



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 05:01 am BST

PDB ID : 6EY6
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

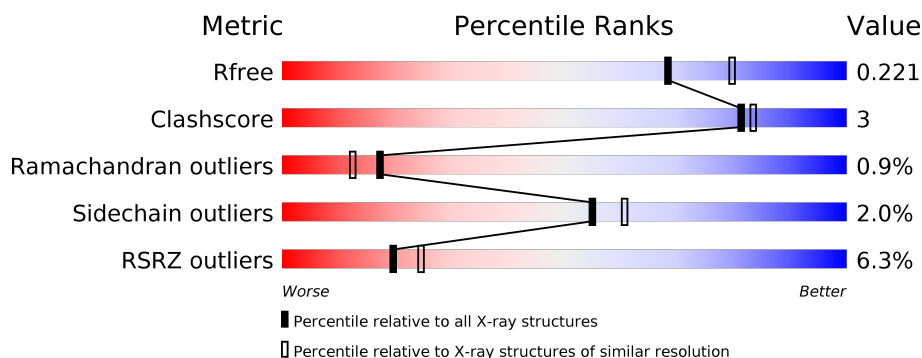
1 Overall quality at a glance

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 on 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	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>5%</div> <div>37%</div> </div> </div>
1	B	315	<div> <div>11%</div> <div> <div></div> <div>55%</div> <div>7%</div> <div>36%</div> </div> </div>
1	C	315	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>•</div> <div>36%</div> </div> </div>
1	D	315	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>• •</div> <div>36%</div> </div> </div>
1	E	315	<div> <div>7%</div> <div> <div></div> <div>57%</div> <div>6%</div> <div>36%</div> </div> </div>
1	F	315	<div> <div>4%</div> <div> <div></div> <div>57%</div> <div>5%</div> <div>37%</div> </div> </div>

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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			

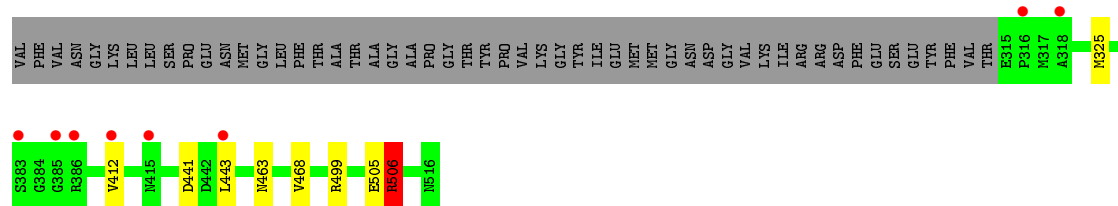
- Molecule 3 is water.

