Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 01:24 pm GMT

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 Full wwPDB X-ray Structure Validation 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:

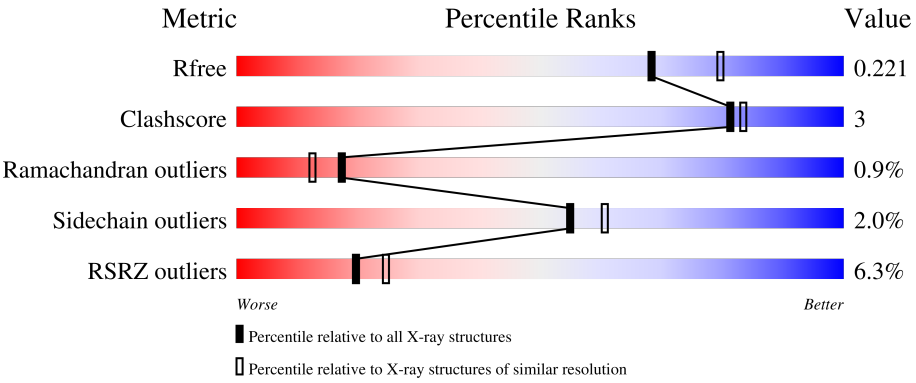
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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 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 <=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	3% 57% 5% 37%
1	B	315	11% 55% 7% 36%
1	C	315	3% 61% 36%
1	D	315	2% 58% 36%
1	E	315	7% 57% 6% 36%

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Mol	Chain	Length	Quality of chain
1	F	315	4% 57% 5% 37%
1	G	315	3% 57% 6% 36%
1	H	315	4% 58% 5% 36%
2	I	138	7% 89% 7%
2	J	138	3% 91% 6%
2	K	138	% 91% 6%
2	L	138	5% 92% 6%
2	M	138	11% 90% 6%
2	N	138	2% 92% 7%
2	O	138	5% 88% 5% 7%
2	P	138	2% 93% 6%

2 Entry composition (i)

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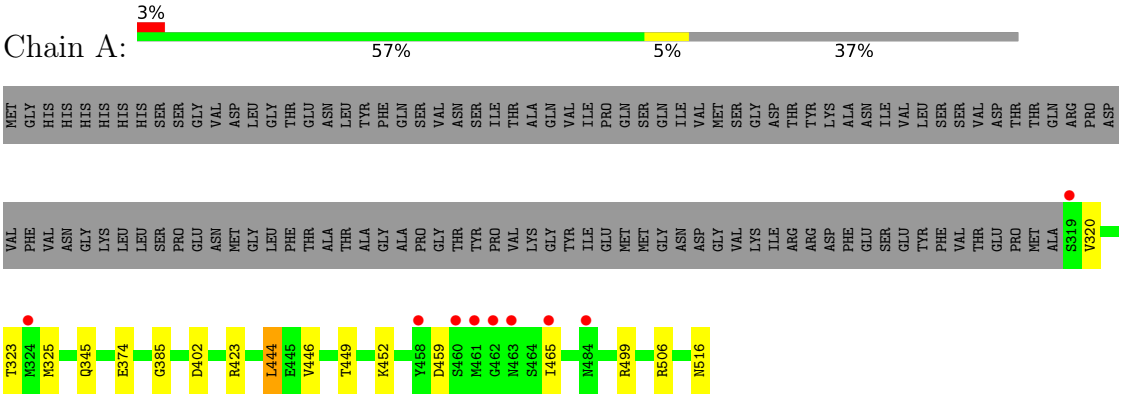
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	35	Total O 35 35	0	0
3	J	65	Total O 65 65	0	0
3	K	107	Total O 107 107	0	0
3	L	64	Total O 64 64	0	0
3	M	40	Total O 40 40	0	0
3	N	71	Total O 71 71	0	0
3	O	39	Total O 39 39	0	0
3	P	79	Total O 79 79	0	0

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.

