



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:38 am GMT

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/EMDatabank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

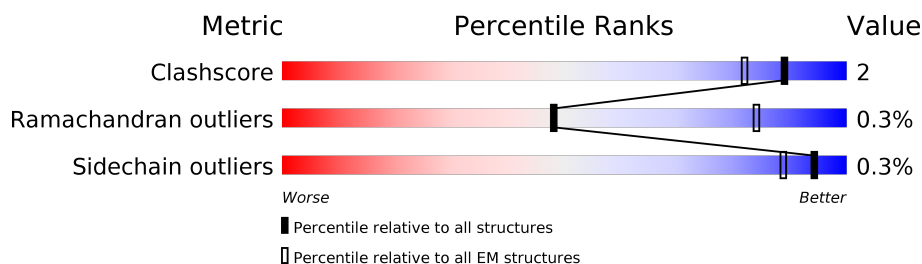
# 1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 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	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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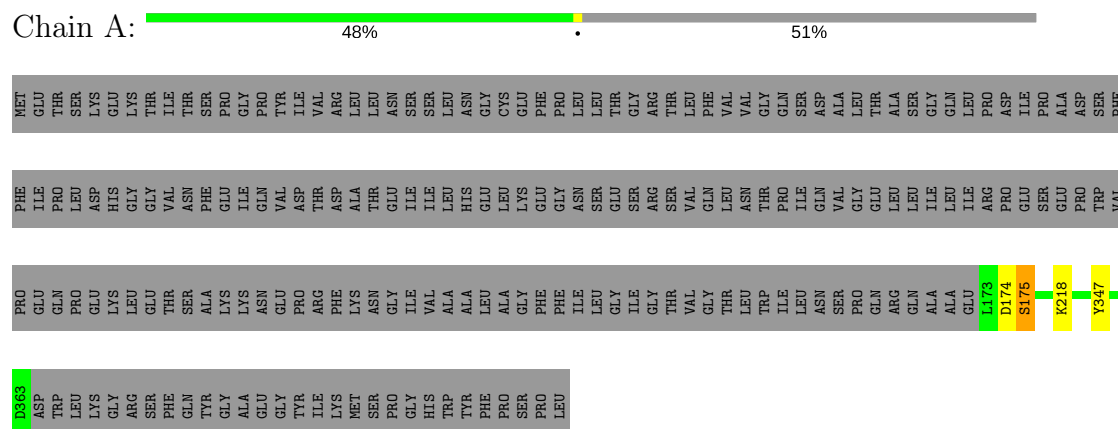
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	m	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	n	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	o	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	p	148	Total	C	N	O	S	0	0
			1170	737	202	229	2		
2	q	148	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		

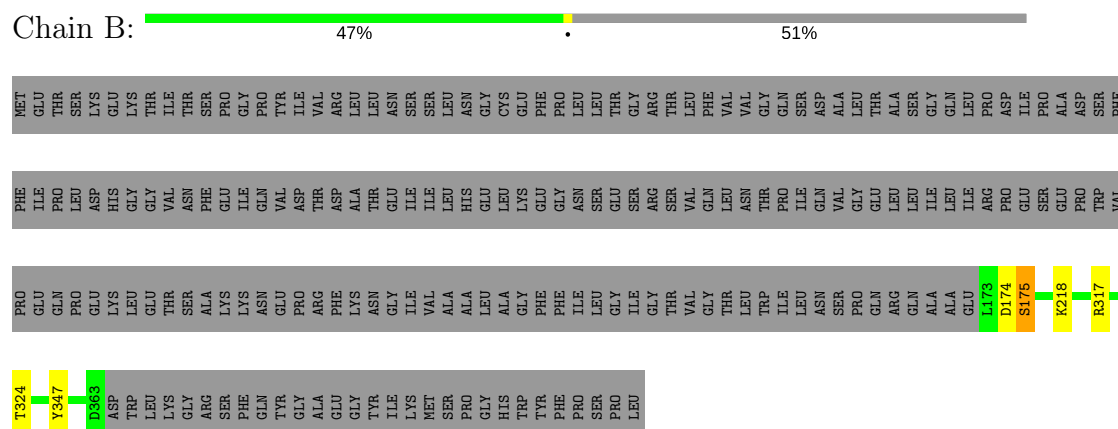
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

