



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 01:22 AM EST

PDB ID : 3J9R
EMDB ID : EMD-6271
Title : Atomic structures of a bactericidal contractile nanotube in its pre- and post-contraction states
Authors : Ge, P.; Scholl, D.; Leiman, P.G.; Yu, X.; Miller, J.F.; Zhou, Z.H.
Deposited on : 2015-02-17
Resolution : 3.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

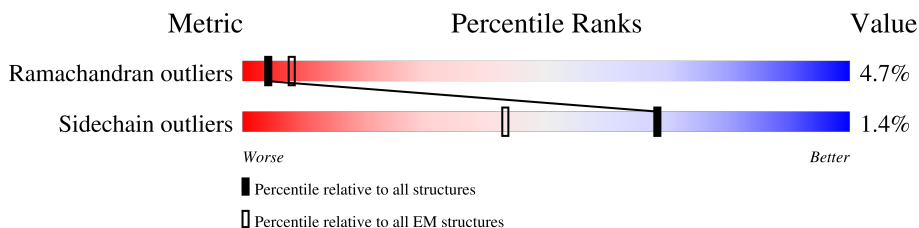
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.90 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.



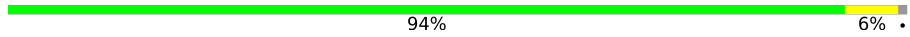


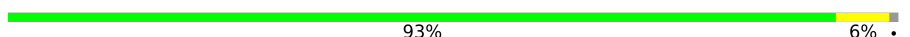

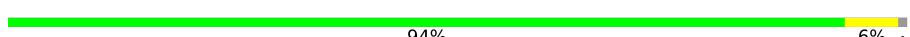




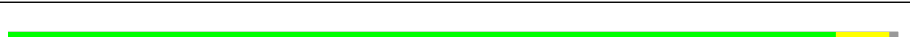


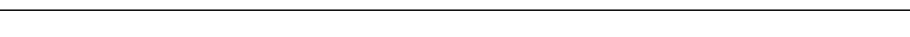
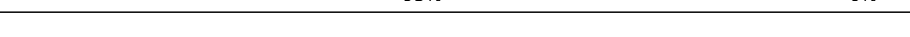
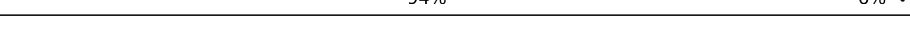
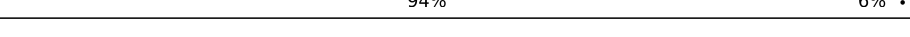
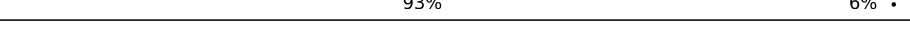
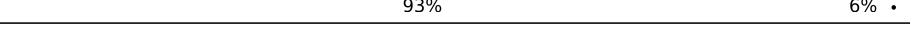
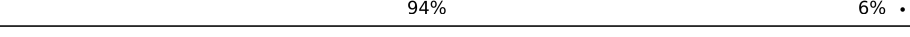
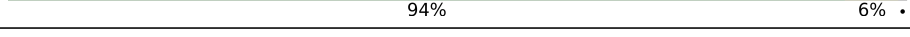
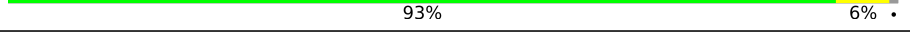
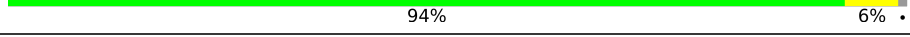
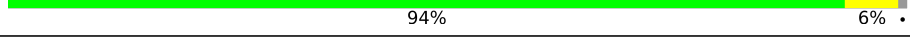
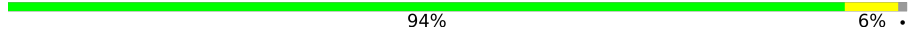
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	386	93% 6% .
1	1	386	93% 6% .
1	2	386	93% 6% .
1	3	386	94% 6% .
1	4	386	94% 6% .
1	5	386	94% 6% .
1	A	386	93% 6% .
1	B	386	93% 6% .
1	C	386	93% 6% .
1	D	386	93% 6% .

