Full wwPDB EM Validation Report ⓘ

Feb 20, 2023 – 06:58 PM EST

PDB ID	:	8FV5
EMDB ID	:	EMD-29451
Title	:	Representation of 16-mer phiPA3 PhuN Lattice, p2
Authors	:	Nieweglowska, E.S.; Brilot, A.F.; Mendez-Moran, M.; Kokontis, C.; Baek, M.; Li, J.; Cheng, Y.; Baker, D.; Bondy-Denomy, J.; Agard, D.A.
Deposited on	:	2023-01-18
Resolution	:	4.21 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

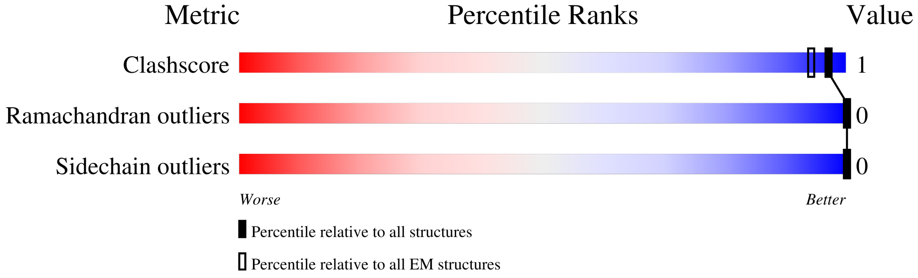
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 4.21 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	996	• 51% • 47%
1	B	996	• 51% • 47%
1	C	996	• 51% • 47%
1	D	996	• 51% • 47%
1	E	996	• 99%
1	F	996	• 99%
1	G	996	• 99%
1	H	996	• 99%

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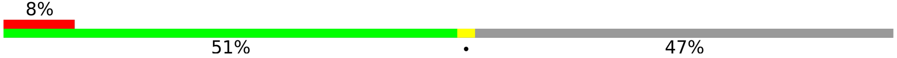
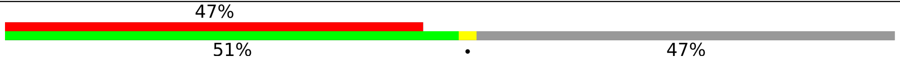
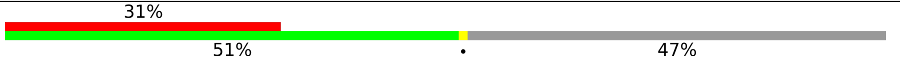
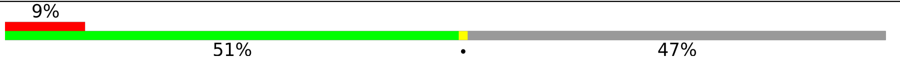
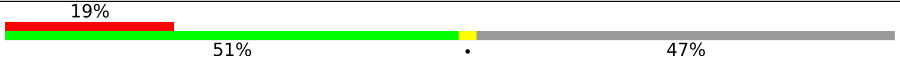
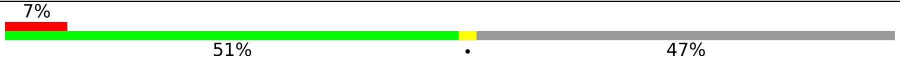
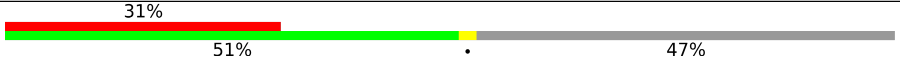
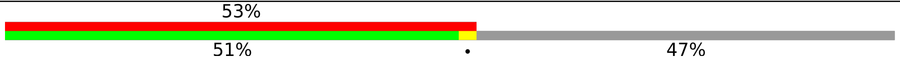
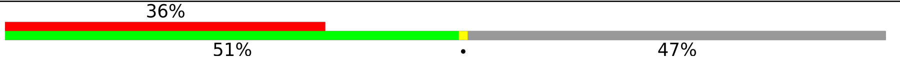
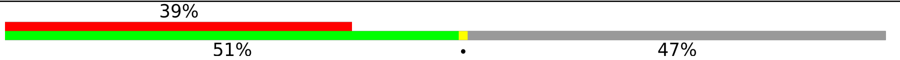
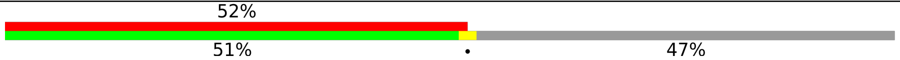
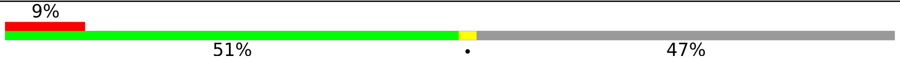
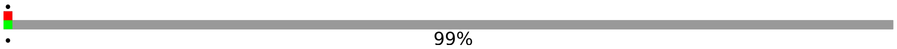
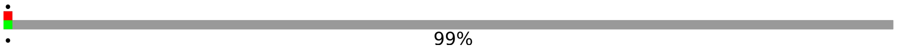
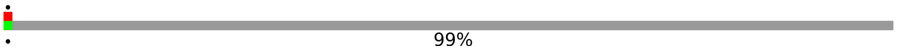
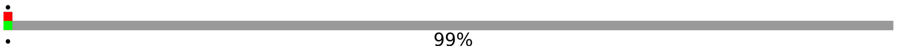
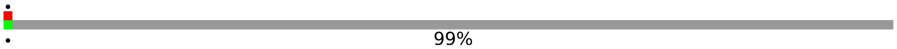
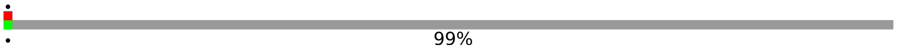
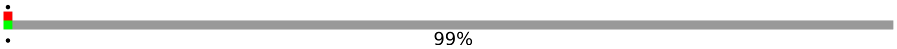
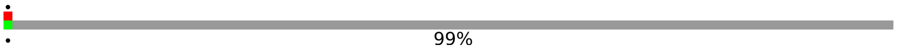
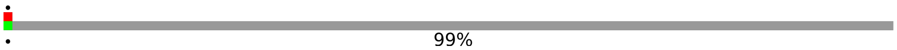
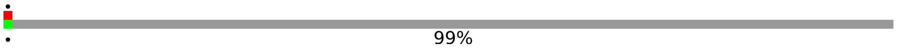
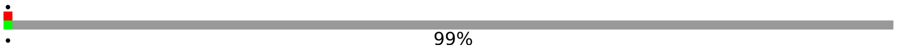
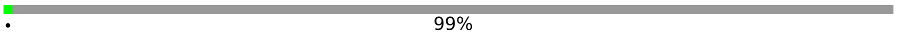
Mol	Chain	Length	Quality of chain
1	I	996	
1	J	996	
1	K	996	
1	L	996	
1	M	996	
1	N	996	
1	O	996	
1	P	996	
1	Q	996	
1	R	996	
1	S	996	
1	T	996	
1	U	996	
1	V	996	
1	W	996	
1	X	996	
1	Y	996	
1	Z	996	
1	a	996	
1	b	996	
1	c	996	
1	d	996	
1	e	996	
1	f	996	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 134032 atoms, of which 66576 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 Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	525	Total C H N O S 8213 2597 4085 727 787 17	0	0
