



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 03:11 PM UTC

PDB ID : 6EY6 / pdb_00006ey6
Title : C-terminal part (residues 315-516) of PorM with the llama nanobody nb130
Authors : Leone, P.; Cambillau, C.; Roussel, A.
Deposited on : 2017-11-10
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

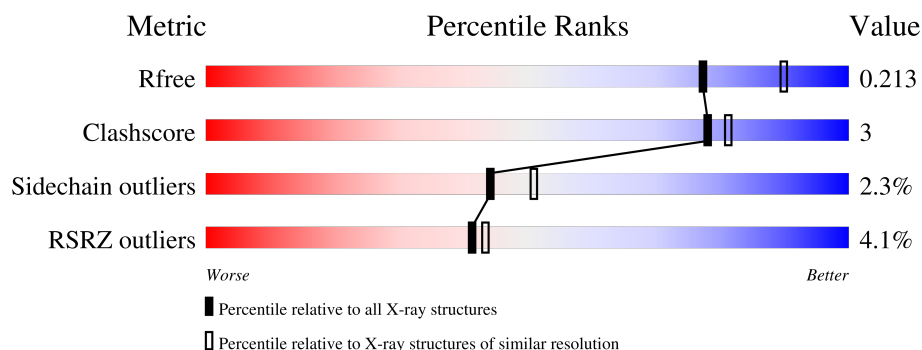
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	2% 56% 6% • 37%
1	B	315	10% 55% 7% • 36%
1	C	315	2% 59% • 36%
1	D	315	3% 56% 6% • 36%
1	E	315	4% 57% 6% • 36%
1	F	315	3% 57% 5% • 37%

