



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 04:01 AM UTC

PDB ID : 9NGW / pdb_00009ngw
EMDB ID : EMD-49395
Title : In-situ cryo-EM structure of Dome of the Legionella Dot/Icm machine
Authors : Yue, J.; Liu, J.
Deposited on : 2025-02-22
Resolution : 3.08 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.dev132
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

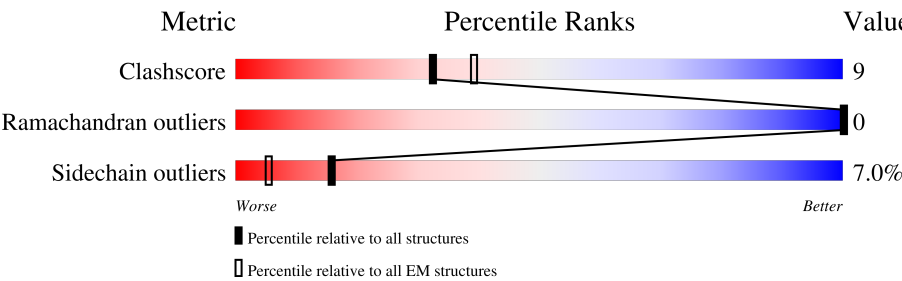
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.08 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	1048	12% • • 84%
1	B	1048	12% • 84%
1	C	1048	12% • 84%
1	D	1048	12% • 84%
1	E	1048	13% • 84%
1	F	1048	12% • 84%
1	G	1048	12% • 84%
1	H	1048	13% • 84%
1	I	1048	12% • 84%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	1048	 12% • 84%
1	K	1048	 13% • 84%
1	L	1048	 12% • 84%
1	M	1048	 12% • 84%
1	N	1048	 13% • 84%
1	O	1048	 12% • 84%
1	P	1048	 13% • 84%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20272 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 IcmE (DotG).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		
1	B	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		
1	C	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		
1	D	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		
1	E	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		
1	F	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		
1	G	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		
1	H	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		
1	I	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		
1	J	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		
1	K	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		
1	L	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		
1	M	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		
1	N	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		
1	O	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		
1	P	170	Total	C	N	O	S	0	0
			1267	802	214	247	4		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	997	ARG	GLY	conflict	UNP Q5ZYC1
B	997	ARG	GLY	conflict	UNP Q5ZYC1
C	997	ARG	GLY	conflict	UNP Q5ZYC1
D	997	ARG	GLY	conflict	UNP Q5ZYC1
E	997	ARG	GLY	conflict	UNP Q5ZYC1
F	997	ARG	GLY	conflict	UNP Q5ZYC1
G	997	ARG	GLY	conflict	UNP Q5ZYC1
H	997	ARG	GLY	conflict	UNP Q5ZYC1
I	997	ARG	GLY	conflict	UNP Q5ZYC1
J	997	ARG	GLY	conflict	UNP Q5ZYC1
K	997	ARG	GLY	conflict	UNP Q5ZYC1
L	997	ARG	GLY	conflict	UNP Q5ZYC1
M	997	ARG	GLY	conflict	UNP Q5ZYC1
N	997	ARG	GLY	conflict	UNP Q5ZYC1
O	997	ARG	GLY	conflict	UNP Q5ZYC1
P	997	ARG	GLY	conflict	UNP Q5ZYC1