1	B	525	Total C H N O S 8213 2597 4085 727 787 17	0	0
1	C	525	Total C H N O S 8213 2597 4085 727 787 17	0	0
1	D	525	Total C H N O S 8213 2597 4085 727 787 17	0	0
1	E	12	Total C H N O 164 58 76 14 16	0	0
1	F	12	Total C H N O 164 58 76 14 16	0	0
1	G	12	Total C H N O 164 58 76 14 16	0	0
1	H	12	Total C H N O 164 58 76 14 16	0	0
1	I	525	Total C H N O S 8213 2597 4085 727 787 17	0	0
1	J	525	Total C H N O S 8213 2597 4085 727 787 17	0	0
1	K	525	Total C H N O S 8213 2597 4085 727 787 17	0	0
1	L	525	Total C H N O S 8213 2597 4085 727 787 17	0	0
1	M	525	Total C H N O S 8213 2597 4085 727 787 17	0	0
1	N	525	Total C H N O S 8213 2597 4085 727 787 17	0	0
1	O	525	Total C H N O S 8213 2597 4085 727 787 17	0	0
1	P	525	Total C H N O S 8213 2597 4085 727 787 17	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	Q	525	Total C H N O S 8213 2597 4085 727 787 17	0	0
1	R	525	Total C H N O S 8213 2597 4085 727 787 17	0	0
1	S	525	Total C H N O S 8213 2597 4085 727 787 17	0	0
1	T	525	Total C H N O S 8213 2597 4085 727 787 17	0	0
1	U	12	Total C H N O 164 58 76 14 16	0	0
1	V	12	Total C H N O 164 58 76 14 16	0	0
1	W	12	Total C H N O 164 58 76 14 16	0	0
1	X	12	Total C H N O 164 58 76 14 16	0	0
1	Y	12	Total C H N O 164 58 76 14 16	0	0
1	Z	12	Total C H N O 164 58 76 14 16	0	0
1	a	12	Total C H N O 164 58 76 14 16	0	0
1	b	12	Total C H N O 164 58 76 14 16	0	0
1	c	12	Total C H N O 164 58 76 14 16	0	0
1	d	12	Total C H N O 164 58 76 14 16	0	0
1	e	12	Total C H N O 164 58 76 14 16	0	0
1	f	12	Total C H N O 164 58 76 14 16	0	0

There are 896 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-393	HIS	-	expression tag	UNP P0AEX9
A	-392	HIS	-	expression tag	UNP P0AEX9
A	-391	HIS	-	expression tag	UNP P0AEX9
A	-390	HIS	-	expression tag	UNP P0AEX9
A	-389	HIS	-	expression tag	UNP P0AEX9
A	-388	HIS	-	expression tag	UNP P0AEX9
A	-387	MET	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	GLY	-	linker	UNP P0AEX9
A	-19	LYS	-	linker	UNP P0AEX9
A	-18	PRO	-	linker	UNP P0AEX9
A	-17	ILE	-	linker	UNP P0AEX9
A	-16	PRO	-	linker	UNP P0AEX9
A	-15	ASN	-	linker	UNP P0AEX9
A	-14	PRO	-	linker	UNP P0AEX9
A	-13	LEU	-	linker	UNP P0AEX9
A	-12	LEU	-	linker	UNP P0AEX9
A	-11	GLY	-	linker	UNP P0AEX9