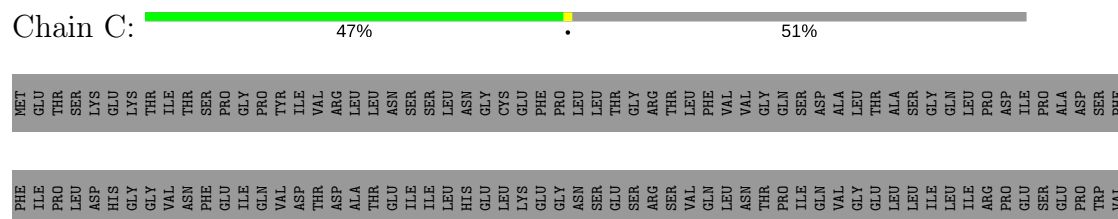
- Molecule 1: Protein PrgH



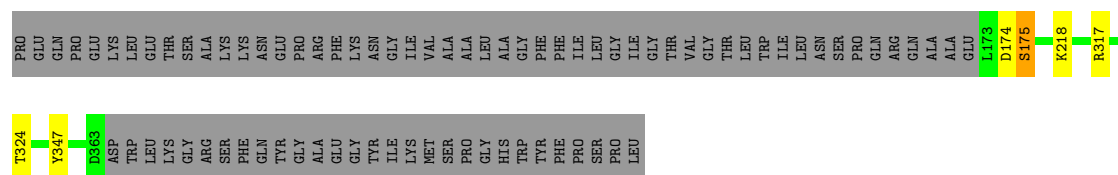
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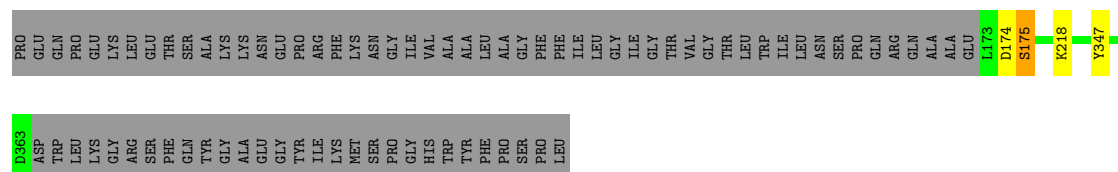
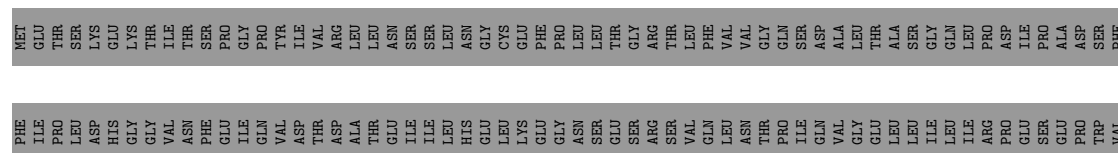
- Molecule 1: Protein PrgH



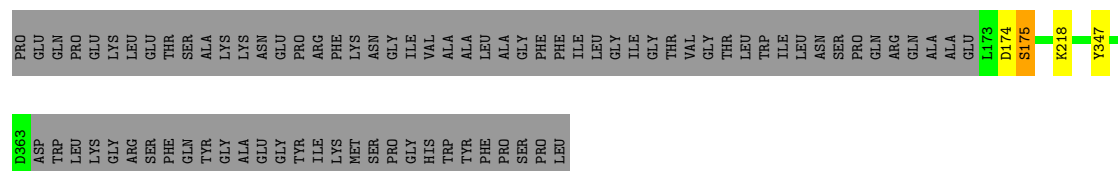
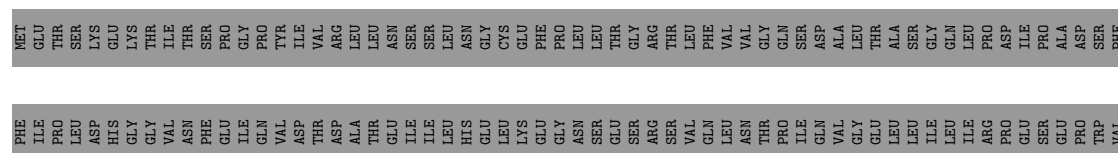




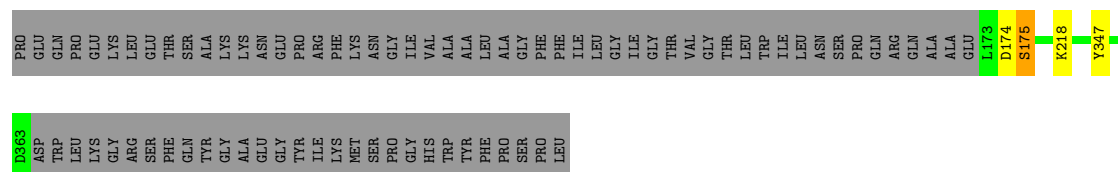
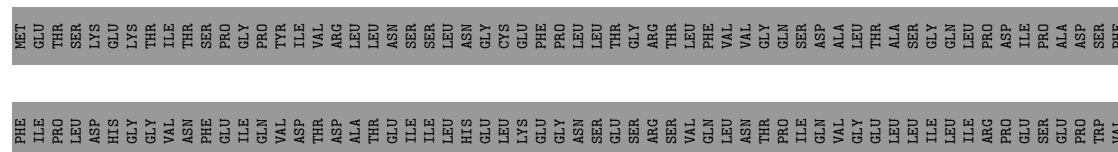
- Molecule 1: Protein PrgH



