



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 01:15 AM EST

PDB ID : 7MUE
EMDB ID : EMD-24006
Title : Legionella pneumophila Dot/Icm T4SS PR
Authors : Sheedlo, M.J.; Durie, C.L.; Swanson, M.; Lacy, D.B.; Ohi, M.D.
Deposited on : 2021-05-14
Resolution : 2.80 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:

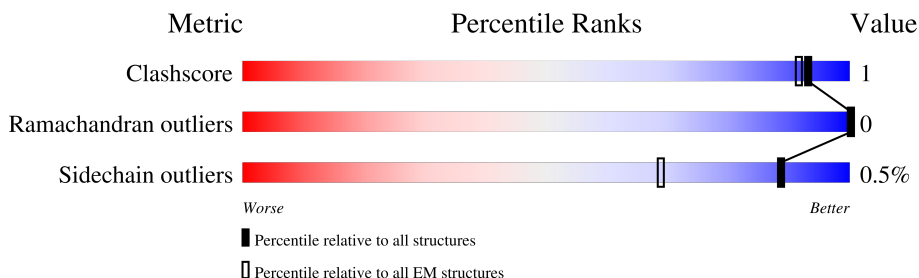
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 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 2.80 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	158937	4297
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	AF	269	22% 77%
1	BF	269	21% 77%
1	CF	269	22% 77%
1	DF	269	22% 77%
1	EF	269	22% 77%
1	FF	269	22% 77%
1	GF	269	22% 77%
1	HF	269	21% 77%
1	IF	269	22% 77%



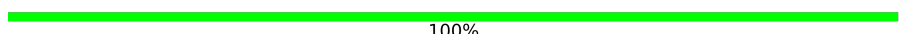
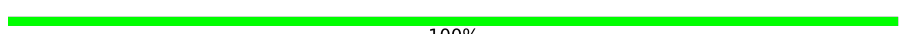


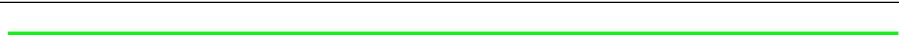
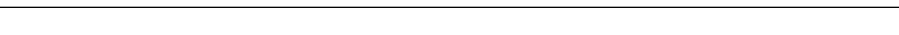
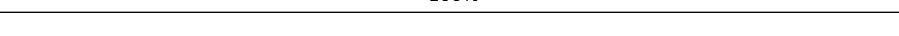
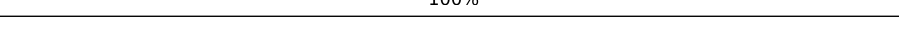
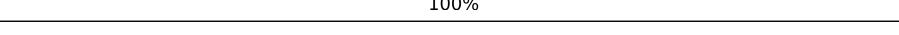
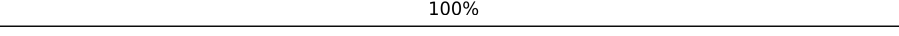
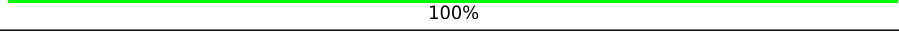
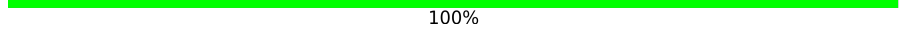
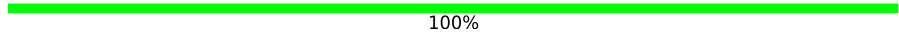
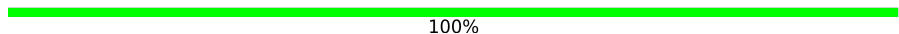
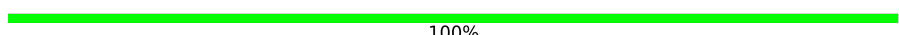
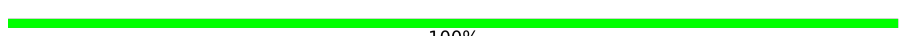





