



Full wwPDB EM Validation Report ⓘ

Mar 3, 2025 – 12:18 pm GMT

PDB ID : 9I0Y
EMDB ID : EMD-52564
Title : Recombinant Ena2A fibers
Authors : Sleutel, M.; Remaut, H.
Deposited on : 2025-01-15
Resolution : 2.74 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) : 2.41

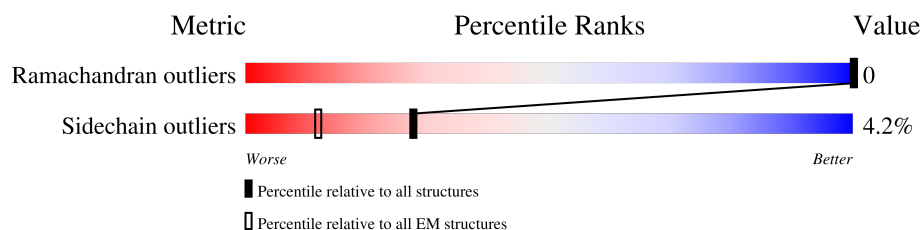
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.74 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.
















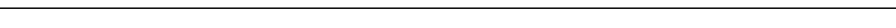











Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	0	122	90% 7%
1	1	122	90% 7%
1	2	122	90% 7%
1	3	122	90% 7%
1	4	122	90% 7%
1	5	122	90% 7%
1	6	122	90% 7%
1	7	122	90% 7%
1	8	122	90% 7%
1	9	122	90% 7%













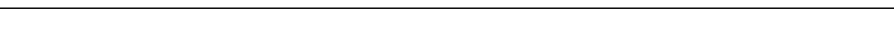
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Mol	Chain	Length	Quality of chain
1	AA	122	 90% • 7%
1	P	122	 90% • 7%
1	Q	122	 90% • 7%
1	R	122	 90% • 7%
1	S	122	 90% • 7%
1	T	122	 90% • 7%
1	U	122	 90% • 7%
1	V	122	 90% • 7%
1	W	122	 90% • 7%
1	X	122	 90% • 7%
1	Y	122	 90% • 7%
1	Z	122	 90% • 7%
1	a	122	 89% • 7%
1	b	122	 90% • 7%
1	c	122	 90% • 7%
1	d	122	 90% • 7%
1	e	122	 90% • 7%
1	f	122	 90% • 7%
1	g	122	 90% • 7%
1	h	122	 90% • 7%
1	i	122	 90% • 7%
1	j	122	 90% • 7%
1	k	122	 90% • 7%
1	l	122	 90% • 7%
1	m	122	 90% • 7%

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Mol	Chain	Length	Quality of chain
1	n	122	 90% • 7%
1	o	122	 90% • 7%
1	p	122	 90% • 7%
1	q	122	 90% • 7%
1	r	122	 90% • 7%
1	s	122	 90% • 7%
1	t	122	 90% • 7%
1	u	122	 90% • 7%
1	v	122	 90% • 7%
1	w	122	 90% • 7%
1	x	122	 90% • 7%
1	y	122	 90% • 7%
1	z	122	 90% • 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 41225 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 DUF3992 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	1	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	2	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	3	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	4	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	5	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	6	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	7	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	8	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	9	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	AA	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	P	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	Q	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	R	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	S	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	T	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	U	114	Total	C	N	O	S	0	0
			859	544	141	169	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	V	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	W	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	X	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	Y	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	Z	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	a	113	Total	C	N	O	S	0	0
			852	541	140	166	5		
1	b	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	c	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	d	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	e	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	f	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	g	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	h	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	i	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	j	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	k	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	l	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	m	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	n	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	o	114	Total	C	N	O	S	0	0
			859	544	141	169	5		
1	p	114	Total	C	N	O	S	0	0
			859	544	141	169	5		

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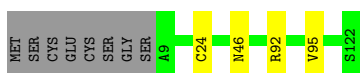
Mol	Chain	Residues	Atoms					AltConf	Trace
1	q	114	Total 859	C 544	N 141	O 169	S 5	0	0
1	r	114	Total 859	C 544	N 141	O 169	S 5	0	0
1	s	114	Total 859	C 544	N 141	O 169	S 5	0	0
1	t	114	Total 859	C 544	N 141	O 169	S 5	0	0
1	u	114	Total 859	C 544	N 141	O 169	S 5	0	0
1	v	114	Total 859	C 544	N 141	O 169	S 5	0	0
1	w	114	Total 859	C 544	N 141	O 169	S 5	0	0
1	x	114	Total 859	C 544	N 141	O 169	S 5	0	0
1	y	114	Total 859	C 544	N 141	O 169	S 5	0	0
1	z	114	Total 859	C 544	N 141	O 169	S 5	0	0

3 Residue-property plots [i](#)


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.