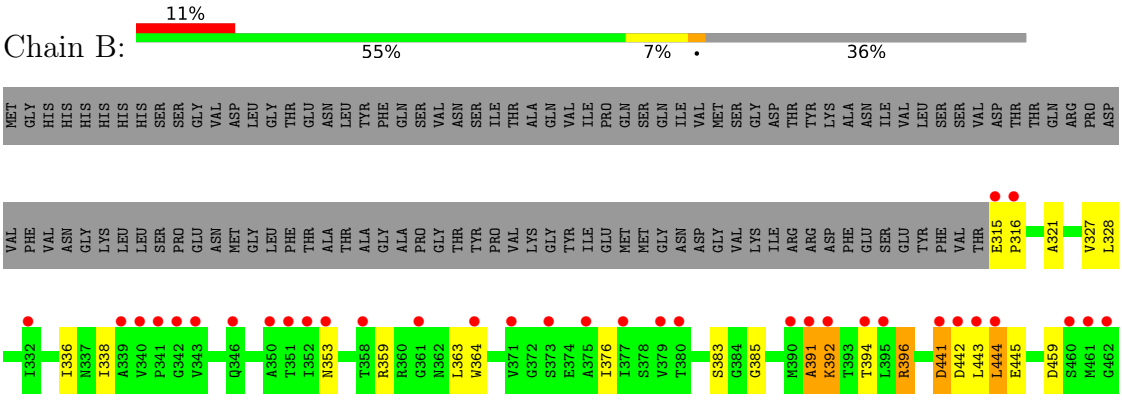
• Molecule 1: T9SS component cytoplasmic membrane protein PorM

Chain A:



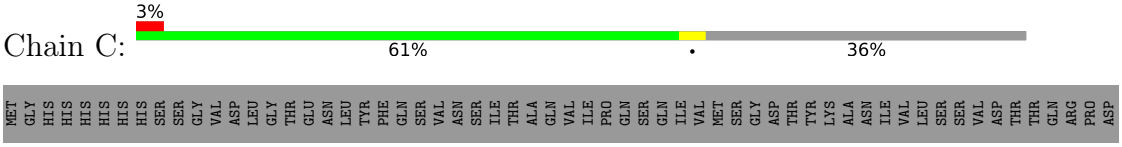
• Molecule 1: T9SS component cytoplasmic membrane protein PorM

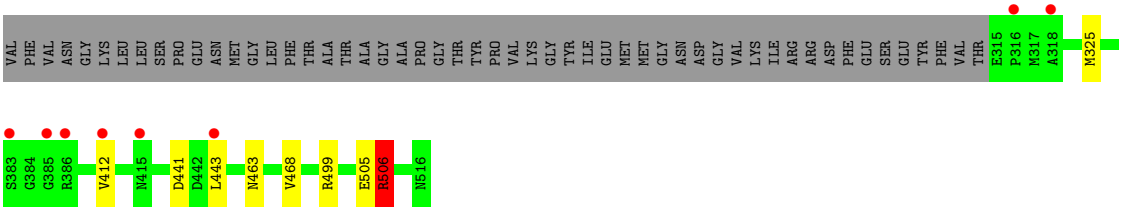
Chain B:



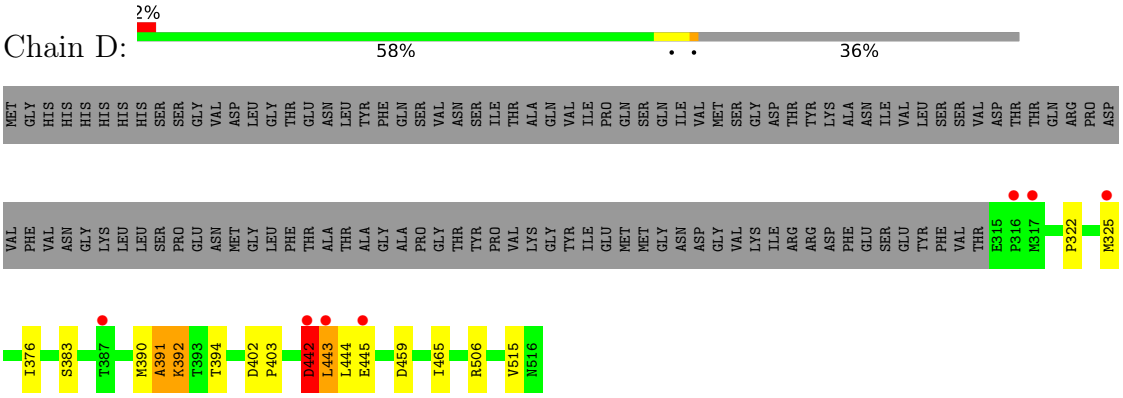
• Molecule 1: T9SS component cytoplasmic membrane protein PorM

Chain C:

