LYS:HG3	2.16	0.46
1:C:417:ARG:NH1	1:D:426:ASN:OD1	2.38	0.46
1:F:425:ASN:OD1	1:F:426:ASN:N	2.47	0.46
1:I:297:GLY:O	1:I:323:GLN:HG3	2.16	0.46
1:L:407:ALA:HA	1:L:410:GLU:OE1	2.15	0.46
1:C:424:ALA:HB2	1:C:481:LEU:HD12	1.96	0.46
1:H:456:LEU:H	1:I:448:GLY:HA2	1.81	0.46
1:J:517:GLY:O	1:J:518:TRP:CD1	2.69	0.46
1:B:296:HIS:ND1	1:B:325:GLU:OE1	2.48	0.46
1:E:290:ALA:HB2	1:E:492:ALA:HB1	1.98	0.46
1:E:339:ILE:HG12	1:E:516:ARG:NH1	2.31	0.46
1:E:527:ASP:OD1	1:E:528:VAL:N	2.41	0.46
1:F:499:VAL:HG22	1:F:520:ALA:HB2	1.98	0.46
1:G:367:THR:HG21	1:L:307:TRP:NE1	2.19	0.46
1:K:418:ARG:HB2	1:K:418:ARG:CZ	2.46	0.46
1:D:307:TRP:CD1	1:E:367:THR:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:432:ILE:HD13	1:H:435:PHE:CE2	2.49	0.45
1:J:392:ILE:HD11	1:J:535:ARG:HD2	1.96	0.45
1:D:320:GLU:N	1:D:320:GLU:OE1	2.50	0.45
1:G:436:ASP:HB2	1:G:442:GLY:O	2.16	0.45
1:J:517:GLY:O	1:J:518:TRP:HD1	1.99	0.45
1:L:422:TRP:CE2	1:L:455:LEU:HD23	2.51	0.45
1:L:503:PRO:O	1:L:516:ARG:HG2	2.15	0.45
1:D:470:TRP:O	1:D:541:THR:HG21	2.16	0.45
1:L:444:TRP:CD2	1:L:452:PRO:HG2	2.52	0.45
1:E:370:THR:HG22	1:E:382:VAL:HG21	1.97	0.45
1:L:259:GLY:O	1:L:262:VAL:HG12	2.17	0.45
1:G:350:GLU:OE1	1:G:350:GLU:N	2.43	0.45
1:E:369:THR:O	1:E:382:VAL:HG22	2.16	0.45
1:G:406:TYR:O	1:G:410:GLU:HG3	2.17	0.45
1:C:535:ARG:HD3	1:C:535:ARG:HA	1.81	0.45
1:K:535:ARG:HD3	1:K:535:ARG:HA	1.77	0.45
1:B:427:LEU:HD22	1:B:468:ALA:HB1	1.99	0.45
1:L:297:GLY:O	1:L:323:GLN:HG3	2.16	0.45
1:B:517:GLY:O	1:B:518:TRP:HD1	2.01	0.44
1:F:368:LEU:HD23	1:F:368:LEU:HA	1.83	0.44
1:H:469:ASN:OD1	1:H:472:THR:HG22	2.17	0.44
1:I:539:VAL:HG13	1:I:539:VAL:O	2.18	0.44
1:E:467:ASP:OD1	1:E:468:ALA:N	2.50	0.44
1:A:279:ASN:OD1	1:A:280:ASP:N	2.50	0.44
1:A:371:GLY:H	1:A:380:GLY:HA3	1.83	0.44
1:H:406:TYR:HD2	1:I:434:GLN:HE21	1.64	0.44
1:A:507:GLY:HA3	1:H:313:GLU:OE2	2.17	0.44
1:D:272:ILE:HG22	1:D:274:SER:H	1.82	0.44
1:F:426:ASN:HB2	1:F:462:GLU:OE2	2.17	0.44
1:H:482:LEU:HD12	1:H:536:LEU:HD13	2.00	0.44
1:K:425:ASN:OD1	1:K:426:ASN:N	2.50	0.44
1:D:279:ASN:OD1	1:D:281:ILE:HD12	2.17	0.44
1:D:368:LEU:HD23	1:D:368:LEU:HA	1.84	0.44
1:G:456:LEU:H	1:H:448:GLY:HA2	1.81	0.44
