



Full wwPDB EM Validation Report ⓘ

May 31, 2026 – 12:18 AM JST

PDB ID : 9V9E / pdb_00009v9e
EMDB ID : EMD-64870
Title : Cryo-EM structure of human RIPK1 DD filament
Authors : Zhao, K.; Liu, J.P.; Liu, C.; Yuan, J.Y.
Deposited on : 2025-05-30
Resolution : 2.87 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 : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

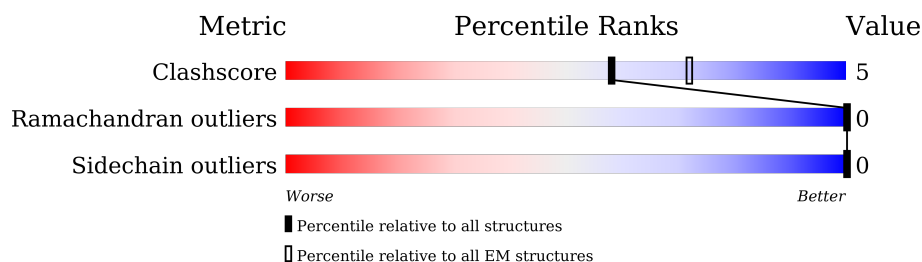
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	115	80% 7% 13%
1	B	115	73% 14% 13%
1	C	115	73% 14% 13%
1	D	115	74% 13% 13%
1	E	115	77% 10% 13%
1	F	115	73% 14% 13%
1	G	115	74% 13% 13%
1	H	115	77% 10% 13%
1	I	115	77% 10% 13%

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Mol	Chain	Length	Quality of chain
1	J	115	 74%13%13%
1	K	115	 77%10%13%
1	L	115	 75%12%13%
1	M	115	 72%15%13%
1	N	115	 75%12%13%
1	O	115	 68%19%13%
1	P	115	 76%11%13%
1	Q	115	 77%10%13%
1	R	115	 78%9%13%
1	S	115	 77%10%13%
1	T	115	 81%6%13%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 16360 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 Receptor-interacting serine/threonine-protein kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	B	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	C	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	D	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	E	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	F	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	G	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	H	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	I	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	J	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	K	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	L	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	M	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	N	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	O	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	P	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	Q	100	Total	C	N	O	S	1	0
			818	515	146	152	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	S	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
1	T	100	Total	C	N	O	S	1	0
			818	515	146	152	5		

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	557	GLY	-	expression tag	UNP Q13546
A	558	PRO	-	expression tag	UNP Q13546
A	559	GLY	-	expression tag	UNP Q13546
A	560	SER	-	expression tag	UNP Q13546
B	557	GLY	-	expression tag	UNP Q13546
B	558	PRO	-	expression tag	UNP Q13546
B	559	GLY	-	expression tag	UNP Q13546
B	560	SER	-	expression tag	UNP Q13546
C	557	GLY	-	expression tag	UNP Q13546
C	558	PRO	-	expression tag	UNP Q13546
C	559	GLY	-	expression tag	UNP Q13546
C	560	SER	-	expression tag	UNP Q13546
D	557	GLY	-	expression tag	UNP Q13546
D	558	PRO	-	expression tag	UNP Q13546
D	559	GLY	-	expression tag	UNP Q13546
D	560	SER	-	expression tag	UNP Q13546
E	557	GLY	-	expression tag	UNP Q13546
E	558	PRO	-	expression tag	UNP Q13546
E	559	GLY	-	expression tag	UNP Q13546
E	560	SER	-	expression tag	UNP Q13546
F	557	GLY	-	expression tag	UNP Q13546
F	558	PRO	-	expression tag	UNP Q13546
F	559	GLY	-	expression tag	UNP Q13546
F	560	SER	-	expression tag	UNP Q13546
G	557	GLY	-	expression tag	UNP Q13546
G	558	PRO	-	expression tag	UNP Q13546
G	559	GLY	-	expression tag	UNP Q13546
G	560	SER	-	expression tag	UNP Q13546
H	557	GLY	-	expression tag	UNP Q13546
H	558	PRO	-	expression tag	UNP Q13546
H	559	GLY	-	expression tag	UNP Q13546
H	560	SER	-	expression tag	UNP Q13546

