



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

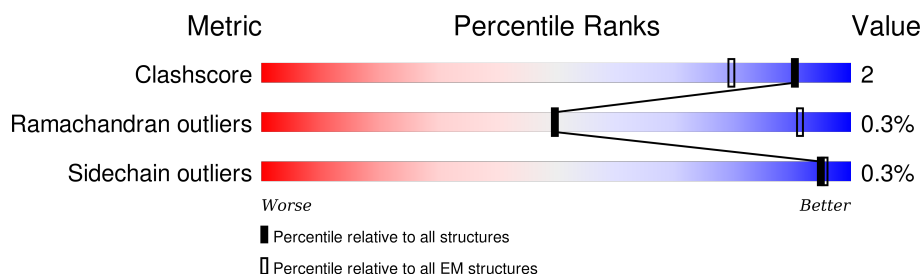
1 Overall quality at a glance

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	 48% 51%
1	K	392	 48% 51%
1	L	392	 48% 51%
1	M	392	 48% 51%
1	N	392	 48% 51%
1	O	392	 48% 51%
1	P	392	 48% 51%
1	Q	392	 48% 51%
1	R	392	 48% 51%
1	S	392	 48% 51%
1	T	392	 48% 51%
1	U	392	 47% 51%
1	V	392	 47% 51%
1	W	392	 48% 51%
1	X	392	 48% 51%
2	Y	252	 56% 41%
2	Z	252	 56% 41%
2	a	252	 59% 41%
2	b	252	 59% 41%
2	c	252	 59% 41%
2	d	252	 59% 41%
2	e	252	 59% 41%
2	f	252	 59% 41%
2	g	252	 59% 41%
2	h	252	 59% 41%

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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 [i](#)

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	C	N	O	S	0	0
			1578	999	285	290	4		
1	B	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	C	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	D	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	E	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	F	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	G	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	H	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	I	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	J	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	K	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	L	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	M	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	N	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	O	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	P	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		
1	Q	191	Total	C	N	O	S	0	0
			1578	999	285	290	4		

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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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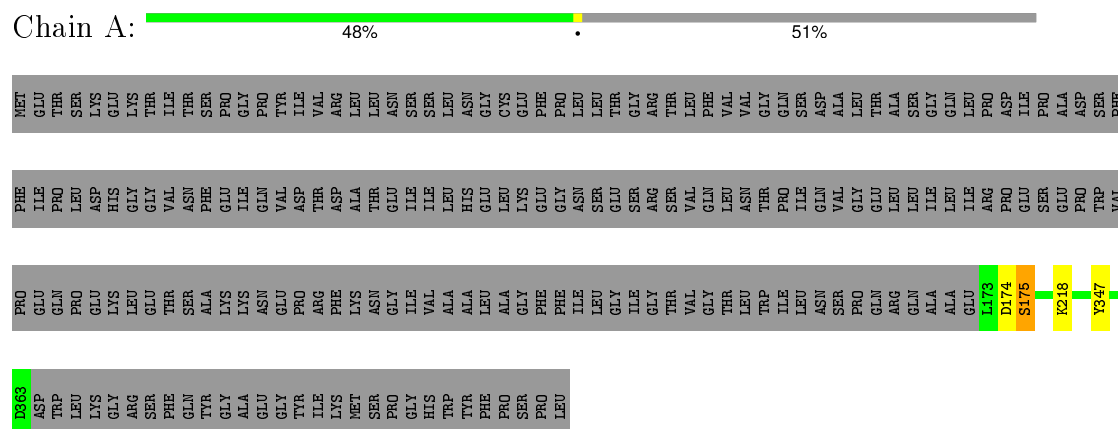
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	m	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	n	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	o	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	p	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	q	148	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		

