



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:06 PM BST

PDB ID : 3J6D
EMDB ID: : EMD-1875
Title : Model of the PrgH-PrgK periplasmic rings
Authors : Bergeron, J.R.C.; Strynadka, N.C.J.
Deposited on : 2014-02-14
Resolution : unknown (reported)
Based on PDB ID : 4G1I, 1MKY, 4OYC

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

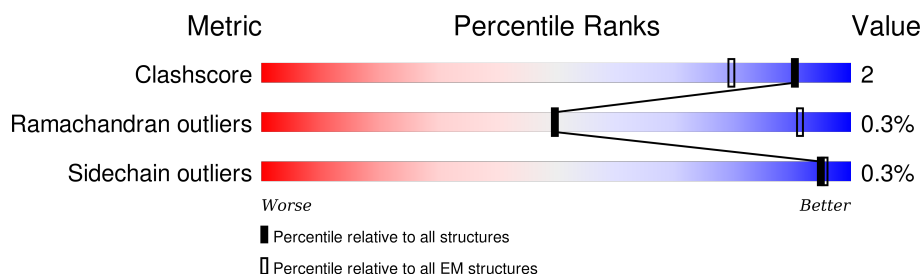
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain	
1	A	392	48%	51%
1	B	392	47%	51%
1	C	392	47%	51%
1	D	392	48%	51%
1	E	392	48%	51%
1	F	392	48%	51%
1	G	392	48%	51%
1	H	392	48%	51%
1	I	392	48%	51%

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Mol	Chain	Length	Quality of chain	
1	J	392		
1	K	392		
1	L	392		
1	M	392		
1	N	392		
1	O	392		
1	P	392		
1	Q	392		
1	R	392		
1	S	392		
1	T	392		
1	U	392		
1	V	392		
1	W	392		
1	X	392		
2	Y	252		
2	Z	252		
2	a	252		
2	b	252		
2	c	252		
2	d	252		
2	e	252		
2	f	252		
2	g	252		
2	h	252		

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Mol	Chain	Length	Quality of chain	
2	i	252		
2	j	252		
2	k	252		
2	l	252		
2	m	252		
2	n	252		
2	o	252		
2	p	252		
2	q	252		
2	r	252		
2	s	252		
2	t	252		
2	u	252		
2	v	252		

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 65952 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein PrgH.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	B	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	C	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	D	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	E	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	F	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	G	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	H	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	I	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	J	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	K	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	L	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	M	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	N	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	O	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	P	191	Total 1578	C 999	N 285	O 290	S 4	0	0
1	Q	191	Total 1578	C 999	N 285	O 290	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	S	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	T	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	U	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	V	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	W	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	X	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		

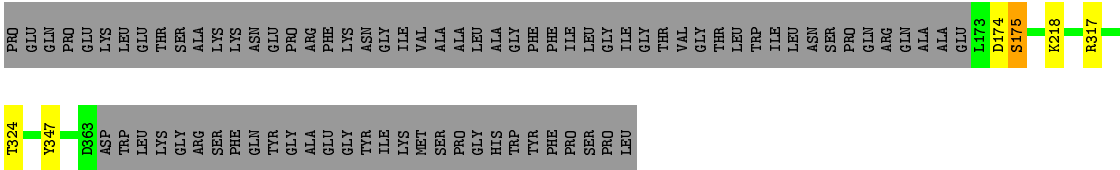
- Molecule 2 is a protein called Pathogenicity 1 island effector protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	b	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	c	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	d	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	e	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	f	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	g	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	h	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	i	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	j	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	k	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	l	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		

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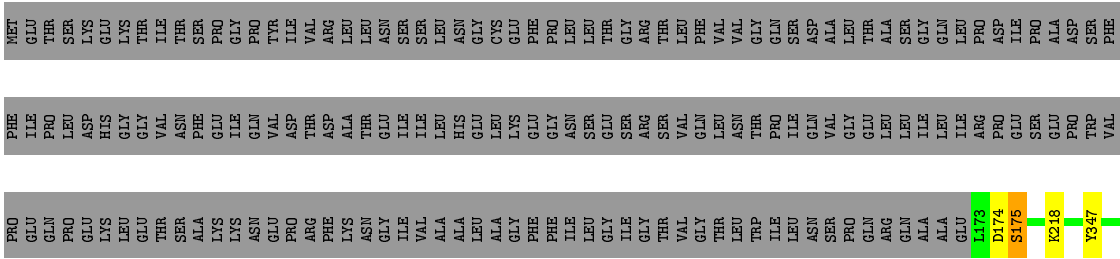
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	m	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	n	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	o	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	p	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	q	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	r	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	s	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	t	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	u	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	v	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	Y	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	Z	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		