A	-10	LEU	-	linker	UNP P0AEX9
A	-9	ASP	-	linker	UNP P0AEX9
A	-8	SER	-	linker	UNP P0AEX9
A	-7	THR	-	linker	UNP P0AEX9
A	-6	GLU	-	linker	UNP P0AEX9
A	-5	ASN	-	linker	UNP P0AEX9
A	-4	LEU	-	linker	UNP P0AEX9
A	-3	TYR	-	linker	UNP P0AEX9
A	-2	PHE	-	linker	UNP P0AEX9
A	-1	GLN	-	linker	UNP P0AEX9
A	0	GLY	-	linker	UNP P0AEX9
B	-393	HIS	-	expression tag	UNP P0AEX9
B	-392	HIS	-	expression tag	UNP P0AEX9
B	-391	HIS	-	expression tag	UNP P0AEX9
B	-390	HIS	-	expression tag	UNP P0AEX9
B	-389	HIS	-	expression tag	UNP P0AEX9
B	-388	HIS	-	expression tag	UNP P0AEX9
B	-387	MET	-	expression tag	UNP P0AEX9
B	-20	GLY	-	linker	UNP P0AEX9
B	-19	LYS	-	linker	UNP P0AEX9
B	-18	PRO	-	linker	UNP P0AEX9
B	-17	ILE	-	linker	UNP P0AEX9
B	-16	PRO	-	linker	UNP P0AEX9
B	-15	ASN	-	linker	UNP P0AEX9
B	-14	PRO	-	linker	UNP P0AEX9
B	-13	LEU	-	linker	UNP P0AEX9
B	-12	LEU	-	linker	UNP P0AEX9
B	-11	GLY	-	linker	UNP P0AEX9
B	-10	LEU	-	linker	UNP P0AEX9
B	-9	ASP	-	linker	UNP P0AEX9
B	-8	SER	-	linker	UNP P0AEX9
B	-7	THR	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	GLU	-	linker	UNP P0AEX9
B	-5	ASN	-	linker	UNP P0AEX9
B	-4	LEU	-	linker	UNP P0AEX9
B	-3	TYR	-	linker	UNP P0AEX9
B	-2	PHE	-	linker	UNP P0AEX9
B	-1	GLN	-	linker	UNP P0AEX9
B	0	GLY	-	linker	UNP P0AEX9
C	-393	HIS	-	expression tag	UNP P0AEX9
C	-392	HIS	-	expression tag	UNP P0AEX9
C	-391	HIS	-	expression tag	UNP P0AEX9
C	-390	HIS	-	expression tag	UNP P0AEX9
C	-389	HIS	-	expression tag	UNP P0AEX9
C	-388	HIS	-	expression tag	UNP P0AEX9
C	-387	MET	-	expression tag	UNP P0AEX9
C	-20	GLY	-	linker	UNP P0AEX9
C	-19	LYS	-	linker	UNP P0AEX9
C	-18	PRO	-	linker	UNP P0AEX9
C	-17	ILE	-	linker	UNP P0AEX9
C	-16	PRO	-	linker	UNP P0AEX9
C	-15	ASN	-	linker	UNP P0AEX9
C	-14	PRO	-	linker	UNP P0AEX9
C	-13	LEU	-	linker	UNP P0AEX9
C	-12	LEU	-	linker	UNP P0AEX9
C	-11	GLY	-	linker	UNP P0AEX9
C	-10	LEU	-	linker	UNP P0AEX9
C	-9	ASP	-	linker	UNP P0AEX9
C	-8	SER	-	linker	UNP P0AEX9
C	-7	THR	-	linker	UNP P0AEX9
C	-6	GLU	-	linker	UNP P0AEX9
C	-5	ASN	-	linker	UNP P0AEX9
C	-4	LEU	-	linker	UNP P0AEX9
C	-3	TYR	-	linker	UNP P0AEX9
C	-2	PHE	-	linker	UNP P0AEX9
C	-1	GLN	-	linker	UNP P0AEX9
C	0	GLY	-	linker	UNP P0AEX9
D	-393	HIS	-	expression tag	UNP P0AEX9
D	-392	HIS	-	expression tag	UNP P0AEX9