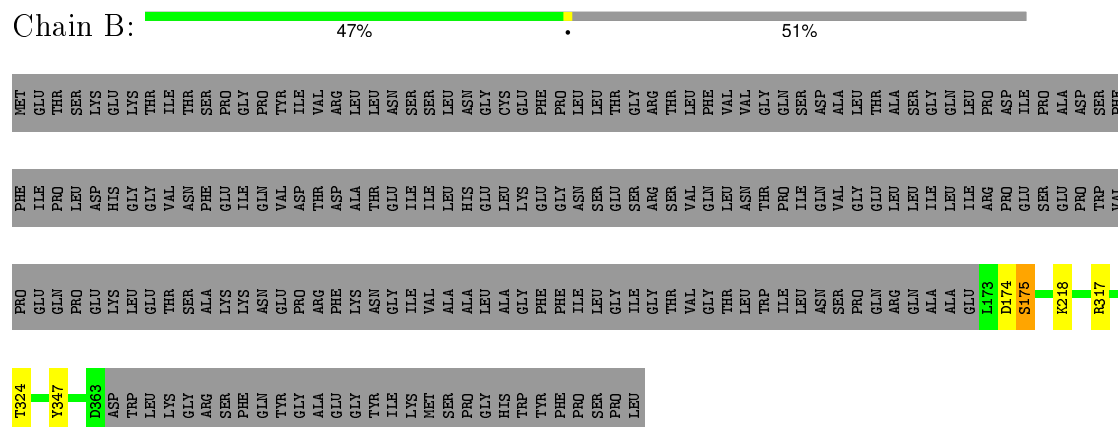
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