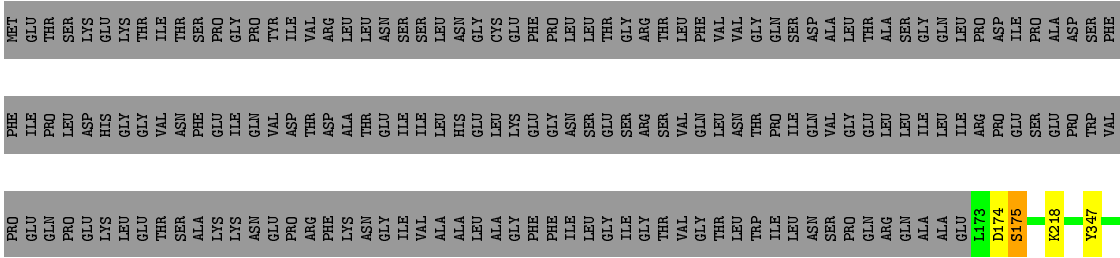
● Molecule 1: Protein PrgH

Chain D: 48% 51%



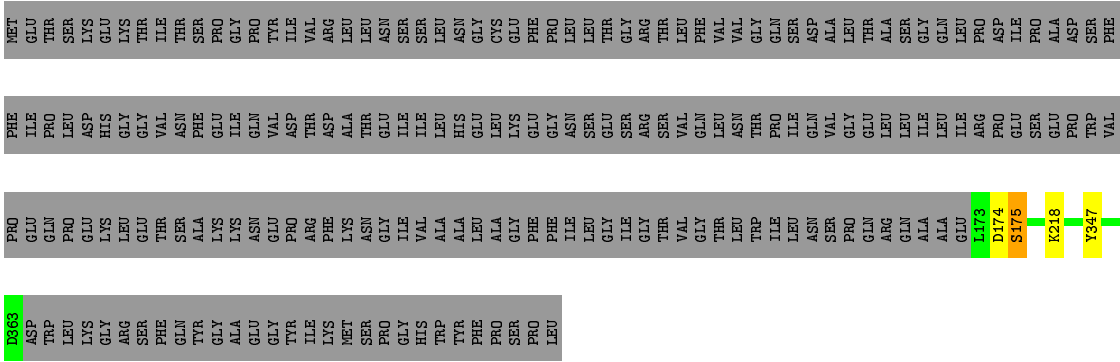
● Molecule 1: Protein PrgH

Chain E: 48% 51%

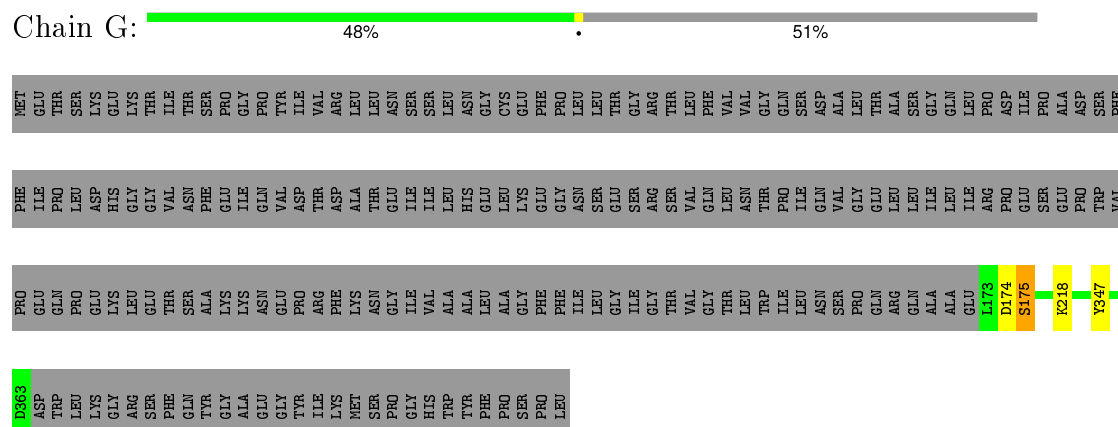


● Molecule 1: Protein PrgH

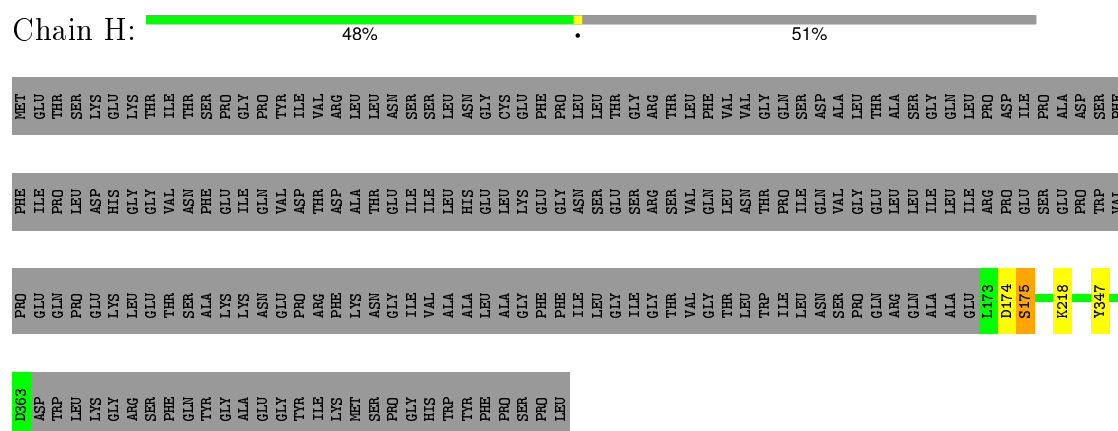
Chain F: 48% 51%



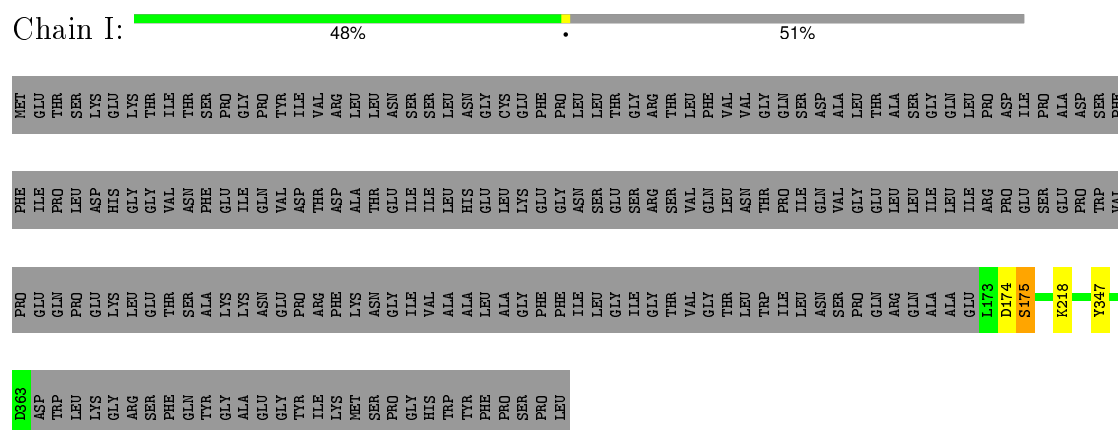
- Molecule 1: Protein PrgH



- Molecule 1: Protein PrgH



- Molecule 1: Protein PrgH



- Molecule 1: Protein PrgH

Chain J: 48% . 51%

1663	ASP	PRO	PHE	MET
	TRP	GLN	ILE	GLU
	LEU	PRO	LEU	SER
	LYS	GLU	ASP	LYS
	GLY	LYS	HIS	GLU
	ARG	LEU	GLY	LYS
	SER	GLU	GLY	THR
	SER	THR	VAL	ILE
	PHE	SER	ASN	THR
	GLN	ALA	PHE	SER
	TYR	LYS	GLU	PRO
	GLY	LYS	ILE	GLY
	ALA	ASN	GLN	PRO
	GLU	GLU	VAL	GLN
	GLY	PRO	ASP	ILE
	TYR	ARG	THR	VAL
	ILE	PHE	ASP	ARG
	LYS	LYS	ALA	LEU
	MET	ASN	THR	LEU
	SER	GLY	GLU	ASN
PRO	ILE	ILE	CYS	
GLY	VAL	LEU	GLU	
HIS	ALA	LEU	PHE	
THR	TRP	GLU	PRO	
TYR	ALA	GLY	LEU	
PHE	LEU	ASN	LEU	
PRO	ALA	GLU	THR	
SER	GLY	SER	GLY	
SER	ILE	SER	ARG	
PRO	GLY	ARG	THR	
LEU	THR	VAL	LEU	
	VAL	GLN	PHE	
	THR	LEU	VAL	
	LEU	ASN	VAL	
	TRP	THR	GLY	
	ILE	PRO	GLN	
	LEU	ILE	SER	
	ASN	GLN	ASP	
	SER	VAL	ALA	
	PRO	GLY	LEU	
	GLN	GLU	THR	
	ARG	LEU	ALA	
	GLN	ILE	SER	
	ALA	LEU	GLN	
	GLU	ILE	LEU	
	1173	ARG	PRO	
	D174	PRO	ASP	
	S175	GLU	ILE	
	+	SER	PRO	
	F218	GLU	ALA	
	+	PRO	ASP	
	Y347	TRP	SER	
	+	VAL	THR	

- Molecule 1: Protein PrgH

Chain K: 48% . 51%

[illegible]

- Molecule 1: Protein PrgH

Chain L: 48% 51%

[illegible]

- Molecule 1: Protein PrgH

Chain M: 48% . 51%

[illegible]

D363 ASP TRP LEU LYS GLY ARG SER PHE GLN TYR GLY ALA GLU GLY TYR ILE LYS MET SER SER PRO GLY HIS TRP TYR PHE PRO SER PRO LEU

- Molecule 1: Protein PrgH

Chain N:  48% . 51%

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

D363 ASP TRP LEU LYS GLY ARG SER PHE GLN TYR GLY ALA GLU GLY TYR ILE LYS MET SER SER PRO GLY HIS TRP TYR PHE PRO SER SER PRO LEU

- Molecule 1: Protein PrgH

Chain O:  48% . 51%

PHE	TLE	PRO	LEU	ASP	HIS	GLY	GLY	VAL	ASN	PHE	GLU	TLE	GLN	VAL	ASP	ASP	ALA	THR	GLU	TLE	TLE	LEU	HIS	GLU	GLU	LEU	LYS	GLU	GLY	ASN	SER	SER	SER	ARG	SER	VAL	VAL	GLN	LEU	LEU	ASN	THR	THR	PRO	TLE	GLN	VAL	GLY	GLY	LEU	LEU	TLE	TLE	ILE	ARG	PRO	GLU	SER	SER	TRP	VAL
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D363 ASP TRP LEU LYS GLY ARG SER PHE GLN TYR GLY ALA GLU GLY TYR ILE LYS MET SER SER PRO GLY HIS TRP TYR PHE PRO SER PRO LEU