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		

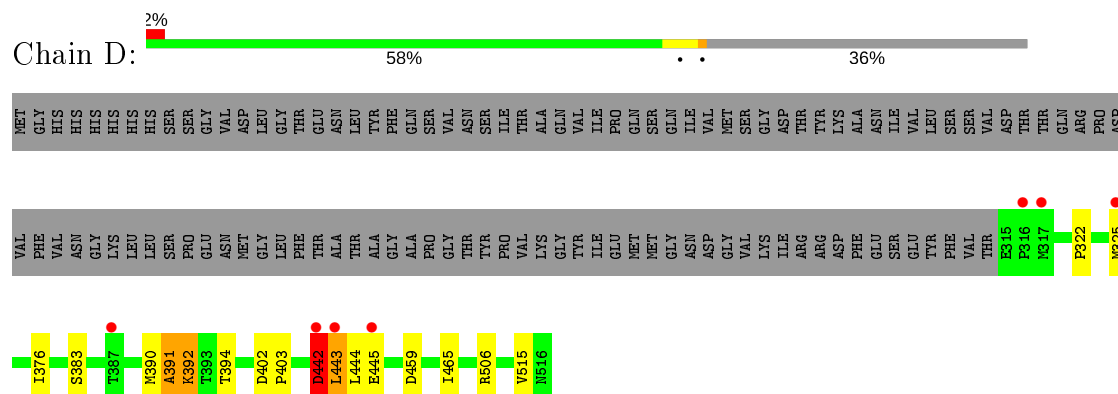
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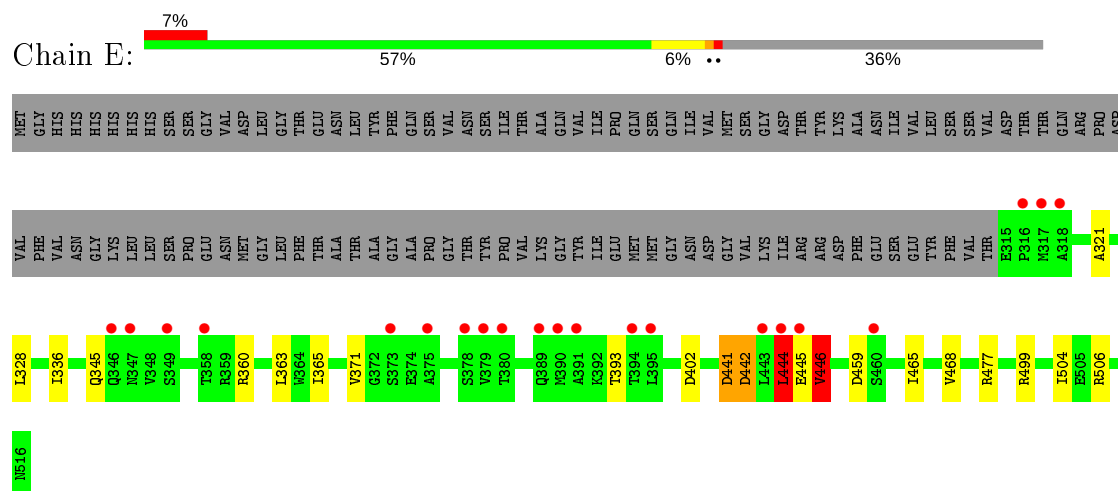
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	35	Total 35	O 35	0	0
3	J	65	Total 65	O 65	0	0
3	K	107	Total 107	O 107	0	0
3	L	64	Total 64	O 64	0	0
3	M	40	Total 40	O 40	0	0
3	N	71	Total 71	O 71	0	0
3	O	39	Total 39	O 39	0	0
3	P	79	Total 79	O 79	0	0



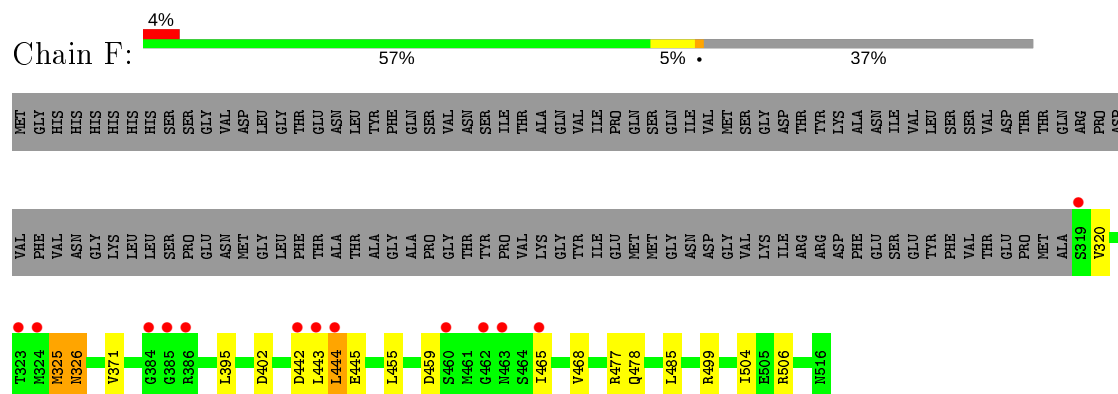
- Molecule 1: T9SS component cytoplasmic membrane protein PorM



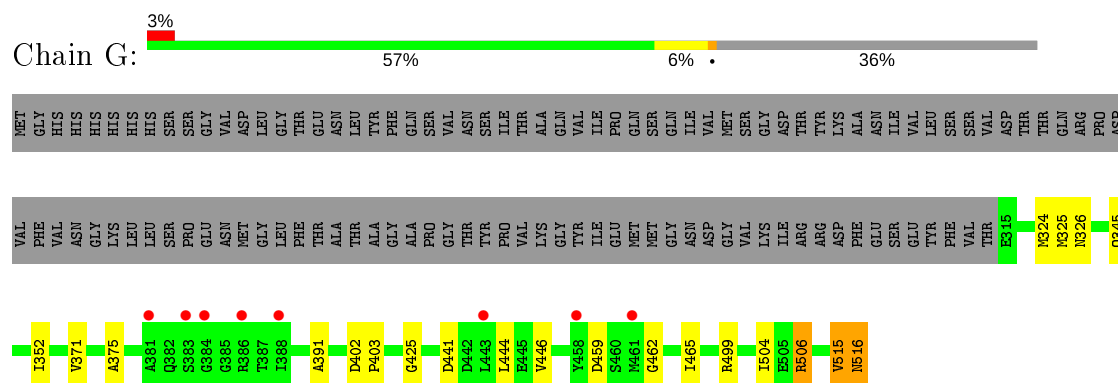
- Molecule 1: T9SS component cytoplasmic membrane protein PorM