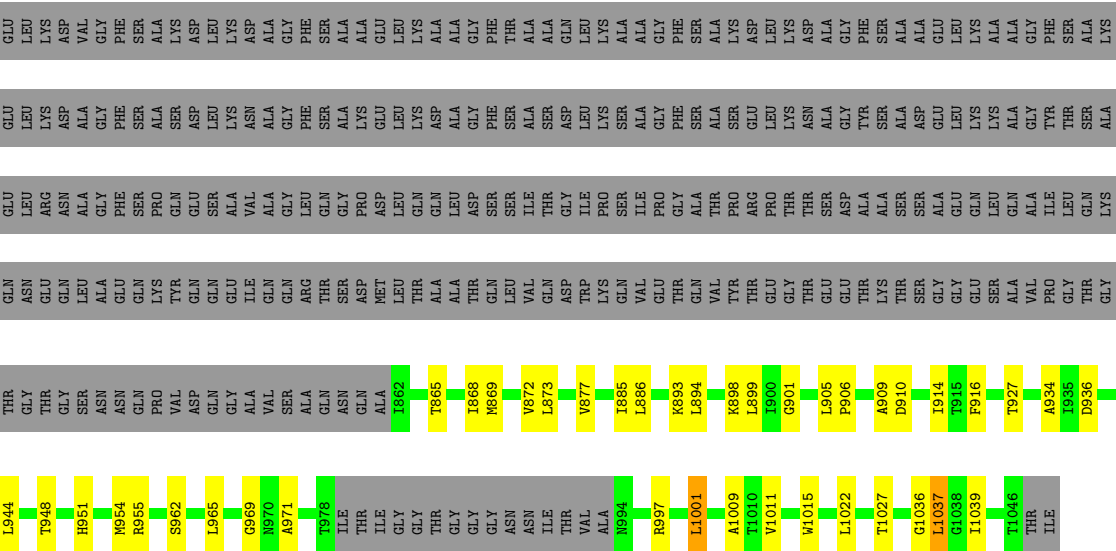


MET	ALA	SER	LYS	LYS	GLU	ASN	LEU	LEU	LYS	SER	LEU	PHE	SER	ASN	THR	THR	THR	ARG	VAL	ILE	ILE	ILE	PHE	THR	ALA	ALA	LEU	LEU	ILE	ILE	ILE	PHE	PHE	PHE	LYS	ILE	ILE	ARG	GLY	ALA	ALA	THR	THR	GLY	SER	ILE	ILE	ALA	ALA	ALA	GLU	VAL	SER	SER	THR	VAL	VAL	PRO	GLY	GLY	ILE	ILE	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