- Molecule 1: Protein PrgH

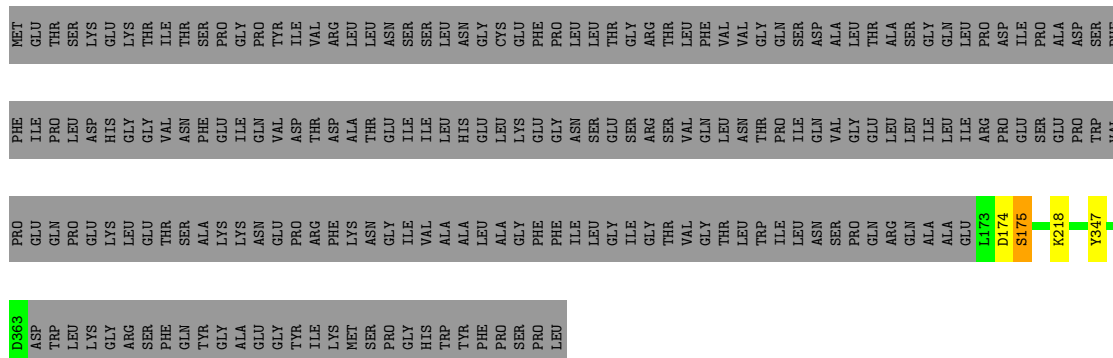


- Molecule 1: Protein PrgH



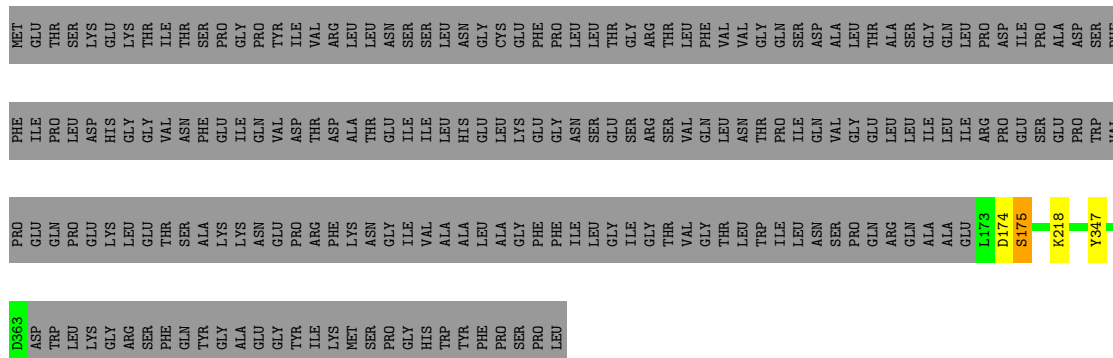
- Molecule 1: Protein PrgH

Chain G:  48% . 51%



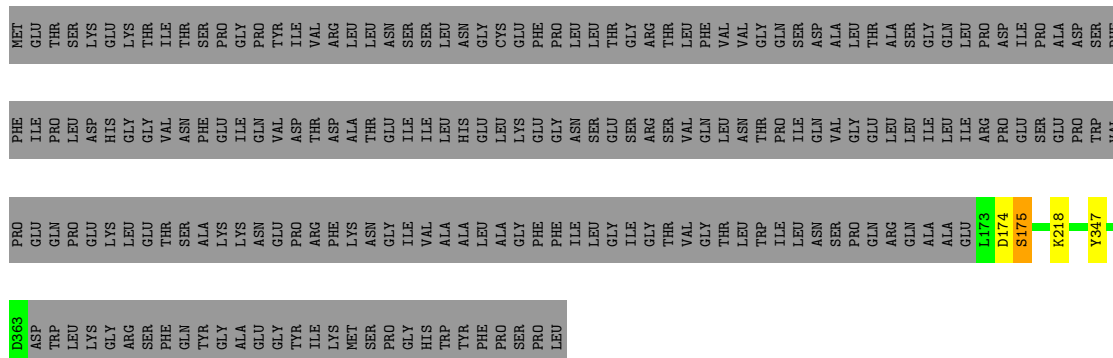
- Molecule 1: Protein PrgH

Chain H:  48% . 51%



- Molecule 1: Protein PrgH

Chain I:  48% 51%



- Molecule 1: Protein PrgH

Chain J:  48% . 51%

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

- Molecule 1: Protein PrgH

Chain K:  48% . 51%

[illegible]

- Molecule 1: Protein PrgH

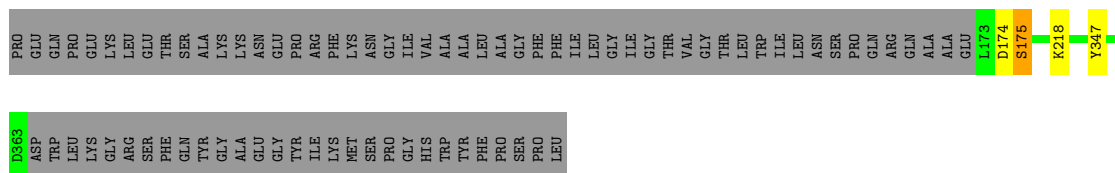
Chain L:  48% 51%

[illegible]