D	-391	HIS	-	expression tag	UNP P0AEX9
D	-390	HIS	-	expression tag	UNP P0AEX9
D	-389	HIS	-	expression tag	UNP P0AEX9
D	-388	HIS	-	expression tag	UNP P0AEX9
D	-387	MET	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	GLY	-	linker	UNP P0AEX9
D	-19	LYS	-	linker	UNP P0AEX9
D	-18	PRO	-	linker	UNP P0AEX9
D	-17	ILE	-	linker	UNP P0AEX9
D	-16	PRO	-	linker	UNP P0AEX9
D	-15	ASN	-	linker	UNP P0AEX9
D	-14	PRO	-	linker	UNP P0AEX9
D	-13	LEU	-	linker	UNP P0AEX9
D	-12	LEU	-	linker	UNP P0AEX9
D	-11	GLY	-	linker	UNP P0AEX9
D	-10	LEU	-	linker	UNP P0AEX9
D	-9	ASP	-	linker	UNP P0AEX9
D	-8	SER	-	linker	UNP P0AEX9
D	-7	THR	-	linker	UNP P0AEX9
D	-6	GLU	-	linker	UNP P0AEX9
D	-5	ASN	-	linker	UNP P0AEX9
D	-4	LEU	-	linker	UNP P0AEX9
D	-3	TYR	-	linker	UNP P0AEX9
D	-2	PHE	-	linker	UNP P0AEX9
D	-1	GLN	-	linker	UNP P0AEX9
D	0	GLY	-	linker	UNP P0AEX9
E	-393	HIS	-	expression tag	UNP P0AEX9
E	-392	HIS	-	expression tag	UNP P0AEX9
E	-391	HIS	-	expression tag	UNP P0AEX9
E	-390	HIS	-	expression tag	UNP P0AEX9
E	-389	HIS	-	expression tag	UNP P0AEX9
E	-388	HIS	-	expression tag	UNP P0AEX9
E	-387	MET	-	expression tag	UNP P0AEX9
E	-20	GLY	-	linker	UNP P0AEX9
E	-19	LYS	-	linker	UNP P0AEX9
E	-18	PRO	-	linker	UNP P0AEX9
E	-17	ILE	-	linker	UNP P0AEX9
E	-16	PRO	-	linker	UNP P0AEX9
E	-15	ASN	-	linker	UNP P0AEX9
E	-14	PRO	-	linker	UNP P0AEX9
E	-13	LEU	-	linker	UNP P0AEX9
E	-12	LEU	-	linker	UNP P0AEX9
E	-11	GLY	-	linker	UNP P0AEX9
E	-10	LEU	-	linker	UNP P0AEX9
E	-9	ASP	-	linker	UNP P0AEX9
E	-8	SER	-	linker	UNP P0AEX9
E	-7	THR	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	GLU	-	linker	UNP P0AEX9
E	-5	ASN	-	linker	UNP P0AEX9
E	-4	LEU	-	linker	UNP P0AEX9
E	-3	TYR	-	linker	UNP P0AEX9
E	-2	PHE	-	linker	UNP P0AEX9
E	-1	GLN	-	linker	UNP P0AEX9
E	0	GLY	-	linker	UNP P0AEX9
F	-393	HIS	-	expression tag	UNP P0AEX9
F	-392	HIS	-	expression tag	UNP P0AEX9
F	-391	HIS	-	expression tag	UNP P0AEX9
F	-390	HIS	-	expression tag	UNP P0AEX9
F	-389	HIS	-	expression tag	UNP P0AEX9
F	-388	HIS	-	expression tag	UNP P0AEX9
F	-387	MET	-	expression tag	UNP P0AEX9
F	-20	GLY	-	linker	UNP P0AEX9
F	-19	LYS	-	linker	UNP P0AEX9
F	-18	PRO	-	linker	UNP P0AEX9
F	-17	ILE	-	linker	UNP P0AEX9
F	-16	PRO	-	linker	UNP P0AEX9