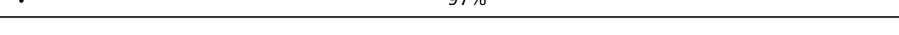
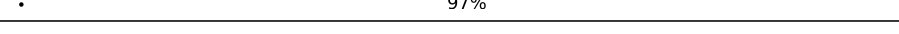
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	JF	269	22%	77%
1	KF	269	23%	77%
1	LF	269	22%	77%
1	MF	269	22%	77%
1	VF	269	23%	77%
1	WF	269	22%	77%
1	XF	269	21%	77%
1	YF	269	22%	77%
1	ZF	269	23%	77%
2	AH	361	41%	56%
2	BH	361	42%	56%
2	CH	361	42%	56%
2	DH	361	42%	56%
2	EH	361	42%	56%
2	FH	361	42%	56%
2	GH	361	43%	56%
2	HH	361	42%	56%
2	IH	361	42%	56%
2	JH	361	43%	56%
2	KH	361	43%	56%
2	LH	361	42%	56%
2	MH	361	42%	56%
2	VH	361	43%	56%
2	WH	361	42%	56%
2	XH	361	43%	56%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	YH	361	 42% 56%
2	ZH	361	 42% 56%
3	AX	48	 100%
3	BX	48	 100%
3	CX	48	 100%
3	DX	48	 100%
3	EX	48	 100%
3	FX	48	 100%
3	GX	48	 100%
3	HX	48	 100%
3	IX	48	 100%
3	JX	48	 100%
3	KX	48	 100%
3	LX	48	 100%
3	MX	48	 100%
3	VX	48	 100%
3	WX	48	 100%
3	XX	48	 100%
3	YX	48	 100%
3	ZX	48	 100%
4	AG	1048	 97%
4	BG	1048	 97%
4	CG	1048	 97%
4	DG	1048	 97%
4	EG	1048	 97%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	FG	1048	97%
4	GG	1048	97%
4	HG	1048	97%
4	IG	1048	97%
4	JG	1048	97%
4	KG	1048	97%
4	LG	1048	97%
4	MG	1048	97%
4	VG	1048	97%
4	WG	1048	97%
4	XG	1048	97%
4	YG	1048	97%
4	ZG	1048	97%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 40266 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 DotF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AF	63	483	308	84	90	1	0	0
1	BF	63	483	308	84	90	1	0	0
1	CF	63	483	308	84	90	1	0	0
1	DF	63	483	308	84	90	1	0	0
1	EF	63	483	308	84	90	1	0	0
1	FF	63	483	308	84	90	1	0	0
1	GF	63	483	308	84	90	1	0	0
1	HF	63	483	308	84	90	1	0	0
1	IF	63	483	308	84	90	1	0	0
1	JF	63	483	308	84	90	1	0	0
1	KF	63	483	308	84	90	1	0	0
1	LF	63	483	308	84	90	1	0	0
1	MF	63	483	308	84	90	1	0	0
1	VF	63	483	308	84	90	1	0	0
1	WF	63	483	308	84	90	1	0	0
1	XF	63	483	308	84	90	1	0	0
1	YF	63	483	308	84	90	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	ZF	63	483	308	84	90	1	0	0

- Molecule 2 is a protein called Type IV secretion protein IcmK.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	XH	160	1238	795	207	233	3	0	0
2	YH	160	1238	795	207	233	3	0	0
2	ZH	160	1238	795	207	233	3	0	0
2	AH	160	1238	795	207	233	3	0	0
2	BH	160	1238	795	207	233	3	0	0
2	CH	160	1238	795	207	233	3	0	0
2	DH	160	1238	795	207	233	3	0	0
2	EH	160	1238	795	207	233	3	0	0
2	FH	160	1238	795	207	233	3	0	0
2	GH	160	1238	795	207	233	3	0	0
2	HH	160	1238	795	207	233	3	0	0
2	IH	160	1238	795	207	233	3	0	0
2	JH	160	1238	795	207	233	3	0	0
2	KH	160	1238	795	207	233	3	0	0
2	LH	160	1238	795	207	233	3	0	0
2	MH	160	1238	795	207	233	3	0	0
2	VH	160	1238	795	207	233	3	0	0
2	WH	160	1238	795	207	233	3	0	0

- Molecule 3 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	AX	48	Total	C	N	O	0	0
			240	144	48	48		
3	BX	48	Total	C	N	O	0	0
			240	144	48	48		
3	CX	48	Total	C	N	O	0	0
			240	144	48	48		
3	DX	48	Total	C	N	O	0	0
			240	144	48	48		
3	EX	48	Total	C	N	O	0	0
			240	144	48	48		
3	FX	48	Total	C	N	O	0	0
			240	144	48	48		
3	GX	48	Total	C	N	O	0	0
			240	144	48	48		
3	HX	48	Total	C	N	O	0	0
			240	144	48	48		
3	IX	48	Total	C	N	O	0	0
			240	144	48	48		
3	JX	48	Total	C	N	O	0	0
			240	144	48	48		
3	KX	48	Total	C	N	O	0	0
			240	144	48	48		
3	LX	48	Total	C	N	O	0	0
			240	144	48	48		
3	MX	48	Total	C	N	O	0	0
			240	144	48	48		
3	VX	48	Total	C	N	O	0	0
			240	144	48	48		
3	WX	48	Total	C	N	O	0	0
			240	144	48	48		
3	XX	48	Total	C	N	O	0	0
			240	144	48	48		
3	YX	48	Total	C	N	O	0	0
			240	144	48	48		
3	ZX	48	Total	C	N	O	0	0
			240	144	48	48		

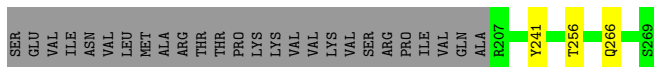
- Molecule 4 is a protein called IcmE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	IG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		

Continued on next page...

