



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 01:49 AM UTC

PDB ID : 9NGY / pdb_00009ngy
EMDB ID : EMD-49396
Title : In situ cryo-EM structure of protochannel (DotA-IcmX) of the Legionella Dot/Icm T4SS machine
Authors : Yue, J.; Liu, J.
Deposited on : 2025-02-22
Resolution : 3.63 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

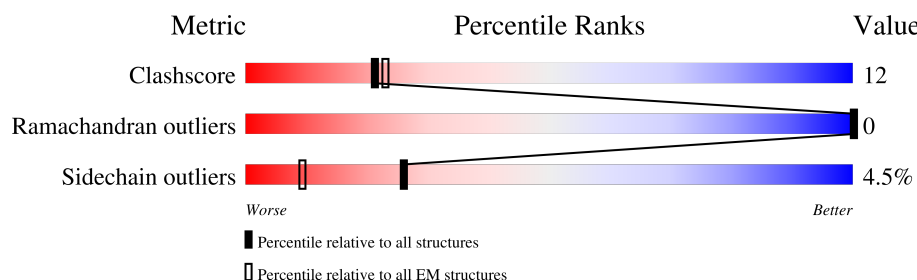
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.63 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.



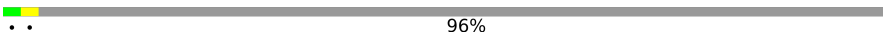
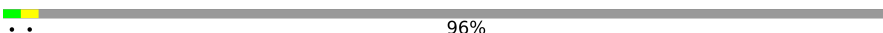
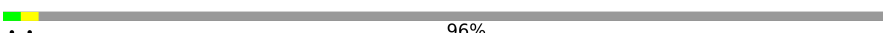
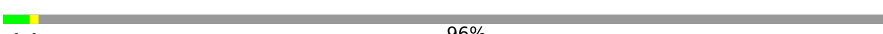
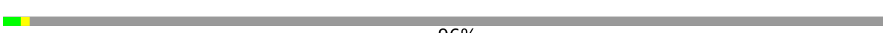
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	AP1	466	69% 19% • 11%
1	BP1	466	67% 22% • 11%
1	CP1	466	70% 19% • 11%
1	DP1	466	69% 20% • 11%
1	EP1	466	70% 19% • 11%
2	FP1	1048	60% 20% • 18%
2	GP1	1048	57% 23% • 18%
2	HP1	1048	57% 23% • 18%
2	IP1	1048	58% 23% • 18%

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Mol	Chain	Length	Quality of chain
2	JP1	1048	 57%23%18%
3	KP1	1048	 96%
3	LP1	1048	 96%
3	MP1	1048	 96%
3	NP1	1048	 96%
3	OP1	1048	 96%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 50535 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 IcmX (IcmY).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AP1	417	Total	C	N	O	S	0	0
			3213	2013	542	646	12		
1	BP1	417	Total	C	N	O	S	0	0
			3213	2013	542	646	12		
1	CP1	417	Total	C	N	O	S	0	0
			3213	2013	542	646	12		
1	DP1	417	Total	C	N	O	S	0	0
			3213	2013	542	646	12		
1	EP1	417	Total	C	N	O	S	0	0
			3213	2013	542	646	12		

- Molecule 2 is a protein called DotA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	FP1	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
2	GP1	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
2	HP1	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
2	IP1	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
2	JP1	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		

- Molecule 3 is a protein called IcmE (DotG).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	KP1	43	Total	C	N	O	S	0	0
			334	221	58	54	1		
3	LP1	43	Total	C	N	O	S	0	0
			334	221	58	54	1		
3	MP1	43	Total	C	N	O	S	0	0
			334	221	58	54	1		