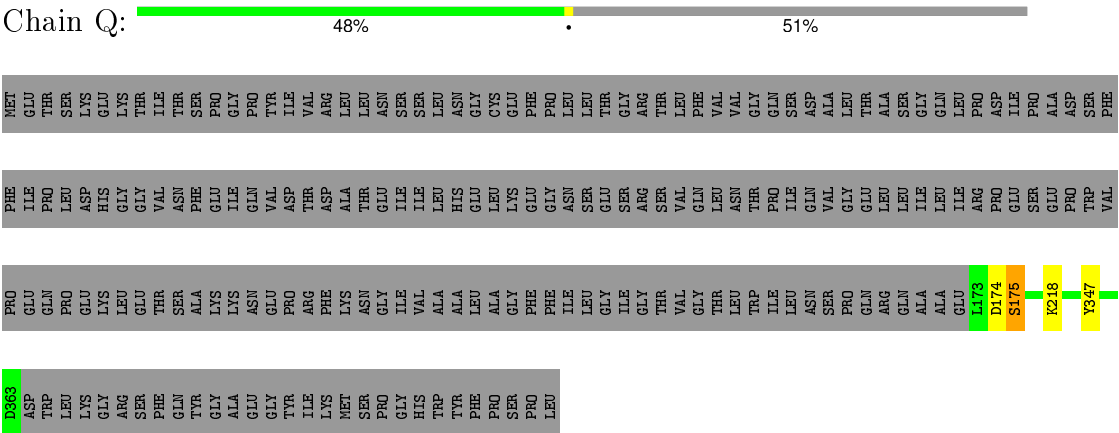
- Molecule 1: Protein PrgH

Chain P:  48% 51%

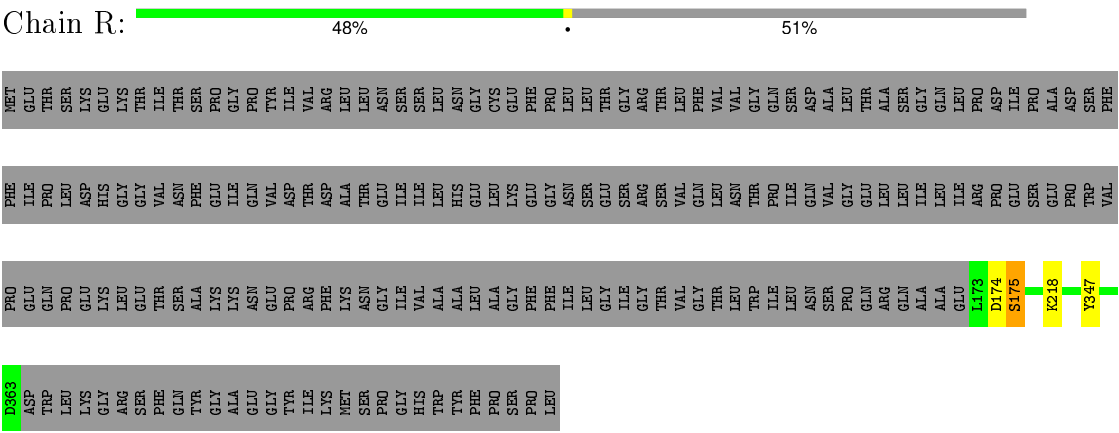
PHE ILE PRO PRO LEU LEU ASP HIS GLY GLY VAL ASN PHE GLU ILE ILE GLN VAL ASP ASP ALA THR GLU ILE ILE LEU LEU HIS GLU LEU LYS GLY GLY ASN SER SER SER ARG SER SER VAL GLN LEU LEU ASN THR THR PRO PRO ILE GLN VAL VAL GLY GLU LEU LEU ILE ILE ARG PRO GLU SER SER GLU PRO TRP VAL

D363 ASP TRP LEU LEU GLY ARG SER PHE GLN TYR GLY ALA GLU GLY TYR ILE LYS MET SER PRO GLY HIS TRP TYR PHE PRO SER PRO LEU

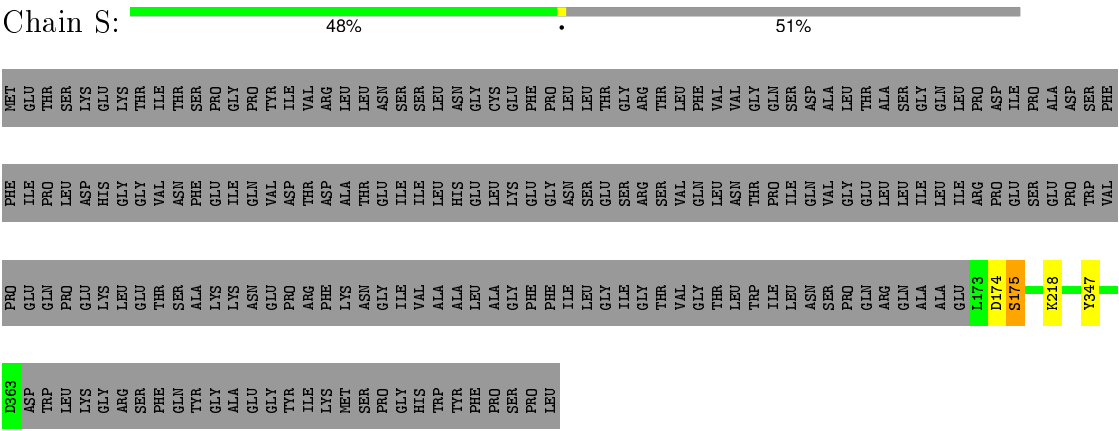
• Molecule 1: Protein PrgH



• Molecule 1: Protein PrgH



• Molecule 1: Protein PrgH



• Molecule 1: Protein PrgH



D363	ASP	TRP	LEU	LYS	GLY	ARG	SER	PHE	GLN	TYR	GLY	ALA	GLU	GLY	TYR	ILE	LYS	MET	SER	SER	PRO	GLY	HIS	TYR	PHE	PRO	SER	PRO	LEU																												
	PHE	ILE	PRO	GLU	LYS	LEU	GLU	THR	SER	ALA	LYS	ASN	GLU	PRO	ARG	PHE	LYS	ASN	GLY	ILE	VAL	ALA	ALA	LEU	PHE	ILE	LEU	GLY	ILE	LEU	GLY	ILE	ARG	PRO	GLU	SER	GLU	PRO	TRP	VAL																	
	PRO	GLU	GLN	PRO	GLU	LEU	GLU	THR	SER	ALA	LYS	ASN	GLU	PRO	ARG	PHE	LYS	ASN	GLY	ILE	VAL	ALA	ALA	LEU	PHE	ILE	LEU	GLY	ILE	LEU	GLY	ILE	ARG	PRO	GLU	SER	GLU	PRO	TRP	VAL																	
	MET	THR	SER	LYS	GLU	THR	ILE	THR	THR	SER	PRO	ARG	VAL	TYR	ILE	VAL	ARG	ASN	SER	GLU	ILE	THR	ALA	LEU	LEU	GLY	PHE	LEU	THR	GLY	THR	ARG	SER	THR	VAL	GLN	ASP	ALA	LEU	THR	SER	GLY	LEU	GLN	LEU	PRO	ASP	ILE	PRO	ASP	SER	PHE					

• Molecule 1: Protein PrgH



T324	GLU	GLN	PRO	GLU	LYS	LEU	GLU	THR	SER	ALA	LYS	ASN	GLU	PRO	ARG	PHE	LYS	ASN	GLY	ILE	VAL	ALA	LEU	ALA	GLY	PHE	PHE	ILE	LEU	GLY	ILE	GLY	THR	THR	VAL	VAL	GLN	LEU	ASN	SER	PRO	GLN	ARG	GLU	THR	THR	ALA	ASP	ILE	PRO	GLU	SER	GLY	CYS	GLU	PHE	PRO	LEU	LEU	THR	GLY	ARG	THR	THR	LEU	LEU	ASN	THR	VAL	VAL	GLN	SER	GLN	GLY	ASP	HIS	GLY	THR	VAL	ASP	ILE	TYR	THR	THR	ASN	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
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• Molecule 1: Protein PrgH