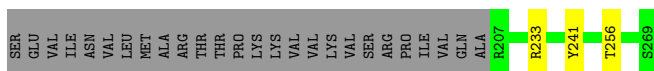
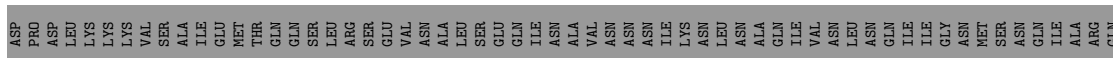
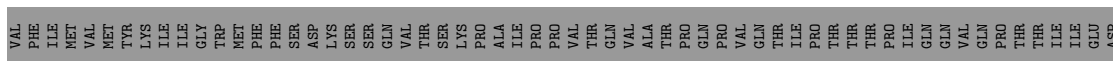
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AG	34	276	168	47	60	1	0	0
4	BG	34	276	168	47	60	1	0	0
4	CG	34	276	168	47	60	1	0	0
4	DG	34	276	168	47	60	1	0	0
4	EG	34	276	168	47	60	1	0	0
4	FG	34	276	168	47	60	1	0	0
4	GG	34	276	168	47	60	1	0	0
4	HG	34	276	168	47	60	1	0	0
4	JG	34	276	168	47	60	1	0	0
4	KG	34	276	168	47	60	1	0	0
4	LG	34	276	168	47	60	1	0	0
4	MG	34	276	168	47	60	1	0	0
4	VG	34	276	168	47	60	1	0	0
4	WG	34	276	168	47	60	1	0	0
4	XG	34	276	168	47	60	1	0	0
4	YG	34	276	168	47	60	1	0	0
4	ZG	34	276	168	47	60	1	0	0



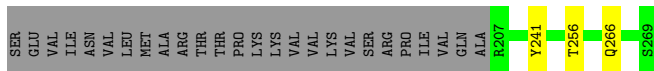
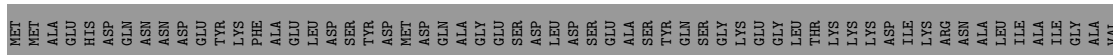
- Molecule 1: DotF

Chain DF: 22% 77%



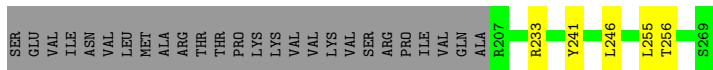
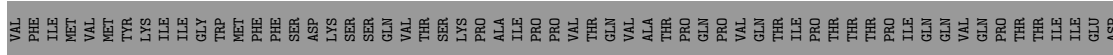
- Molecule 1: DotF

Chain EF: 22% 77%



- Molecule 1: DotF

Chain FF: 22% 77%



- Molecule 1: DotF

Chain GF: 22% 77%

SER	GLU	VAL	ILE	HIS	ASN	ASP	VAL	LEU	MET	ALA	ALA	R207	Y241	L246	L285	T256	S269
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------

● Molecule 1: DotF

Chain KF:  23%  77%

MET	MET	ALA	GLU	HIS	ASP	ASN	GLN	TYR	THR	PRO	LYS	VAL	VAL	LEU	VAL	VAL	SER	TYR	ASP	ASP	GLN	VAL	VAL	GLY	GLU	ILE	SER	GLN	ALA	SER	TYR	GLN	SER	GLY	LYS	LYS	LYS	ASP	ILE	LYS	ARG	ASN	VAL	ALA	GLN	LEU	ILE	THR	THR	ALA	ILE	GLY	GLY	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

VAL	PHE	ILE	MET	VAL	MET	LYS	TYR	LYS	VAL	SER	ILE	ILE	TRP	THR	MET	PHE	PHE	ALA	GLU	SER	ASP	LEU	LYS	SER	VAL	VAL	VAL	ARG	SER	TYR	GLN	ASP	GLY	VAL	VAL	ASN	ASN	ASN	VAL	VAL	ASP	LEU	VAL	GLN	VAL	VAL	ASP	GLY	ILE	LYS	GLN	VAL	VAL	GLN	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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

SER	GLU	VAL	ILE	ASN	GLN	MET	MET	LEU	MET	ALA	ALA	R207	Y241	T256	S269
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------

● Molecule 1: DotF

Chain LF:  22%  77%

MET	MET	ALA	GLU	HIS	ASN	ASP	GLN	TYR	THR	PRO	LYS	VAL	VAL	LEU	VAL	VAL	SER	TYR	ASP	ASP	GLN	VAL	VAL	VAL	VAL	VAL	ARG	SER	TYR	GLY	VAL	VAL	ASN	ASN	ASN	VAL	VAL	ASN	ASN	ASN	VAL	VAL	ASP	LEU	VAL	GLN	VAL	VAL	GLY	GLY	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

VAL	PHE	ILE	MET	VAL	MET	LYS	TYR	LYS	VAL	SER	ILE	ILE	TRP	THR	MET	PHE	PHE	ALA	GLU	SER	ASP	LEU	LYS	SER	VAL	VAL	VAL	ARG	SER	TYR	GLN	ASP	GLY	VAL	VAL	ASN	ASN	ASN	VAL	VAL	ASP	LEU	VAL	GLN	VAL	VAL	ASP	LEU	VAL	GLN	VAL	VAL	GLN	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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