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Chain	Residue	Modelled	Actual	Comment	Reference
I	557	GLY	-	expression tag	UNP Q13546
I	558	PRO	-	expression tag	UNP Q13546
I	559	GLY	-	expression tag	UNP Q13546
I	560	SER	-	expression tag	UNP Q13546
J	557	GLY	-	expression tag	UNP Q13546
J	558	PRO	-	expression tag	UNP Q13546
J	559	GLY	-	expression tag	UNP Q13546
J	560	SER	-	expression tag	UNP Q13546
K	557	GLY	-	expression tag	UNP Q13546
K	558	PRO	-	expression tag	UNP Q13546
K	559	GLY	-	expression tag	UNP Q13546
K	560	SER	-	expression tag	UNP Q13546
L	557	GLY	-	expression tag	UNP Q13546
L	558	PRO	-	expression tag	UNP Q13546
L	559	GLY	-	expression tag	UNP Q13546
L	560	SER	-	expression tag	UNP Q13546
M	557	GLY	-	expression tag	UNP Q13546
M	558	PRO	-	expression tag	UNP Q13546
M	559	GLY	-	expression tag	UNP Q13546
M	560	SER	-	expression tag	UNP Q13546
N	557	GLY	-	expression tag	UNP Q13546
N	558	PRO	-	expression tag	UNP Q13546
N	559	GLY	-	expression tag	UNP Q13546
N	560	SER	-	expression tag	UNP Q13546
O	557	GLY	-	expression tag	UNP Q13546
O	558	PRO	-	expression tag	UNP Q13546
O	559	GLY	-	expression tag	UNP Q13546
O	560	SER	-	expression tag	UNP Q13546
P	557	GLY	-	expression tag	UNP Q13546
P	558	PRO	-	expression tag	UNP Q13546
P	559	GLY	-	expression tag	UNP Q13546
P	560	SER	-	expression tag	UNP Q13546
Q	557	GLY	-	expression tag	UNP Q13546
Q	558	PRO	-	expression tag	UNP Q13546
Q	559	GLY	-	expression tag	UNP Q13546
Q	560	SER	-	expression tag	UNP Q13546
R	557	GLY	-	expression tag	UNP Q13546
R	558	PRO	-	expression tag	UNP Q13546
R	559	GLY	-	expression tag	UNP Q13546
R	560	SER	-	expression tag	UNP Q13546
S	557	GLY	-	expression tag	UNP Q13546
S	558	PRO	-	expression tag	UNP Q13546

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Chain	Residue	Modelled	Actual	Comment	Reference
S	559	GLY	-	expression tag	UNP Q13546
S	560	SER	-	expression tag	UNP Q13546
T	557	GLY	-	expression tag	UNP Q13546
T	558	PRO	-	expression tag	UNP Q13546
T	559	GLY	-	expression tag	UNP Q13546
T	560	SER	-	expression tag	UNP Q13546

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: Receptor-interacting serine/threonine-protein kinase 1

Chain A: 



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain B: 



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain C: 



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain D: 



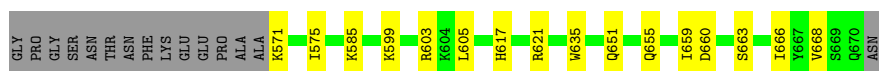
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain E: 



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain F: 