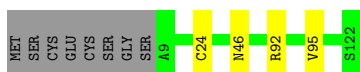
- Molecule 1: DUF3992 domain-containing protein

Chain 0:  90% 7%



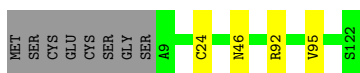
- Molecule 1: DUF3992 domain-containing protein

Chain 1:  90% 7%




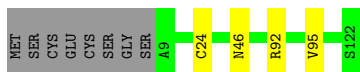
- Molecule 1: DUF3992 domain-containing protein

Chain 2:  90% 7%




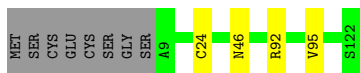
- Molecule 1: DUF3992 domain-containing protein

Chain 3:  90% 7%




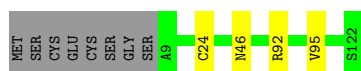
- Molecule 1: DUF3992 domain-containing protein

Chain 4:  90% 7%



- Molecule 1: DUF3992 domain-containing protein

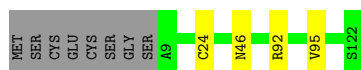
Chain 5:  90% 7%



- Molecule 1: DUF3992 domain-containing protein

Chain 6:
90% 7%

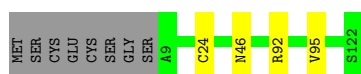
A horizontal bar chart showing validation metrics for Chain 6. The bar is 90% green and 7% yellow, indicating a high level of validation.



- Molecule 1: DUF3992 domain-containing protein

Chain 7:
90% 7%

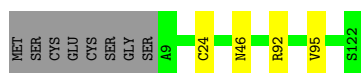
A horizontal bar chart showing validation metrics for Chain 7. The bar is 90% green and 7% yellow, indicating a high level of validation.



- Molecule 1: DUF3992 domain-containing protein

Chain 8:
90% 7%

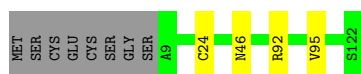
A horizontal bar chart showing validation metrics for Chain 8. The bar is 90% green and 7% yellow, indicating a high level of validation.



- Molecule 1: DUF3992 domain-containing protein

Chain 9:
90% 7%

A horizontal bar chart showing validation metrics for Chain 9. The bar is 90% green and 7% yellow, indicating a high level of validation.



- Molecule 1: DUF3992 domain-containing protein

Chain AA:
90% 7%

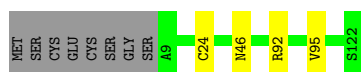
A horizontal bar chart showing validation metrics for Chain AA. The bar is 90% green and 7% yellow, indicating a high level of validation.



- Molecule 1: DUF3992 domain-containing protein

Chain P:
90% 7%

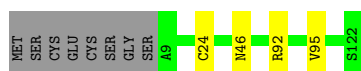
A horizontal bar chart showing validation metrics for Chain P. The bar is 90% green and 7% yellow, indicating a high level of validation.



- Molecule 1: DUF3992 domain-containing protein

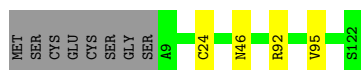
Chain Q:
90% 7%

A horizontal bar chart showing validation metrics for Chain Q. The bar is 90% green and 7% yellow, indicating a high level of validation.