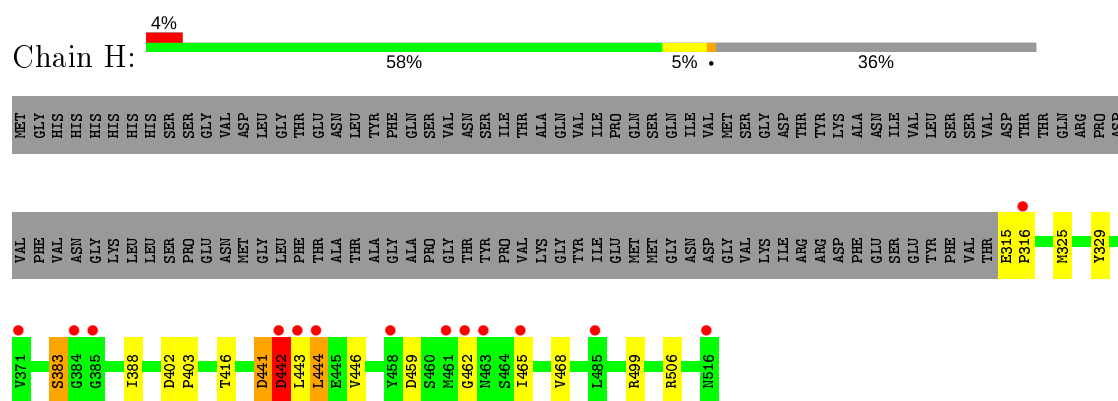
- Molecule 1: T9SS component cytoplasmic membrane protein PorM



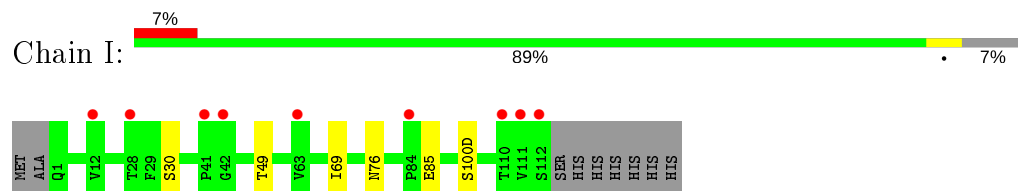
- Molecule 1: T9SS component cytoplasmic membrane protein PorM



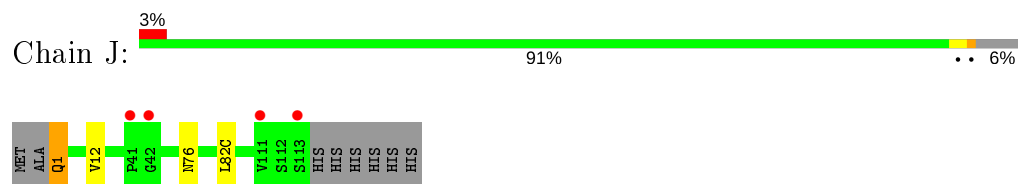
- Molecule 1: T9SS component cytoplasmic membrane protein PorM



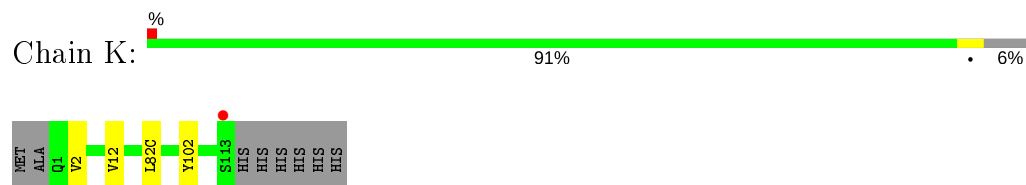
- Molecule 2: nb130



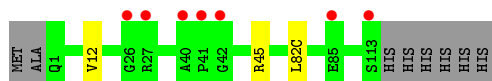
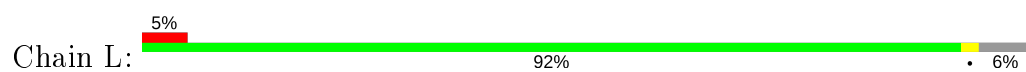
- Molecule 2: nb130