- Molecule 1: Protein PrgH

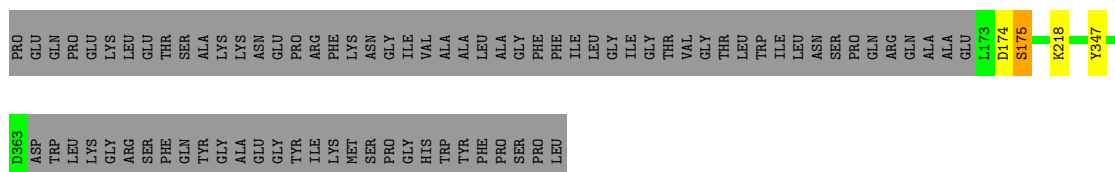
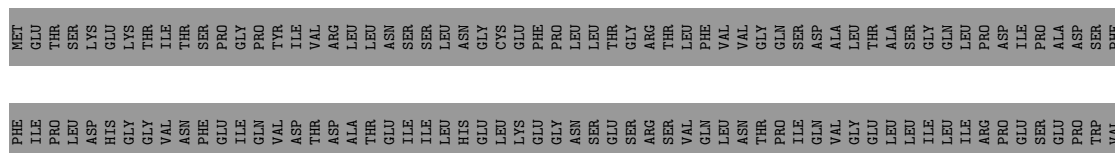
Chain M:  48% . 51%

[illegible]



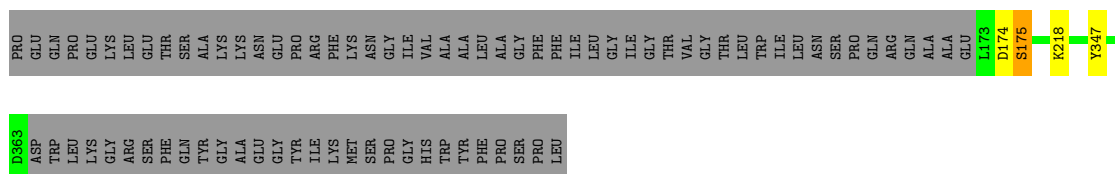
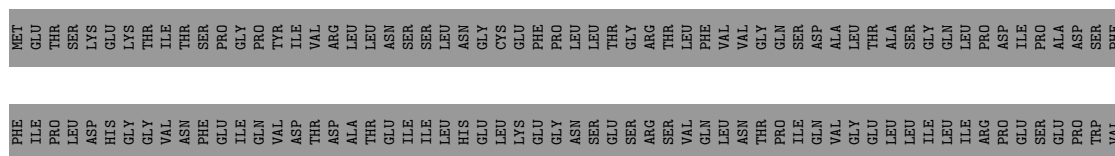
- Molecule 1: Protein PrgH

Chain N:  48% 51%



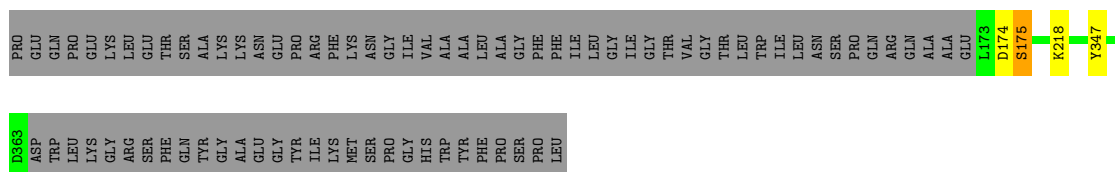
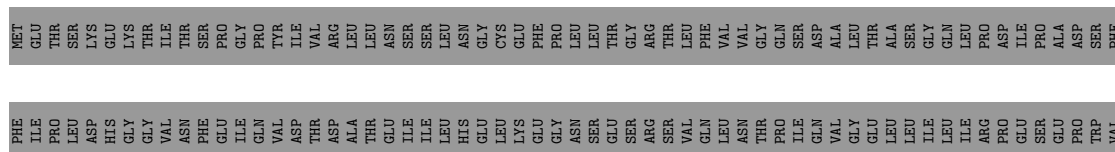
- Molecule 1: Protein PrgH