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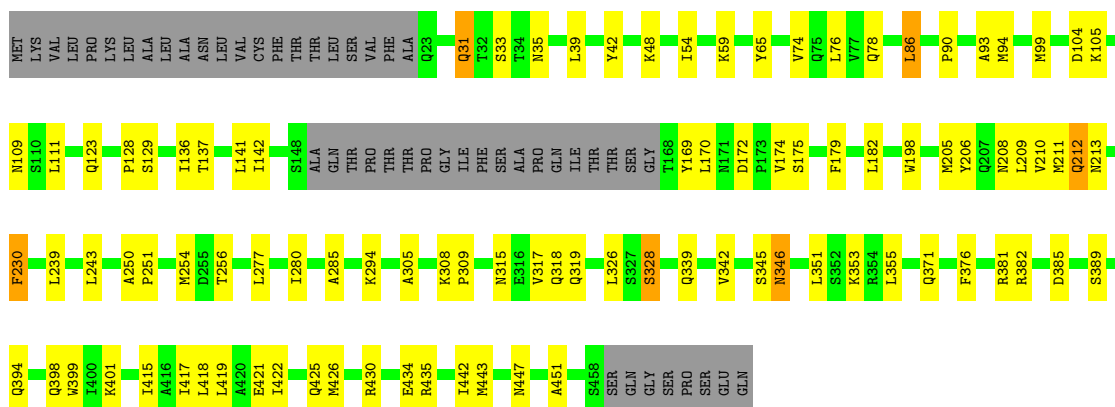
Mol	Chain	Residues	Atoms					AltConf	Trace
3	NP1	43	Total	C	N	O	S	0	0
			334	221	58	54	1		
3	OP1	43	Total	C	N	O	S	0	0
			334	221	58	54	1		

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.

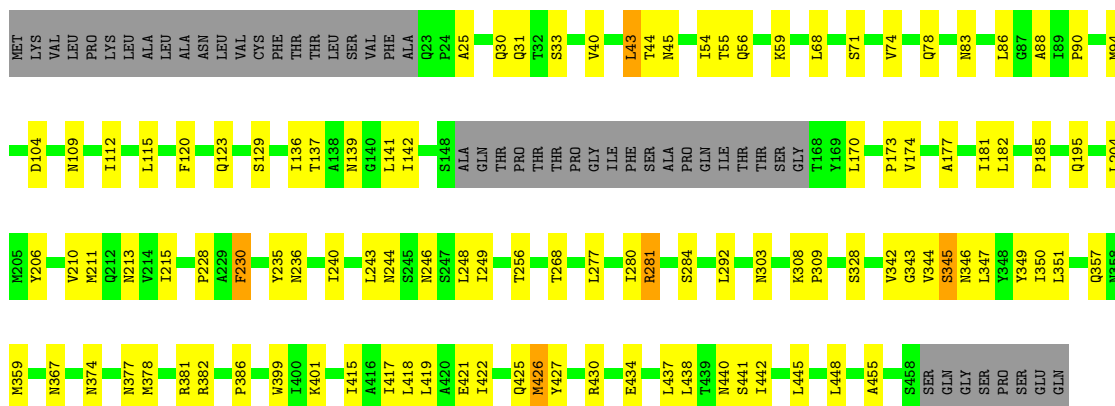
- Molecule 1: IcmX (IcmY)

Chain AP1: 



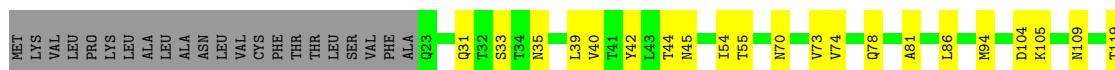
- Molecule 1: IcmX (IcmY)

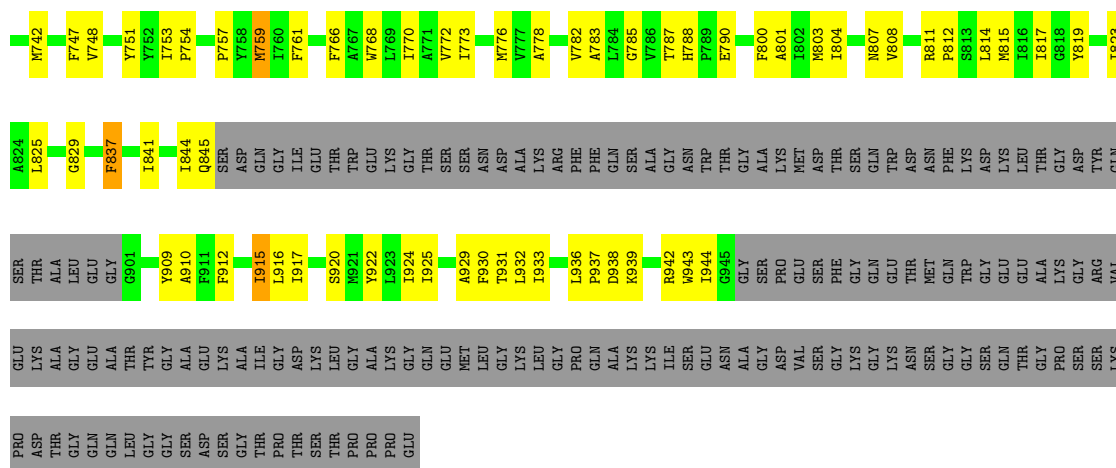
Chain BP1: 