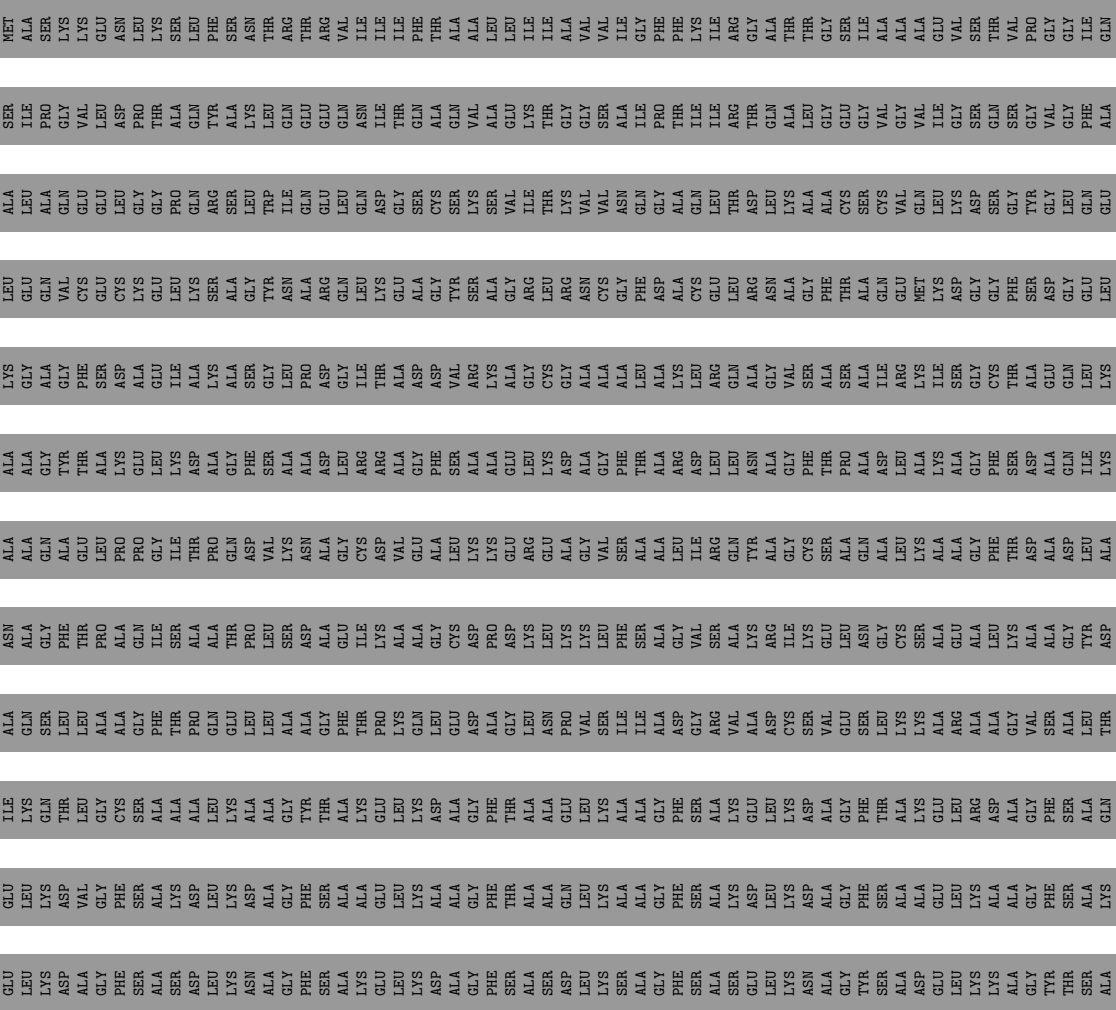








● Molecule 1: IcmE (DotG)

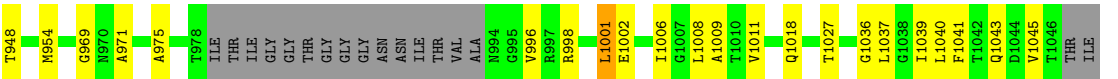


[illegible]