SER	GLU	VAL	ILE	ASN	GLN	MET	MET	LEU	MET	ALA	ALA	R207	R233	Y241	T256	S269
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------

● Molecule 1: DotF

Chain MF:  22%  77%

MET	MET	ALA	GLU	HIS	ASP	ASN	GLN	TYR	THR	PRO	LYS	VAL	VAL	LEU	VAL	VAL	SER	TYR	ASP	ASP	GLN	VAL	VAL	VAL	VAL	VAL	ARG	SER	TYR	GLY	VAL	VAL	ASN	ASN	ASN	VAL	VAL	ASN	ASN	ASN	VAL	VAL	ASP	LEU	VAL	GLN	VAL	VAL	GLY	GLY	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

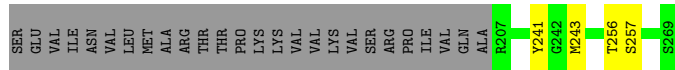
VAL	PHE	ILE	MET	VAL	MET	LYS	TYR	LYS	VAL	SER	ILE	ILE	TRP	THR	MET	PHE	PHE	ALA	GLU	SER	ASP	LEU	LYS	SER	VAL	VAL	VAL	ARG	SER	TYR	GLN	ASP	GLY	VAL	VAL	ASN	ASN	ASN	VAL	VAL	ASP	LEU	VAL	GLN	VAL	VAL	ASP	LEU	VAL	GLN	VAL	VAL	GLN	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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

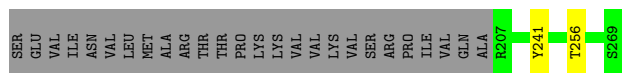
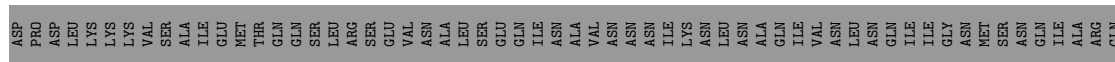
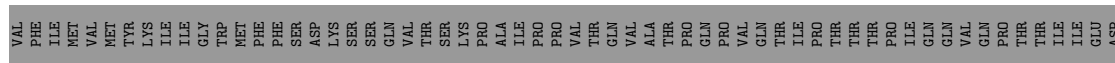
SER	GLU	VAL	ILE	ASN	GLN	MET	MET	LEU	MET	ALA	ALA	R207	Y241	T256	Q286	S269
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------

● Molecule 1: DotF

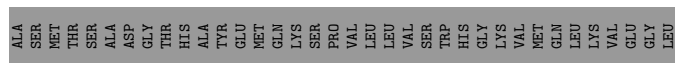
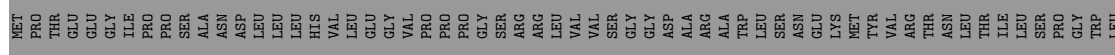
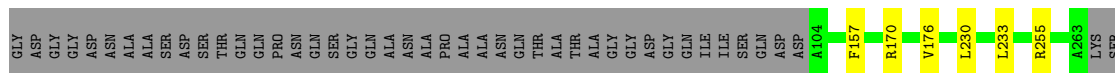
Chain VF:  23%  77%



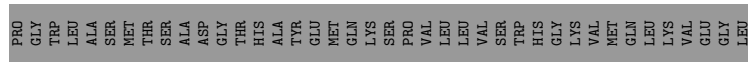
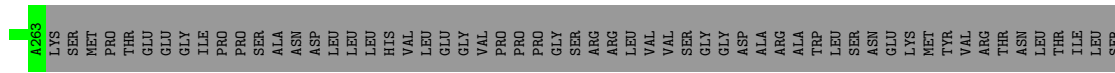
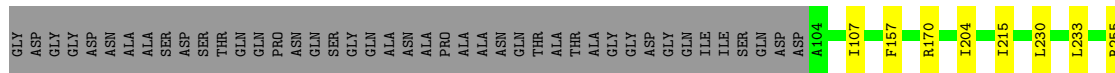
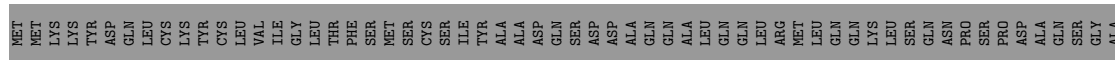
• Molecule 1: DotF