T324	Y347	D363	ASP	TRP	LEU	LYS	GLY	THR	VAL	VAL	ASN	PHE	GLU	ILE	ILE	LYS	MET	SER	PRO	GLY	HIS	TRP	PHE	PRO	SER	PRO	PRO	LEU	LEU	THR	GLY	ILE	ILE	ARG	GLY	THR	VAL	VAL	GLN	LEU	ASN	THR	PRO	ILE	ILE	GLN	VAL	GLY	LEU	LEU	ILE	LEU	ARG	PRO	ASP	ILE	PRO	ALA	ASP	SER	PHE																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
PRO	GLU	GLN	PRO	GLU	LYS	LEU	GLU	THR	SER	ALA	LYS	PHE	LYS	ASN	GLU	PRO	ARG	PHE	LYS	ASN	ASN	GLY	ILE	VAL	ALA	ALA	LEU	ALA	GLY	PHE	PHE	ILE	LEU	GLY	ILE	GLY	THR	VAL	VAL	GLY	THR	LEU	TRAP	ILE	ILE	LEU	ASN	SER	PRO	GLN	ARG	GLN	ALA	ALA	GLU	L173	D174	S175	K218	R317																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		

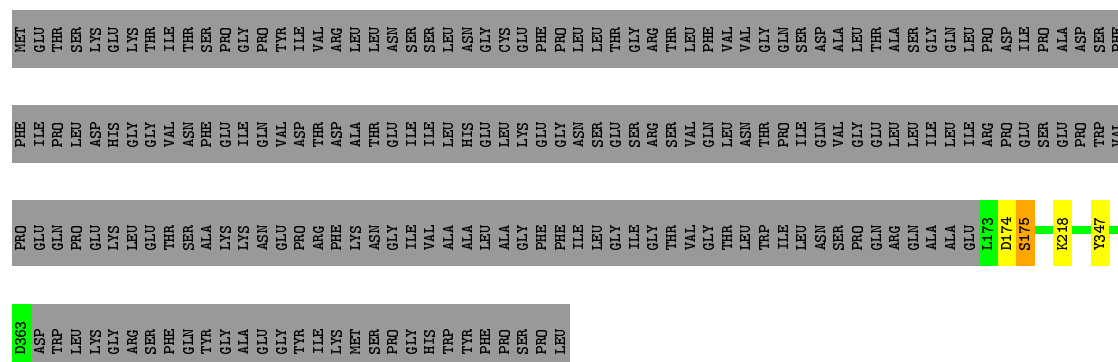
• Molecule 1: Protein PrgH



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

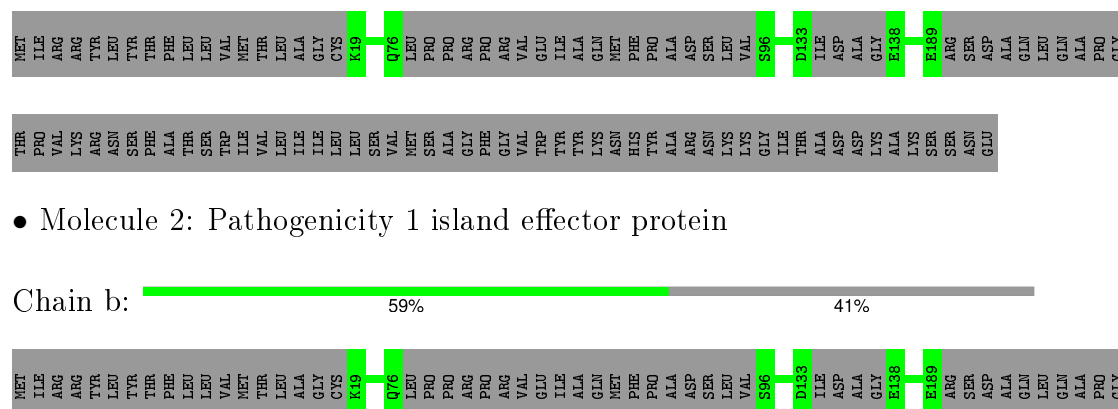
- Molecule 1: Protein PrgH

Chain X: 48% 51%



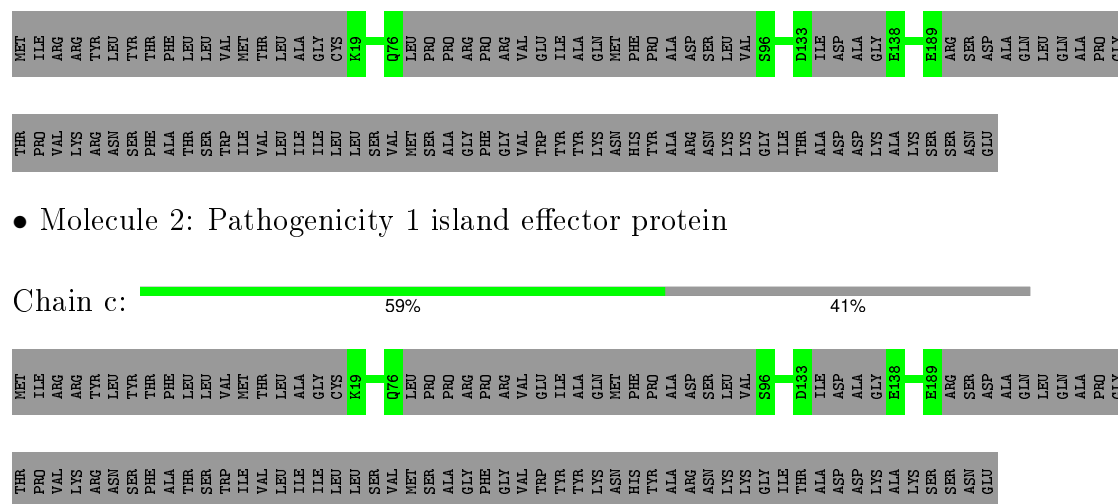
- Molecule 2: Pathogenicity 1 island effector protein

Chain a: 59% 41%



- Molecule 2: Pathogenicity 1 island effector protein

Chain b: 59% 41%




- Molecule 2: Pathogenicity 1 island effector protein

Chain d:  59% 41%

THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	LEU	TRP	ILE	VAL	LEU	ILE	ILE	LEU	LEU	CYS	K19	Q76	LEU	PRO	PRO	ARG	PRO	ARG	VAL	GLU	TRP	TYR	TYR	LYS	ASN	HIS	PHE	PRO	TYR	ASP	SER	LEU	VAL	S96	D133	ILE	ASP	ALA	GLY	E138	E189	ARG	SER	ASN	GLU
MET	ILE	ARG	TRP	LEU	THR	THR	PHE	LEU	LEU	VAL	MET	THR	LEU	ALA	GLY	CYS	K19	Q76	LEU	PRO	PRO	ARG	PRO	ARG	VAL	GLU	ILE	ALA	GLN	MET	PHE	PRO	ASP	SER	LEU	VAL	S96	D133	ILE	ASP	ALA	GLY	E138	E189	ARG	SER	ASP	ALA	GLN	LEU	GLN	ALA	PRO		

- Molecule 2: Pathogenicity 1 island effector protein

Chain e:  59% 41%

THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	LEU	TRP	ILE	VAL	LEU	ILE	ILE	LEU	LEU	CYS	K19	Q76	LEU	PRO	PRO	ARG	PRO	ARG	VAL	GLU	TRP	TYR	TYR	LYS	ASN	HIS	PHE	PRO	TYR	ASP	SER	LEU	VAL	S96	D133	ILE	ASP	ALA	GLY	E138	E189	ARG	SER	ASP	ALA	GLN	LEU	GLN	ALA	PRO	PRO	GLY
MET	ILE	ARG	VAL	ARG	TYR	LEU	THR	THR	PHE	LEU	LEU	VAL	MET	THR	LEU	ALA	GLY	CYS	K19	Q76	LEU	PRO	PRO	ARG	PRO	ARG	VAL	GLU	ILE	ILE	ALA	GLN	MET	PHE	PRO	TYR	ASP	SER	LEU	VAL	S96	D133	ILE	ASP	ALA	GLY	E138	E189	ARG	SER	ASP	ALA	GLN	LEU	GLN	ALA	PRO	PRO	GLY			