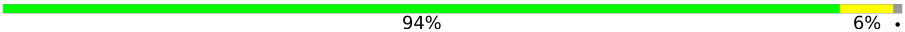
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Mol	Chain	Length	Quality of chain
1	E	386	 94% 6%
1	F	386	 93% 6%
1	G	386	 93% 6%
1	H	386	 93% 6%
1	I	386	 93% 6%
1	J	386	 94% 6%
1	K	386	 93% 6%
1	L	386	 93% 6%
1	M	386	 93% 6%
1	N	386	 93% 6%
1	O	386	 93% 6%
1	P	386	 93% 6%
1	Q	386	 93% 6%
1	R	386	 93% 6%
1	a	386	 94% 6%
1	b	386	 94% 6%
1	c	386	 93% 6%
1	d	386	 93% 6%
1	e	386	 94% 6%
1	f	386	 94% 6%
1	g	386	 93% 6%
1	h	386	 94% 6%
1	i	386	 94% 6%
1	j	386	 94% 6%
1	k	386	 94% 6%

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Mol	Chain	Length	Quality of chain
1	1	386	 94% 6%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 103824 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 sheath.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	383	2884	1817	504	555	8	0	0
1	B	383	2884	1817	504	555	8	0	0
1	F	383	2884	1817	504	555	8	0	0
1	E	383	2884	1817	504	555	8	0	0
1	D	383	2884	1817	504	555	8	0	0
1	C	383	2884	1817	504	555	8	0	0
1	0	383	2884	1817	504	555	8	0	0
1	1	383	2884	1817	504	555	8	0	0
1	5	383	2884	1817	504	555	8	0	0
1	4	383	2884	1817	504	555	8	0	0
1	3	383	2884	1817	504	555	8	0	0
1	2	383	2884	1817	504	555	8	0	0
1	G	383	2884	1817	504	555	8	0	0
1	H	383	2884	1817	504	555	8	0	0
1	L	383	2884	1817	504	555	8	0	0
1	K	383	2884	1817	504	555	8	0	0
1	J	383	2884	1817	504	555	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	M	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	N	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	R	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	Q	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	P	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	O	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	a	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	b	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	f	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	e	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	d	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	c	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	g	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	h	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	l	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	k	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	j	383	Total 2884	C 1817	N 504	O 555	S 8	0	0
1	i	383	Total 2884	C 1817	N 504	O 555	S 8	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: sheath