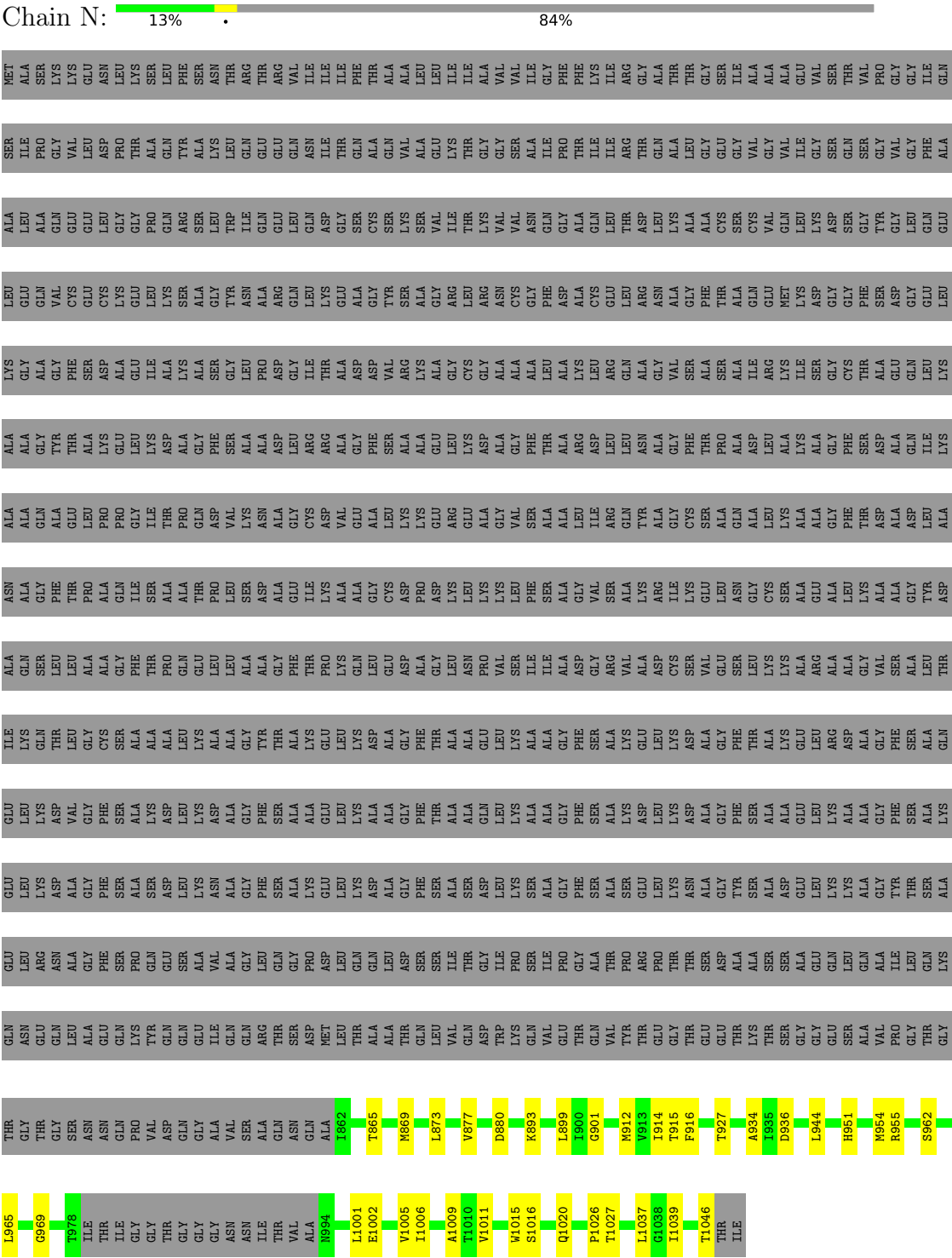
- Molecule 1: IcmE (DotG)

[illegible]