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain G: 74% 13% 13%



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain H: 77% 10% 13%



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain I: 77% 10% 13%



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain J: 74% 13% 13%



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain K: 77% 10% 13%



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain L: 75% 12% 13%



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain M: 72% 15% 13%



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain N: 75% 12% 13%



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain O: 68% 19% 13%



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain P: 76% 11% 13%



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain Q: 77% 10% 13%



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain R: 78% 9% 13%



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain S: 77% 10% 13%



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 1

Chain T: 81% 6% 13%

GLY	PRO	GLY	SER	ASN	THR	ASN	PHE	LYS	GLU	GLU	PRO	ALA	ALA	K571	L594	K599	R603	K604	L605	H617	V628	W635	Q670	ASN
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4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=139.359°, rise=5.22311 Å, axial sym=C1	Depositor
Number of segments used	392912	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.12	0/835	0.32	0/1121
1	B	0.12	0/835	0.32	0/1121
1	C	0.11	0/835	0.27	0/1121
1	D	0.11	0/835	0.28	0/1121
1	E	0.12	0/835	0.32	0/1121
1	F	0.12	0/835	0.29	0/1121
1	G	0.11	0/835	0.30	0/1121
1	H	0.12	0/835	0.31	0/1121
1	I	0.12	0/835	0.31	0/1121
1	J	0.12	0/835	0.28	0/1121
1	K	0.12	0/835	0.29	0/1121
1	L	0.12	0/835	0.28	0/1121
1	M	0.12	0/835	0.31	0/1121
1	N	0.12	0/835	0.31	0/1121
1	O	0.12	0/835	0.33	0/1121
1	P	0.12	0/835	0.32	0/1121
1	Q	0.12	0/835	0.30	0/1121
1	R	0.12	0/835	0.31	0/1121
1	S	0.12	0/835	0.31	0/1121
1	T	0.11	0/835	0.28	0/1121
All	All	0.12	0/16700	0.30	0/22420

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	818	0	820	5	0
1	B	818	0	820	10	0
1	C	818	0	820	10	0
1	D	818	0	820	10	0
1	E	818	0	820	7	0
1	F	818	0	820	10	0
1	G	818	0	820	10	0
1	H	818	0	820	7	0
1	I	818	0	820	8	0
1	J	818	0	820	9	0
1	K	818	0	820	8	0
1	L	818	0	820	11	0
1	M	818	0	820	13	0
1	N	818	0	820	11	0
1	O	818	0	820	14	0
1	P	818	0	820	8	0
1	Q	818	0	820	7	0
1	R	818	0	820	6	0
1	S	818	0	820	8	0
1	T	818	0	820	5	0
All	All	16360	0	16400	155	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 5.