- Molecule 2: Pathogenicity 1 island effector protein

Chain f:  59% 41%

THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	LEU	TRP	ILE	VAL	LEU	ILE	ILE	LEU	LEU	CYS	K19	Q76	LEU	PRO	PRO	ARG	PRO	ARG	VAL	GLU	TRP	TYR	TYR	LYS	ASN	HIS	PHE	PRO	TYR	ASP	SER	LEU	VAL	S96	D133	ILE	ASP	ALA	GLY	E138	E189	ARG	SER	ASP	ALA	GLN	LEU	GLN	ALA	PRO	PRO	GLY
MET	ILE	ARG	VAL	ARG	TYR	LEU	THR	THR	PHE	LEU	LEU	VAL	MET	THR	LEU	ALA	GLY	CYS	K19	Q76	LEU	PRO	PRO	ARG	PRO	ARG	VAL	GLU	ILE	ILE	ALA	GLN	MET	PHE	PRO	TYR	ASP	SER	LEU	VAL	S96	D133	ILE	ASP	ALA	GLY	E138	E189	ARG	SER	ASP	ALA	GLN	LEU	GLN	ALA	PRO	PRO	GLY			

- Molecule 2: Pathogenicity 1 island effector protein

Chain g:  59% 41%

MET	ILE	ARG	VAL	ARG	TYR	LEU	THR	THR	PHE	LEU	LEU	VAL	MET	THR	LEU	ALA	GLY	CYS	K19	Q76	LEU	PRO	PRO	ARG	PRO	ARG	VAL	GLU	TRP	ILE	ILE	ALA	GLN	MET	PHE	PRO	TYR	ASP	SER	LEU	VAL	S96	D133	ILE	ASP	ALA	GLY	E138	E189	ARG	SER	ASP	ALA	GLN	LEU	GLN	ALA	PRO	PRO	GLY
THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	LEU	TRP	ILE	VAL	LEU	ILE	ILE	LEU	LEU	CYS	K19	Q76	LEU	PRO	PRO	ARG	PRO	ARG	VAL	GLU	TRP	TYR	TYR	LYS	ASN	HIS	PHE	PRO	TYR	ASP	SER	LEU	VAL	S96	D133	ILE	THR	ALA	ASP	ASP	LYS	ALA	LYS	SER	SER	ASN	GLU			

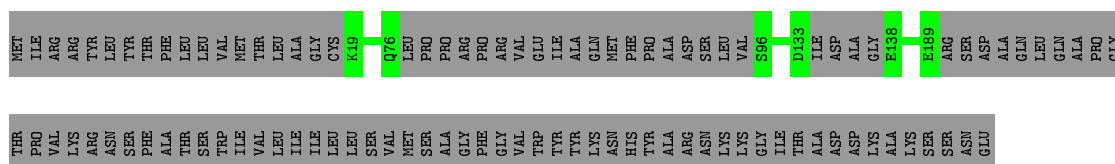
- Molecule 2: Pathogenicity 1 island effector protein

Chain h:  59% 41%

MET	ILE	ARG	ARG	TYR	LEU	TYR	THR	PHE	LEU	LEU	VAL	MET	MET	THR	LEU	ALA	GLY	CYS	K19	Q76	LEU	PRO	PRO	ARG	ARG	PRO	PRO	ARG	VAL	VAL	GLU	ILE	ILE	ALA	GLN	MET	PHE	PRO	PRO	ALA	ASP	SER	LEU	LEU	VAL	S96	D133	ILE	ASP	ASP	ALA	ALA	GLY	E138	E189	ARG	SER	ASP	ALA	ALA	GLN	LEU	GLN	ALA	ALA	PRO
THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	LEU	CYS	K19	Q76	LEU	PRO	PRO	ARG	ARG	PRO	PRO	ARG	VAL	VAL	GLU	TRP	TYR	TYR	LYS	ASN	HIS	PHE	PRO	TYR	ASP	SER	LEU	VAL	S96	D133	ILE	THR	ALA	ASP	ASP	LYS	ALA	LYS	SER	SER	ASN	GLU						

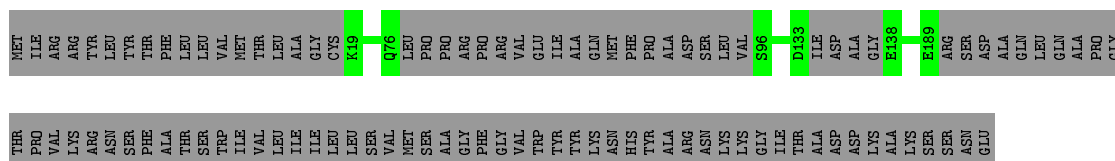
- Molecule 2: Pathogenicity 1 island effector protein

Chain i:  59% 41%



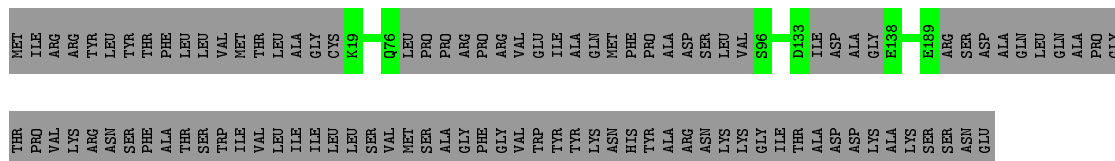
- Molecule 2: Pathogenicity 1 island effector protein

Chain j:



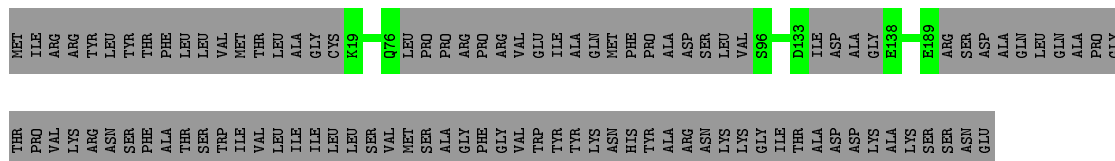
- Molecule 2: Pathogenicity 1 island effector protein

Chain k:



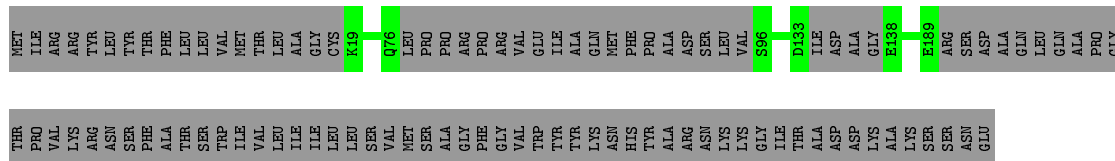
- Molecule 2: Pathogenicity 1 island effector protein

Chain l:



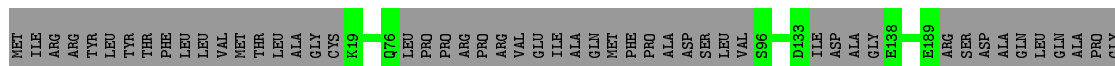
- Molecule 2: Pathogenicity 1 island effector protein

Chain m:



- Molecule 2: Pathogenicity 1 island effector protein

Chain n:



THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	SER	VAL
THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	SER	VAL