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Mol	Chain	Length	Quality of chain
1	G	315	
1	H	315	
2	I	138	
2	J	138	
2	K	138	
2	L	138	
2	M	138	
2	N	138	
2	O	138	
2	P	138	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21404 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 T9SS component cytoplasmic membrane protein PorM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	30	0	0
			1515	953	274	284	4			
1	B	202	Total	C	N	O	S	131	0	0
			1544	971	278	290	5			
1	C	202	Total	C	N	O	S	47	0	0
			1544	971	278	290	5			
1	D	202	Total	C	N	O	S	57	0	0
			1544	971	278	290	5			
1	E	202	Total	C	N	O	S	170	0	0
			1544	971	278	290	5			
1	F	198	Total	C	N	O	S	49	0	0
			1515	953	274	284	4			
1	G	202	Total	C	N	O	S	38	0	0
			1544	971	278	290	5			
1	H	202	Total	C	N	O	S	105	0	0
			1544	971	278	290	5			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	MET	-	initiating methionine	UNP A0A1R4DSC1
A	203	GLY	-	expression tag	UNP A0A1R4DSC1
A	204	HIS	-	expression tag	UNP A0A1R4DSC1
A	205	HIS	-	expression tag	UNP A0A1R4DSC1
A	206	HIS	-	expression tag	UNP A0A1R4DSC1
A	207	HIS	-	expression tag	UNP A0A1R4DSC1
A	208	HIS	-	expression tag	UNP A0A1R4DSC1
A	209	HIS	-	expression tag	UNP A0A1R4DSC1
A	210	SER	-	expression tag	UNP A0A1R4DSC1
A	211	SER	-	expression tag	UNP A0A1R4DSC1
A	212	GLY	-	expression tag	UNP A0A1R4DSC1
A	213	VAL	-	expression tag	UNP A0A1R4DSC1
A	214	ASP	-	expression tag	UNP A0A1R4DSC1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	215	LEU	-	expression tag	UNP A0A1R4DSC1
A	216	GLY	-	expression tag	UNP A0A1R4DSC1
A	217	THR	-	expression tag	UNP A0A1R4DSC1
A	218	GLU	-	expression tag	UNP A0A1R4DSC1
A	219	ASN	-	expression tag	UNP A0A1R4DSC1
A	220	LEU	-	expression tag	UNP A0A1R4DSC1
A	221	TYR	-	expression tag	UNP A0A1R4DSC1
A	222	PHE	-	expression tag	UNP A0A1R4DSC1
A	223	GLN	-	expression tag	UNP A0A1R4DSC1
A	224	SER	-	expression tag	UNP A0A1R4DSC1
B	202	MET	-	initiating methionine	UNP A0A1R4DSC1
B	203	GLY	-	expression tag	UNP A0A1R4DSC1
B	204	HIS	-	expression tag	UNP A0A1R4DSC1
B	205	HIS	-	expression tag	UNP A0A1R4DSC1
B	206	HIS	-	expression tag	UNP A0A1R4DSC1
B	207	HIS	-	expression tag	UNP A0A1R4DSC1
B	208	HIS	-	expression tag	UNP A0A1R4DSC1
B	209	HIS	-	expression tag	UNP A0A1R4DSC1
B	210	SER	-	expression tag	UNP A0A1R4DSC1
B	211	SER	-	expression tag	UNP A0A1R4DSC1
B	212	GLY	-	expression tag	UNP A0A1R4DSC1
B	213	VAL	-	expression tag	UNP A0A1R4DSC1
B	214	ASP	-	expression tag	UNP A0A1R4DSC1
B	215	LEU	-	expression tag	UNP A0A1R4DSC1
B	216	GLY	-	expression tag	UNP A0A1R4DSC1
B	217	THR	-	expression tag	UNP A0A1R4DSC1
B	218	GLU	-	expression tag	UNP A0A1R4DSC1
B	219	ASN	-	expression tag	UNP A0A1R4DSC1
B	220	LEU	-	expression tag	UNP A0A1R4DSC1
B	221	TYR	-	expression tag	UNP A0A1R4DSC1
B	222	PHE	-	expression tag	UNP A0A1R4DSC1
B	223	GLN	-	expression tag	UNP A0A1R4DSC1
B	224	SER	-	expression tag	UNP A0A1R4DSC1
C	202	MET	-	initiating methionine	UNP A0A1R4DSC1
C	203	GLY	-	expression tag	UNP A0A1R4DSC1
C	204	HIS	-	expression tag	UNP A0A1R4DSC1
C	205	HIS	-	expression tag	UNP A0A1R4DSC1
C	206	HIS	-	expression tag	UNP A0A1R4DSC1
C	207	HIS	-	expression tag	UNP A0A1R4DSC1
C	208	HIS	-	expression tag	UNP A0A1R4DSC1
C	209	HIS	-	expression tag	UNP A0A1R4DSC1
C	210	SER	-	expression tag	UNP A0A1R4DSC1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	211	SER	-	expression tag	UNP A0A1R4DSC1
C	212	GLY	-	expression tag	UNP A0A1R4DSC1
C	213	VAL	-	expression tag	UNP A0A1R4DSC1
C	214	ASP	-	expression tag	UNP A0A1R4DSC1
C	215	LEU	-	expression tag	UNP A0A1R4DSC1
C	216	GLY	-	expression tag	UNP A0A1R4DSC1
C	217	THR	-	expression tag	UNP A0A1R4DSC1
C	218	GLU	-	expression tag	UNP A0A1R4DSC1
C	219	ASN	-	expression tag	UNP A0A1R4DSC1
C	220	LEU	-	expression tag	UNP A0A1R4DSC1
C	221	TYR	-	expression tag	UNP A0A1R4DSC1
C	222	PHE	-	expression tag	UNP A0A1R4DSC1
C	223	GLN	-	expression tag	UNP A0A1R4DSC1
C	224	SER	-	expression tag	UNP A0A1R4DSC1
D	202	MET	-	initiating methionine	UNP A0A1R4DSC1
D	203	GLY	-	expression tag	UNP A0A1R4DSC1
D	204	HIS	-	expression tag	UNP A0A1R4DSC1
D	205	HIS	-	expression tag	UNP A0A1R4DSC1
D	206	HIS	-	expression tag	UNP A0A1R4DSC1
D	207	HIS	-	expression tag	UNP A0A1R4DSC1
D	208	HIS	-	expression tag	UNP A0A1R4DSC1
D	209	HIS	-	expression tag	UNP A0A1R4DSC1
D	210	SER	-	expression tag	UNP A0A1R4DSC1
D	211	SER	-	expression tag	UNP A0A1R4DSC1
D	212	GLY	-	expression tag	UNP A0A1R4DSC1
D	213	VAL	-	expression tag	UNP A0A1R4DSC1
D	214	ASP	-	expression tag	UNP A0A1R4DSC1