All (155) 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:E:592:GLU:OE2	1:E:625:LYS:NZ	2.28	0.67
1:D:592:GLU:OE1	1:D:625:LYS:NZ	2.27	0.65
1:B:592:GLU:OE1	1:B:625:LYS:NZ	2.27	0.65
1:R:621:ARG:HD3	1:S:617:HIS:CD2	2.36	0.60
1:B:609:GLN:HB2	1:I:633:GLN:HE22	1.67	0.59
1:C:621:ARG:HD3	1:D:617:HIS:HD2	1.70	0.57
1:K:621:ARG:HD3	1:L:617:HIS:CD2	2.41	0.55
1:G:609:GLN:HB2	1:N:633:GLN:HE22	1.71	0.55
1:E:588:ASP:O	1:E:592:GLU:HG2	2.06	0.55
1:H:651:GLN:O	1:H:655:GLN:HG2	2.07	0.55
1:F:617:HIS:CD2	1:O:621:ARG:HD3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:ASP:O	1:B:592:GLU:HG2	2.07	0.54
1:O:651:GLN:O	1:O:655:GLN:HG2	2.09	0.53
1:B:578:ASN:OD1	1:B:580:THR:OG1	2.22	0.53
1:D:588:ASP:O	1:D:592:GLU:HG2	2.07	0.53
1:Q:651:GLN:O	1:Q:655:GLN:HG2	2.09	0.52
1:M:616:ASP:O	1:M:620:GLU:HG2	2.09	0.52
1:J:585:LYS:HE2	1:J:668:VAL:HG22	1.92	0.52
1:G:651:GLN:O	1:G:655:GLN:HG2	2.11	0.51
1:P:594:LEU:HD23	1:P:628:VAL:HG13	1.92	0.51
1:M:651:GLN:O	1:M:655:GLN:HG2	2.11	0.51
1:M:575:ILE:HG12	1:M:666:ILE:HG12	1.92	0.51
1:F:651:GLN:O	1:F:655:GLN:HG2	2.10	0.51
1:H:660:ASP:N	1:H:660:ASP:OD1	2.44	0.51
1:M:621:ARG:HD3	1:N:617:HIS:CD2	2.47	0.50
1:C:605:LEU:HD22	1:C:635:TRP:CE2	2.47	0.50
1:T:605:LEU:HD22	1:T:635:TRP:CE2	2.46	0.50
1:F:599:LYS:O	1:F:603:ARG:HG3	2.12	0.50
1:N:594:LEU:HD23	1:N:628:VAL:HG13	1.94	0.49
1:L:651:GLN:O	1:L:655:GLN:HG2	2.13	0.49
1:D:638:ARG:NH2	1:D:639:GLU:OE2	2.46	0.49
1:K:651:GLN:O	1:K:655:GLN:HG2	2.13	0.48
1:M:578:ASN:OD1	1:M:579:THR:N	2.47	0.48
1:G:660:ASP:OD1	1:G:660:ASP:N	2.46	0.48
1:J:651:GLN:O	1:J:655:GLN:HG2	2.14	0.48
1:M:609:GLN:NE2	1:M:613:ASP:OD1	2.47	0.48
1:N:616:ASP:O	1:N:620:GLU:HG2	2.14	0.48
1:N:573:GLN:NE2	1:N:577:ASP:OD1	2.47	0.48
1:S:605:LEU:HD22	1:S:635:TRP:CE2	2.48	0.48
1:O:599:LYS:O	1:O:603:ARG:HG3	2.13	0.48
1:D:594:LEU:HD23	1:D:628:VAL:HG13	1.96	0.48
1:J:599:LYS:O	1:J:603:ARG:HG3	2.14	0.48
1:S:594:LEU:HD23	1:S:628:VAL:HG13	1.95	0.48
1:F:621:ARG:HD3	1:G:617:HIS:HD2	1.79	0.47
1:O:605:LEU:HD22	1:O:635:TRP:CE2	2.49	0.47
1:G:605:LEU:HD22	1:G:635:TRP:CE2	2.50	0.47
1:J:594:LEU:HD23	1:J:628:VAL:HG13	1.95	0.47
1:J:660:ASP:OD1	1:J:660:ASP:N	2.47	0.47
1:Q:621:ARG:HD3	1:R:617:HIS:CD2	2.49	0.47
1:H:621:ARG:HD3	1:I:617:HIS:CD2	2.49	0.47
1:Q:594:LEU:HD23	1:Q:628:VAL:HG13	1.95	0.47