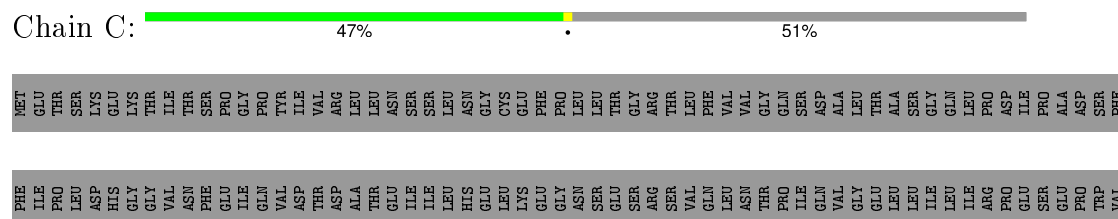
- Molecule 1: Protein PrgH

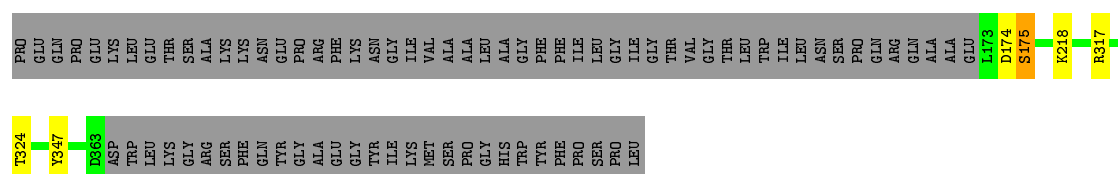


- Molecule 1: Protein PrgH

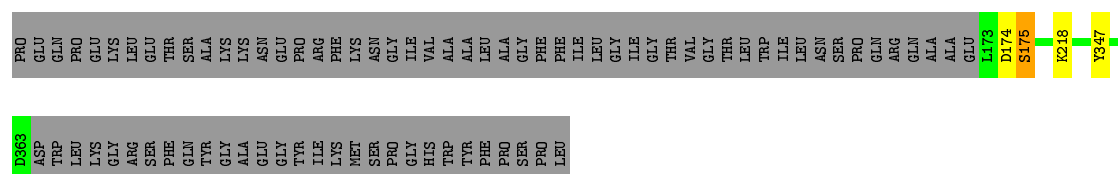


- Molecule 1: Protein PrgH

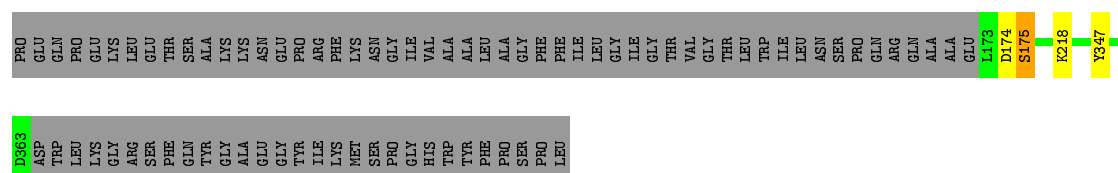




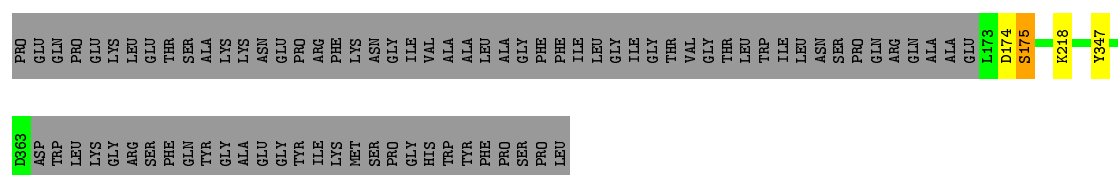
- Molecule 1: Protein PrgH