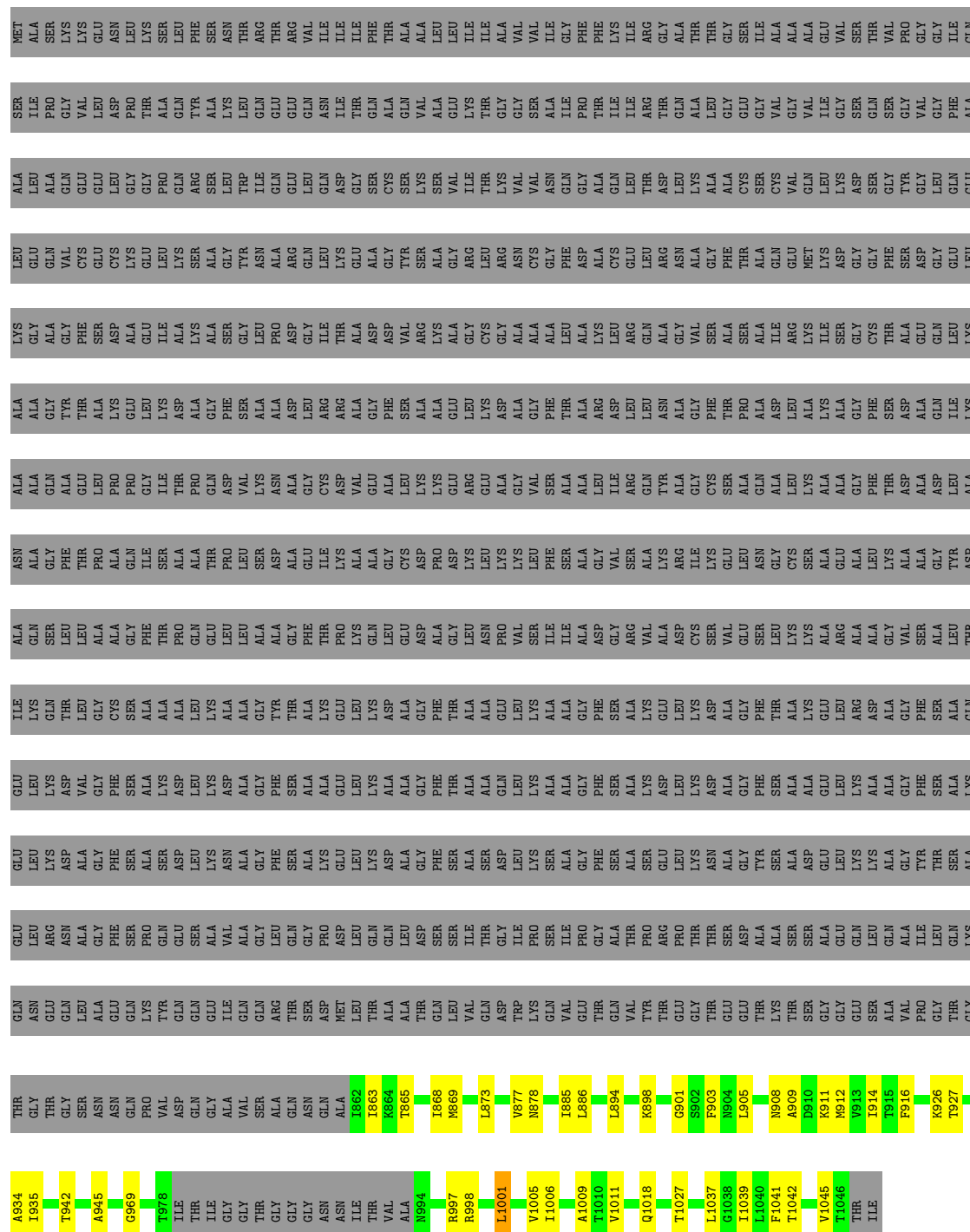




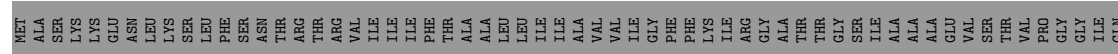
• Molecule 1: IcmE (DotG)



• Molecule 1: IcmE (DotG)



- Molecule 1: IcmE (DotG)





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76400	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	73	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	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	0.17	0/1288	0.34	0/1749
1	B	0.17	0/1288	0.38	0/1749
1	C	0.17	0/1288	0.35	0/1749
1	D	0.16	0/1288	0.31	0/1749
1	E	0.16	0/1288	0.29	0/1749
1	F	0.17	0/1288	0.31	0/1749
1	G	0.16	0/1288	0.30	0/1749
1	H	0.16	0/1288	0.31	0/1749
1	I	0.16	0/1288	0.33	0/1749
1	J	0.17	0/1288	0.35	0/1749
1	K	0.16	0/1288	0.29	0/1749
1	L	0.16	0/1288	0.33	0/1749
1	M	0.16	0/1288	0.32	0/1749
1	N	0.17	0/1288	0.34	0/1749
1	O	0.17	0/1288	0.32	0/1749
1	P	0.17	0/1288	0.31	0/1749
All	All	0.17	0/20608	0.32	0/27984

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	1267	0	1271	25	0
1	B	1267	0	1271	20	0
1	C	1267	0	1271	30	0
1	D	1267	0	1271	19	0
1	E	1267	0	1271	15	0
1	F	1267	0	1271	23	0
1	G	1267	0	1271	28	0
1	H	1267	0	1271	23	0
1	I	1267	0	1271	26	0
1	J	1267	0	1271	29	0
1	K	1267	0	1271	21	0
1	L	1267	0	1271	27	0
1	M	1267	0	1271	23	0
1	N	1267	0	1271	16	0
1	O	1267	0	1271	25	0
1	P	1267	0	1271	20	0
All	All	20272	0	20336	346	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 9.