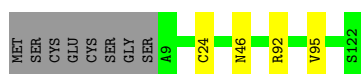
- Molecule 1: DUF3992 domain-containing protein

Chain R: 90% 7%



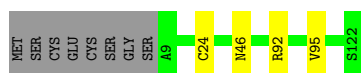
- Molecule 1: DUF3992 domain-containing protein

Chain S: 90% 7%



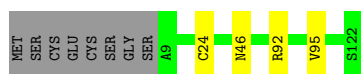
- Molecule 1: DUF3992 domain-containing protein

Chain T: 90% 7%



- Molecule 1: DUF3992 domain-containing protein

Chain U: 90% 7%



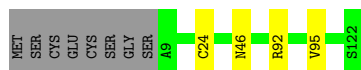
- Molecule 1: DUF3992 domain-containing protein

Chain V: 90% 7%



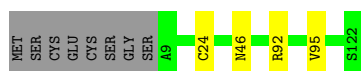
- Molecule 1: DUF3992 domain-containing protein

Chain W: 90% 7%



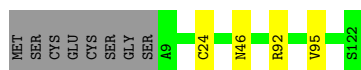
- Molecule 1: DUF3992 domain-containing protein

Chain X: 90% 7%



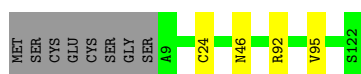
- Molecule 1: DUF3992 domain-containing protein

Chain Y: 90% 7%



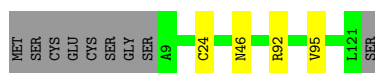
- Molecule 1: DUF3992 domain-containing protein

Chain Z: 90% 7%



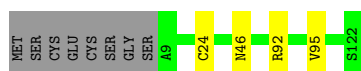
- Molecule 1: DUF3992 domain-containing protein

Chain a: 89% 7%



- Molecule 1: DUF3992 domain-containing protein

Chain b: 90% 7%



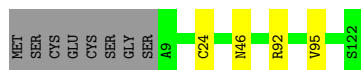
- Molecule 1: DUF3992 domain-containing protein

Chain c: 90% 7%



- Molecule 1: DUF3992 domain-containing protein

Chain d: 90% 7%



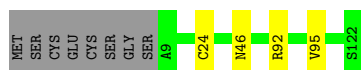
- Molecule 1: DUF3992 domain-containing protein

Chain e: 90% 7%



- Molecule 1: DUF3992 domain-containing protein

Chain f: 90% 7%



- Molecule 1: DUF3992 domain-containing protein

Chain g: 90% 7%



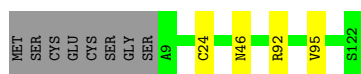
- Molecule 1: DUF3992 domain-containing protein

Chain h: 90% 7%



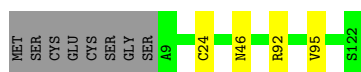
- Molecule 1: DUF3992 domain-containing protein

Chain i: 90% 7%



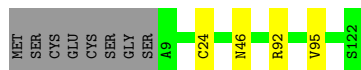
- Molecule 1: DUF3992 domain-containing protein

Chain j: 90% 7%



- Molecule 1: DUF3992 domain-containing protein

Chain k: 90% 7%



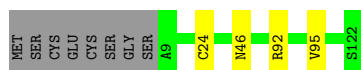
- Molecule 1: DUF3992 domain-containing protein

Chain l: 90% 7%



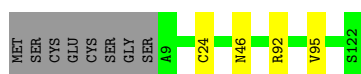
- Molecule 1: DUF3992 domain-containing protein

Chain m: 90% 7%



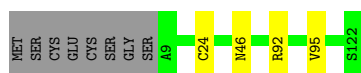
- Molecule 1: DUF3992 domain-containing protein

Chain n: 90% 7%



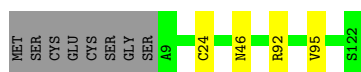
- Molecule 1: DUF3992 domain-containing protein

Chain o: 90% 7%



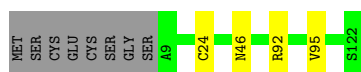
- Molecule 1: DUF3992 domain-containing protein

Chain p: 90% 7%



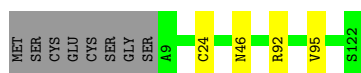
- Molecule 1: DUF3992 domain-containing protein