• Molecule 2: Type IV secretion protein IcmK

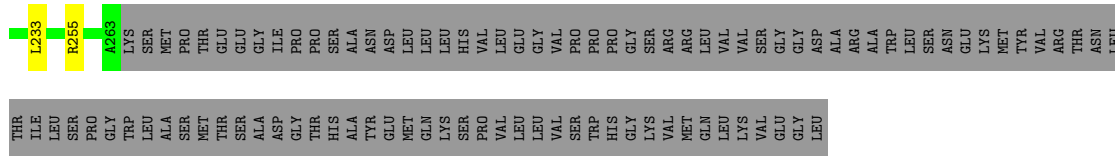


• Molecule 2: Type IV secretion protein IcmK

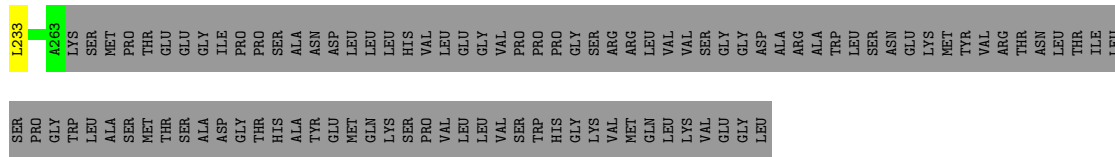
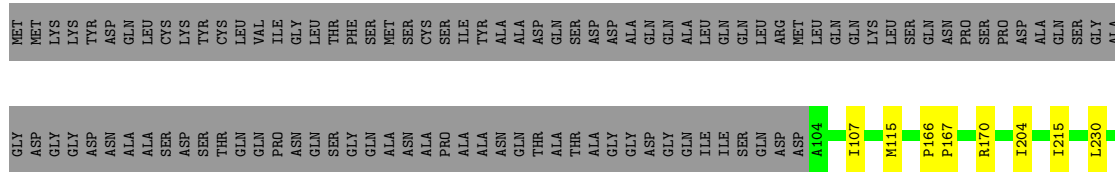


• Molecule 2: Type IV secretion protein IcmK

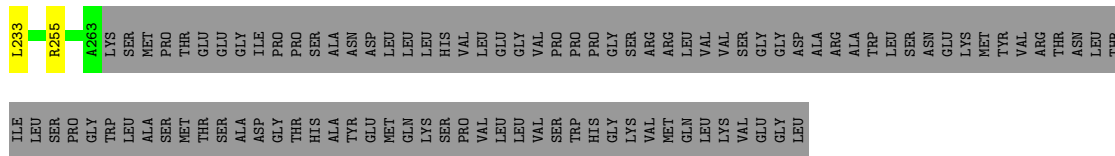
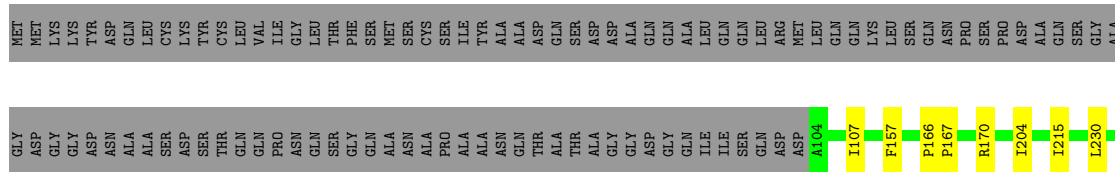




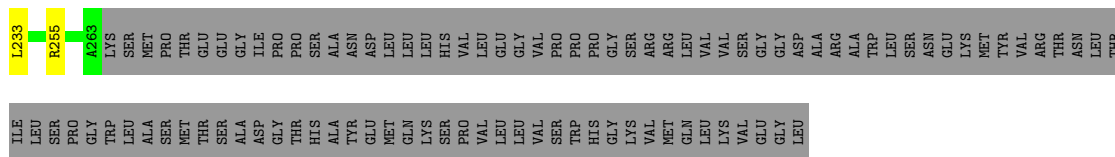
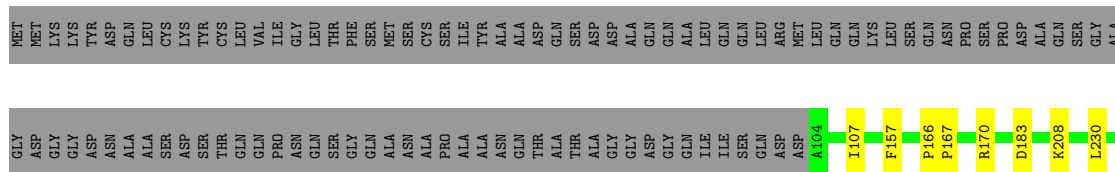
● Molecule 2: Type IV secretion protein IcmK