D	215	LEU	-	expression tag	UNP A0A1R4DSC1
D	216	GLY	-	expression tag	UNP A0A1R4DSC1
D	217	THR	-	expression tag	UNP A0A1R4DSC1
D	218	GLU	-	expression tag	UNP A0A1R4DSC1
D	219	ASN	-	expression tag	UNP A0A1R4DSC1
D	220	LEU	-	expression tag	UNP A0A1R4DSC1
D	221	TYR	-	expression tag	UNP A0A1R4DSC1
D	222	PHE	-	expression tag	UNP A0A1R4DSC1
D	223	GLN	-	expression tag	UNP A0A1R4DSC1
D	224	SER	-	expression tag	UNP A0A1R4DSC1
E	202	MET	-	initiating methionine	UNP A0A1R4DSC1
E	203	GLY	-	expression tag	UNP A0A1R4DSC1
E	204	HIS	-	expression tag	UNP A0A1R4DSC1
E	205	HIS	-	expression tag	UNP A0A1R4DSC1
E	206	HIS	-	expression tag	UNP A0A1R4DSC1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	207	HIS	-	expression tag	UNP A0A1R4DSC1
E	208	HIS	-	expression tag	UNP A0A1R4DSC1
E	209	HIS	-	expression tag	UNP A0A1R4DSC1
E	210	SER	-	expression tag	UNP A0A1R4DSC1
E	211	SER	-	expression tag	UNP A0A1R4DSC1
E	212	GLY	-	expression tag	UNP A0A1R4DSC1
E	213	VAL	-	expression tag	UNP A0A1R4DSC1
E	214	ASP	-	expression tag	UNP A0A1R4DSC1
E	215	LEU	-	expression tag	UNP A0A1R4DSC1
E	216	GLY	-	expression tag	UNP A0A1R4DSC1
E	217	THR	-	expression tag	UNP A0A1R4DSC1
E	218	GLU	-	expression tag	UNP A0A1R4DSC1
E	219	ASN	-	expression tag	UNP A0A1R4DSC1
E	220	LEU	-	expression tag	UNP A0A1R4DSC1
E	221	TYR	-	expression tag	UNP A0A1R4DSC1
E	222	PHE	-	expression tag	UNP A0A1R4DSC1
E	223	GLN	-	expression tag	UNP A0A1R4DSC1
E	224	SER	-	expression tag	UNP A0A1R4DSC1
F	202	MET	-	initiating methionine	UNP A0A1R4DSC1
F	203	GLY	-	expression tag	UNP A0A1R4DSC1
F	204	HIS	-	expression tag	UNP A0A1R4DSC1
F	205	HIS	-	expression tag	UNP A0A1R4DSC1
F	206	HIS	-	expression tag	UNP A0A1R4DSC1
F	207	HIS	-	expression tag	UNP A0A1R4DSC1
F	208	HIS	-	expression tag	UNP A0A1R4DSC1
F	209	HIS	-	expression tag	UNP A0A1R4DSC1
F	210	SER	-	expression tag	UNP A0A1R4DSC1
F	211	SER	-	expression tag	UNP A0A1R4DSC1
F	212	GLY	-	expression tag	UNP A0A1R4DSC1
F	213	VAL	-	expression tag	UNP A0A1R4DSC1
F	214	ASP	-	expression tag	UNP A0A1R4DSC1
F	215	LEU	-	expression tag	UNP A0A1R4DSC1
F	216	GLY	-	expression tag	UNP A0A1R4DSC1
F	217	THR	-	expression tag	UNP A0A1R4DSC1
F	218	GLU	-	expression tag	UNP A0A1R4DSC1
F	219	ASN	-	expression tag	UNP A0A1R4DSC1
F	220	LEU	-	expression tag	UNP A0A1R4DSC1
F	221	TYR	-	expression tag	UNP A0A1R4DSC1
F	222	PHE	-	expression tag	UNP A0A1R4DSC1
F	223	GLN	-	expression tag	UNP A0A1R4DSC1
F	224	SER	-	expression tag	UNP A0A1R4DSC1
G	202	MET	-	initiating methionine	UNP A0A1R4DSC1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	203	GLY	-	expression tag	UNP A0A1R4DSC1
G	204	HIS	-	expression tag	UNP A0A1R4DSC1
G	205	HIS	-	expression tag	UNP A0A1R4DSC1
G	206	HIS	-	expression tag	UNP A0A1R4DSC1
G	207	HIS	-	expression tag	UNP A0A1R4DSC1
G	208	HIS	-	expression tag	UNP A0A1R4DSC1
G	209	HIS	-	expression tag	UNP A0A1R4DSC1
G	210	SER	-	expression tag	UNP A0A1R4DSC1
G	211	SER	-	expression tag	UNP A0A1R4DSC1
G	212	GLY	-	expression tag	UNP A0A1R4DSC1
G	213	VAL	-	expression tag	UNP A0A1R4DSC1
G	214	ASP	-	expression tag	UNP A0A1R4DSC1
G	215	LEU	-	expression tag	UNP A0A1R4DSC1
G	216	GLY	-	expression tag	UNP A0A1R4DSC1
G	217	THR	-	expression tag	UNP A0A1R4DSC1
G	218	GLU	-	expression tag	UNP A0A1R4DSC1
G	219	ASN	-	expression tag	UNP A0A1R4DSC1
G	220	LEU	-	expression tag	UNP A0A1R4DSC1
G	221	TYR	-	expression tag	UNP A0A1R4DSC1
G	222	PHE	-	expression tag	UNP A0A1R4DSC1
G	223	GLN	-	expression tag	UNP A0A1R4DSC1
G	224	SER	-	expression tag	UNP A0A1R4DSC1
H	202	MET	-	initiating methionine	UNP A0A1R4DSC1
H	203	GLY	-	expression tag	UNP A0A1R4DSC1
H	204	HIS	-	expression tag	UNP A0A1R4DSC1
H	205	HIS	-	expression tag	UNP A0A1R4DSC1
H	206	HIS	-	expression tag	UNP A0A1R4DSC1
H	207	HIS	-	expression tag	UNP A0A1R4DSC1
H	208	HIS	-	expression tag	UNP A0A1R4DSC1
H	209	HIS	-	expression tag	UNP A0A1R4DSC1
H	210	SER	-	expression tag	UNP A0A1R4DSC1
H	211	SER	-	expression tag	UNP A0A1R4DSC1
H	212	GLY	-	expression tag	UNP A0A1R4DSC1
H	213	VAL	-	expression tag	UNP A0A1R4DSC1
H	214	ASP	-	expression tag	UNP A0A1R4DSC1
H	215	LEU	-	expression tag	UNP A0A1R4DSC1
H	216	GLY	-	expression tag	UNP A0A1R4DSC1
H	217	THR	-	expression tag	UNP A0A1R4DSC1
H	218	GLU	-	expression tag	UNP A0A1R4DSC1
H	219	ASN	-	expression tag	UNP A0A1R4DSC1
H	220	LEU	-	expression tag	UNP A0A1R4DSC1
H	221	TYR	-	expression tag	UNP A0A1R4DSC1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	222	PHE	-	expression tag	UNP A0A1R4DSC1
H	223	GLN	-	expression tag	UNP A0A1R4DSC1
H	224	SER	-	expression tag	UNP A0A1R4DSC1