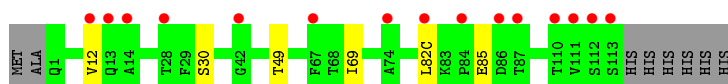
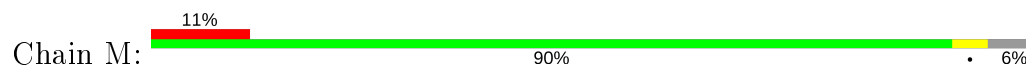
- Molecule 2: nb130



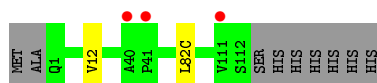
- Molecule 2: nb130



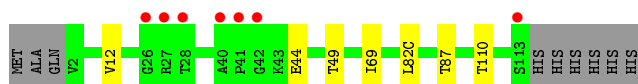
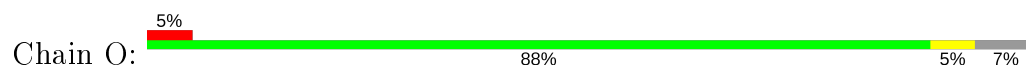
• Molecule 2: nb130



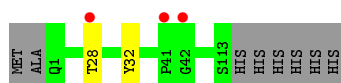
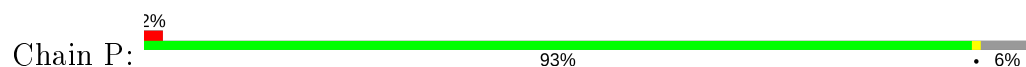
• Molecule 2: nb130



• 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 0.187 , 0.221	Depositor DCC
R_{free} test set	7242 reflections (4.98%)	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)	0.32 , 52.5	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 [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	0.51	0/1537	0.70	0/2078
1	B	0.49	0/1567	0.75	2/2119 (0.1%)
1	C	0.53	0/1567	0.70	1/2119 (0.0%)
1	D	0.54	0/1567	0.82	4/2119 (0.2%)
1	E	0.49	0/1567	0.70	1/2119 (0.0%)
1	F	0.50	0/1537	0.71	1/2078 (0.0%)
1	G	0.51	0/1567	0.73	1/2119 (0.0%)
1	H	0.53	0/1567	0.76	4/2119 (0.2%)
2	I	0.46	0/1002	0.63	0/1352
2	J	0.49	0/1008	0.61	0/1360
2	K	0.56	0/1008	0.62	0/1360
2	L	0.51	0/1008	0.63	0/1360
2	M	0.48	0/1008	0.61	0/1360
2	N	0.50	0/1002	0.62	0/1352
2	O	0.49	0/999	0.63	0/1348
2	P	0.53	0/1008	0.63	0/1360
All	All	0.51	0/20519	0.69	14/27722 (0.1%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	442	ASP	C-N-CA	9.78	146.14	121.70
1	B	391	ALA	C-N-CA	7.01	139.22	121.70
1	C	506	ARG	CG-CD-NE	-6.57	98.01	111.80
1	E	444	LEU	C-N-CA	6.48	137.89	121.70
1	H	441	ASP	C-N-CA	6.48	137.90	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	20	0
1	C	1544	0	1592	3	0
1	D	1544	0	1592	13	0
1	E	1544	0	1592	12	0
1	F	1515	0	1565	9	0
1	G	1544	0	1592	17	0
1	H	1544	0	1592	14	0
2	I	981	0	941	1	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	2	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	0	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
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	99	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 99 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](#)