• Molecule 2: Pathogenicity 1 island effector protein



MET	ILE	ARG	ARG	TYR	TYR	THR	PHE	LEU	VAL	MET	THR	LEU	ALA	GLY	CYS	K19	Q76	LEU	PRO
MET	ILE	ARG	ARG	TYR	TYR	THR	PHE	LEU	VAL	MET	THR	LEU	ALA	GLY	CYS	K19	Q76	LEU	PRO

THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	SER	VAL
THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	SER	VAL

• Molecule 2: Pathogenicity 1 island effector protein



MET	ILE	ARG	ARG	TYR	TYR	THR	PHE	LEU	VAL	MET	THR	LEU	ALA	GLY	CYS	K19	Q76	LEU	PRO
MET	ILE	ARG	ARG	TYR	TYR	THR	PHE	LEU	VAL	MET	THR	LEU	ALA	GLY	CYS	K19	Q76	LEU	PRO

THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	SER	VAL
THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	SER	VAL

• Molecule 2: Pathogenicity 1 island effector protein



MET	ILE	ARG	ARG	TYR	TYR	THR	PHE	LEU	VAL	MET	THR	LEU	ALA	GLY	CYS	K19	Q76	LEU	PRO
MET	ILE	ARG	ARG	TYR	TYR	THR	PHE	LEU	VAL	MET	THR	LEU	ALA	GLY	CYS	K19	Q76	LEU	PRO

THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	SER	VAL
THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	SER	VAL

• Molecule 2: Pathogenicity 1 island effector protein



MET	ILE	ARG	ARG	TYR	TYR	THR	PHE	LEU	VAL	MET	THR	LEU	ALA	GLY	CYS	K19	Q76	LEU	PRO
MET	ILE	ARG	ARG	TYR	TYR	THR	PHE	LEU	VAL	MET	THR	LEU	ALA	GLY	CYS	K19	Q76	LEU	PRO


THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	SER	VAL
THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	SER	VAL

• Molecule 2: Pathogenicity 1 island effector protein



MET	ILE	ARG	ARG	TYR	TYR	THR	PHE	LEU	VAL	MET	THR	LEU	ALA	GLY	CYS	K19	Q76	LEU	PRO
MET	ILE	ARG	ARG	TYR	TYR	THR	PHE	LEU	VAL	MET	THR	LEU	ALA	GLY	CYS	K19	Q76	LEU	PRO

THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	SER	VAL
THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	SER	VAL

- Chain Z:  56% 41%
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|-----|-----|-----|-----|------|------|------|
| MET | ILE | ARG | ARG | TRR | LEU | THR | PHE | GLY | LEU | VAL | MET | THR | LEU | ALA | GLY | CYS | K19 | H42 | N43 | Y75 | Q76 | LEU | PRO | PRO | ARG | PRO | ARG | VAL | GLU | ILE | ALA | GLN | MET | PHE | PRO | PRO | ALA | ASP | SER | LEU | VAL | S96 | E121 | G122 | V123 | D133 | ILE | ASP | ALA | GLY | E138 | V153 | E155 |
| ARG | SER | ASP | ALA | GLN | LEU | GLN | PRO | GLY | THR | PRO | VAL | LYS | ARG | ASN | SER | PHE | ALA | THR | SER | ILE | VAL | LEU | ILE | LEU | LEU | SER | VAL | SER | ALA | GLY | PHE | GLY | VAL | TRP | TRR | LYS | ASN | THR | LYS | ALA | ARG | ASN | LYS | LYS | GLY | ILE | THR | ALA | ASP | LYS | ALA | LYS | |

SER
ASN
GLU

4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.82	0/1610	0.72	0/2174
1	B	0.82	0/1610	0.72	0/2174
1	C	0.81	0/1610	0.72	0/2174
1	D	0.82	0/1610	0.72	0/2174
1	E	0.81	0/1610	0.72	0/2174
1	F	0.82	0/1610	0.72	0/2174
1	G	0.81	0/1610	0.72	0/2174
1	H	0.82	0/1610	0.72	0/2174
1	I	0.82	0/1610	0.72	0/2174
1	J	0.82	0/1610	0.72	0/2174
1	K	0.82	0/1610	0.72	0/2174
1	L	0.82	0/1610	0.72	0/2174
1	M	0.82	0/1610	0.72	0/2174
1	N	0.82	0/1610	0.72	0/2174
1	O	0.81	0/1610	0.72	0/2174
1	P	0.81	0/1610	0.72	0/2174
1	Q	0.82	0/1610	0.72	0/2174
1	R	0.81	0/1610	0.72	0/2174
1	S	0.82	0/1610	0.72	0/2174
1	T	0.81	0/1610	0.72	0/2174
1	U	0.82	0/1610	0.72	0/2174
1	V	0.82	0/1610	0.72	0/2174
1	W	0.82	0/1610	0.72	0/2174
1	X	0.82	0/1610	0.72	0/2174
2	Y	0.71	0/1189	0.56	0/1606
2	Z	0.71	0/1189	0.56	0/1606
2	a	0.71	0/1189	0.56	0/1606
2	b	0.71	0/1189	0.56	0/1606
2	c	0.71	0/1189	0.56	0/1606
2	d	0.71	0/1189	0.56	0/1606
2	e	0.71	0/1189	0.56	0/1606
2	f	0.71	0/1189	0.56	0/1606
2	g	0.71	0/1189	0.56	0/1606
2	h	0.71	0/1189	0.56	0/1606

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
2	i	0.71	0/1189	0.56	0/1606
2	j	0.71	0/1189	0.56	0/1606
2	k	0.71	0/1189	0.56	0/1606
2	l	0.71	0/1189	0.56	0/1606
2	m	0.71	0/1189	0.56	0/1606
2	n	0.71	0/1189	0.56	0/1606
2	o	0.71	0/1189	0.56	0/1606
2	p	0.71	0/1189	0.56	0/1606
2	q	0.71	0/1189	0.56	0/1606
2	r	0.71	0/1189	0.56	0/1606
2	s	0.71	0/1189	0.56	0/1606
2	t	0.71	0/1189	0.56	0/1606
2	u	0.71	0/1189	0.56	0/1606
2	v	0.71	0/1189	0.56	0/1606
All	All	0.77	0/67176	0.66	0/90720

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1578	0	1565	5	0
1	B	1578	0	1565	7	0
1	C	1578	0	1565	6	0
1	D	1578	0	1565	5	0
1	E	1578	0	1565	5	0
1	F	1578	0	1565	5	0
1	G	1578	0	1565	5	0
1	H	1578	0	1565	5	0
1	I	1578	0	1565	6	0
1	J	1578	0	1565	5	0
1	K	1578	0	1565	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1578	0	1565	6	0
1	M	1578	0	1565	6	0
1	N	1578	0	1565	6	0
1	O	1578	0	1565	5	0
1	P	1578	0	1565	5	0
1	Q	1578	0	1565	6	0
1	R	1578	0	1565	6	0
1	S	1578	0	1565	5	0
1	T	1578	0	1565	5	0
1	U	1578	0	1565	6	0
1	V	1578	0	1565	6	0
1	W	1578	0	1565	6	0
1	X	1578	0	1565	5	0
2	Y	1170	0	1161	6	0
2	Z	1170	0	1161	6	0
2	a	1170	0	1161	0	0
2	b	1170	0	1161	0	0
2	c	1170	0	1161	0	0
2	d	1170	0	1161	0	0
2	e	1170	0	1161	0	0
2	f	1170	0	1161	0	0
2	g	1170	0	1161	0	0
2	h	1170	0	1161	0	0
2	i	1170	0	1161	0	0
2	j	1170	0	1161	0	0
2	k	1170	0	1161	0	0
2	l	1170	0	1161	0	0
2	m	1170	0	1161	0	0
2	n	1170	0	1161	0	0
2	o	1170	0	1161	0	0
2	p	1170	0	1161	0	0
2	q	1170	0	1161	0	0
2	r	1170	0	1161	0	0
2	s	1170	0	1161	0	0
2	t	1170	0	1161	0	0
2	u	1170	0	1161	0	0
2	v	1170	0	1161	0	0
All	All	65952	0	65424	144	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 2.