Chain O:  48% . 51%



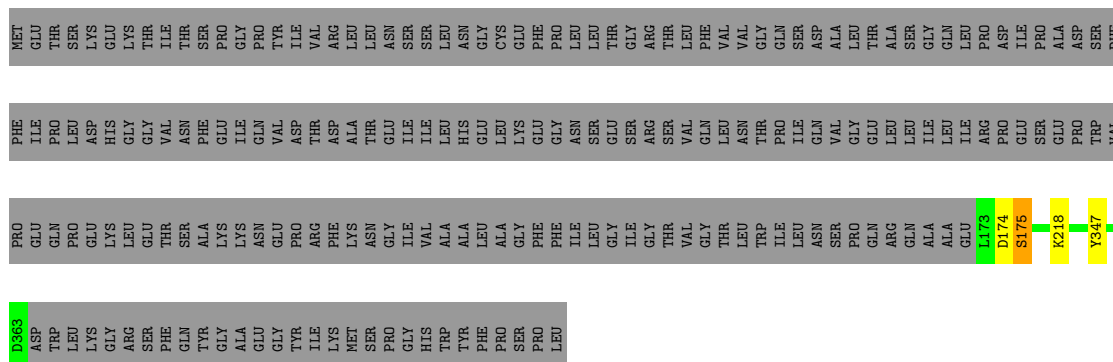
- Molecule 1: Protein PrgH

Chain P:  48% 51%



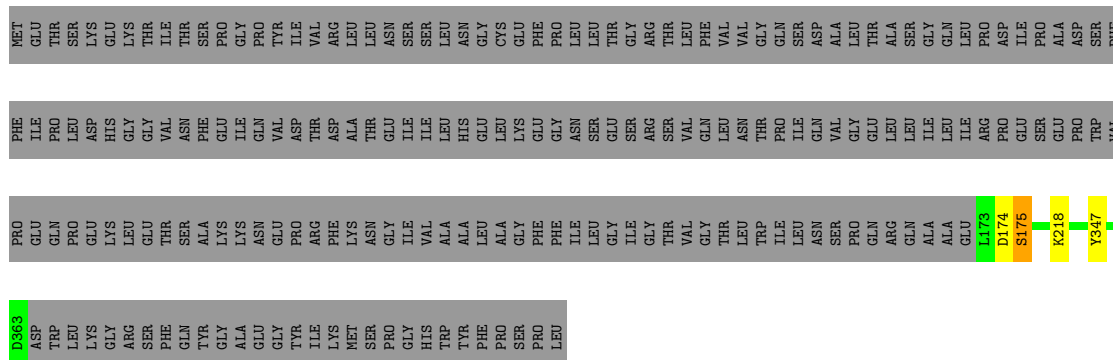
- Molecule 1: Protein PrgH

Chain Q:  48% . 51%



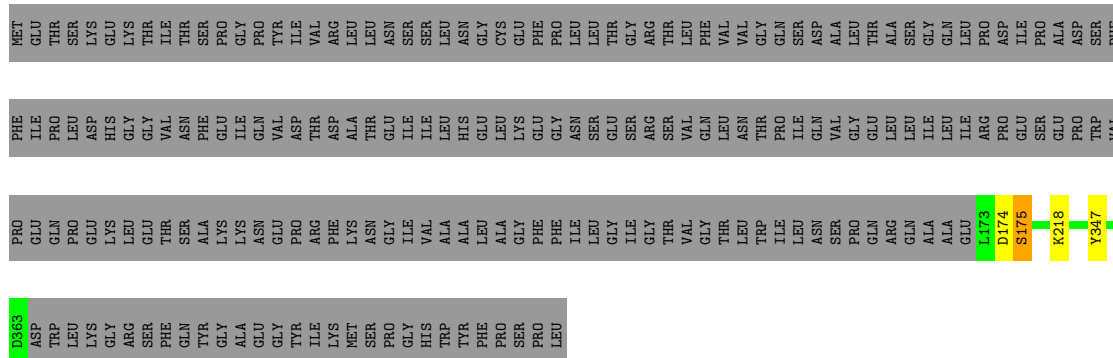
- Molecule 1: Protein PrgH

Chain R:  48% 51%



- Molecule 1: Protein PrgH

Chain S:  48% 51%



- Molecule 1: Protein PrgH

Chain T:  48% 51%

[illegible]

- Molecule 1: Protein PrgH

Chain U:  47% 51%

[illegible]

- Molecule 1: Protein PrgH

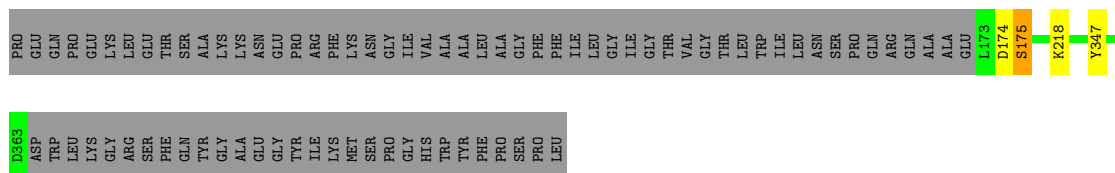
Chain V:  47% . 51%

[illegible]