- Molecule 2 is a protein called nb130.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	129	Total	C	N	O	S	23	0	0
			981	613	173	191	4			
2	J	130	Total	C	N	O	S	17	0	0
			987	616	174	193	4			
2	K	130	Total	C	N	O	S	16	0	0
			987	616	174	193	4			
2	L	130	Total	C	N	O	S	25	0	0
			987	616	174	193	4			
2	M	130	Total	C	N	O	S	32	0	0
			987	616	174	193	4			
2	N	129	Total	C	N	O	S	13	0	0
			981	613	173	191	4			
2	O	129	Total	C	N	O	S	32	0	0
			978	611	172	191	4			
2	P	130	Total	C	N	O	S	23	0	0
			987	616	174	193	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	105	Total	O	0	0
			105	105		
3	B	45	Total	O	0	0
			45	45		
3	C	117	Total	O	0	0
			117	117		
3	D	123	Total	O	0	0
			123	123		
3	E	77	Total	O	0	0
			77	77		
3	F	82	Total	O	0	0
			82	82		
3	G	89	Total	O	0	0
			89	89		
3	H	97	Total	O	0	0
			97	97		

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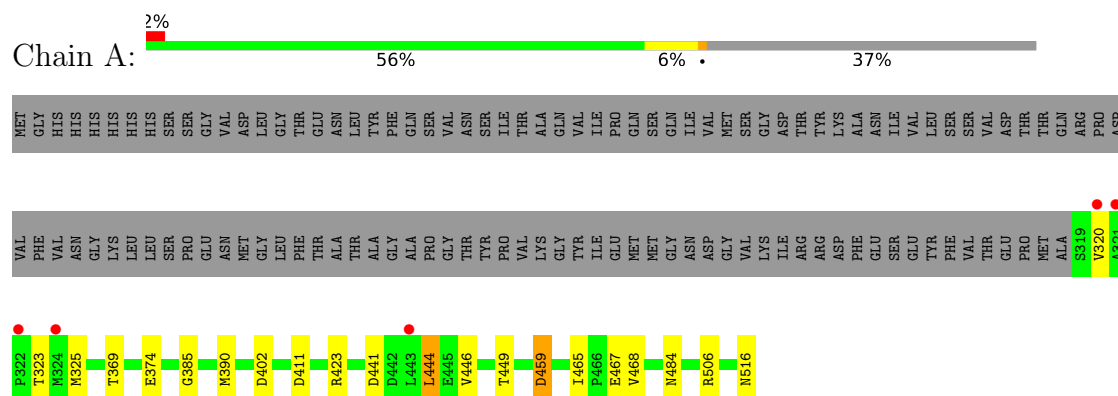
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	35	Total 35	O 35	0	0
3	J	65	Total 65	O 65	0	0
3	K	107	Total 107	O 107	0	0
3	L	64	Total 64	O 64	0	0
3	M	40	Total 40	O 40	0	0
3	N	71	Total 71	O 71	0	0
3	O	39	Total 39	O 39	0	0
3	P	79	Total 79	O 79	0	0