- Molecule 1: IcmX (IcmY)

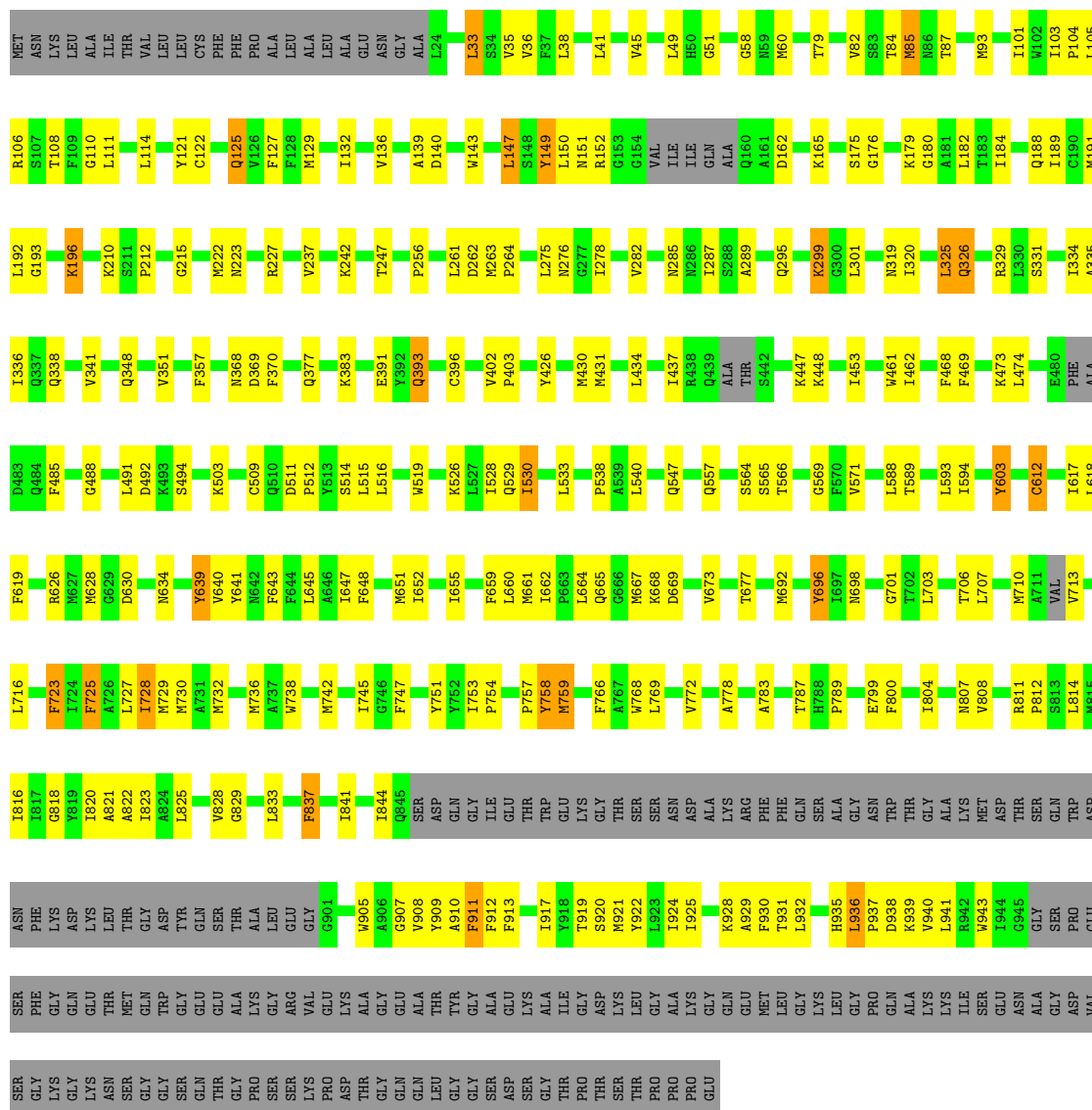
Chain CP1: 





• Molecule 2: DotA

Chain HP1:



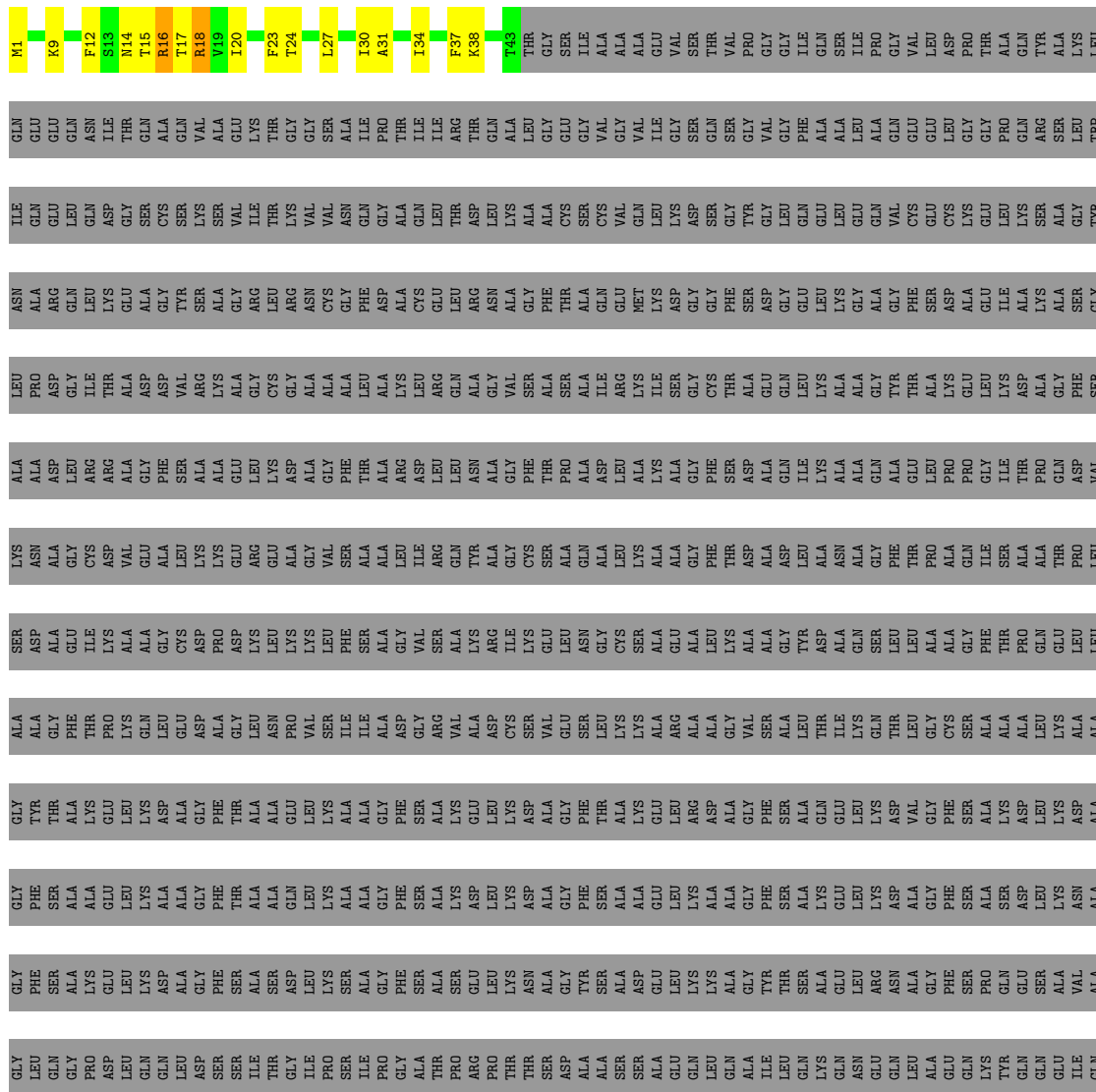
Tyr	Phe	Met	Gln	Glu	Ser	Leu	Leu
Ser	Gln	Val	Gly	Glu	Ala	Asn	Lys
Gly	Ser	Ile	Ala	Ile	Val	Asp	Ala
Thr	Ala	Thr	Val	Gln	Gly	Gly	Ala
Leu	Asn	Phe	Ser	Gln	Arg	Phe	Thr
Gly	Thr	Thr	Gln	Thr	Gln	Ser	Thr
Ile	Thr	Met	Asn	Ser	Gly	Ala	Ala
Leu	Thr	Ser	Gln	Asp	Pro	Lys	Glu
Phe	Ile	Ile	Ala	Met	Asp	Glu	Lys
Thr	Gly	Pro	Ile	Leu	Ile	Leu	Leu
Gln	Gly	Gly	Ile	Thr	Gln	Lys	Lys
Asp	Thr	Ala	Lys	Ala	Gln	Asp	Asp
Val	Gly	Glu	Thr	Ala	Leu	Ala	Ala
Thr	Gly	Lys	Gly	Thr	Asp	Gly	Gly
Thr	Gly	Thr	Asp	Gln	Ser	Phe	Thr
Ile	Asn	Ile	Ile	Leu	Ser	Ser	Phe
	Asn	Ser	Met	Val	Ile	Ala	Ala
	Ile	Ile	Phe	Gln	Thr	Ser	Ala
	Thr	Ser	Ala	Asp	Gly	Asp	Glu
	Val	Ala	Leu	Trp	Ile	Leu	Leu
	Ala	Tyr	Leu	Lys	Pro	Lys	Lys
	Asn	Ala	Ala	Ser	Ser	Ser	Ala
	Gly	Ile	Thr	Val	Ile	Ala	Ala
	Val	Asp	Ser	Glu	Pro	Gly	Gly
	Gly	Ile	Thr	Val	Ile	Ala	Ala
	Val	Pro	Val	Thr	Gly	Ser	Ala
	Arg	Asn	Asn	Val	Thr	Ala	Ala
	Arg	Thr	Ser	Val	Thr	Ser	Ala