The worst 5 of 346 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:P:998:ARG:HG2	1:P:1001:LEU:HB2	1.59	0.82
1:E:998:ARG:HG3	1:E:1001:LEU:HB2	1.66	0.77
1:F:998:ARG:HG2	1:F:1001:LEU:HB2	1.65	0.77
1:I:998:ARG:HG2	1:I:1001:LEU:HB2	1.68	0.76
1:K:869:MET:HG3	1:K:1041:PHE:HE2	1.51	0.74

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	166/1048 (16%)	158 (95%)	8 (5%)	0	100	100
1	B	166/1048 (16%)	155 (93%)	11 (7%)	0	100	100
1	C	166/1048 (16%)	154 (93%)	12 (7%)	0	100	100
1	D	166/1048 (16%)	157 (95%)	9 (5%)	0	100	100
1	E	166/1048 (16%)	160 (96%)	6 (4%)	0	100	100
1	F	166/1048 (16%)	160 (96%)	6 (4%)	0	100	100
1	G	166/1048 (16%)	157 (95%)	9 (5%)	0	100	100
1	H	166/1048 (16%)	154 (93%)	12 (7%)	0	100	100
1	I	166/1048 (16%)	157 (95%)	9 (5%)	0	100	100
1	J	166/1048 (16%)	157 (95%)	9 (5%)	0	100	100
1	K	166/1048 (16%)	158 (95%)	8 (5%)	0	100	100
1	L	166/1048 (16%)	156 (94%)	10 (6%)	0	100	100
1	M	166/1048 (16%)	155 (93%)	11 (7%)	0	100	100
1	N	166/1048 (16%)	156 (94%)	10 (6%)	0	100	100
1	O	166/1048 (16%)	155 (93%)	11 (7%)	0	100	100
1	P	166/1048 (16%)	155 (93%)	11 (7%)	0	100	100
All	All	2656/16768 (16%)	2504 (94%)	152 (6%)	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	138/766 (18%)	124 (90%)	14 (10%)	7	26
1	B	138/766 (18%)	125 (91%)	13 (9%)	8	29
1	C	138/766 (18%)	130 (94%)	8 (6%)	18	46
1	D	138/766 (18%)	122 (88%)	16 (12%)	5	20
1	E	138/766 (18%)	133 (96%)	5 (4%)	31	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	138/766 (18%)	128 (93%)	10 (7%)	13	38
1	G	138/766 (18%)	128 (93%)	10 (7%)	13	38
1	H	138/766 (18%)	129 (94%)	9 (6%)	15	42
1	I	138/766 (18%)	131 (95%)	7 (5%)	21	50
1	J	138/766 (18%)	133 (96%)	5 (4%)	31	58
1	K	138/766 (18%)	129 (94%)	9 (6%)	15	42
1	L	138/766 (18%)	125 (91%)	13 (9%)	8	29
1	M	138/766 (18%)	131 (95%)	7 (5%)	21	50
1	N	138/766 (18%)	127 (92%)	11 (8%)	11	35
1	O	138/766 (18%)	130 (94%)	8 (6%)	18	46
1	P	138/766 (18%)	128 (93%)	10 (7%)	13	38
All	All	2208/12256 (18%)	2053 (93%)	155 (7%)	16	39

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1028	THR
1	O	1027	THR
1	M	874	ASP
1	N	954	MET
1	P	1001	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	908	ASN
1	K	949	ASN
1	P	904	ASN
1	K	908	ASN
1	K	951	HIS

5.3.3 RNA ⓘ

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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-49395. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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 standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 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.