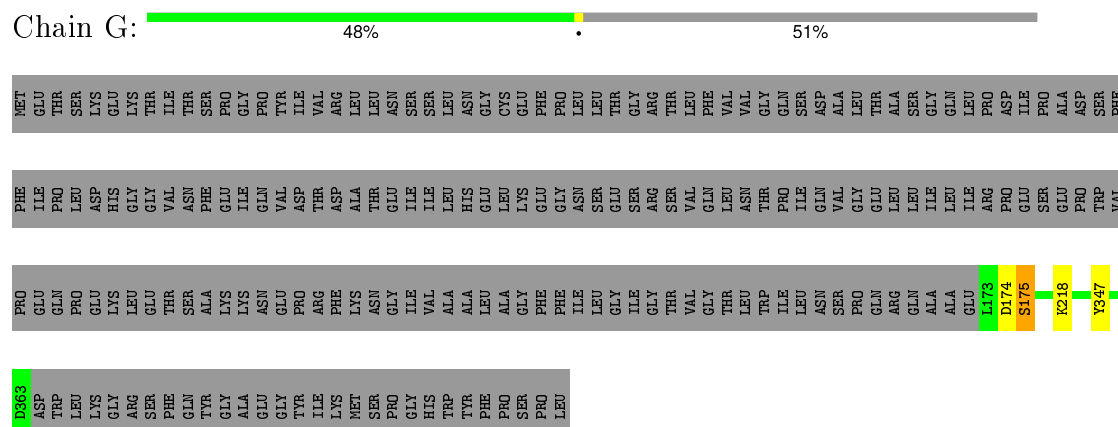
- Molecule 1: Protein PrgH



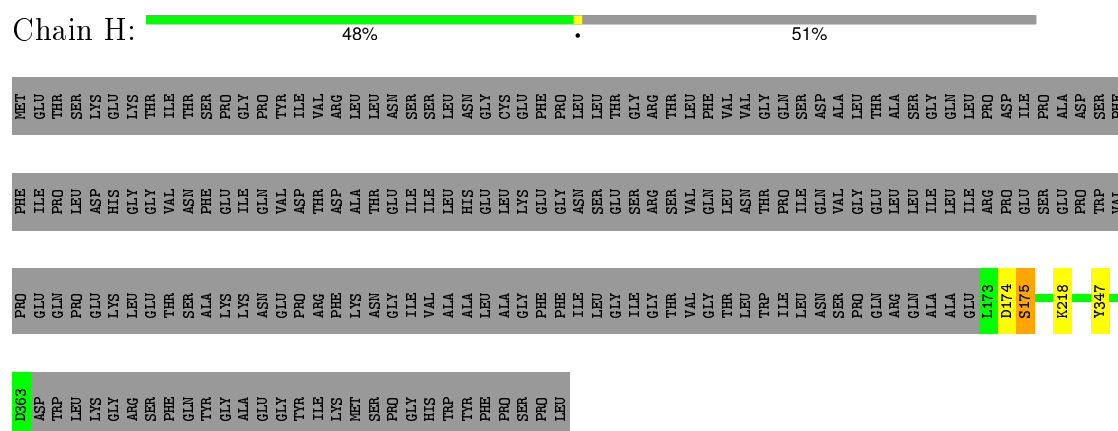
- Molecule 1: Protein PrgH



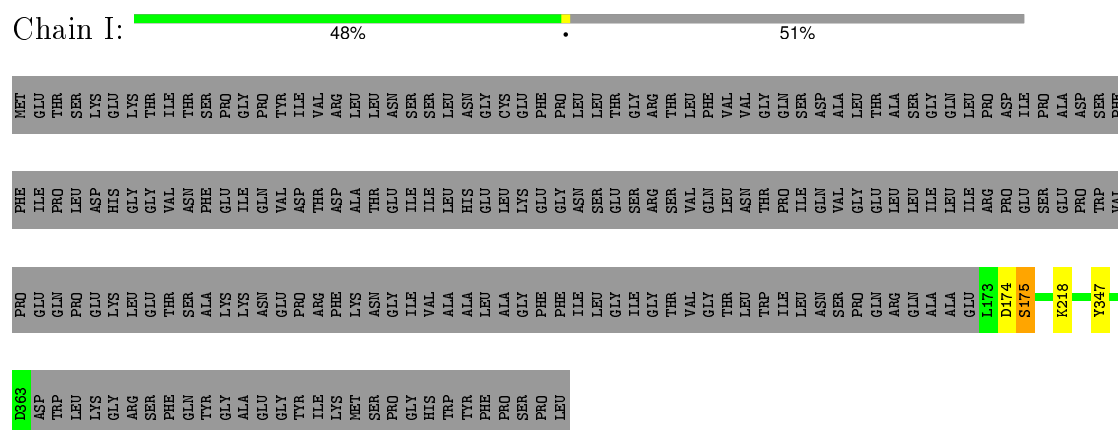
- Molecule 1: Protein PrgH



- Molecule 1: Protein PrgH



- Molecule 1: Protein PrgH



- Molecule 1: Protein PrgH

Chain J:  48% . 51%

[illegible]