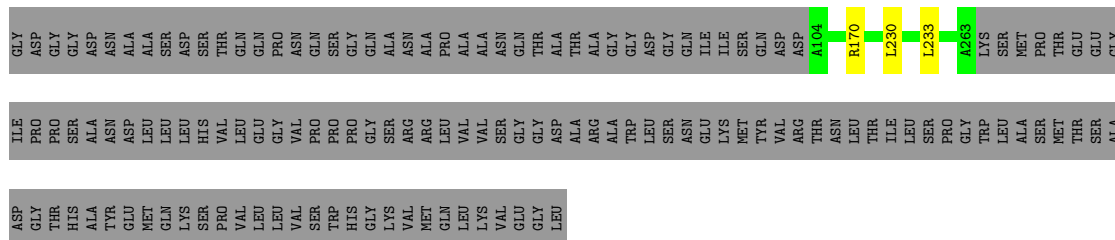


● Molecule 2: Type IV secretion protein IcmK

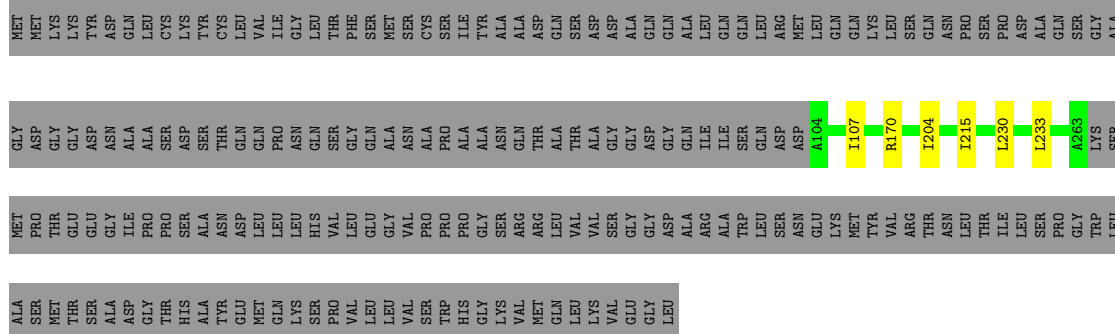


● Molecule 2: Type IV secretion protein IcmK





• Molecule 2: Type IV secretion protein IcmK



• Molecule 2: Type IV secretion protein IcmK



• Molecule 2: Type IV secretion protein IcmK



Chain DX:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown protein fragment

Chain EX:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown protein fragment

Chain FX:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown protein fragment

Chain GX:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown protein fragment

Chain HX:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown protein fragment

Chain IX:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown protein fragment

Chain JX:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown protein fragment

Chain KX:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown protein fragment

Chain LX:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown protein fragment

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

ALA
TYR
ALA
GLY
ILE
VAL
PRO
ASN
THR
SER
ALA
ARG
THR
GLU
ALA
ASN
LEU
ALA
SER
ILE
ARG
THR
ASN
ASN
HIS
HIS
TYR
GLY
LYS
MET
MET
TRP
ARG
TYR
GLY
SER
SER
PHE
ALA
GLN
GLY
PHE
GLY
ASN
ASN
ALA
PHE
GLN
SER
GLN
ALA
THR
ALA
ASN
PHE
THR
THR
THR
ILE
ILE
ILE
GLY
THR
THR
GLY
GLY
ASN
ASN
THR

VAL
ALA
ASN
ASN
GLY
VAL
GLY
ARG
SER
SER
THR
LEU
GLU
THR
ASN
ALA
VAL
ILE
GLY
LEU
ALA
THR
VAL
VAL
GLY
LYS
ALA
ALA
TRP
SER
GLN
GLN
ALA
GLN
GLN
LEU
PHE
ASN
ASN
THR
PRO
THR
THR
THR
VAL
VAL
GLU
TYR
SER
GLY
THR
GLY
LEU
ILE
ILE
PHE
THR
GLN
GLN
VAL
THR
THR
THR
ILE

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43907	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
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	AF	0.26	0/490	0.63	1/660 (0.2%)
1	BF	0.25	0/490	0.62	0/660
1	CF	0.26	0/490	0.63	0/660
1	DF	0.25	0/490	0.59	0/660
1	EF	0.26	0/490	0.61	0/660
1	FF	0.26	0/490	0.60	0/660
1	GF	0.26	0/490	0.58	0/660
1	HF	0.26	0/490	0.63	1/660 (0.2%)
1	IF	0.25	0/490	0.59	0/660
1	JF	0.26	0/490	0.60	0/660
1	KF	0.26	0/490	0.59	0/660
1	LF	0.26	0/490	0.62	0/660
1	MF	0.26	0/490	0.60	0/660
1	VF	0.26	0/490	0.61	0/660
1	WF	0.26	0/490	0.60	0/660
1	XF	0.26	0/490	0.63	0/660
1	YF	0.26	0/490	0.60	0/660
1	ZF	0.25	0/490	0.59	0/660
2	AH	0.26	0/1269	0.58	1/1734 (0.1%)
2	BH	0.26	0/1269	0.53	0/1734
2	CH	0.26	0/1269	0.58	1/1734 (0.1%)
2	DH	0.26	0/1269	0.52	0/1734
2	EH	0.26	0/1269	0.55	0/1734
2	FH	0.26	0/1269	0.55	1/1734 (0.1%)
2	GH	0.26	0/1269	0.57	1/1734 (0.1%)
2	HH	0.26	0/1269	0.57	1/1734 (0.1%)
2	IH	0.26	0/1269	0.54	0/1734
2	JH	0.25	0/1269	0.52	0/1734
2	KH	0.26	0/1269	0.52	0/1734
2	LH	0.26	0/1269	0.56	1/1734 (0.1%)
2	MH	0.26	0/1269	0.56	1/1734 (0.1%)
2	VH	0.25	0/1269	0.53	0/1734
2	WH	0.26	0/1269	0.56	1/1734 (0.1%)
2	XH	0.26	0/1269	0.53	0/1734