In the following table, the Percentiles column shows the percent Ramachandran 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 backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	196/315 (62%)	193 (98%)	3 (2%)	0	100	100
1	B	200/315 (64%)	189 (94%)	7 (4%)	4 (2%)	7	3
1	C	200/315 (64%)	194 (97%)	5 (2%)	1 (0%)	29	26
1	D	200/315 (64%)	189 (94%)	6 (3%)	5 (2%)	5	2
1	E	200/315 (64%)	190 (95%)	6 (3%)	4 (2%)	7	3
1	F	196/315 (62%)	189 (96%)	2 (1%)	5 (3%)	5	2
1	G	200/315 (64%)	195 (98%)	4 (2%)	1 (0%)	29	26
1	H	200/315 (64%)	192 (96%)	5 (2%)	3 (2%)	10	5
2	I	127/138 (92%)	127 (100%)	0	0	100	100
2	J	128/138 (93%)	128 (100%)	0	0	100	100
2	K	128/138 (93%)	127 (99%)	1 (1%)	0	100	100
2	L	128/138 (93%)	128 (100%)	0	0	100	100
2	M	128/138 (93%)	126 (98%)	2 (2%)	0	100	100
2	N	127/138 (92%)	126 (99%)	1 (1%)	0	100	100
2	O	127/138 (92%)	127 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	128/138 (93%)	127 (99%)	1 (1%)	0	100	100
All	All	2613/3624 (72%)	2547 (98%)	43 (2%)	23 (1%)	17	12

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	392	LYS
1	D	443	LEU
1	E	442	ASP
1	E	445	GLU
1	F	442	ASP

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 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%)	157 (97%)	5 (3%)	40	43
1	B	165/262 (63%)	162 (98%)	3 (2%)	59	65
1	C	165/262 (63%)	160 (97%)	5 (3%)	41	44
1	D	165/262 (63%)	164 (99%)	1 (1%)	86	90
1	E	165/262 (63%)	159 (96%)	6 (4%)	35	36
1	F	162/262 (62%)	157 (97%)	5 (3%)	40	43
1	G	165/262 (63%)	160 (97%)	5 (3%)	41	44
1	H	165/262 (63%)	162 (98%)	3 (2%)	59	65
2	I	102/110 (93%)	98 (96%)	4 (4%)	32	33
2	J	103/110 (94%)	101 (98%)	2 (2%)	57	63
2	K	103/110 (94%)	103 (100%)	0	100	100
2	L	103/110 (94%)	103 (100%)	0	100	100
2	M	103/110 (94%)	101 (98%)	2 (2%)	57	63
2	N	102/110 (93%)	102 (100%)	0	100	100
2	O	102/110 (93%)	101 (99%)	1 (1%)	76	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	103/110 (94%)	103 (100%)	0	100	100
All	All	2135/2976 (72%)	2093 (98%)	42 (2%)	55	60

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	468	VAL
1	F	485	LEU
2	J	76	ASN
1	E	499	ARG
1	F	468	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
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 carbohydrates 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 ⓘ

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%)	0.15	9 (4%) 33 38	31, 44, 77, 94	9 (4%)
1	B	194/315 (61%)	0.76	36 (18%) 1 1	31, 59, 110, 146	22 (11%)
1	C	202/315 (64%)	0.09	8 (3%) 38 44	27, 47, 84, 124	14 (6%)
1	D	199/315 (63%)	0.21	7 (3%) 44 50	24, 45, 84, 124	13 (6%)
1	E	187/315 (59%)	0.52	21 (11%) 5 6	30, 52, 103, 146	19 (10%)
1	F	198/315 (62%)	0.26	13 (6%) 18 23	30, 50, 81, 96	17 (8%)
1	G	202/315 (64%)	0.18	8 (3%) 38 44	30, 51, 83, 109	14 (6%)
1	H	196/315 (62%)	0.21	14 (7%) 16 20	29, 50, 82, 105	17 (8%)
2	I	129/138 (93%)	0.46	9 (6%) 16 20	32, 50, 82, 104	8 (6%)
2	J	130/138 (94%)	0.10	4 (3%) 49 55	33, 44, 68, 108	7 (5%)
2	K	130/138 (94%)	0.02	1 (0%) 86 88	25, 33, 56, 88	6 (4%)
2	L	130/138 (94%)	0.35	7 (5%) 25 31	30, 47, 75, 102	8 (6%)
2	M	130/138 (94%)	0.71	15 (11%) 4 6	32, 58, 101, 186	11 (8%)
2	N	129/138 (93%)	0.12	3 (2%) 60 65	31, 42, 67, 86	5 (3%)
2	O	129/138 (93%)	0.39	7 (5%) 25 31	32, 54, 80, 107	10 (7%)
2	P	130/138 (94%)	-0.03	3 (2%) 60 65	31, 41, 62, 88	8 (6%)
All	All	2613/3624 (72%)	0.28	165 (6%) 20 24	24, 48, 87, 186	188 (7%)

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	444	LEU	9.7
1	F	442	ASP	6.4
2	O	41	PRO	6.2
1	B	341	PRO	6.1
1	E	445	GLU	6.0

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 carbohydrates 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.