- 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 PRO LEU

- Molecule 1: Protein PrgH

Chain O:  48% . 51%

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

- Molecule 1: Protein PrgH

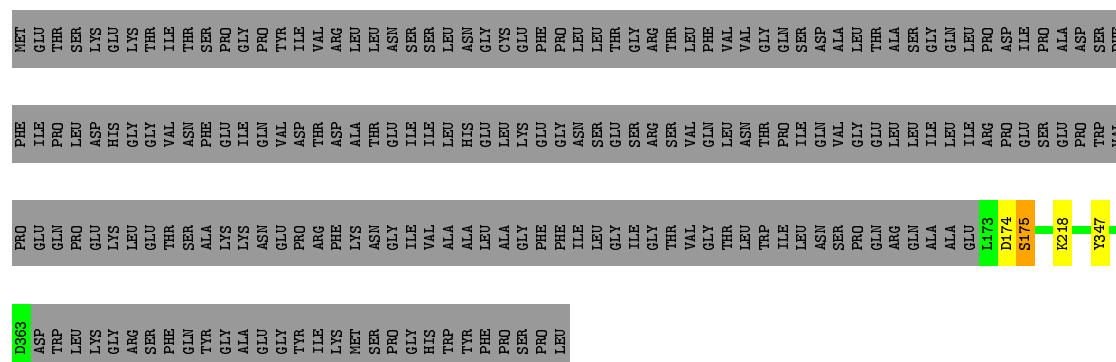
Chain P:  48% 51%

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 GLU 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