1:H:410:GLU:CD	1:I:427:LEU:HD12	2.38	0.44
1:J:259:GLY:O	1:J:262:VAL:HG12	2.17	0.44
1:J:310:GLU:HG2	1:J:311:PHE:CD2	2.52	0.44
1:D:444:TRP:CE2	1:D:452:PRO:HG2	2.53	0.44
1:E:303:VAL:HG23	1:F:355:LEU:HB3	2.00	0.44
1:C:316:ASP:N	1:C:316:ASP:OD1	2.50	0.44
1:C:410:GLU:OE2	1:D:427:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:364:GLU:HA	1:L:367:THR:HG22	1.99	0.44
1:K:428:ILE:O	1:K:432:ILE:HG12	2.18	0.44
1:F:427:LEU:HD23	1:F:431:LYS:HD2	2.00	0.43
1:L:479:PHE:HB3	1:L:536:LEU:HD11	2.00	0.43
1:A:392:ILE:HD13	1:A:392:ILE:HA	1.86	0.43
1:I:470:TRP:O	1:I:541:THR:HG21	2.17	0.43
1:J:395:VAL:HG12	1:J:396:THR:HG23	2.01	0.43
1:C:351:THR:O	1:C:355:LEU:HG	2.18	0.43
1:E:424:ALA:HA	1:E:466:MET:SD	2.58	0.43
1:A:444:TRP:CE2	1:A:452:PRO:HG2	2.53	0.43
1:B:410:GLU:HB3	1:C:430:ASN:ND2	2.34	0.43
1:F:349:THR:HG22	1:F:518:TRP:HZ2	1.84	0.43
1:H:479:PHE:HB3	1:H:536:LEU:HD11	2.01	0.43
1:F:350:GLU:O	1:F:354:LEU:HD13	2.18	0.43
1:J:279:ASN:ND2	1:J:365:ALA:HB1	2.33	0.43
1:E:305:TRP:HB2	1:F:363:LEU:HD22	2.01	0.43
1:D:381:ILE:HD13	1:D:489:TYR:CD1	2.54	0.43
1:E:489:TYR:HD1	1:E:528:VAL:HG22	1.83	0.43
1:G:456:LEU:HD23	1:G:456:LEU:HA	1.83	0.43
1:A:427:LEU:HD13	1:F:410:GLU:CD	2.39	0.43
1:C:368:LEU:HD23	1:C:368:LEU:HA	1.81	0.43
1:E:494:ARG:HG3	1:E:495:ILE:HG13	2.01	0.43
1:G:355:LEU:HB3	1:L:303:VAL:HG23	2.00	0.43
1:H:379:THR:HG22	1:H:384:ALA:HB2	2.01	0.43
1:L:535:ARG:HD3	1:L:535:ARG:HA	1.86	0.43
1:A:259:GLY:O	1:A:262:VAL:HG12	2.18	0.43
1:A:350:GLU:H	1:A:350:GLU:CD	2.21	0.43
1:B:303:VAL:HG23	1:C:355:LEU:HB3	2.01	0.43
1:D:282:ARG:HH21	1:D:368:LEU:HD11	1.83	0.43
1:K:352:VAL:HG21	1:K:518:TRP:CZ3	2.54	0.43
1:A:392:ILE:O	1:A:537:LEU:HD12	2.19	0.42
1:H:351:THR:O	1:H:355:LEU:HG	2.19	0.42
1:J:527:ASP:OD1	1:J:528:VAL:N	2.46	0.42
1:K:305:TRP:HB2	1:L:363:LEU:HD22	2.00	0.42
1:B:419:GLN:HA	1:B:458:ARG:NH2	2.34	0.42
1:C:402:LEU:HD23	1:C:402:LEU:H	1.85	0.42
1:E:310:GLU:HG2	1:E:311:PHE:CD2	2.55	0.42
1:E:427:LEU:HG	1:E:468:ALA:HB1	2.02	0.42
1:F:430:ASN:O	1:F:434:GLN:HG3	2.19	0.42
1:G:330:LYS:HG3	1:G:523:ARG:HG2	2.00	0.42