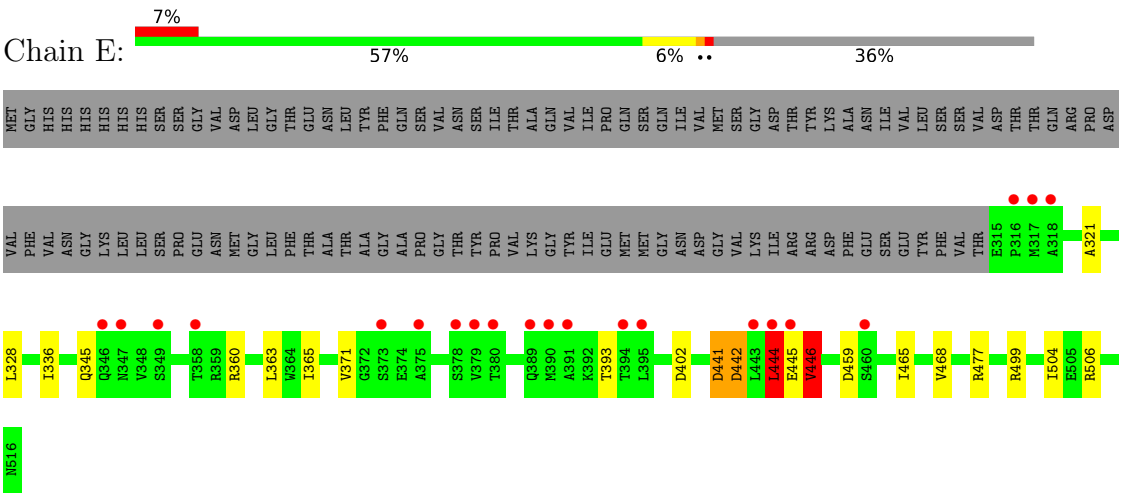




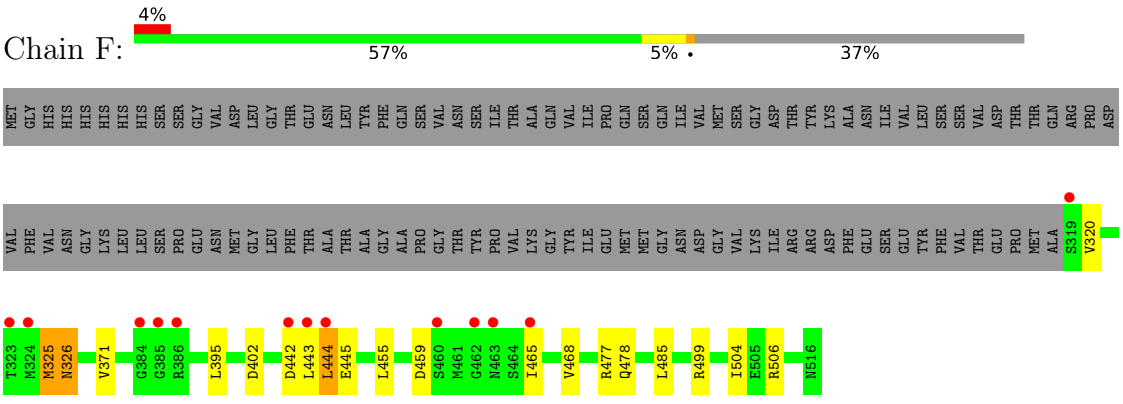
• Molecule 1: T9SS component cytoplasmic membrane protein PorM