- Molecule 1: Protein PrgH

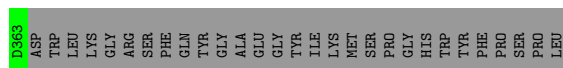
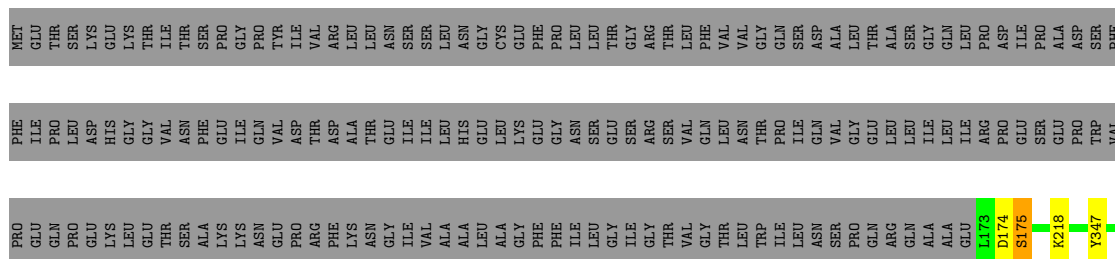
Chain W:  48% 51%

[illegible]



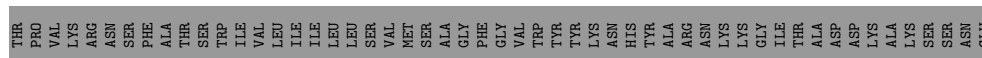
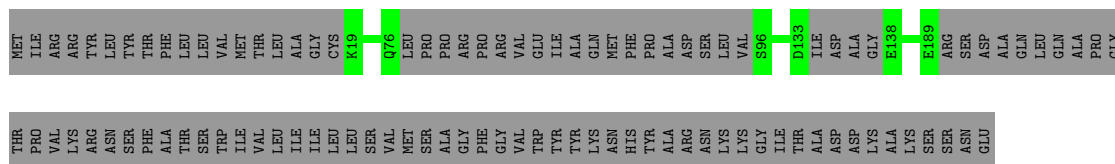
- Molecule 1: Protein PrgH

Chain X:  48% 51%



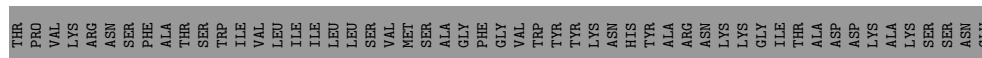
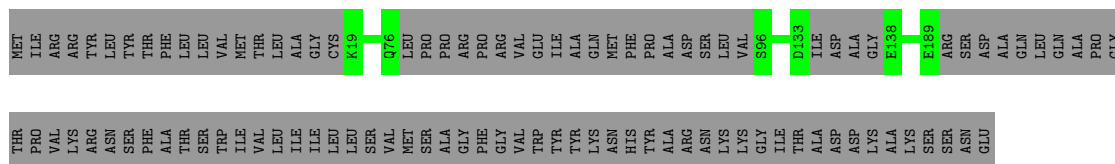
- Molecule 2: Pathogenicity 1 island effector protein

Chain a:  59% 41%



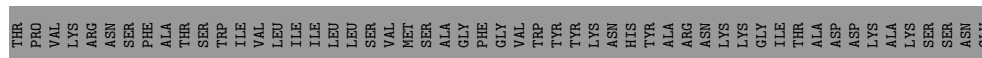
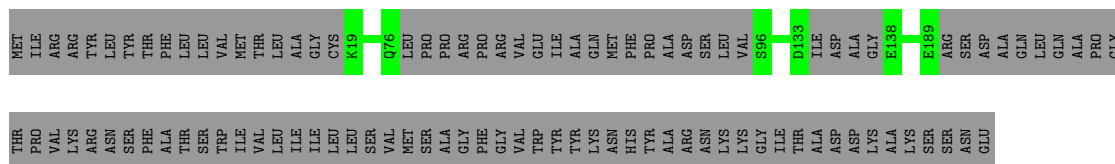
- Molecule 2: Pathogenicity 1 island effector protein

Chain b:  59% 41%



- Molecule 2: Pathogenicity 1 island effector protein

Chain c:  59% 41%



- Molecule 2: Pathogenicity 1 island effector protein

Chain d:  59% 41%

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

- Molecule 2: Pathogenicity 1 island effector protein

Chain e:  59% 41%

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

- Molecule 2: Pathogenicity 1 island effector protein

Chain f:  59% 41%

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

- Molecule 2: Pathogenicity 1 island effector protein

Chain g:  59% 41%

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

- Molecule 2: Pathogenicity 1 island effector protein

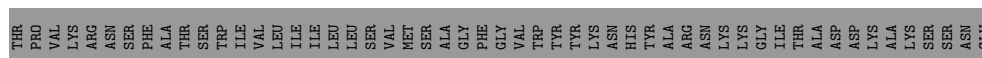
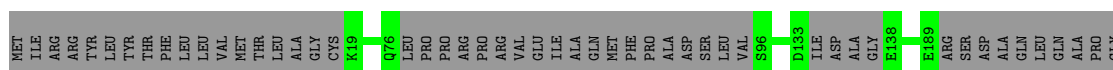
Chain h:  59% 41%