1:E:596:LYS:HE3	1:E:597:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:605:LEU:HD22	1:L:635:TRP:CE2	2.49	0.47
1:S:621:ARG:HD3	1:T:617:HIS:CD2	2.50	0.47
1:L:621:ARG:HD3	1:M:617:HIS:CD2	2.50	0.46
1:R:605:LEU:HD22	1:R:635:TRP:CE2	2.50	0.46
1:P:621:ARG:HD3	1:Q:617:HIS:CD2	2.50	0.46
1:G:621:ARG:HD3	1:H:617:HIS:CD2	2.51	0.46
1:E:605:LEU:HD22	1:E:635:TRP:CE2	2.51	0.46
1:M:605:LEU:HD22	1:M:635:TRP:CE2	2.50	0.46
1:C:638:ARG:NH2	1:C:639:GLU:OE2	2.49	0.46
1:D:605:LEU:HD22	1:D:635:TRP:CE2	2.51	0.46
1:S:651:GLN:O	1:S:655:GLN:HG2	2.17	0.45
1:N:620:GLU:CD	1:N:627:LYS:HZ1	2.24	0.45
1:O:575:ILE:HG12	1:O:666:ILE:HG12	1.98	0.45
1:E:594:LEU:HD23	1:E:628:VAL:HG13	1.98	0.45
1:P:651:GLN:O	1:P:655:GLN:HG2	2.16	0.45
1:O:660:ASP:OD1	1:O:660:ASP:N	2.47	0.45
1:P:605:LEU:HD22	1:P:635:TRP:CE2	2.51	0.45
1:I:664:SER:O	1:I:668:VAL:HG22	2.17	0.44
1:B:594:LEU:HD23	1:B:628:VAL:HG13	2.00	0.44
1:B:605:LEU:HD22	1:B:635:TRP:CE2	2.52	0.44
1:F:660:ASP:OD1	1:F:660:ASP:N	2.46	0.44
1:G:594:LEU:HD23	1:G:628:VAL:HG13	1.99	0.44
1:N:621:ARG:HD3	1:O:617:HIS:HD2	1.82	0.44
1:K:605:LEU:HD22	1:K:635:TRP:CE2	2.53	0.44
1:K:609:GLN:NE2	1:K:613:ASP:OD1	2.50	0.44
1:N:621:ARG:HD3	1:O:617:HIS:CD2	2.52	0.44
1:A:585:LYS:HE3	1:A:585:LYS:HB3	1.80	0.44
1:I:660:ASP:OD1	1:I:660:ASP:N	2.50	0.44
1:N:599:LYS:O	1:N:603:ARG:HG3	2.17	0.44
1:R:594:LEU:HD23	1:R:628:VAL:HG13	1.99	0.44
1:C:621:ARG:HD3	1:D:617:HIS:CD2	2.52	0.44
1:F:575:ILE:HG12	1:F:666:ILE:HG12	2.00	0.44
1:S:621:ARG:HD3	1:T:617:HIS:HD2	1.83	0.44
1:B:651:GLN:O	1:B:655:GLN:HG2	2.17	0.44
1:C:594:LEU:HD23	1:C:628:VAL:HG13	1.99	0.44
1:N:605:LEU:HD22	1:N:635:TRP:CE2	2.53	0.44
1:Q:605:LEU:HD22	1:Q:635:TRP:CE2	2.53	0.44
1:A:651:GLN:O	1:A:655:GLN:HG2	2.18	0.43
1:O:616:ASP:O	1:O:620:GLU:HG2	2.18	0.43
1:B:660:ASP:N	1:B:660:ASP:OD1	2.52	0.43
1:K:616:ASP:O	1:K:620:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:585:LYS:HE3	1:Q:586:HIS:CE1	2.54	0.43
1:B:623:GLY:O	1:B:627:LYS:HG3	2.17	0.43
1:H:605:LEU:HD22	1:H:635:TRP:CE2	2.53	0.43
1:J:605:LEU:HD22	1:J:635:TRP:CE2	2.54	0.43
1:K:620:GLU:CD	1:K:627:LYS:HZ1	2.26	0.43
1:L:594:LEU:HD23	1:L:628:VAL:HG13	2.01	0.43
1:F:571:LYS:HB2	1:F:571:LYS:HE3	1.77	0.43
1:O:594:LEU:HD23	1:O:628:VAL:HG13	2.00	0.43
1:M:594:LEU:HD23	1:M:628:VAL:HG13	2.00	0.43
1:O:616:ASP:OD1	1:O:627:LYS:NZ	2.52	0.43
1:C:664:SER:O	1:C:668:VAL:HG22	2.19	0.42