• Molecule 1: T9SS component cytoplasmic membrane protein PorM

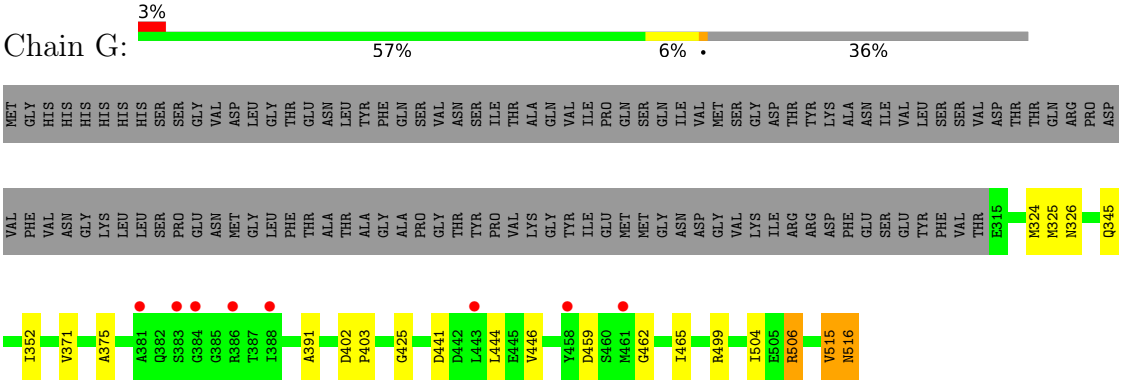


• Molecule 1: T9SS component cytoplasmic membrane protein PorM



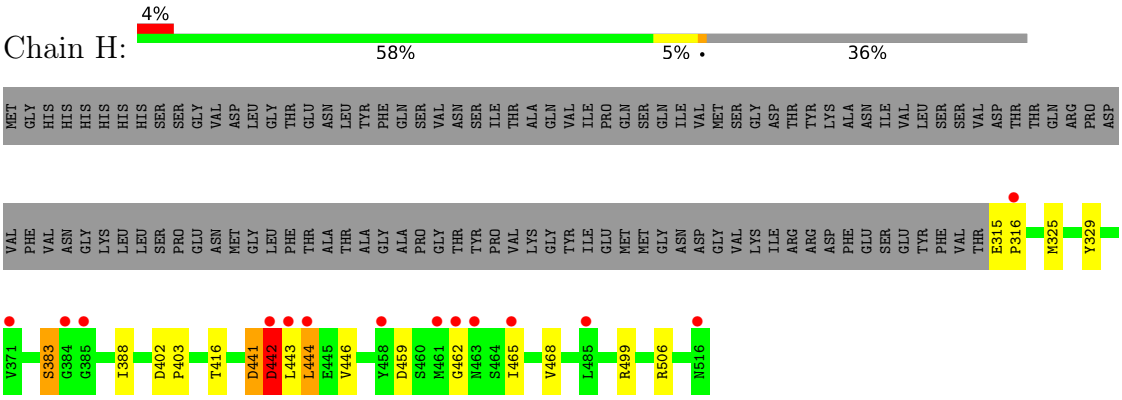
• Molecule 1: T9SS component cytoplasmic membrane protein PorM

Chain G:



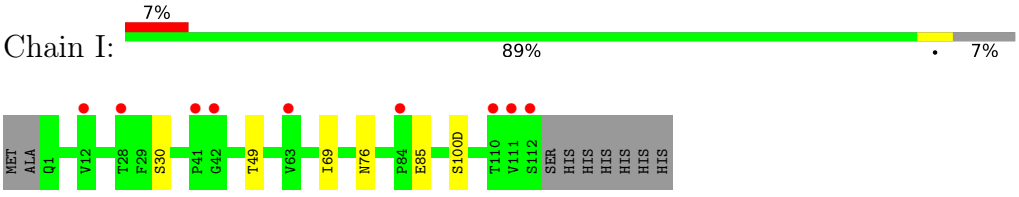
• Molecule 1: T9SS component cytoplasmic membrane protein PorM

Chain H:



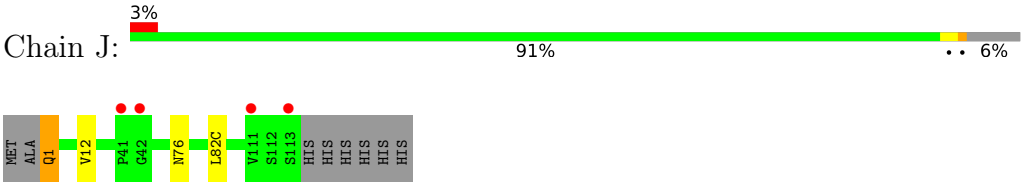
• Molecule 2: nb130

Chain I:



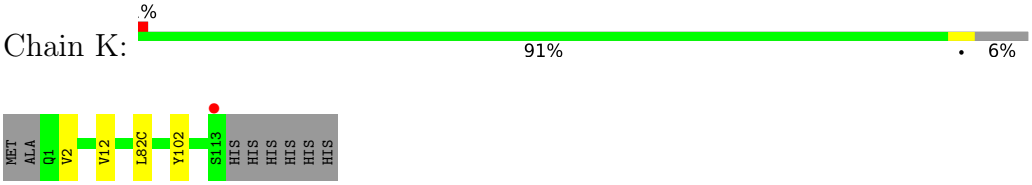
• Molecule 2: nb130

Chain J:



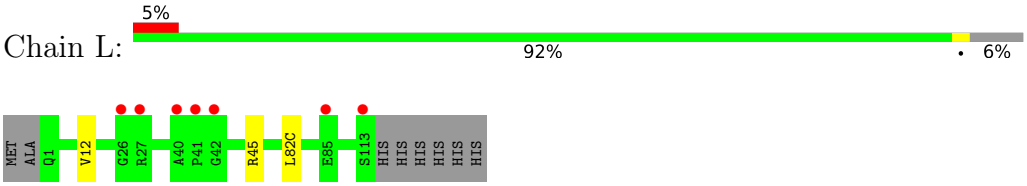
• Molecule 2: nb130

Chain K:



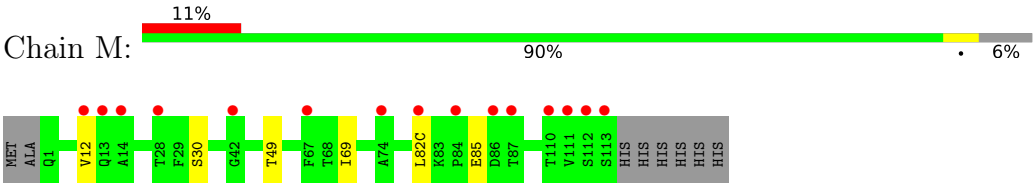
• Molecule 2: nb130

Chain L:



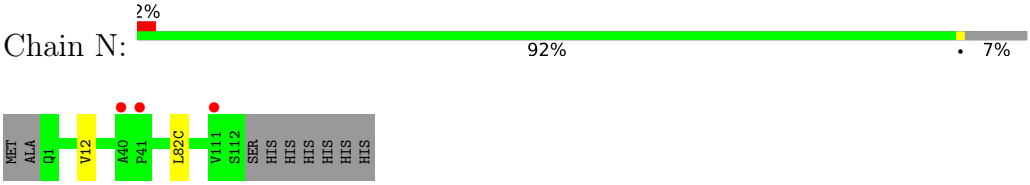
• Molecule 2: nb130

Chain M:



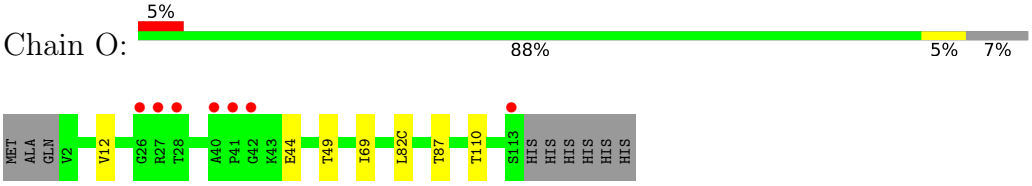
• Molecule 2: nb130

Chain N:



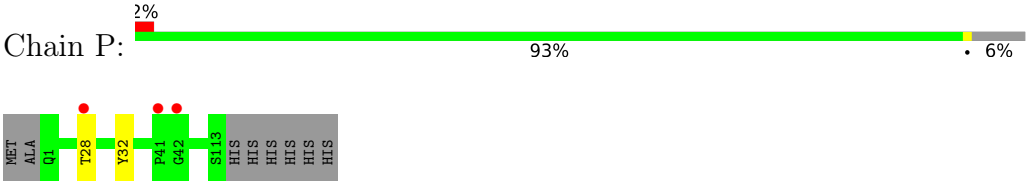
• Molecule 2: nb130

Chain O:



• Molecule 2: nb130

Chain P:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	D	444	LEU	C-N-CA	6.25	137.32	121.70
1	H	316	PRO	C-N-CA	6.21	137.22	121.70
1	H	444	LEU	C-N-CA	6.08	136.89	121.70
1	F	444	LEU	C-N-CA	6.02	136.74	121.70
1	D	391	ALA	C-N-CA	5.89	136.43	121.70
1	G	515	VAL	C-N-CA	5.64	135.79	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	442	ASP	N-CA-C	-5.56	95.99	111.00
1	D	515	VAL	C-N-CA	5.30	134.96	121.70
1	B	444	LEU	C-N-CA	5.20	134.69	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:D:322:PRO:O	1:D:325:MET:HB3	1.89	0.72
1:B:459:ASP:HB3	1:B:465:ILE:HD11	1.71	0.72
1:E:402:ASP:OD1	1:E:506:ARG:HD3	1.88	0.72
1:B:376:ILE:HG13	1:B:394:THR:HG22	1.73	0.71
1:A:402:ASP:OD1	1:A:506:ARG:HD3	1.91	0.69
1:G:325:MET:HB3	1:H:325:MET:HB3	1.74	0.69
1:B:444:LEU:HB2	1:B:445:GLU:HA	1.73	0.69
1:D:402:ASP:OD1	1:D:506:ARG:HD3	1.94	0.67
1:E:371:VAL:HG21	1:E:504:ILE:CD1	2.23	0.67
1:D:391:ALA:HA	1:D:392:LYS:HB2	1.75	0.67
1:G:402:ASP:OD1	1:G:506:ARG:HD3	1.95	0.67
1:H:442:ASP:HB2	1:H:443:LEU:HA	1.77	0.66
1:B:327:VAL:HG12	1:B:396:ARG:HG3	1.77	0.66
1:F:402:ASP:OD1	1:F:506:ARG:HD3	1.95	0.65
1:D:442:ASP:HB2	3:D:636:HOH:O	1.94	0.65
1:E:459:ASP:HB3	1:E:465:ILE:HD11	1.79	0.65
1:D:442:ASP:HB3	1:D:443:LEU:CB	2.28	0.64
1:F:371:VAL:HG21	1:F:504:ILE:HD11	1.79	0.63
1:A:444:LEU:HB2	1:A:446:VAL:HG23	1.81	0.62
2:J:1:GLN:HE21	2:J:1:GLN:N	1.97	0.62
1:H:402:ASP:OD1	1:H:506:ARG:HD3	1.99	0.61
1:E:444:LEU:HA	1:E:446:VAL:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:ILE:HG12	1:D:394:THR:HG22	1.82	0.61
1:E:328:LEU:HD21	1:E:336:ILE:HD11	1.84	0.60
1:B:315:GLU:HB2	1:B:316:PRO:HD3	1.86	0.58
1:E:441:ASP:O	1:E:442:ASP:HB2	2.03	0.58
1:B:363:LEU:HD23	1:B:364:TRP:N	2.20	0.56
2:K:2:VAL:HG12	2:K:102:TYR:CG	2.41	0.55
1:E:321:ALA:HB1	1:F:325:MET:CE	2.36	0.55
1:G:444:LEU:HB3	1:G:446:VAL:HG23	1.89	0.55
1:G:324:MET:HE1	1:H:444:LEU:HD21	1.88	0.54
1:H:444:LEU:HB3	1:H:446:VAL:HG23	1.89	0.54
1:D:442:ASP:HB3	1:D:443:LEU:HB3	1.87	0.54
1:H:383:SER:HB2	1:H:388:ILE:HD11	1.88	0.54
2:O:49:THR:HG23	2:O:69:ILE:HD12	1.88	0.54
1:C:505:GLU:C	1:C:506:ARG:HG3	2.28	0.53
1:D:442:ASP:HB3	1:D:443:LEU:HB2	1.91	0.53
1:C:325:MET:HB3	1:D:325:MET:HA	1.90	0.53
1:F:459:ASP:HB3	1:F:465:ILE:HD11	1.90	0.52
1:A:449:THR:HG23	3:A:681:HOH:O	2.09	0.52
1:B:441:ASP:HB3	1:B:442:ASP:O	2.11	0.51
1:F:326:ASN:HA	1:F:395:LEU:HD22	1.92	0.51
1:H:459:ASP:HB3	1:H:465:ILE:HD11	1.91	0.50
1:F:371:VAL:HG21	1:F:504:ILE:CD1	2.42	0.50
1:G:371:VAL:HG21	1:G:504:ILE:CD1	2.40	0.49
2:O:12:VAL:HG11	2:O:82(C):LEU:HD13	1.95	0.48
2:L:12:VAL:HG11	2:L:82(C):LEU:HD13	1.94	0.48
1:B:391:ALA:CA	1:B:392:LYS:HB2	2.40	0.48
2:J:12:VAL:HG11	2:J:82(C):LEU:HD13	1.96	0.48
2:K:12:VAL:HG11	2:K:82(C):LEU:HD13	1.96	0.48
1:G:403:PRO:HD2	1:G:506:ARG:HD2	1.95	0.47
1:H:444:LEU:CB	1:H:446:VAL:HG23	2.45	0.47
1:A:459:ASP:HB3	1:A:465:ILE:HD11	1.97	0.47
1:D:403:PRO:HD2	1:D:506:ARG:HD2	1.97	0.47
1:B:444:LEU:HB2	1:B:445:GLU:CA	2.45	0.47
1:D:459:ASP:HB3	1:D:465:ILE:HD11	1.97	0.47
2:N:12:VAL:HG11	2:N:82(C):LEU:HD13	1.97	0.47
1:G:462:GLY:HA2	1:H:462:GLY:HA2	1.97	0.46
2:M:12:VAL:HG11	2:M:82(C):LEU:HD13	1.96	0.46
2:J:1:GLN:HE21	2:J:1:GLN:H1	1.62	0.46
1:A:423:ARG:HB3	1:A:516:ASN:HB2	1.98	0.46
2:M:49:THR:HG23	2:M:69:ILE:HD12	1.96	0.46
1:E:321:ALA:HB1	1:F:325:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:455:LEU:HD12	1:F:478:GLN:HB3	1.99	0.45
1:A:320:VAL:HG13	1:B:336:ILE:HG21	1.99	0.45
1:B:353:ASN:HD21	1:B:376:ILE:HD13	1.82	0.45
1:H:442:ASP:CB	1:H:443:LEU:HA	2.44	0.45
1:G:391:ALA:HB2	1:H:315:GLU:O	2.18	0.44
1:B:359:ARG:HD3	2:L:45:ARG:HH21	1.82	0.44
1:A:444:LEU:HB2	1:A:446:VAL:CG2	2.46	0.44
1:D:442:ASP:CB	1:D:443:LEU:HB3	2.48	0.43
1:E:360:ARG:HD3	1:E:365:ILE:HG13	1.99	0.43
1:H:403:PRO:HD2	1:H:506:ARG:HD2	2.00	0.43
1:B:328:LEU:CD2	1:B:336:ILE:HD11	2.49	0.43
1:B:442:ASP:HB3	1:B:443:LEU:HA	2.00	0.42
1:G:325:MET:CE	1:H:329:TYR:CE2	3.01	0.42
1:G:425:GLY:CA	1:G:516:ASN:HB2	2.28	0.42
1:A:323:THR:HB	1:C:412:VAL:O	2.19	0.42
2:P:28:THR:HG23	2:P:32:TYR:CE2	2.55	0.42
1:A:325:MET:HE1	1:B:321:ALA:HB1	2.01	0.42
1:A:320:VAL:HG22	1:B:338:ILE:HG12	2.02	0.42
1:G:425:GLY:HA2	1:G:516:ASN:CB	2.28	0.42
2:I:49:THR:HG23	2:I:69:ILE:HD12	2.02	0.42
1:D:391:ALA:HA	1:D:392:LYS:CB	2.46	0.41
1:G:352:ILE:HD11	1:G:375:ALA:HB1	2.02	0.41
2:O:87:THR:HG23	2:O:110:THR:HA	2.03	0.41
1:E:393:THR:HG21	1:F:320:VAL:HB	2.02	0.41
1:G:444:LEU:HB3	1:G:446:VAL:CG2	2.51	0.41
1:H:442:ASP:CB	1:H:443:LEU:CA	2.98	0.41
1:A:385:GLY:HA3	1:E:477:ARG:HH22	1.85	0.41
1:B:396:ARG:H	1:B:396:ARG:HG2	1.40	0.40
1:B:505:GLU:C	1:B:506:ARG:HG3	2.40	0.40
1:B:459:ASP:HB3	1:B:465:ILE:CD1	2.48	0.40
1:G:515:VAL:CG1	1:G:516:ASN:HB3	2.51	0.40