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	YH	0.26	0/1269	0.54	0/1734
2	ZH	0.26	0/1269	0.58	1/1734 (0.1%)
4	AG	0.24	0/278	0.44	0/377
4	BG	0.23	0/278	0.45	0/377
4	CG	0.24	0/278	0.49	0/377
4	DG	0.23	0/278	0.43	0/377
4	EG	0.23	0/278	0.43	0/377
4	FG	0.23	0/278	0.43	0/377
4	GG	0.23	0/278	0.44	0/377
4	HG	0.29	0/278	0.49	0/377
4	IG	0.25	0/278	0.47	0/377
4	JG	0.24	0/278	0.45	0/377
4	KG	0.23	0/278	0.43	0/377
4	LG	0.23	0/278	0.43	0/377
4	MG	0.26	0/278	0.46	0/377
4	VG	0.25	0/278	0.45	0/377
4	WG	0.23	0/278	0.44	0/377
4	XG	0.27	0/278	0.48	0/377
4	YG	0.24	0/278	0.43	0/377
4	ZG	0.23	0/278	0.44	0/377
All	All	0.26	0/36666	0.55	11/49878 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	WH	183	ASP	CB-CG-OD1	7.75	125.28	118.30
2	CH	183	ASP	CB-CG-OD1	7.73	125.26	118.30
2	MH	183	ASP	CB-CG-OD1	7.72	125.25	118.30
2	ZH	183	ASP	CB-CG-OD1	7.70	125.23	118.30
2	GH	183	ASP	CB-CG-OD1	7.62	125.15	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	AF	483	0	502	1	0
1	BF	483	0	502	4	0
1	CF	483	0	502	2	0
1	DF	483	0	502	2	0
1	EF	483	0	502	2	0
1	FF	483	0	502	3	0
1	GF	483	0	502	3	0
1	HF	483	0	502	4	0
1	IF	483	0	502	2	0
1	JF	483	0	502	2	0
1	KF	483	0	502	1	0
1	LF	483	0	502	2	0
1	MF	483	0	502	3	0
1	VF	483	0	502	1	0
1	WF	483	0	502	3	0
1	XF	483	0	502	4	0
1	YF	483	0	502	2	0
1	ZF	483	0	502	1	0
2	AH	1238	0	1252	6	0
2	BH	1238	0	1252	4	0
2	CH	1238	0	1252	5	0
2	DH	1238	0	1252	5	0
2	EH	1238	0	1252	5	0
2	FH	1238	0	1252	5	0
2	GH	1238	0	1252	2	0
2	HH	1238	0	1252	5	0
2	IH	1238	0	1252	4	0
2	JH	1238	0	1252	1	0
2	KH	1238	0	1252	3	0
2	LH	1238	0	1252	4	0
2	MH	1238	0	1252	3	0
2	VH	1238	0	1252	3	0
2	WH	1238	0	1252	4	0
2	XH	1238	0	1252	3	0
2	YH	1238	0	1252	4	0
2	ZH	1238	0	1252	3	0
3	AX	240	0	55	0	0
3	BX	240	0	55	0	0
3	CX	240	0	55	0	0
3	DX	240	0	54	0	0
3	EX	240	0	54	0	0
3	FX	240	0	55	0	0
3	GX	240	0	55	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	HX	240	0	54	0	0
3	IX	240	0	54	0	0
3	JX	240	0	55	0	0
3	KX	240	0	55	0	0
3	LX	240	0	55	0	0
3	MX	240	0	55	0	0
3	VX	240	0	55	0	0
3	WX	240	0	54	0	0
3	XX	240	0	55	0	0
3	YX	240	0	54	0	0
3	ZX	240	0	55	0	0
4	AG	276	0	263	1	0
4	BG	276	0	263	2	0
4	CG	276	0	263	2	0
4	DG	276	0	263	1	0
4	EG	276	0	263	1	0
4	FG	276	0	263	1	0
4	GG	276	0	263	0	0
4	HG	276	0	263	1	0
4	IG	276	0	263	1	0
4	JG	276	0	263	1	0
4	KG	276	0	263	1	0
4	LG	276	0	263	1	0
4	MG	276	0	263	2	0
4	VG	276	0	263	1	0
4	WG	276	0	263	2	0
4	XG	276	0	263	0	0
4	YG	276	0	263	1	0
4	ZG	276	0	263	0	0
All	All	40266	0	37290	103	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 1.

The worst 5 of 103 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:DH:204:ILE:HG12	2:DH:215:ILE:HG12	1.81	0.63
2:KH:204:ILE:HG12	2:KH:215:ILE:HG12	1.81	0.62
2:CH:204:ILE:HG12	2:CH:215:ILE:HG12	1.83	0.61
2:IH:204:ILE:HG12	2:IH:215:ILE:HG12	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:YH:204:ILE:HG12	2:YH:215:ILE:HG12	1.84	0.60