Chain q: 90% 7%



- Molecule 1: DUF3992 domain-containing protein

Chain r: 90% 7%

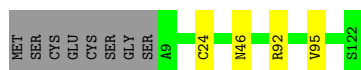
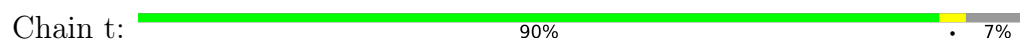


- Molecule 1: DUF3992 domain-containing protein

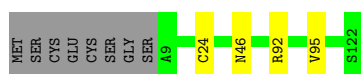
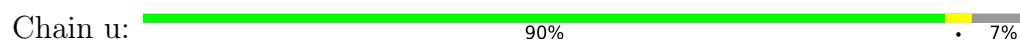
Chain s: 90% 7%



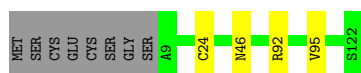
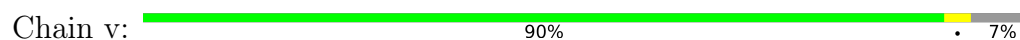
- Molecule 1: DUF3992 domain-containing protein



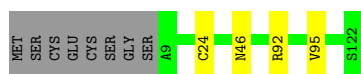
- Molecule 1: DUF3992 domain-containing protein



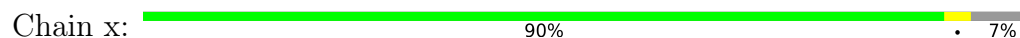
- Molecule 1: DUF3992 domain-containing protein



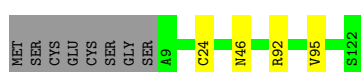
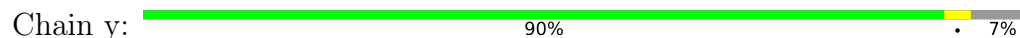
- Molecule 1: DUF3992 domain-containing protein



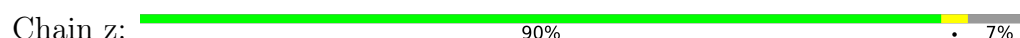
- Molecule 1: DUF3992 domain-containing protein



- Molecule 1: DUF3992 domain-containing protein



- Molecule 1: DUF3992 domain-containing protein



MET	SER	CYS	GLU	CYS	SER	GLY	SER	A9	C24	M46	R92	V95	S122
-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	------

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-31.03°, rise=3.16 Å, axial sym=C1	Depositor
Number of segments used	388452	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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	0	0.26	0/877	0.52	0/1205
1	1	0.26	0/877	0.52	0/1205
1	2	0.26	0/877	0.52	0/1205
1	3	0.26	0/877	0.52	0/1205
1	4	0.26	0/877	0.52	0/1205
1	5	0.26	0/877	0.52	0/1205
1	6	0.26	0/877	0.52	0/1205
1	7	0.26	0/877	0.52	0/1205
1	8	0.26	0/877	0.52	0/1205
1	9	0.26	0/877	0.52	0/1205
1	AA	0.26	0/877	0.52	0/1205
1	P	0.26	0/877	0.52	0/1205
1	Q	0.26	0/877	0.52	0/1205
1	R	0.26	0/877	0.52	0/1205
1	S	0.26	0/877	0.52	0/1205
1	T	0.26	0/877	0.52	0/1205
1	U	0.26	0/877	0.52	0/1205
1	V	0.26	0/877	0.52	0/1205
1	W	0.26	0/877	0.52	0/1205
1	X	0.26	0/877	0.52	0/1205
1	Y	0.26	0/877	0.52	0/1205
1	Z	0.26	0/877	0.52	0/1205
1	a	0.26	0/870	0.52	0/1197
1	b	0.26	0/877	0.52	0/1205
1	c	0.26	0/877	0.52	0/1205
1	d	0.26	0/877	0.52	0/1205
1	e	0.26	0/877	0.53	0/1205
1	f	0.26	0/877	0.52	0/1205
1	g	0.26	0/877	0.52	0/1205
1	h	0.26	0/877	0.52	0/1205
1	i	0.26	0/877	0.52	0/1205
1	j	0.26	0/877	0.52	0/1205
1	k	0.26	0/877	0.52	0/1205
1	l	0.26	0/877	0.52	0/1205