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

- Molecule 2: Pathogenicity 1 island effector protein

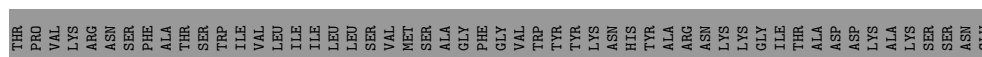
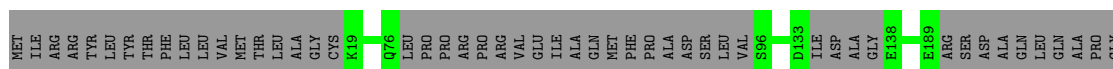
Chain i:  59% 41%






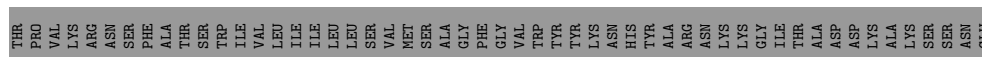
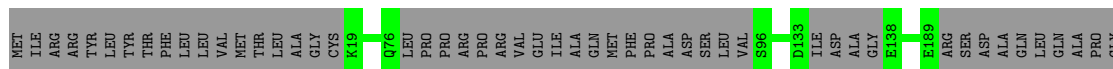
- Molecule 2: Pathogenicity 1 island effector protein

Chain j:  59% 41%



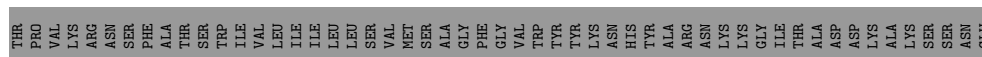
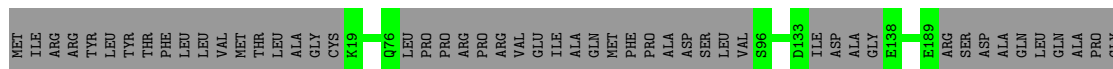
- Molecule 2: Pathogenicity 1 island effector protein

Chain k:  59% 41%



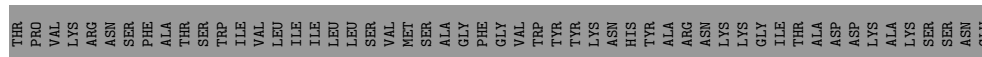
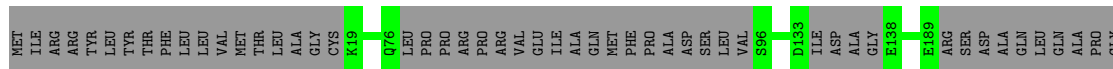
- Molecule 2: Pathogenicity 1 island effector protein

Chain l:  59% 41%



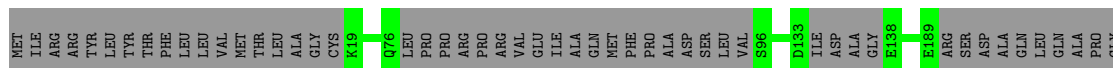
- Molecule 2: Pathogenicity 1 island effector protein

Chain m:  59% 41%



- Molecule 2: Pathogenicity 1 island effector protein

Chain n:  59% 41%



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

• Molecule 2: Pathogenicity 1 island effector protein



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

THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	LEU	SER	VAL
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• Molecule 2: Pathogenicity 1 island effector protein



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

THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	LEU	SER	VAL
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• Molecule 2: Pathogenicity 1 island effector protein



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

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

• Molecule 2: Pathogenicity 1 island effector protein



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

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

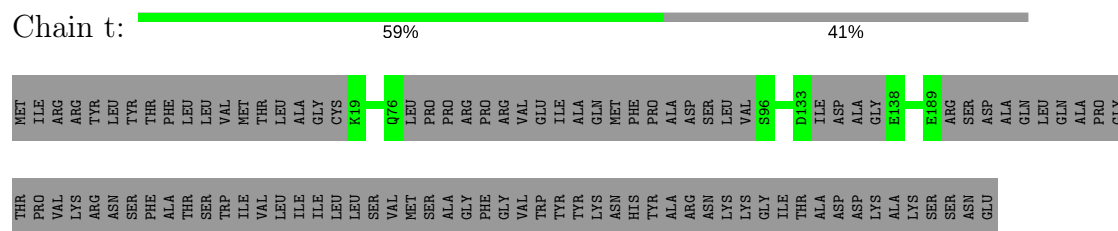
• Molecule 2: Pathogenicity 1 island effector protein