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	AF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	BF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	CF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	DF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	EF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	FF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	GF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	HF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	IF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	JF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
1	KF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	LF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	MF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	VF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
1	WF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	XF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	YF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	ZF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
2	AH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	CH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	DH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	EH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	FH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	GH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	HH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	IH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	JH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	KH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	LH	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
2	MH	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
2	VH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	WH	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
2	XH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	YH	158/361 (44%)	153 (97%)	5 (3%)	0	100	100
2	ZH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
4	AG	32/1048 (3%)	32 (100%)	0	0	100	100
4	BG	32/1048 (3%)	32 (100%)	0	0	100	100
4	CG	32/1048 (3%)	32 (100%)	0	0	100	100
4	DG	32/1048 (3%)	32 (100%)	0	0	100	100
4	EG	32/1048 (3%)	32 (100%)	0	0	100	100
4	FG	32/1048 (3%)	32 (100%)	0	0	100	100
4	GG	32/1048 (3%)	32 (100%)	0	0	100	100
4	HG	32/1048 (3%)	32 (100%)	0	0	100	100
4	IG	32/1048 (3%)	32 (100%)	0	0	100	100
4	JG	32/1048 (3%)	32 (100%)	0	0	100	100
4	KG	32/1048 (3%)	32 (100%)	0	0	100	100
4	LG	32/1048 (3%)	32 (100%)	0	0	100	100
4	MG	32/1048 (3%)	32 (100%)	0	0	100	100
4	VG	32/1048 (3%)	32 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	WG	32/1048 (3%)	32 (100%)	0	0	100	100
4	XG	32/1048 (3%)	32 (100%)	0	0	100	100
4	YG	32/1048 (3%)	32 (100%)	0	0	100	100
4	ZG	32/1048 (3%)	32 (100%)	0	0	100	100
All	All	4518/30204 (15%)	4378 (97%)	140 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AF	53/237 (22%)	53 (100%)	0	100	100
1	BF	53/237 (22%)	53 (100%)	0	100	100
1	CF	53/237 (22%)	53 (100%)	0	100	100
1	DF	53/237 (22%)	53 (100%)	0	100	100
1	EF	53/237 (22%)	53 (100%)	0	100	100
1	FF	53/237 (22%)	53 (100%)	0	100	100
1	GF	53/237 (22%)	53 (100%)	0	100	100
1	HF	53/237 (22%)	53 (100%)	0	100	100
1	IF	53/237 (22%)	53 (100%)	0	100	100
1	JF	53/237 (22%)	53 (100%)	0	100	100
1	KF	53/237 (22%)	53 (100%)	0	100	100
1	LF	53/237 (22%)	53 (100%)	0	100	100
1	MF	53/237 (22%)	53 (100%)	0	100	100
1	VF	53/237 (22%)	53 (100%)	0	100	100
1	WF	53/237 (22%)	53 (100%)	0	100	100
1	XF	53/237 (22%)	53 (100%)	0	100	100
1	YF	53/237 (22%)	53 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	ZF	53/237 (22%)	53 (100%)	0	100	100
2	AH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	BH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	CH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	DH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	EH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	FH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	GH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	HH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	IH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	JH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	KH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	LH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	MH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	VH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	WH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	XH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	YH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	ZH	137/300 (46%)	136 (99%)	1 (1%)	84	95
4	AG	31/765 (4%)	31 (100%)	0	100	100
4	BG	31/765 (4%)	31 (100%)	0	100	100
4	CG	31/765 (4%)	31 (100%)	0	100	100
4	DG	31/765 (4%)	31 (100%)	0	100	100
4	EG	31/765 (4%)	31 (100%)	0	100	100
4	FG	31/765 (4%)	31 (100%)	0	100	100
4	GG	31/765 (4%)	31 (100%)	0	100	100
4	HG	31/765 (4%)	31 (100%)	0	100	100
4	IG	31/765 (4%)	31 (100%)	0	100	100
4	JG	31/765 (4%)	31 (100%)	0	100	100
4	KG	31/765 (4%)	31 (100%)	0	100	100
4	LG	31/765 (4%)	31 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	MG	31/765 (4%)	31 (100%)	0	100	100
4	VG	31/765 (4%)	31 (100%)	0	100	100
4	WG	31/765 (4%)	31 (100%)	0	100	100
4	XG	31/765 (4%)	31 (100%)	0	100	100
4	YG	31/765 (4%)	31 (100%)	0	100	100
4	ZG	31/765 (4%)	31 (100%)	0	100	100
All	All	3978/23436 (17%)	3960 (100%)	18 (0%)	89	96

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	LH	170	ARG
2	WH	170	ARG
2	VH	170	ARG
2	FH	170	ARG
2	KH	170	ARG

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

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	ZX	1
3	GX	1
3	CX	1
3	KX	1
3	BX	1
3	HX	1
3	YX	1
3	MX	1
3	XX	1
3	IX	1
3	LX	1
3	WX	1
3	FX	1
3	AX	1
3	EX	1
3	DX	1
3	JX	1
3	VX	1

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	ZX	38:UNK	C	70:UNK	N	24.53
1	GX	38:UNK	C	70:UNK	N	24.52
1	CX	38:UNK	C	70:UNK	N	24.51
1	KX	38:UNK	C	70:UNK	N	24.51
1	BX	38:UNK	C	70:UNK	N	24.49

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24006. 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.