1:K:621:ARG:HD3	1:L:617:HIS:HD2	1.84	0.42
1:D:660:ASP:N	1:D:660:ASP:OD1	2.51	0.42
1:L:616:ASP:O	1:L:620:GLU:HG2	2.19	0.42
1:L:599:LYS:O	1:L:603:ARG:HG3	2.20	0.42
1:F:659:ILE:O	1:F:663:SER:OG	2.29	0.42
1:J:596:LYS:HE3	1:J:597:HIS:CE1	2.54	0.42
1:P:585:LYS:HE3	1:P:586:HIS:CE1	2.55	0.42
1:C:651:GLN:O	1:C:655:GLN:HG2	2.20	0.42
1:J:575:ILE:HG12	1:J:666:ILE:HG12	2.02	0.42
1:O:639:GLU:HB2	1:O:644:ALA:HB2	2.02	0.42
1:A:605:LEU:HD22	1:A:635:TRP:CE2	2.54	0.42
1:F:585:LYS:HE2	1:F:668:VAL:HG22	2.01	0.42
1:I:631:MET:HE3	1:I:631:MET:HB3	1.99	0.42
1:M:579:THR:HG22	1:M:579:THR:O	2.20	0.41
1:M:621:ARG:HD3	1:N:617:HIS:HD2	1.85	0.41
1:P:585:LYS:O	1:P:668:VAL:HG21	2.20	0.41
1:S:642:LYS:HB2	1:S:642:LYS:HE2	1.97	0.41
1:H:585:LYS:NZ	1:H:668:VAL:O	2.41	0.41
1:T:599:LYS:O	1:T:603:ARG:HG3	2.20	0.41
1:C:578:ASN:OD1	1:C:580:THR:OG1	2.23	0.41
1:L:621:ARG:HD3	1:M:617:HIS:HD2	1.84	0.41
1:E:585:LYS:HE3	1:E:585:LYS:HB2	1.80	0.41
1:B:621:ARG:HD3	1:C:617:HIS:HD2	1.85	0.41
1:G:579:THR:HG22	1:G:579:THR:O	2.21	0.41
1:G:596:LYS:HE3	1:G:597:HIS:CE1	2.55	0.41
1:O:585:LYS:HE2	1:O:668:VAL:HG22	2.03	0.41
1:P:660:ASP:OD1	1:P:660:ASP:N	2.52	0.41
1:R:599:LYS:O	1:R:603:ARG:HG3	2.21	0.41
1:I:623:GLY:O	1:I:627:LYS:HG3	2.20	0.41
1:K:594:LEU:HD23	1:K:628:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:623:GLY:O	1:C:627:LYS:HG3	2.21	0.41
1:D:664:SER:O	1:D:668:VAL:HG22	2.21	0.41
1:L:641:ILE:HD12	1:L:641:ILE:HA	1.96	0.41
1:Q:660:ASP:OD1	1:Q:660:ASP:N	2.53	0.41
1:R:651:GLN:O	1:R:655:GLN:HG2	2.21	0.41
1:I:592:GLU:OE2	1:I:625:LYS:NZ	2.42	0.41
1:O:615:ILE:HD11	1:O:634:LYS:HD2	2.03	0.41
1:D:604:LYS:HD2	1:D:655:GLN:HB3	2.03	0.40
1:F:605:LEU:HD22	1:F:635:TRP:CE2	2.55	0.40
1:S:630:GLN:O	1:S:634:LYS:HG3	2.21	0.40
1:A:575:ILE:HG12	1:A:666:ILE:HG12	2.02	0.40
1:J:585:LYS:HE3	1:J:585:LYS:HB2	1.89	0.40
1:L:604:LYS:HA	1:L:604:LYS:HD3	1.86	0.40
1:M:604:LYS:HD3	1:M:604:LYS:HA	1.83	0.40
1:A:660:ASP:N	1:A:660:ASP:OD1	2.54	0.40
1:G:585:LYS:NZ	1:G:668:VAL:O	2.53	0.40
1:T:594:LEU:HD23	1:T:628:VAL:HG13	2.04	0.40
1:P:616:ASP:O	1:P:620:GLU:HG2	2.22	0.40
1:E:571:LYS:HB2	1:E:571:LYS:HE3	1.90	0.40
1:H:623:GLY:O	1:H:627:LYS:HG3	2.21	0.40
1:I:594:LEU:HD23	1:I:628:VAL:HG13	2.03	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	99/115 (86%)	96 (97%)	3 (3%)	0	100	100
1	B	99/115 (86%)	97 (98%)	2 (2%)	0	100	100