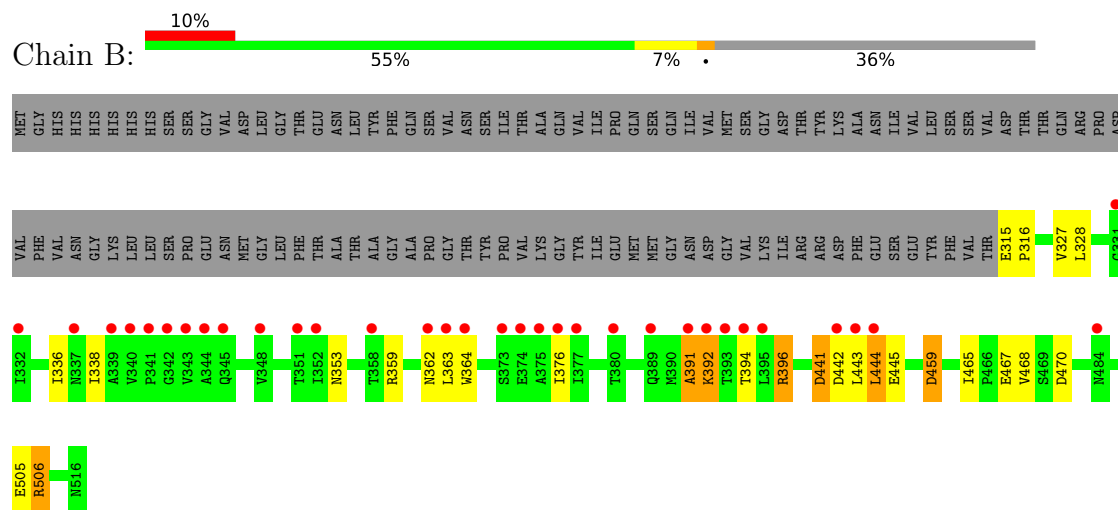
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

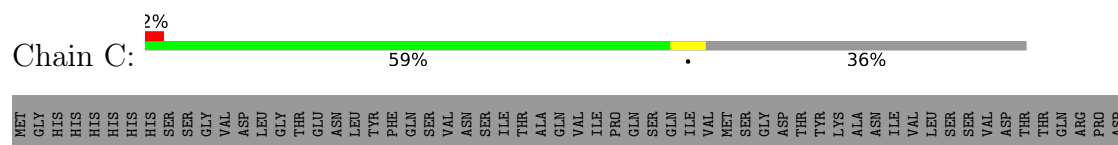
- Molecule 1: T9SS component cytoplasmic membrane protein PorM

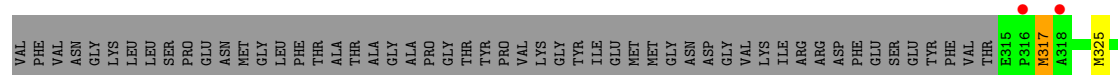


- Molecule 1: T9SS component cytoplasmic membrane protein PorM

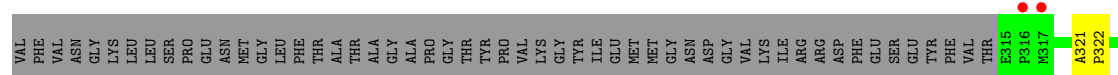
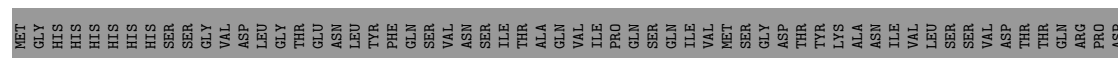


- Molecule 1: T9SS component cytoplasmic membrane protein PorM

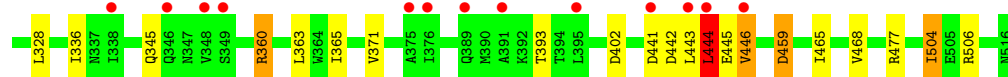
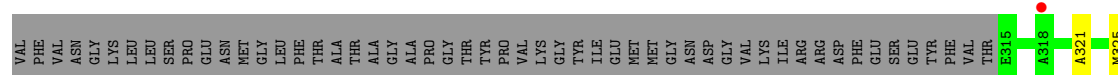
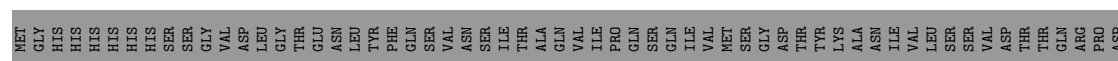