Chain A:  93% 6%



- Molecule 1: sheath

Chain B:  93% 6%



- Molecule 1: sheath

Chain F:  93% 6%



- Molecule 1: sheath

Chain E:  94% 6%



- Molecule 1: sheath

Chain D:  93% 6%



- Molecule 1: sheath

Chain C:  93% 6%



• Molecule 1: sheath



• Molecule 1: sheath



• Molecule 1: sheath



• Molecule 1: sheath



• Molecule 1: sheath



• Molecule 1: sheath



• Molecule 1: sheath





• Molecule 1: sheath



• Molecule 1: sheath



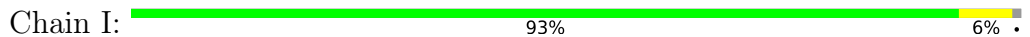
• Molecule 1: sheath



• Molecule 1: sheath



• Molecule 1: sheath



• Molecule 1: sheath



• Molecule 1: sheath





- Molecule 1: sheath

Chain R: 93% 6%



- Molecule 1: sheath

Chain Q: 93% 6%



- Molecule 1: sheath

Chain P: 93% 6%



- Molecule 1: sheath

Chain O: 93% 6%



- Molecule 1: sheath

Chain a: 94% 6%



- Molecule 1: sheath

Chain b: 94% 6%



- Molecule 1: sheath

Chain f: 94% 6%



- Molecule 1: sheath

Chain e: 94% 6%



- Molecule 1: sheath

Chain d: 93% 6%



- Molecule 1: sheath

Chain c: 93% 6%



- Molecule 1: sheath

Chain g: 93% 6%



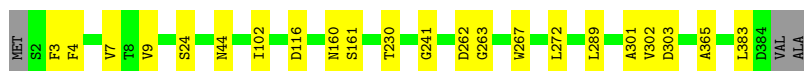
- Molecule 1: sheath

Chain h: 94% 6%



- Molecule 1: sheath

Chain i: 94% 6%

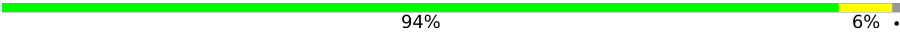


- Molecule 1: sheath

Chain k: 94% 6%



- Molecule 1: sheath

Chain j:  94% 6%



- Molecule 1: sheath

Chain i:  94% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=33.1°, rise=16.2 Å, axial sym=C6	Depositor
Number of segments used	Not provided	
Resolution determination method	OTHER	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	25	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	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	0	0.35	3/2942 (0.1%)	0.37	0/4010
1	1	0.32	3/2942 (0.1%)	0.37	0/4010
1	2	0.36	4/2942 (0.1%)	0.37	0/4010
1	3	0.31	1/2942 (0.0%)	0.37	0/4010
1	4	0.29	1/2942 (0.0%)	0.37	0/4010
1	5	0.29	1/2942 (0.0%)	0.37	0/4010
1	A	0.28	1/2942 (0.0%)	0.37	0/4010
1	B	0.31	3/2942 (0.1%)	0.37	0/4010
1	C	0.29	1/2942 (0.0%)	0.37	0/4010
1	D	0.29	1/2942 (0.0%)	0.37	0/4010
1	E	0.36	2/2942 (0.1%)	0.37	0/4010
1	F	0.35	3/2942 (0.1%)	0.37	0/4010
1	G	0.29	1/2942 (0.0%)	0.37	0/4010
1	H	0.30	1/2942 (0.0%)	0.37	0/4010
1	I	0.29	2/2942 (0.1%)	0.37	0/4010
1	J	0.29	0/2942	0.37	0/4010
1	K	0.29	1/2942 (0.0%)	0.37	0/4010
1	L	0.30	1/2942 (0.0%)	0.37	0/4010
1	M	0.31	2/2942 (0.1%)	0.36	0/4010
1	N	0.30	1/2942 (0.0%)	0.37	0/4010
1	O	0.30	1/2942 (0.0%)	0.36	0/4010
1	P	0.29	1/2942 (0.0%)	0.37	0/4010
1	Q	0.29	1/2942 (0.0%)	0.37	0/4010
1	R	0.29	2/2942 (0.1%)	0.37	0/4010
1	a	0.28	0/2942	0.37	0/4010
1	b	0.28	0/2942	0.37	0/4010
1	c	0.29	1/2942 (0.0%)	0.37	0/4010
1	d	0.28	1/2942 (0.0%)	0.37	0/4010
1	e	0.27	0/2942	0.37	0/4010
1	f	0.27	0/2942	0.37	0/4010
1	g	0.28	1/2942 (0.0%)	0.37	0/4010
1	h	0.27	0/2942	0.37	0/4010
1	i	0.28	0/2942	0.37	0/4010
1	j	0.27	0/2942	0.37	0/4010

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	k	0.28	0/2942	0.37	0/4010
1	l	0.28	0/2942	0.36	0/4010
All	All	0.30	41/105912 (0.0%)	0.37	0/144360

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
1	B	0	1
All	All	0	2

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	193	ASN	CG-ND2	-9.37	1.09	1.32
1	E	193	ASN	CG-ND2	-9.23	1.09	1.32
1	F	193	ASN	CG-ND2	-8.72	1.11	1.32
1	0	193	ASN	CG-ND2	-8.42	1.11	1.32
1	2	193	ASN	CG-OD1	-8.29	1.05	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	193	ASN	Sidechain
1	B	193	ASN	Sidechain

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

5.3.1 Protein backbone

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	381/386 (99%)	307 (81%)	57 (15%)	17 (4%)	2	25
1	1	381/386 (99%)	307 (81%)	57 (15%)	17 (4%)	2	25
1	2	381/386 (99%)	307 (81%)	57 (15%)	17 (4%)	2	25
1	3	381/386 (99%)	307 (81%)	57 (15%)	17 (4%)	2	25
1	4	381/386 (99%)	308 (81%)	56 (15%)	17 (4%)	2	25
1	5	381/386 (99%)	309 (81%)	55 (14%)	17 (4%)	2	25
1	A	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	2	24
1	B	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	24
1	C	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	24
1	D	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	24
1	E	381/386 (99%)	308 (81%)	56 (15%)	17 (4%)	2	25
1	F	381/386 (99%)	306 (80%)	57 (15%)	18 (5%)	2	24
1	G	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	24
1	H	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	2	24
1	I	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	24
1	J	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	24
1	K	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	2	24
1	L	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	24
1	M	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	2	24
1	N	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	24
1	O	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	2	24
1	P	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	2	24
1	Q	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	24
1	R	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	24
1	a	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	2	24
1	c	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	24
1	d	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	24
1	e	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	24
1	f	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	24
1	g	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	24
1	h	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	24
1	i	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	24
1	j	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	24
1	k	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	24
1	l	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	24
All	All	13716/13896 (99%)	11082 (81%)	1993 (14%)	641 (5%)	4	24

5 of 641 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	B	9	VAL
1	F	9	VAL
1	E	9	VAL
1	D	9	VAL

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	0	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	1	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	2	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	3	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	4	296/298 (99%)	292 (99%)	4 (1%)	67	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	A	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	B	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	C	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	D	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	E	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	F	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	G	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	H	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	I	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	J	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	K	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	L	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	M	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	N	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	O	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	P	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	Q	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	R	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	a	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	b	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	c	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	d	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	e	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	f	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	g	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	h	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	i	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	j	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	k	296/298 (99%)	292 (99%)	4 (1%)	67	81
1	l	296/298 (99%)	292 (99%)	4 (1%)	67	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	10656/10728 (99%)	10512 (99%)	144 (1%)	68 81

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	d	303	ASP
1	i	303	ASP
1	c	303	ASP
1	l	289	LEU
1	G	116	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	137	GLN
1	L	172	ASN
1	O	172	ASN
1	M	347	GLN
1	N	172	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 monosaccharides 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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6271. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.