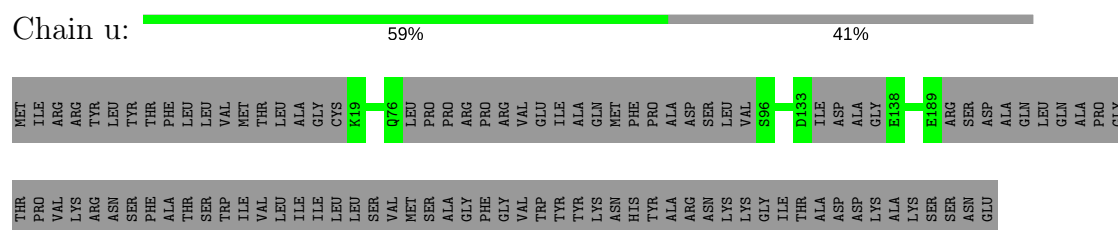
MET	ILE	ARG	ARG	TYR	THR	THR	PHE	ALA	THR	SER	LEU	VAL	MET	THR	LEU	ALA	GLY	CYS	K19	Q76
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

THR	PRO	VAL	LYS	ARG	ASN	SER	PHE	ALA	THR	SER	TRP	ILE	VAL	LEU	ILE	ILE	LEU	LEU	SER	VAL
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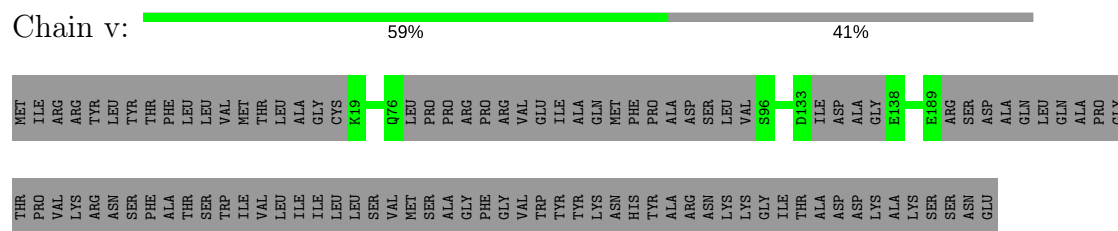
- Molecule 2: Pathogenicity 1 island effector protein



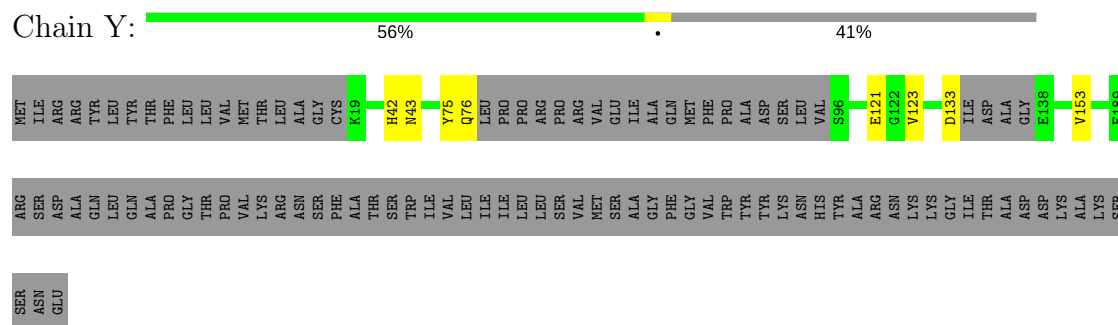
- Molecule 2: Pathogenicity 1 island effector protein



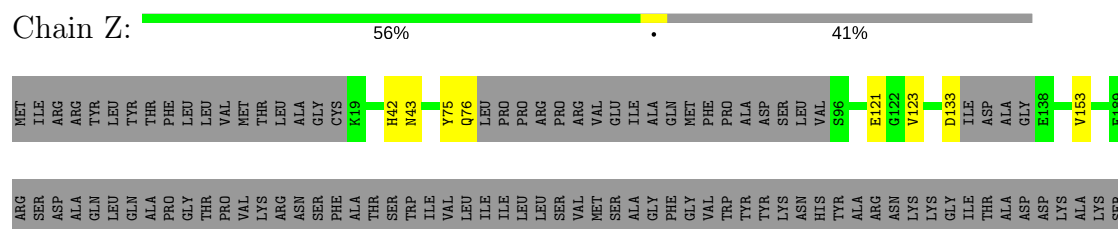
- Molecule 2: Pathogenicity 1 island effector protein



- Molecule 2: Pathogenicity 1 island effector protein



- Molecule 2: Pathogenicity 1 island effector protein



SER  
ASN  
GLU

## 4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	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 ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >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 ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	32	32
1	B	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	C	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	D	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	E	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	F	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	G	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	H	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	I	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	J	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	K	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	L	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	M	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	N	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	O	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	P	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	R	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	S	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	T	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	U	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	V	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	W	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
1	X	189/392 (48%)	174 (92%)	14 (7%)	1 (0%)	32	32
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%)	48	44

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%)	89	89
1	B	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	C	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	D	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	E	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	F	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	G	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	H	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	I	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	J	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	K	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	L	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	M	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	N	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	O	165/337 (49%)	164 (99%)	1 (1%)	89	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	Q	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	R	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	S	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	T	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	U	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	V	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	W	165/337 (49%)	164 (99%)	1 (1%)	89	89
1	X	165/337 (49%)	164 (99%)	1 (1%)	89	89
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%)	94	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.