	Thr	Ala	Ser	Tyr	Pro	Ser	Lys
	Leu	Arg	Glu	Thr	Arg	Glu	Asp
	Gln	Thr	Pro	Glu	Pro	Leu	Leu
	Asn	Ala	Gly	Gly	Thr	Lys	Lys
	Ala	Leu	Ala	Thr	Thr	Asn	Asp
	Val	Ala	Ile	Glu	Ser	Ala	Ala
	Ile	Ser	Leu	Glu	Asp	Gly	Gly
	Gly	Arg	Ala	Thr	Ala	Phe	Phe
	Leu	Thr	Thr	Lys	Ala	Ser	Thr
	Ala	Asn	Ile	Thr	Ser	Ala	Ala
	His	His	Val	Ser	Ser	Gly	Lys
	Val	Tyr	Thr	Ala	Ala	Tyr	Ala
	Gly	Tyr	Gly	Gly	Glu	Thr	Thr
	Lys	Leu	Lys	Glu	Gln	Lys	Arg
	Ala	Met	Leu	Ser	Lys	Lys	Asp
	Ala	Arg	Leu	Leu	Leu	Ala	Ala
	Trp	Thr	Lys	Ala	Ala	Ala	Ala
	Ser	Tyr	Val	Val	Gly	Gly	Gly
	Gln	Gly	Ser	Pro	Ile	Phe	Phe
	Ala	Ser	Lys	Gly	Thr	Ser	Ser
	Ala	Leu	Leu	Thr	Gln	Ala	Ala
	Gln	Phe	Ile	Gly	Lys	Lys	Gln
	Gln	Ala	Gly	Thr	Lys	Leu	Leu
	Leu	Ser	Ser	Gly	Asn	Leu	Lys
	Phe	Phe	Phe	Gly	Gln	Asp	Ala
	Thr	Leu	Leu	Ser	Leu	Ala	Val
	Pro	Gln	Pro	Asn	Ala	Gly	Gly
	Thr	Gly	Ser	Asn	Glu	Phe	Phe
	Thr	Phe	Ser	Gln	Thr	Ser	Ser
	Val	Gly	Ala	Pro	Lys	Ala	Ala
	Glu	Asn	Val	Val	Thr	Ser	Lys
	Val	Ala	Lys	Val	Cys	Ser	Asp