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
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

All (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
1	F	445	GLU
1	H	442	ASP
1	B	441	ASP
1	D	383	SER
1	D	392	LYS
1	E	441	ASP
1	G	441	ASP
1	D	442	ASP
1	H	383	SER

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Mol	Chain	Res	Type
1	F	326	ASN
1	F	443	LEU
1	H	441	ASP
1	B	383	SER
1	B	385	GLY
1	D	445	GLU
1	C	441	ASP
1	F	444	LEU
1	E	446	VAL

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%)	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
2	P	103/110 (94%)	103 (100%)	0	100	100
All	All	2135/2976 (72%)	2093 (98%)	42 (2%)	55	60

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	GLN
1	A	374	GLU
1	A	444	LEU
1	A	452	LYS
1	A	499	ARG
1	B	396	ARG
1	B	499	ARG
1	B	506	ARG
1	C	443	LEU
1	C	463	ASN
1	C	468	VAL
1	C	499	ARG
1	C	506	ARG
1	D	390	MET
1	E	345	GLN
1	E	363	LEU
1	E	444	LEU
1	E	446	VAL
1	E	468	VAL
1	E	499	ARG
1	F	325	MET
1	F	468	VAL
1	F	477	ARG
1	F	485	LEU
1	F	499	ARG
1	G	326	ASN
1	G	345	GLN
1	G	499	ARG
1	G	506	ARG
1	G	516	ASN
1	H	416	THR
1	H	468	VAL
1	H	499	ARG
2	I	30	SER
2	I	76	ASN
2	I	85	GLU
2	I	100(D)	SER
2	J	1	GLN
2	J	76	ASN
2	M	30	SER
2	M	85	GLU
2	O	44	GLU

Sometimes 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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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, 95^{th} 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%)