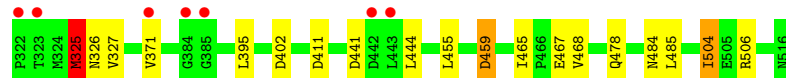
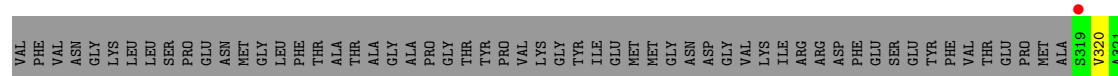
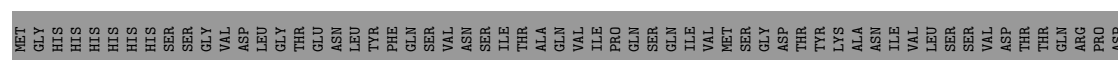
- Molecule 1: T9SS component cytoplasmic membrane protein PorM



- Molecule 1: T9SS component cytoplasmic membrane protein PorM

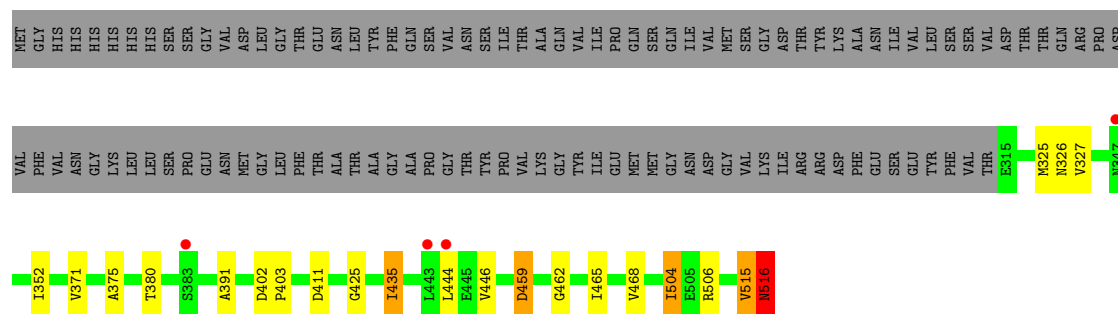


- Molecule 1: T9SS component cytoplasmic membrane protein PorM

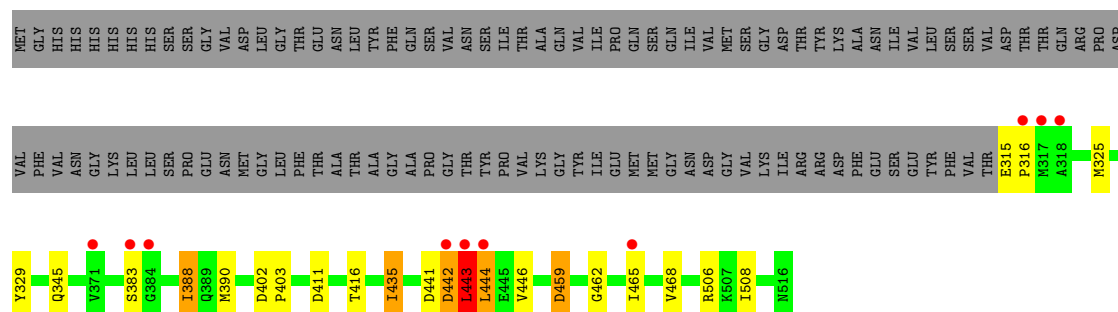


- Molecule 1: T9SS component cytoplasmic membrane protein PorM

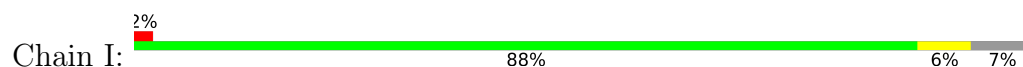




- Molecule 1: T9SS component cytoplasmic membrane protein PorM



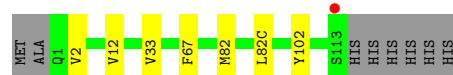
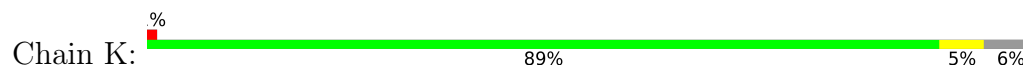
- Molecule 2: nb130