1:G:501:PHE:HD1	1:G:518:TRP:CD1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:436:ASP:OD1	1:J:437:THR:N	2.52	0.42
1:F:407:ALA:HA	1:F:410:GLU:HG2	2.01	0.42
1:G:351:THR:O	1:G:355:LEU:HG	2.18	0.42
1:I:291:THR:OG1	1:J:265:GLN:OE1	2.26	0.42
1:L:426:ASN:O	1:L:426:ASN:ND2	2.50	0.42
1:D:484:GLY:HA3	1:D:534:PHE:CD1	2.54	0.42
1:G:517:GLY:O	1:G:518:TRP:CD1	2.71	0.42
1:B:388:THR:HG22	1:B:389:ALA:N	2.34	0.42
1:F:456:LEU:HD23	1:F:456:LEU:HA	1.88	0.42
1:J:410:GLU:HB3	1:K:430:ASN:ND2	2.34	0.42
1:K:398:GLU:OE1	1:K:541:THR:OG1	2.32	0.42
1:B:499:VAL:HG22	1:B:520:ALA:HB2	2.02	0.42
1:E:423:LEU:HD23	1:E:466:MET:SD	2.60	0.42
1:L:495:ILE:HG22	1:L:496:GLY:O	2.20	0.42
1:D:314:VAL:HG11	1:E:519:PHE:HE1	1.84	0.42
1:G:314:VAL:HG11	1:H:519:PHE:CE1	2.55	0.42
1:H:444:TRP:CE2	1:H:452:PRO:HG2	2.54	0.42
1:I:425:ASN:OD1	1:I:426:ASN:N	2.52	0.42
1:L:527:ASP:OD1	1:L:528:VAL:N	2.45	0.42
1:F:370:THR:HG22	1:F:370:THR:O	2.19	0.42
1:I:433:ARG:NH2	1:I:451:GLU:HA	2.35	0.42
1:A:438:GLN:HG2	1:F:438:GLN:OE1	2.20	0.41
1:C:354:LEU:O	1:C:357:ALA:N	2.53	0.41
1:D:351:THR:O	1:D:355:LEU:HG	2.19	0.41
1:F:482:LEU:HD12	1:F:536:LEU:HD13	2.02	0.41
1:G:293:ASP:OD1	1:G:293:ASP:N	2.50	0.41
1:A:436:ASP:OD1	1:A:437:THR:N	2.54	0.41
1:A:502:ILE:HA	1:A:503:PRO:HD3	1.94	0.41
1:L:339:ILE:HG12	1:L:514:GLY:O	2.20	0.41
1:C:438:GLN:OE1	1:D:438:GLN:HB3	2.20	0.41
1:B:419:GLN:O	1:B:419:GLN:HG2	2.20	0.41
1:I:477:ASP:OD1	1:I:477:ASP:N	2.51	0.41
1:C:419:GLN:HA	1:C:458:ARG:NH2	2.35	0.41
1:J:280:ASP:OD2	1:J:283:ARG:NH2	2.54	0.41
1:L:431:LYS:HE2	1:L:431:LYS:HB3	1.84	0.41
1:G:527:ASP:OD1	1:G:528:VAL:N	2.46	0.41
1:D:428:ILE:HD12	1:D:428:ILE:H	1.85	0.41
1:E:535:ARG:HD3	1:E:535:ARG:HA	1.85	0.41
1:H:412:LEU:HD13	1:H:535:ARG:HG2	2.03	0.41
1:A:479:PHE:HA	1:A:537:LEU:O	2.20	0.41
1:C:430:ASN:O	1:C:434:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:425:ASN:ND2	1:F:468:ALA:HB2	2.34	0.41
1:C:354:LEU:O	1:C:358:GLU:OE1	2.39	0.41
1:D:455:LEU:HA	1:E:448:GLY:HA2	2.03	0.41
1:E:318:SER:HA	1:F:335:VAL:HG23	2.03	0.41
1:K:476:ALA:O	1:K:478:ASN:ND2	2.54	0.41
1:L:406:TYR:O	1:L:410:GLU:HG3	2.21	0.41
1:F:537:LEU:HD23	1:F:538:ASN:N	2.37	0.40
1:K:280:ASP:OD1	1:K:283:ARG:NE	2.54	0.40