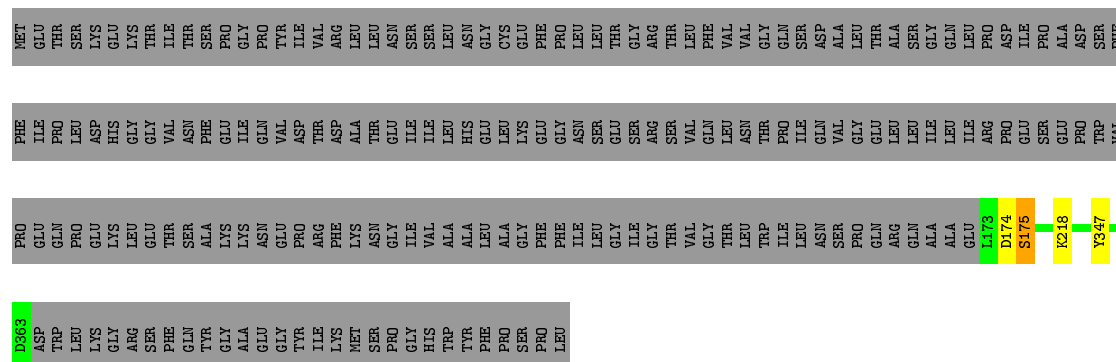
- Molecule 1: Protein PrgH

Chain Q:  48% 51%



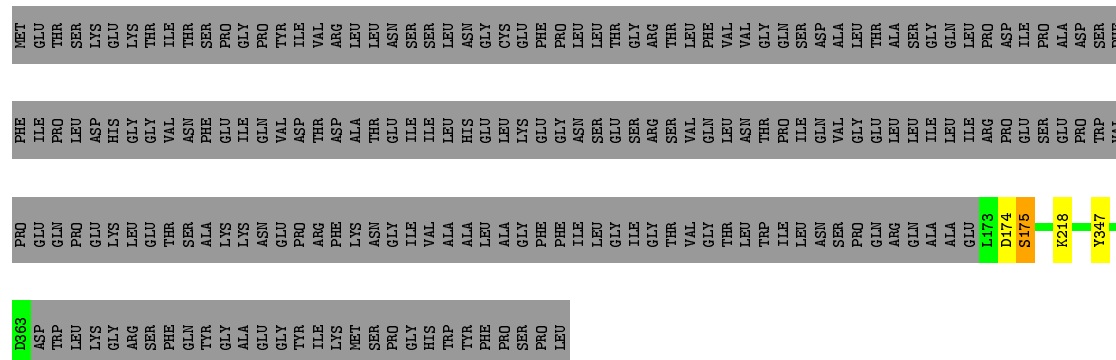
- Molecule 1: Protein PrgH

Chain R: 48% 51%



- Molecule 1: Protein PrgH

Chain S:  48% 51%



- Molecule 1: Protein PrgH

Chain T: 48% 51%

D363	ASP	TRP	LEU	LYS	GLY	ARG	SER	PHE	GLN	TYR	GLY	ALA	ALA	GLU	GLY	TYR	ILE	LYS	MET	SER	PRO	GLY	HIS	TYR	PHE	PRO	SER	PRO	LEU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
	PHE	ILE	PRO	GLU	LYS	GLY	GLY	VAL	ASN	SER	PHE	LYS	LYS	GLU	PRO	ARG	PHE	ASN	GLY	ILE	VAL	ALA	ALA	LEU	LEU	PHE	ILE	LEU	GLY	THR	GLY	ILE	LEU	GLN	ASP	ALA	LEU	THR	ALA	SER	GLY	LEU	ILE	ARG	PRO	GLU	SER	GLU	PRO	GLU	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
	PRO	GLU	GLN	PRO	GLU	LEU	GLU	THR	SER	ALA	LYS	LYS	ASN	GLU	PRO	ARG	PHE	ASN	GLY	ILE	VAL	ALA	ALA	LEU	LEU	PHE	ILE	LEU	GLY	THR	GLY	ILE	LEU	GLN	ASN	VAL	GLY	GLU	LEU	ALA	ALA	SER	GLY	LEU	ILE	ARG	PRO	GLU	SER	GLU	PRO	TRP	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
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• Molecule 1: Protein PrgH



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

• Molecule 1: Protein PrgH



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

• Molecule 1: Protein PrgH



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

THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	THR	THR	SER	TRP	TRP	ILE	ILE	VAL	LEU	LEU	ILE	ILE	LEU	SER	SER	VAL	VAL	MET	SER	SER	ALA	GLY	PHE	GLY	VAL	TRP	TRP	TYR	TYR	LYS	ASN	HIS	TYR	TYR	ALA	ALA	ARG	ASN	LYS	LYS	GLY	ILE	THR	ALA	ASP	ASP	LYS	LYS	LYS	SER	SER	ASN	THR
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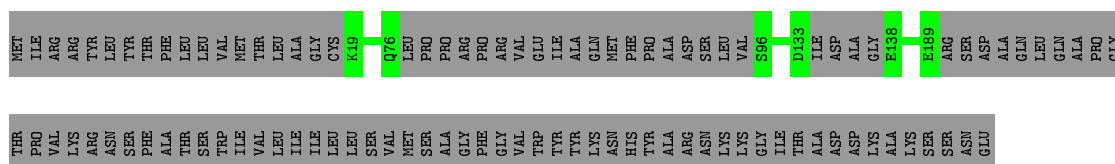
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| THR | PRO | VAL | LYS | ARG | ASN | SER | PHE | THR | THR | SER | TRP | ILE | VAL | LEU | ILE | ILE | LEU | SER | VAL | MET | SER | SER | ALA | GLY | PHE | GLY | VAL | TRP | TYR | TYR | LYS | ASN | HIS | TYR | ALA | ARG | ASN | LYS | LYS | GLY | ILE | THR | ASP | ASP | LYS | ALA | LYS | SER | SER | ASN | TRP |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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| THR | PRO | VAL | LYS | ARG | ASN | SER | PHE | ALA | THR | SER | TRP | ILE | VAL | LEU | ILE | ILE | LEU | LEU | SER | SER | VAL | NET | SER | SER | ALA | GLY | PHE | GLY | GLY | VAL | TRP | TRP | TYR | TYR | LYS | ASN | HIS | TYR | ALA | ARG | ASN | LYS | LYS | GLY | ILE | THR | ASP | ASP | LYS | ALA | LYS | SER | SER | ASN | ILE |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