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	m	0.26	0/877	0.52	0/1205
1	n	0.26	0/877	0.52	0/1205
1	o	0.26	0/877	0.52	0/1205
1	p	0.26	0/877	0.52	0/1205
1	q	0.26	0/877	0.52	0/1205
1	r	0.26	0/877	0.52	0/1205
1	s	0.26	0/877	0.52	0/1205
1	t	0.26	0/877	0.52	0/1205
1	u	0.26	0/877	0.52	0/1205
1	v	0.26	0/877	0.52	0/1205
1	w	0.26	0/877	0.53	0/1205
1	x	0.26	0/877	0.52	0/1205
1	y	0.26	0/877	0.52	0/1205
1	z	0.26	0/877	0.52	0/1205
All	All	0.26	0/42089	0.52	0/57832

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	0	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	1	112/122 (92%)	106 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	3	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	4	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	5	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	6	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	7	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	8	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	9	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	AA	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	P	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	Q	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	R	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	S	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	T	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	U	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	V	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	W	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	X	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	Y	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	Z	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	a	111/122 (91%)	106 (96%)	5 (4%)	0	100	100
1	b	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	c	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	d	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	e	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	f	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	g	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	h	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	i	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	j	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	k	112/122 (92%)	106 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	l	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	m	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	n	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	o	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	p	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	q	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	r	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	s	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	t	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	u	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	v	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	w	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	x	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	y	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
1	z	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
All	All	5375/5856 (92%)	5088 (95%)	287 (5%)	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	0	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	1	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	2	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	3	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	4	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	5	95/102 (93%)	91 (96%)	4 (4%)	25	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	7	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	8	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	9	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	AA	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	P	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	Q	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	R	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	S	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	T	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	U	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	V	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	W	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	X	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	Y	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	Z	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	a	94/102 (92%)	90 (96%)	4 (4%)	25	43
1	b	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	c	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	d	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	e	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	f	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	g	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	h	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	i	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	j	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	k	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	l	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	m	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	n	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	o	95/102 (93%)	91 (96%)	4 (4%)	25	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	p	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	q	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	r	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	s	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	t	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	u	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	v	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	w	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	x	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	y	95/102 (93%)	91 (96%)	4 (4%)	25	44
1	z	95/102 (93%)	91 (96%)	4 (4%)	25	44
All	All	4559/4896 (93%)	4367 (96%)	192 (4%)	27	44

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	24	CYS
1	0	46	ASN
1	0	92	ARG
1	0	95	VAL
1	1	24	CYS
1	1	46	ASN
1	1	92	ARG
1	1	95	VAL
1	2	24	CYS
1	2	46	ASN
1	2	92	ARG
1	2	95	VAL
1	3	24	CYS
1	3	46	ASN
1	3	92	ARG
1	3	95	VAL
1	4	24	CYS
1	4	46	ASN
1	4	92	ARG
1	4	95	VAL
1	5	24	CYS
1	5	46	ASN

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Mol	Chain	Res	Type
1	5	92	ARG
1	5	95	VAL
1	6	24	CYS
1	6	46	ASN
1	6	92	ARG
1	6	95	VAL
1	7	24	CYS
1	7	46	ASN
1	7	92	ARG
1	7	95	VAL
1	8	24	CYS
1	8	46	ASN
1	8	92	ARG
1	8	95	VAL
1	9	24	CYS
1	9	46	ASN
1	9	92	ARG
1	9	95	VAL
1	AA	24	CYS
1	AA	46	ASN
1	AA	92	ARG
1	AA	95	VAL
1	P	24	CYS
1	P	46	ASN
1	P	92	ARG
1	P	95	VAL
1	Q	24	CYS
1	Q	46	ASN
1	Q	92	ARG
1	Q	95	VAL
1	R	24	CYS
1	R	46	ASN
1	R	92	ARG
1	R	95	VAL
1	S	24	CYS
1	S	46	ASN
1	S	92	ARG
1	S	95	VAL
1	T	24	CYS
1	T	46	ASN
1	T	92	ARG
1	T	95	VAL