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:76:GLN:O	2:Y:76:GLN:HG3	2.10	0.52
2:Z:76:GLN:O	2:Z:76:GLN:HG3	2.10	0.51
2:Y:123:VAL:HG13	2:Y:153:VAL:H	1.76	0.50
2:Z:123:VAL:HG13	2:Z:153:VAL:H	1.76	0.50
1:L:174:ASP:CA	1:L:175:SER:CB	2.93	0.47
1:B:174:ASP:CA	1:B:175:SER:CB	2.93	0.47
1:C:174:ASP:CA	1:C:175:SER:CB	2.93	0.47
2:Z:121:GLU:OE1	2:Z:121:GLU:N	2.44	0.47
1:G:174:ASP:CA	1:G:175:SER:CB	2.93	0.47
1:K:174:ASP:CA	1:K:175:SER:CB	2.93	0.47
1:M:174:ASP:CA	1:M:175:SER:CB	2.93	0.47
1:A:174:ASP:CA	1:A:175:SER:CB	2.93	0.47
1:R:174:ASP:CA	1:R:175:SER:CB	2.93	0.47
1:H:174:ASP:CA	1:H:175:SER:CB	2.93	0.47
1:Q:174:ASP:CA	1:Q:175:SER:CB	2.93	0.47
1:K:347:TYR:C	1:K:347:TYR:CD1	2.89	0.47
1:D:174:ASP:CA	1:D:175:SER:CB	2.93	0.47
1:S:174:ASP:CA	1:S:175:SER:CB	2.93	0.47
1:R:347:TYR:CD1	1:R:347:TYR:C	2.89	0.47
1:M:347:TYR:CD1	1:M:347:TYR:C	2.89	0.47
1:F:174:ASP:CA	1:F:175:SER:CB	2.93	0.47
1:T:174:ASP:CA	1:T:175:SER:CB	2.93	0.47
2:Y:133:ASP:O	2:Y:133:ASP:OD1	2.32	0.46
2:Z:133:ASP:O	2:Z:133:ASP:OD1	2.32	0.46
1:T:347:TYR:CD1	1:T:347:TYR:C	2.89	0.46
1:I:347:TYR:CD1	1:I:347:TYR:C	2.89	0.46
1:P:347:TYR:C	1:P:347:TYR:CD1	2.89	0.46
1:X:174:ASP:CA	1:X:175:SER:CB	2.93	0.46
1:N:174:ASP:CA	1:N:175:SER:CB	2.93	0.46
1:P:174:ASP:CA	1:P:175:SER:CB	2.93	0.46
1:J:174:ASP:CA	1:J:175:SER:CB	2.93	0.46
1:O:347:TYR:C	1:O:347:TYR:CD1	2.89	0.46
1:U:174:ASP:CA	1:U:175:SER:CB	2.93	0.46
1:I:174:ASP:CA	1:I:175:SER:CB	2.93	0.46
1:H:347:TYR:C	1:H:347:TYR:CD1	2.89	0.46
1:V:347:TYR:CD1	1:V:347:TYR:C	2.89	0.46
1:G:347:TYR:C	1:G:347:TYR:CD1	2.89	0.46
1:N:347:TYR:CD1	1:N:347:TYR:C	2.89	0.46
1:O:174:ASP:CA	1:O:175:SER:CB	2.93	0.46
1:R:174:ASP:N	1:R:175:SER:CB	2.79	0.46
1:D:174:ASP:N	1:D:175:SER:CB	2.79	0.46
1:F:347:TYR:CD1	1:F:347:TYR:C	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:347:TYR:CD1	1:J:347:TYR:C	2.89	0.46
1:E:174:ASP:CA	1:E:175:SER:CB	2.93	0.46
1:V:174:ASP:CA	1:V:175:SER:CB	2.93	0.46
1:A:174:ASP:N	1:A:175:SER:CB	2.79	0.46
1:U:174:ASP:N	1:U:175:SER:CB	2.79	0.46
1:Q:347:TYR:C	1:Q:347:TYR:CD1	2.89	0.46
1:X:347:TYR:CD1	1:X:347:TYR:C	2.89	0.46
1:X:174:ASP:N	1:X:175:SER:CB	2.79	0.46
1:E:174:ASP:N	1:E:175:SER:CB	2.79	0.46
1:V:174:ASP:N	1:V:175:SER:CB	2.79	0.46
1:D:347:TYR:CD1	1:D:347:TYR:C	2.89	0.46
1:W:174:ASP:CA	1:W:175:SER:CB	2.93	0.46
1:S:174:ASP:N	1:S:175:SER:CB	2.79	0.46
1:N:174:ASP:N	1:N:175:SER:CB	2.79	0.46
1:E:347:TYR:CD1	1:E:347:TYR:C	2.89	0.46
1:B:347:TYR:CD1	1:B:347:TYR:C	2.89	0.46
1:U:347:TYR:C	1:U:347:TYR:CD1	2.89	0.46
1:H:174:ASP:N	1:H:175:SER:CB	2.79	0.46
1:O:174:ASP:N	1:O:175:SER:CB	2.79	0.46
1:L:347:TYR:C	1:L:347:TYR:CD1	2.89	0.46
1:Q:174:ASP:N	1:Q:175:SER:CB	2.79	0.45
1:I:174:ASP:N	1:I:175:SER:CB	2.79	0.45
1:W:347:TYR:C	1:W:347:TYR:CD1	2.89	0.45
1:S:347:TYR:C	1:S:347:TYR:CD1	2.89	0.45
1:C:174:ASP:N	1:C:175:SER:CB	2.79	0.45
1:G:174:ASP:N	1:G:175:SER:CB	2.79	0.45
1:M:174:ASP:N	1:M:175:SER:CB	2.79	0.45
1:A:347:TYR:C	1:A:347:TYR:CD1	2.89	0.45
1:C:347:TYR:CD1	1:C:347:TYR:C	2.89	0.45
1:B:174:ASP:N	1:B:175:SER:CB	2.79	0.45
1:J:174:ASP:N	1:J:175:SER:CB	2.79	0.45
1:K:174:ASP:N	1:K:175:SER:CB	2.79	0.45
1:T:174:ASP:N	1:T:175:SER:CB	2.79	0.45
1:P:174:ASP:N	1:P:175:SER:CB	2.79	0.45
1:F:174:ASP:N	1:F:175:SER:CB	2.79	0.45
1:W:174:ASP:N	1:W:175:SER:CB	2.79	0.45
1:L:174:ASP:N	1:L:175:SER:CB	2.79	0.45
1:E:174:ASP:HA	1:E:175:SER:HB3	2.00	0.44
1:L:174:ASP:HA	1:L:175:SER:HB3	2.00	0.44
1:G:174:ASP:HA	1:G:175:SER:HB3	2.00	0.44
1:J:174:ASP:HA	1:J:175:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:174:ASP:HA	1:K:175:SER:HB3	2.00	0.44
1:M:174:ASP:HA	1:M:175:SER:HB3	2.00	0.44
1:F:174:ASP:HA	1:F:175:SER:HB3	2.00	0.44
1:O:174:ASP:HA	1:O:175:SER:HB3	2.00	0.44
1:C:174:ASP:HA	1:C:175:SER:HB3	2.00	0.44
1:H:174:ASP:HA	1:H:175:SER:HB3	2.00	0.44
1:D:174:ASP:HA	1:D:175:SER:HB3	2.00	0.44
1:N:174:ASP:HA	1:N:175:SER:HB3	2.00	0.44
1:B:174:ASP:HA	1:B:175:SER:HB3	2.00	0.44
1:P:174:ASP:HA	1:P:175:SER:HB3	2.00	0.44
1:I:174:ASP:HA	1:I:175:SER:HB3	2.00	0.44
1:R:174:ASP:HA	1:R:175:SER:HB3	2.00	0.44
1:Q:174:ASP:HA	1:Q:175:SER:HB3	2.00	0.44
1:X:174:ASP:HA	1:X:175:SER:HB3	2.00	0.44
1:A:174:ASP:HA	1:A:175:SER:HB3	2.00	0.44
1:V:174:ASP:HA	1:V:175:SER:HB3	2.00	0.44
1:W:174:ASP:HA	1:W:175:SER:HB3	2.00	0.44
1:T:174:ASP:HA	1:T:175:SER:HB3	2.00	0.43
1:S:174:ASP:HA	1:S:175:SER:HB3	2.00	0.43
1:U:174:ASP:HA	1:U:175:SER:HB3	2.00	0.43
2:Y:75:TYR:O	2:Y:76:GLN:C	2.58	0.42
1:B:174:ASP:N	1:B:175:SER:HB3	2.35	0.42
1:X:174:ASP:N	1:X:175:SER:HB3	2.35	0.42
1:C:174:ASP:N	1:C:175:SER:HB3	2.35	0.41
1:A:174:ASP:N	1:A:175:SER:HB3	2.35	0.41
1:W:174:ASP:N	1:W:175:SER:HB3	2.35	0.41
1:V:174:ASP:N	1:V:175:SER:HB3	2.35	0.41
1:D:174:ASP:N	1:D:175:SER:HB3	2.35	0.41
2:Y:42:HIS:O	2:Y:43:ASN:HB2	2.20	0.41
1:U:174:ASP:N	1:U:175:SER:HB3	2.35	0.41
1:Q:174:ASP:N	1:Q:175:SER:HB3	2.35	0.41
2:Y:121:GLU:OE1	2:Y:121:GLU:N	2.44	0.41
1:G:174:ASP:N	1:G:175:SER:HB3	2.35	0.41
1:R:174:ASP:N	1:R:175:SER:HB3	2.35	0.41
1:F:174:ASP:N	1:F:175:SER:HB3	2.35	0.41
1:P:174:ASP:N	1:P:175:SER:HB3	2.35	0.41
1:E:174:ASP:N	1:E:175:SER:HB3	2.35	0.41
2:Z:42:HIS:O	2:Z:43:ASN:HB2	2.20	0.41
1:S:174:ASP:N	1:S:175:SER:HB3	2.35	0.41
1:T:174:ASP:N	1:T:175:SER:HB3	2.35	0.41
1:O:174:ASP:N	1:O:175:SER:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:174:ASP:HA	1:M:175:SER:C	2.42	0.40
1:H:174:ASP:N	1:H:175:SER:HB3	2.35	0.40
1:N:174:ASP:N	1:N:175:SER:HB3	2.35	0.40
1:N:174:ASP:HA	1:N:175:SER:C	2.42	0.40
1:B:317:ARG:O	1:B:324:THR:N	2.55	0.40
1:U:317:ARG:O	1:U:324:THR:N	2.55	0.40
1:L:174:ASP:HA	1:L:175:SER:C	2.42	0.40
1:L:174:ASP:N	1:L:175:SER:HB3	2.35	0.40
1:B:174:ASP:HA	1:B:175:SER:C	2.42	0.40
1:R:174:ASP:HA	1:R:175:SER:C	2.42	0.40
2:Z:75:TYR:O	2:Z:76:GLN:C	2.58	0.40
1:M:174:ASP:N	1:M:175:SER:HB3	2.35	0.40
1:I:174:ASP:N	1:I:175:SER:HB3	2.35	0.40
1:V:317:ARG:O	1:V:324:THR:N	2.55	0.40
1:K:174:ASP:N	1:K:175:SER:HB3	2.35	0.40
1:Q:174:ASP:HA	1:Q:175:SER:C	2.42	0.40
1:J:174:ASP:N	1:J:175:SER:HB3	2.35	0.40
1:I:174:ASP:HA	1:I:175:SER:C	2.42	0.40
1:W:174:ASP:HA	1:W:175:SER:C	2.42	0.40
1:C:317:ARG:O	1:C:324:THR:N	2.55	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	B	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	C	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	D	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	F	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	G	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	H	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	I	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	J	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	K	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	L	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	M	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	N	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	O	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	P	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	Q	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	R	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	S	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	T	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	U	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	V	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	W	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
1	X	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	34	34
2	Y	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	Z	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	a	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	b	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	c	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	d	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	e	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	f	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	g	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	h	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	i	142/252 (56%)	129 (91%)	13 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	j	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	k	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	l	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	m	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	n	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	o	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	p	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	q	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	r	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	s	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	t	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	u	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
2	v	142/252 (56%)	129 (91%)	13 (9%)	0	100	100
All	All	7944/15456 (51%)	7272 (92%)	648 (8%)	24 (0%)	50	46