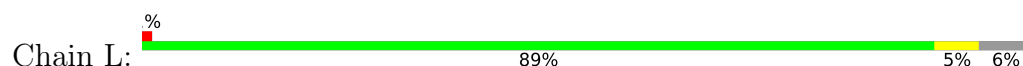
- Molecule 2: nb130



- Molecule 2: nb130

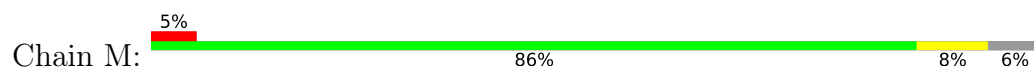


- Molecule 2: nb130

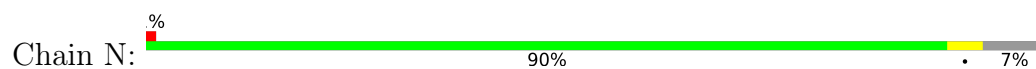




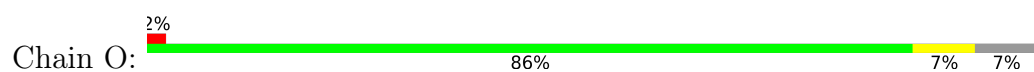
• Molecule 2: nb130



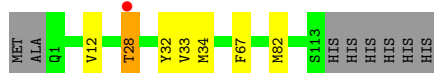
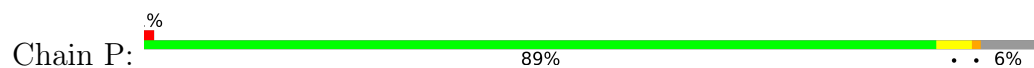
• Molecule 2: nb130



• Molecule 2: nb130



• Molecule 2: nb130



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.24Å 77.18Å 156.30Å 90.24° 91.76° 97.16°	Depositor
Resolution (Å)	38.35 – 2.10 38.35 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (38.35-2.10) 97.4 (38.35-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.181 , 0.215 (Not available) , 0.213	Depositor DCC
R_{free} test set	7242 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.117 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21404	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.86	1/1537 (0.1%)	1.15	9/2078 (0.4%)
1	B	0.85	0/1567	1.26	14/2119 (0.7%)
1	C	0.88	1/1567 (0.1%)	1.11	5/2119 (0.2%)
1	D	0.90	1/1567 (0.1%)	1.33	21/2119 (1.0%)
1	E	0.83	1/1567 (0.1%)	1.14	4/2119 (0.2%)
1	F	0.86	2/1537 (0.1%)	1.18	9/2078 (0.4%)
1	G	0.89	3/1567 (0.2%)	1.18	6/2119 (0.3%)
1	H	0.90	3/1567 (0.2%)	1.24	14/2119 (0.7%)
2	I	0.75	0/1002	1.02	2/1352 (0.1%)
2	J	0.76	0/1008	1.01	2/1360 (0.1%)
2	K	0.89	1/1008 (0.1%)	0.99	2/1360 (0.1%)
2	L	0.82	0/1008	1.04	2/1360 (0.1%)
2	M	0.77	0/1008	1.02	3/1360 (0.2%)
2	N	0.78	0/1002	1.01	2/1352 (0.1%)
2	O	0.79	0/999	1.07	2/1348 (0.1%)
2	P	0.83	2/1008 (0.2%)	1.03	4/1360 (0.3%)
All	All	0.84	15/20519 (0.1%)	1.13	101/27722 (0.4%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	82	MET	SD-CE	-9.11	1.56	1.79
1	F	325	MET	SD-CE	-7.92	1.59	1.79
1	G	435	ILE	CG1-CD1	-7.74	1.21	1.51
1	H	435	ILE	CG1-CD1	-7.70	1.21	1.51
1	H	390	MET	SD-CE	-7.10	1.61	1.79

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	442	ASP	CA-C-N	13.58	146.14	121.70
1	D	442	ASP	C-N-CA	13.58	146.14	121.70
1	B	391	ALA	CA-C-N	9.73	139.22	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	391	ALA	C-N-CA	9.73	139.22	121.70
1	E	444	LEU	CA-C-N	9.00	137.89	121.70

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	A	1515	0	1565	11	0
1	B	1544	0	1592	19	0
1	C	1544	0	1592	4	0
1	D	1544	0	1592	14	0
1	E	1544	0	1592	14	0
1	F	1515	0	1565	10	0
1	G	1544	0	1592	17	0
1	H	1544	0	1592	15	0
2	I	981	0	941	2	0
2	J	987	0	946	3	0
2	K	987	0	946	2	0
2	L	987	0	946	2	0
2	M	987	0	946	3	0
2	N	981	0	941	1	0
2	O	978	0	935	3	0
2	P	987	0	946	1	0
3	A	105	0	0	1	0
3	B	45	0	0	0	0
3	C	117	0	0	1	0
3	D	123	0	0	1	0
3	E	77	0	0	0	0
3	F	82	0	0	0	0
3	G	89	0	0	0	0
3	H	97	0	0	0	0
3	I	35	0	0	0	0
3	J	65	0	0	0	0
3	K	107	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	64	0	0	0	0
3	M	40	0	0	0	0
3	N	71	0	0	0	0
3	O	39	0	0	0	0
3	P	79	0	0	0	0
All	All	21404	0	20229	106	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 3.