1	C	99/115 (86%)	96 (97%)	3 (3%)	0	100	100
1	D	99/115 (86%)	97 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
1	F	99/115 (86%)	97 (98%)	2 (2%)	0	100	100
1	G	99/115 (86%)	99 (100%)	0	0	100	100
1	H	99/115 (86%)	99 (100%)	0	0	100	100
1	I	99/115 (86%)	97 (98%)	2 (2%)	0	100	100
1	J	99/115 (86%)	96 (97%)	3 (3%)	0	100	100
1	K	99/115 (86%)	97 (98%)	2 (2%)	0	100	100
1	L	99/115 (86%)	99 (100%)	0	0	100	100
1	M	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
1	N	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
1	O	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
1	P	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
1	Q	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
1	R	99/115 (86%)	99 (100%)	0	0	100	100
1	S	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
1	T	99/115 (86%)	97 (98%)	2 (2%)	0	100	100
All	All	1980/2300 (86%)	1952 (99%)	28 (1%)	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	90/100 (90%)	90 (100%)	0	100	100
1	B	90/100 (90%)	90 (100%)	0	100	100
1	C	90/100 (90%)	90 (100%)	0	100	100
1	D	90/100 (90%)	90 (100%)	0	100	100
1	E	90/100 (90%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	90/100 (90%)	90 (100%)	0	100	100
1	G	90/100 (90%)	90 (100%)	0	100	100
1	H	90/100 (90%)	90 (100%)	0	100	100
1	I	90/100 (90%)	90 (100%)	0	100	100
1	J	90/100 (90%)	90 (100%)	0	100	100
1	K	90/100 (90%)	90 (100%)	0	100	100
1	L	90/100 (90%)	90 (100%)	0	100	100
1	M	90/100 (90%)	90 (100%)	0	100	100
1	N	90/100 (90%)	90 (100%)	0	100	100
1	O	90/100 (90%)	90 (100%)	0	100	100
1	P	90/100 (90%)	90 (100%)	0	100	100
1	Q	90/100 (90%)	90 (100%)	0	100	100
1	R	90/100 (90%)	90 (100%)	0	100	100
1	S	90/100 (90%)	90 (100%)	0	100	100
1	T	90/100 (90%)	90 (100%)	0	100	100
All	All	1800/2000 (90%)	1800 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	597	HIS
1	A	633	GLN
1	B	573	GLN
1	D	573	GLN
1	E	597	HIS
1	F	633	GLN
1	G	597	HIS
1	I	597	HIS
1	I	609	GLN
1	I	633	GLN
1	J	597	HIS
1	K	573	GLN
1	L	611	GLN
1	M	573	GLN

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Mol	Chain	Res	Type
1	M	600	ASN
1	M	609	GLN
1	M	611	GLN
1	N	573	GLN
1	N	633	GLN
1	O	611	GLN
1	P	633	GLN
1	Q	611	GLN
1	Q	633	GLN
1	R	600	ASN
1	R	609	GLN
1	R	633	GLN
1	R	651	GLN
1	S	609	GLN
1	T	611	GLN
1	T	633	GLN

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.