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	LYS
1	B	218	LYS
1	C	218	LYS
1	D	218	LYS
1	E	218	LYS
1	F	218	LYS
1	G	218	LYS
1	H	218	LYS
1	I	218	LYS
1	J	218	LYS
1	K	218	LYS
1	L	218	LYS
1	M	218	LYS
1	N	218	LYS
1	O	218	LYS
1	P	218	LYS
1	Q	218	LYS
1	R	218	LYS
1	S	218	LYS

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Mol	Chain	Res	Type
1	T	218	LYS
1	U	218	LYS
1	V	218	LYS
1	W	218	LYS
1	X	218	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	B	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	C	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	D	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	E	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	F	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	G	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	H	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	I	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	J	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	K	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	L	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	M	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	N	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	O	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	P	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	Q	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	R	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	S	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	T	165/337 (49%)	164 (99%)	1 (1%)	90	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	V	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	W	165/337 (49%)	164 (99%)	1 (1%)	90	90
1	X	165/337 (49%)	164 (99%)	1 (1%)	90	90
2	Y	128/215 (60%)	128 (100%)	0	100	100
2	Z	128/215 (60%)	128 (100%)	0	100	100
2	a	128/215 (60%)	128 (100%)	0	100	100
2	b	128/215 (60%)	128 (100%)	0	100	100
2	c	128/215 (60%)	128 (100%)	0	100	100
2	d	128/215 (60%)	128 (100%)	0	100	100
2	e	128/215 (60%)	128 (100%)	0	100	100
2	f	128/215 (60%)	128 (100%)	0	100	100
2	g	128/215 (60%)	128 (100%)	0	100	100
2	h	128/215 (60%)	128 (100%)	0	100	100
2	i	128/215 (60%)	128 (100%)	0	100	100
2	j	128/215 (60%)	128 (100%)	0	100	100
2	k	128/215 (60%)	128 (100%)	0	100	100
2	l	128/215 (60%)	128 (100%)	0	100	100
2	m	128/215 (60%)	128 (100%)	0	100	100
2	n	128/215 (60%)	128 (100%)	0	100	100
2	o	128/215 (60%)	128 (100%)	0	100	100
2	p	128/215 (60%)	128 (100%)	0	100	100
2	q	128/215 (60%)	128 (100%)	0	100	100
2	r	128/215 (60%)	128 (100%)	0	100	100
2	s	128/215 (60%)	128 (100%)	0	100	100
2	t	128/215 (60%)	128 (100%)	0	100	100
2	u	128/215 (60%)	128 (100%)	0	100	100
2	v	128/215 (60%)	128 (100%)	0	100	100
All	All	7032/13248 (53%)	7008 (100%)	24 (0%)	95	94

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	SER
1	B	175	SER
1	C	175	SER
1	D	175	SER
1	E	175	SER
1	F	175	SER
1	G	175	SER
1	H	175	SER
1	I	175	SER
1	J	175	SER
1	K	175	SER
1	L	175	SER
1	M	175	SER
1	N	175	SER
1	O	175	SER
1	P	175	SER
1	Q	175	SER
1	R	175	SER
1	S	175	SER
1	T	175	SER
1	U	175	SER
1	V	175	SER
1	W	175	SER
1	X	175	SER

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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 [i](#)

There are no chain breaks in this entry.