1:C:350:GLU:H	1:C:350:GLU:CD	2.24	0.40
1:F:445:THR:OG1	1:F:452:PRO:HG3	2.20	0.40
1:F:495:ILE:HG22	1:F:523:ARG:HB2	2.04	0.40
1:B:259:GLY:O	1:B:262:VAL:HG22	2.22	0.40
1:D:426:ASN:ND2	1:D:462:GLU:OE1	2.55	0.40
1:L:425:ASN:HD22	1:L:468:ALA:HB2	1.85	0.40
1:B:438:GLN:NE2	1:C:438:GLN:HE21	2.19	0.40
1:D:318:SER:HA	1:E:335:VAL:HG23	2.02	0.40
1:D:491:ILE:HD13	1:D:526:ALA:HB2	2.02	0.40
1:G:488:ASN:O	1:G:529:VAL:HG22	2.22	0.40
1:G:517:GLY:O	1:G:518:TRP:HD1	2.04	0.40
1:I:286:ARG:O	1:I:490:VAL:HA	2.22	0.40
1:K:332:GLN:HA	1:K:521:TYR:HA	2.04	0.40
1:A:529:VAL:HG11	1:B:271:ILE:HD13	2.04	0.40
1:H:410:GLU:HB3	1:I:430:ASN:HD22	1.86	0.40
1:I:424:ALA:HA	1:I:466:MET:CE	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	291/543 (54%)	278 (96%)	13 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	291/543 (54%)	278 (96%)	13 (4%)	0	100	100
1	C	291/543 (54%)	284 (98%)	7 (2%)	0	100	100
1	D	291/543 (54%)	284 (98%)	7 (2%)	0	100	100
1	E	291/543 (54%)	284 (98%)	7 (2%)	0	100	100
1	F	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	G	291/543 (54%)	282 (97%)	9 (3%)	0	100	100
1	H	291/543 (54%)	278 (96%)	13 (4%)	0	100	100
1	I	291/543 (54%)	282 (97%)	9 (3%)	0	100	100
1	J	291/543 (54%)	282 (97%)	9 (3%)	0	100	100
1	K	291/543 (54%)	278 (96%)	13 (4%)	0	100	100
1	L	291/543 (54%)	280 (96%)	11 (4%)	0	100	100
All	All	3492/6516 (54%)	3376 (97%)	116 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/432 (53%)	229 (100%)	0	100	100
1	B	229/432 (53%)	228 (100%)	1 (0%)	89	94
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%)	228 (100%)	1 (0%)	89	94
1	I	229/432 (53%)	229 (100%)	0	100	100
1	J	229/432 (53%)	229 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	229/432 (53%)	227 (99%)	2 (1%)	75	86
1	L	229/432 (53%)	228 (100%)	1 (0%)	89	94
All	All	2748/5184 (53%)	2743 (100%)	5 (0%)	91	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	426	ASN
1	H	426	ASN
1	K	426	ASN
1	K	510	ARG
1	L	426	ASN

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

Mol	Chain	Res	Type
1	C	438	GLN
1	D	287	GLN
1	E	425	ASN
1	J	279	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.