- Molecule 3: IcmE (DotG)

Chain LP1: 96%

[illegible]





[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37503	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	AP1	0.17	0/3277	0.35	0/4473
1	BP1	0.17	0/3277	0.35	0/4473
1	CP1	0.16	0/3277	0.32	0/4473
1	DP1	0.16	0/3277	0.32	0/4473
1	EP1	0.17	0/3277	0.32	0/4473
2	FP1	0.16	0/6715	0.36	0/9115
2	GP1	0.16	0/6715	0.39	0/9115
2	HP1	0.16	0/6715	0.39	0/9115
2	IP1	0.16	0/6715	0.39	0/9115
2	JP1	0.16	0/6715	0.36	0/9115
3	KP1	0.16	0/337	0.52	0/451
3	LP1	0.09	0/337	0.27	0/451
3	MP1	0.12	0/337	0.38	0/451
3	NP1	0.14	0/337	0.41	0/451
3	OP1	0.18	0/337	0.54	0/451
All	All	0.16	0/51645	0.37	0/70195

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	AP1	3213	0	3131	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BP1	3213	0	3131	91	0
1	CP1	3213	0	3131	74	0
1	DP1	3213	0	3131	75	0
1	EP1	3213	0	3131	78	0
2	FP1	6560	0	6545	165	0
2	GP1	6560	0	6545	208	0
2	HP1	6560	0	6545	198	0
2	IP1	6560	0	6545	185	0
2	JP1	6560	0	6545	174	0
3	KP1	334	0	378	15	0
3	LP1	334	0	378	14	0
3	MP1	334	0	378	12	0
3	NP1	334	0	378	11	0
3	OP1	334	0	378	13	0
All	All	50535	0	50270	1188	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 12.

The worst 5 of 1188 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)
2:FP1:671:PHE:HE1	2:FP1:915:ILE:HD13	1.29	0.97
2:HP1:193:GLY:HA3	2:HP1:530:ILE:HD11	1.51	0.92
1:DP1:443:MET:HE2	1:EP1:443:MET:HE1	1.53	0.91
2:GP1:929:ALA:O	2:GP1:932:LEU:HB3	1.73	0.88
2:GP1:193:GLY:HA3	2:GP1:530:ILE:HD11	1.55	0.87

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	AP1	413/466 (89%)	401 (97%)	12 (3%)	0	100	100
1	BP1	413/466 (89%)	405 (98%)	8 (2%)	0	100	100
1	CP1	413/466 (89%)	406 (98%)	7 (2%)	0	100	100
1	DP1	413/466 (89%)	402 (97%)	11 (3%)	0	100	100
1	EP1	413/466 (89%)	406 (98%)	7 (2%)	0	100	100
2	FP1	847/1048 (81%)	816 (96%)	31 (4%)	0	100	100
2	GP1	847/1048 (81%)	813 (96%)	34 (4%)	0	100	100
2	HP1	847/1048 (81%)	807 (95%)	40 (5%)	0	100	100
2	IP1	847/1048 (81%)	813 (96%)	34 (4%)	0	100	100
2	JP1	847/1048 (81%)	811 (96%)	36 (4%)	0	100	100
3	KP1	41/1048 (4%)	41 (100%)	0	0	100	100
3	LP1	41/1048 (4%)	41 (100%)	0	0	100	100
3	MP1	41/1048 (4%)	41 (100%)	0	0	100	100
3	NP1	41/1048 (4%)	41 (100%)	0	0	100	100
3	OP1	41/1048 (4%)	41 (100%)	0	0	100	100
All	All	6505/12810 (51%)	6285 (97%)	220 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AP1	360/401 (90%)	347 (96%)	13 (4%)	31	52
1	BP1	360/401 (90%)	350 (97%)	10 (3%)	38	57
1	CP1	360/401 (90%)	350 (97%)	10 (3%)	38	57
1	DP1	360/401 (90%)	350 (97%)	10 (3%)	38	57
1	EP1	360/401 (90%)	352 (98%)	8 (2%)	45	61
2	FP1	715/858 (83%)	683 (96%)	32 (4%)	24	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	GP1	715/858 (83%)	683 (96%)	32 (4%)	24	48
2	HP1	715/858 (83%)	674 (94%)	41 (6%)	18	43
2	IP1	715/858 (83%)	678 (95%)	37 (5%)	21	45
2	JP1	715/858 (83%)	677 (95%)	38 (5%)	20	44
3	KP1	36/765 (5%)	32 (89%)	4 (11%)	6	24
3	LP1	36/765 (5%)	35 (97%)	1 (3%)	38	57
3	MP1	36/765 (5%)	32 (89%)	4 (11%)	6	24
3	NP1	36/765 (5%)	31 (86%)	5 (14%)	3	17
3	OP1	36/765 (5%)	31 (86%)	5 (14%)	3	17
All	All	5555/10120 (55%)	5305 (96%)	250 (4%)	26	48

5 of 250 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	HP1	33	LEU
2	JP1	696	TYR
2	HP1	603	TYR
2	JP1	624	LEU
3	MP1	7	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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-49396. 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.