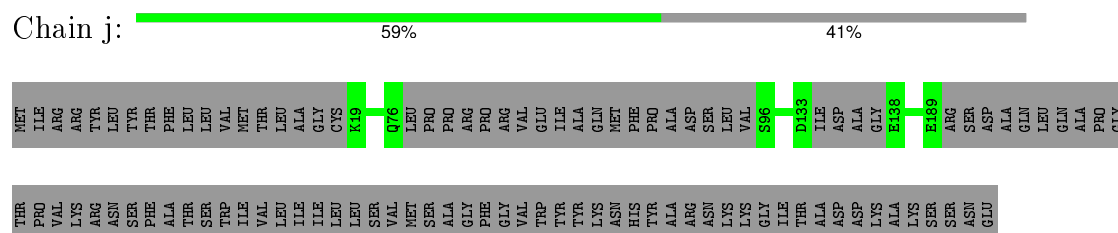
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| THR | PRO | VAL | LYS | ARG | ASN | SER | PHE | ALA | THR | SER | TRP | ILE | VAL | LEU | ILE | ILE | LEU | LEU | SER | VAL | VAL | NET | SER | SER | ALA | GLY | PHE | GLY | GLY | VAL | TRP | TRP | TYR | LYS | ASN | HIS | TYR | ALA | ARG | ASN | LYS | LYS | GLY | ILE | THR | ALA | ASP | LYS | LYS | SER | ASN | THR |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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| THR | PRO | VAL | LYS | ARG | ASN | SER | PHE | ALA | THR | SER | TRP | ILE | VAL | LEU | ILE | ILE | LEU | LEU | SER | VAL | NET | SER | SER | ALA | GLY | PHE | GLY | VAL | TRP | TYR | TYR | LYS | ASN | HIS | TYR | ALA | ARG | ASN | LYS | LYS | GLY | ILE | THR | ASP | ASP | LYS | ALA | LYS | SER | SER | ASN | THR |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

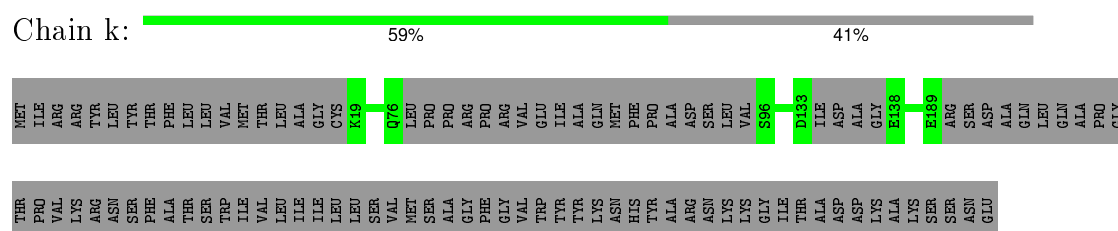
- Chain i: 59% 41%



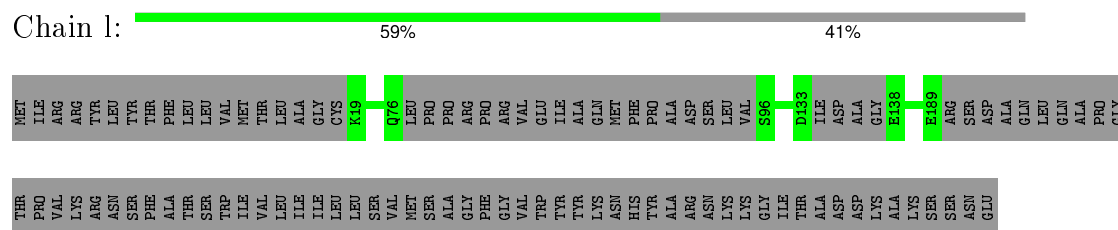
- Molecule 2: Pathogenicity 1 island effector protein



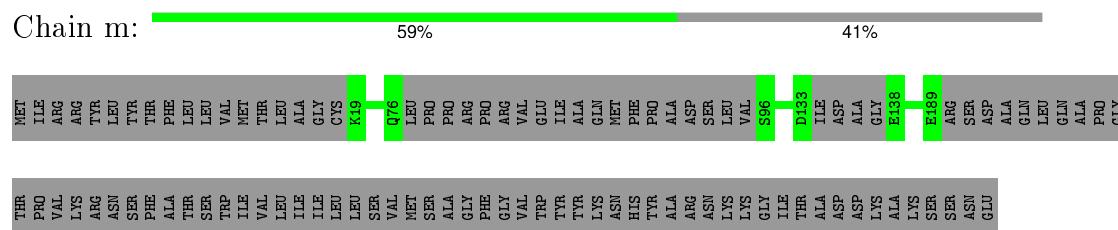
- Molecule 2: Pathogenicity 1 island effector protein