The worst 5 of 106 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:G:425:GLY:HA2	1:G:516:ASN:HB2	1.38	1.03
1:E:371:VAL:HG21	1:E:504:ILE:HD11	1.49	0.92
1:G:459:ASP:HB3	1:G:465:ILE:HD11	1.62	0.80
1:B:391:ALA:HA	1:B:392:LYS:HB2	1.65	0.78
1:G:371:VAL:HG21	1:G:504:ILE:HD11	1.68	0.74

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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 X-ray entries followed by that with respect to entries of similar resolution.

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	162/262 (62%)	159 (98%)	3 (2%)	50	58
1	B	165/262 (63%)	162 (98%)	3 (2%)	51	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	165/262 (63%)	157 (95%)	8 (5%)	23	23
1	D	165/262 (63%)	162 (98%)	3 (2%)	51	60
1	E	165/262 (63%)	159 (96%)	6 (4%)	31	34
1	F	162/262 (62%)	159 (98%)	3 (2%)	50	58
1	G	165/262 (63%)	159 (96%)	6 (4%)	31	34
1	H	165/262 (63%)	159 (96%)	6 (4%)	31	34
2	I	102/110 (93%)	100 (98%)	2 (2%)	48	56
2	J	103/110 (94%)	101 (98%)	2 (2%)	50	58
2	K	103/110 (94%)	103 (100%)	0	100	100
2	L	103/110 (94%)	101 (98%)	2 (2%)	50	58
2	M	103/110 (94%)	101 (98%)	2 (2%)	50	58
2	N	102/110 (93%)	101 (99%)	1 (1%)	68	76
2	O	102/110 (93%)	100 (98%)	2 (2%)	48	56
2	P	103/110 (94%)	102 (99%)	1 (1%)	68	76
All	All	2135/2976 (72%)	2085 (98%)	50 (2%)	44	51

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	380	THR
1	H	435	ILE
2	P	12	VAL
1	G	435	ILE
1	H	345	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	389	GLN
2	M	3	GLN
1	F	483	GLN
2	N	105	GLN
2	J	1	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	198/315 (62%)	0.07	5 (2%) 58 61	31, 44, 76, 94	9 (4%)
1	B	194/315 (61%)	0.66	33 (17%) 4 4	25, 55, 100, 137	22 (11%)
1	C	202/315 (64%)	0.19	7 (3%) 47 49	22, 45, 83, 124	14 (6%)
1	D	199/315 (63%)	0.13	8 (4%) 42 44	24, 43, 81, 118	13 (6%)
1	E	187/315 (59%)	0.45	14 (7%) 20 21	25, 50, 93, 128	19 (10%)
1	F	198/315 (62%)	0.19	8 (4%) 42 44	30, 48, 78, 96	17 (8%)
1	G	202/315 (64%)	0.19	4 (1%) 65 67	29, 50, 83, 109	14 (6%)
1	H	196/315 (62%)	0.30	10 (5%) 33 35	21, 48, 78, 102	17 (8%)
2	I	129/138 (93%)	0.27	3 (2%) 61 64	30, 49, 82, 104	8 (6%)
2	J	130/138 (94%)	0.03	2 (1%) 72 74	28, 44, 68, 90	7 (5%)
2	K	130/138 (94%)	-0.30	1 (0%) 82 84	25, 33, 53, 73	6 (4%)
2	L	130/138 (94%)	0.17	1 (0%) 82 84	30, 46, 74, 102	8 (6%)
2	M	130/138 (94%)	0.59	7 (5%) 31 33	28, 55, 101, 155	11 (8%)
2	N	129/138 (93%)	-0.07	1 (0%) 82 84	31, 42, 65, 86	5 (3%)
2	O	129/138 (93%)	0.22	3 (2%) 61 64	32, 51, 76, 100	10 (7%)
2	P	130/138 (94%)	-0.12	1 (0%) 82 84	26, 41, 62, 73	8 (6%)
All	All	2613/3624 (72%)	0.20	108 (4%) 41 43	21, 46, 84, 155	188 (7%)

The worst 5 of 108 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	443	LEU	4.7
1	F	442	ASP	4.7
2	M	113	SER	4.5
1	C	412	VAL	4.4
1	E	443	LEU	4.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.