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Mol	Chain	Res	Type
1	U	24	CYS
1	U	46	ASN
1	U	92	ARG
1	U	95	VAL
1	V	24	CYS
1	V	46	ASN
1	V	92	ARG
1	V	95	VAL
1	W	24	CYS
1	W	46	ASN
1	W	92	ARG
1	W	95	VAL
1	X	24	CYS
1	X	46	ASN
1	X	92	ARG
1	X	95	VAL
1	Y	24	CYS
1	Y	46	ASN
1	Y	92	ARG
1	Y	95	VAL
1	Z	24	CYS
1	Z	46	ASN
1	Z	92	ARG
1	Z	95	VAL
1	a	24	CYS
1	a	46	ASN
1	a	92	ARG
1	a	95	VAL
1	b	24	CYS
1	b	46	ASN
1	b	92	ARG
1	b	95	VAL
1	c	24	CYS
1	c	46	ASN
1	c	92	ARG
1	c	95	VAL
1	d	24	CYS
1	d	46	ASN
1	d	92	ARG
1	d	95	VAL
1	e	24	CYS
1	e	46	ASN

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Mol	Chain	Res	Type
1	e	92	ARG
1	e	95	VAL
1	f	24	CYS
1	f	46	ASN
1	f	92	ARG
1	f	95	VAL
1	g	24	CYS
1	g	46	ASN
1	g	92	ARG
1	g	95	VAL
1	h	24	CYS
1	h	46	ASN
1	h	92	ARG
1	h	95	VAL
1	i	24	CYS
1	i	46	ASN
1	i	92	ARG
1	i	95	VAL
1	j	24	CYS
1	j	46	ASN
1	j	92	ARG
1	j	95	VAL
1	k	24	CYS
1	k	46	ASN
1	k	92	ARG
1	k	95	VAL
1	l	24	CYS
1	l	46	ASN
1	l	92	ARG
1	l	95	VAL
1	m	24	CYS
1	m	46	ASN
1	m	92	ARG
1	m	95	VAL
1	n	24	CYS
1	n	46	ASN
1	n	92	ARG
1	n	95	VAL
1	o	24	CYS
1	o	46	ASN
1	o	92	ARG
1	o	95	VAL

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Mol	Chain	Res	Type
1	p	24	CYS
1	p	46	ASN
1	p	92	ARG
1	p	95	VAL
1	q	24	CYS
1	q	46	ASN
1	q	92	ARG
1	q	95	VAL
1	r	24	CYS
1	r	46	ASN
1	r	92	ARG
1	r	95	VAL
1	s	24	CYS
1	s	46	ASN
1	s	92	ARG
1	s	95	VAL
1	t	24	CYS
1	t	46	ASN
1	t	92	ARG
1	t	95	VAL
1	u	24	CYS
1	u	46	ASN
1	u	92	ARG
1	u	95	VAL
1	v	24	CYS
1	v	46	ASN
1	v	92	ARG
1	v	95	VAL
1	w	24	CYS
1	w	46	ASN
1	w	92	ARG
1	w	95	VAL
1	x	24	CYS
1	x	46	ASN
1	x	92	ARG
1	x	95	VAL
1	y	24	CYS
1	y	46	ASN
1	y	92	ARG
1	y	95	VAL
1	z	24	CYS
1	z	46	ASN

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Mol	Chain	Res	Type
1	z	92	ARG
1	z	95	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	20	GLN
1	1	20	GLN
1	2	20	GLN
1	3	20	GLN
1	4	20	GLN
1	5	20	GLN
1	6	20	GLN
1	7	20	GLN
1	8	20	GLN
1	9	20	GLN
1	AA	20	GLN
1	Z	20	GLN
1	a	20	GLN
1	b	20	GLN
1	c	20	GLN
1	d	20	GLN
1	e	20	GLN
1	f	20	GLN
1	g	20	GLN
1	h	20	GLN
1	i	20	GLN
1	j	20	GLN
1	k	20	GLN
1	l	20	GLN
1	m	20	GLN
1	n	20	GLN
1	o	20	GLN
1	p	20	GLN
1	q	20	GLN
1	r	20	GLN
1	s	20	GLN
1	t	20	GLN
1	u	20	GLN
1	v	20	GLN
1	w	20	GLN
1	x	20	GLN

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Mol	Chain	Res	Type
1	y	20	GLN
1	z	20	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 [i](#)

There are no chain breaks in this entry.