All (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

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Mol	Chain	Res	Type	RSRZ
1	G	383	SER	5.9
2	L	42	GLY	5.7
2	O	42	GLY	5.7
1	B	343	VAL	5.4
1	B	339	ALA	5.3
1	E	380	THR	5.2
1	B	460	SER	5.0
2	O	40	ALA	5.0
1	B	443	LEU	4.9
1	F	444	LEU	4.8
1	B	351	THR	4.7
1	H	443	LEU	4.7
1	G	388	ILE	4.6
2	M	82(C)	LEU	4.6
2	M	111	VAL	4.5
2	M	14	ALA	4.5
1	H	444	LEU	4.5
2	I	42	GLY	4.4
2	L	41	PRO	4.3
1	A	463	ASN	4.3
1	F	443	LEU	4.2
2	N	41	PRO	4.2
1	H	462	GLY	4.2
1	F	460	SER	4.2
1	E	346	GLN	4.0
2	L	40	ALA	4.0
1	E	389	GLN	3.9
1	B	390	MET	3.9
1	E	379	VAL	3.9
1	B	373	SER	3.9
1	E	443	LEU	3.9
2	I	111	VAL	3.8
1	B	462	GLY	3.8
1	D	387	THR	3.8
1	E	375	ALA	3.8
1	B	332	ILE	3.7
1	B	375	ALA	3.7
2	L	113	SER	3.6
2	M	112	SER	3.6
1	H	442	ASP	3.6
1	E	391	ALA	3.5
1	C	386	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	461	MET	3.5
1	F	319	SER	3.5
1	G	384	GLY	3.5
1	B	342	GLY	3.3
2	J	113	SER	3.2
1	B	352	ILE	3.2
1	B	442	ASP	3.2
1	A	465	ILE	3.2
1	E	390	MET	3.2
1	F	463	ASN	3.2
2	I	12	VAL	3.2
1	B	377	ILE	3.2
1	C	412	VAL	3.1
1	F	385	GLY	3.1
2	M	13	GLN	3.1
1	H	465	ILE	3.1
1	B	465	ILE	3.1
1	F	462	GLY	3.0
1	E	347	ASN	3.0
1	F	324	MET	3.0
1	B	391	ALA	3.0
1	F	465	ILE	3.0
1	A	458	TYR	3.0
1	A	462	GLY	2.9
1	G	461	MET	2.9
1	E	378	SER	2.9
1	E	444	LEU	2.9
2	I	41	PRO	2.9
1	E	318	ALA	2.9
1	B	346	GLN	2.9
2	I	84	PRO	2.9
1	F	323	THR	2.9
2	M	84	PRO	2.9
1	B	379	VAL	2.8
1	H	371	VAL	2.8
2	N	111	VAL	2.8
1	A	324	MET	2.8
1	H	316	PRO	2.8
1	C	385	GLY	2.8
1	E	373	SER	2.8
1	B	461	MET	2.8
1	A	319	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	M	86	ASP	2.7
1	C	383	SER	2.7
1	B	353	ASN	2.7
2	M	74	ALA	2.7
2	O	27	ARG	2.7
1	B	350	ALA	2.6
2	P	28	THR	2.6
1	B	371	VAL	2.6
2	L	27	ARG	2.6
2	N	40	ALA	2.6
1	B	316	PRO	2.6
1	D	317	MET	2.6
1	E	317	MET	2.6
2	O	28	THR	2.6
2	O	113	SER	2.6
1	B	395	LEU	2.6
2	M	113	SER	2.6
1	H	384	GLY	2.5
1	E	316	PRO	2.5
1	D	443	LEU	2.5
1	E	395	LEU	2.5
2	P	42	GLY	2.5
1	H	463	ASN	2.5
1	B	358	THR	2.5
1	C	443	LEU	2.4
2	I	63	VAL	2.4
1	E	394	THR	2.4
2	M	87	THR	2.4
1	G	443	LEU	2.4
1	A	484	ASN	2.4
2	L	26	GLY	2.4
2	M	42	GLY	2.4
2	M	28	THR	2.4
1	H	458	TYR	2.4
2	K	113	SER	2.4
2	I	112	SER	2.3
1	F	384	GLY	2.3
1	H	385	GLY	2.3
2	O	26	GLY	2.3
1	G	386	ARG	2.3
1	B	361	GLY	2.3
1	E	460	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	380	THR	2.3
1	A	460	SER	2.3
1	B	364	TRP	2.3
1	C	318	ALA	2.3
1	E	349	SER	2.3
2	M	67	PHE	2.3
1	B	394	THR	2.3
1	B	441	ASP	2.3
1	B	484	ASN	2.2
2	I	110	THR	2.2
2	M	12	VAL	2.2
2	J	42	GLY	2.2
1	E	358	THR	2.2
2	M	110	THR	2.2
1	C	316	PRO	2.2
2	P	41	PRO	2.2
1	D	316	PRO	2.2
1	D	325	MET	2.2
1	G	458	TYR	2.2
1	B	315	GLU	2.1
2	L	85	GLU	2.1
1	C	415	ASN	2.1
2	J	41	PRO	2.1
1	F	386	ARG	2.1
2	I	28	THR	2.1
1	B	392	LYS	2.1
1	H	485	LEU	2.1
1	H	516	ASN	2.1
1	G	381	ALA	2.1
1	H	461	MET	2.0
1	B	340	VAL	2.0
1	D	445	GLU	2.0
1	D	442	ASP	2.0
2	J	111	VAL	2.0

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 monosaccharides 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.