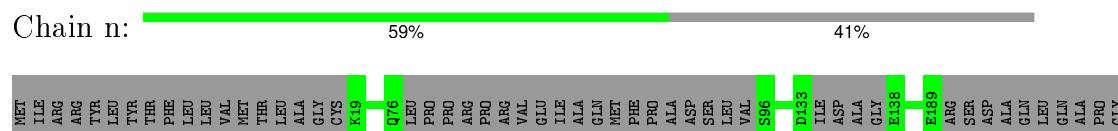
- Molecule 2: Pathogenicity 1 island effector protein



- Molecule 2: Pathogenicity 1 island effector protein



- Molecule 2: Pathogenicity 1 island effector protein



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

• Molecule 2: Pathogenicity 1 island effector protein

Chain o: 59% 41%

MET ILE ARG ARG TYR TYR PHE LEU LEU VAL MET THR LEU ILE ALA GLY CYS K149 Q76 LEU PRO PRO ARG PRO ARG VAL VAL GLU TYR ILE ILE GLN MET PHE PRO TYR ALA ASP SER LEU VAL S96 D133 ILE ASP ALA GLY E138 E189 ARG SER ASP ALA GLN LEU GLN ALA PRO GLY

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

• Molecule 2: Pathogenicity 1 island effector protein

Chain p: 59% 41%

MET ILE ARG ARG TYR TYR PHE LEU LEU VAL MET THR LEU ILE ALA GLY CYS K149 Q76 LEU PRO PRO ARG PRO ARG VAL VAL GLU TYR ILE ILE GLN MET PHE PRO TYR ALA ASP SER LEU VAL S96 D133 ILE ASP ALA GLY E138 E189 ARG SER ASP ALA GLN LEU GLN ALA PRO GLY

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

• Molecule 2: Pathogenicity 1 island effector protein

Chain q: 59% 41%

MET ILE ARG ARG TYR TYR PHE LEU LEU VAL MET THR LEU ILE ALA GLY CYS K149 Q76 LEU PRO PRO ARG PRO ARG VAL VAL GLU TYR ILE ILE GLN MET PHE PRO TYR ALA ASP SER LEU VAL S96 D133 ILE ASP ALA GLY E138 E189 ARG SER ASP ALA GLN LEU GLN ALA PRO GLY

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

• Molecule 2: Pathogenicity 1 island effector protein

Chain r: 59% 41%

MET ILE ARG ARG TYR TYR PHE LEU LEU VAL MET THR LEU ILE ALA GLY CYS K149 Q76 LEU PRO PRO ARG PRO ARG VAL VAL GLU TYR ILE ILE GLN MET PHE PRO TYR ALA ASP SER LEU VAL S96 D133 ILE ASP ALA GLY E138 E189 ARG SER ASP ALA GLN LEU GLN ALA PRO GLY


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

• Molecule 2: Pathogenicity 1 island effector protein

Chain s: 59% 41%

MET ILE ARG ARG TYR TYR PHE LEU LEU VAL MET THR LEU ILE ALA GLY CYS K149 Q76 LEU PRO PRO ARG PRO ARG VAL VAL GLU TYR ILE ILE GLN MET PHE PRO TYR ALA ASP SER LEU VAL S96 D133 ILE ASP ALA GLY E138 E189 ARG SER ASP ALA GLN LEU GLN ALA PRO GLY

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

- 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 | ALA | PRO | GLY | THR | PRO | VAL | LYS | ARG | ASN | SER | PHE | THR | SER | ILE | VAL | LEU | ILE | ILE | LEU | LEU | SER | VAL | SER | ALA | GLY | PHE | GLY | VAL | TRP | TRR | LYS | ASN | THR | 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.

The worst 5 of 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

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	175	SER
1	N	175	SER
1	W	175	SER
1	L	175	SER
1	M	175	SER

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.