F	-15	ASN	-	linker	UNP P0AEX9
F	-14	PRO	-	linker	UNP P0AEX9
F	-13	LEU	-	linker	UNP P0AEX9
F	-12	LEU	-	linker	UNP P0AEX9
F	-11	GLY	-	linker	UNP P0AEX9
F	-10	LEU	-	linker	UNP P0AEX9
F	-9	ASP	-	linker	UNP P0AEX9
F	-8	SER	-	linker	UNP P0AEX9
F	-7	THR	-	linker	UNP P0AEX9
F	-6	GLU	-	linker	UNP P0AEX9
F	-5	ASN	-	linker	UNP P0AEX9
F	-4	LEU	-	linker	UNP P0AEX9
F	-3	TYR	-	linker	UNP P0AEX9
F	-2	PHE	-	linker	UNP P0AEX9
F	-1	GLN	-	linker	UNP P0AEX9
F	0	GLY	-	linker	UNP P0AEX9
G	-393	HIS	-	expression tag	UNP P0AEX9
G	-392	HIS	-	expression tag	UNP P0AEX9
G	-391	HIS	-	expression tag	UNP P0AEX9
G	-390	HIS	-	expression tag	UNP P0AEX9
G	-389	HIS	-	expression tag	UNP P0AEX9
G	-388	HIS	-	expression tag	UNP P0AEX9
G	-387	MET	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-20	GLY	-	linker	UNP P0AEX9
G	-19	LYS	-	linker	UNP P0AEX9
G	-18	PRO	-	linker	UNP P0AEX9
G	-17	ILE	-	linker	UNP P0AEX9
G	-16	PRO	-	linker	UNP P0AEX9
G	-15	ASN	-	linker	UNP P0AEX9
G	-14	PRO	-	linker	UNP P0AEX9
G	-13	LEU	-	linker	UNP P0AEX9
G	-12	LEU	-	linker	UNP P0AEX9
G	-11	GLY	-	linker	UNP P0AEX9
G	-10	LEU	-	linker	UNP P0AEX9
G	-9	ASP	-	linker	UNP P0AEX9
G	-8	SER	-	linker	UNP P0AEX9
G	-7	THR	-	linker	UNP P0AEX9
G	-6	GLU	-	linker	UNP P0AEX9
G	-5	ASN	-	linker	UNP P0AEX9
G	-4	LEU	-	linker	UNP P0AEX9
G	-3	TYR	-	linker	UNP P0AEX9
G	-2	PHE	-	linker	UNP P0AEX9
G	-1	GLN	-	linker	UNP P0AEX9
G	0	GLY	-	linker	UNP P0AEX9
H	-393	HIS	-	expression tag	UNP P0AEX9
H	-392	HIS	-	expression tag	UNP P0AEX9
H	-391	HIS	-	expression tag	UNP P0AEX9
H	-390	HIS	-	expression tag	UNP P0AEX9
H	-389	HIS	-	expression tag	UNP P0AEX9
H	-388	HIS	-	expression tag	UNP P0AEX9
H	-387	MET	-	expression tag	UNP P0AEX9
H	-20	GLY	-	linker	UNP P0AEX9
H	-19	LYS	-	linker	UNP P0AEX9
H	-18	PRO	-	linker	UNP P0AEX9
H	-17	ILE	-	linker	UNP P0AEX9
H	-16	PRO	-	linker	UNP P0AEX9
H	-15	ASN	-	linker	UNP P0AEX9
H	-14	PRO	-	linker	UNP P0AEX9
H	-13	LEU	-	linker	UNP P0AEX9
H	-12	LEU	-	linker	UNP P0AEX9
H	-11	GLY	-	linker	UNP P0AEX9
H	-10	LEU	-	linker	UNP P0AEX9
H	-9	ASP	-	linker	UNP P0AEX9
H	-8	SER	-	linker	UNP P0AEX9
H	-7	THR	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-6	GLU	-	linker	UNP P0AEX9
H	-5	ASN	-	linker	UNP P0AEX9
H	-4	LEU	-	linker	UNP P0AEX9
H	-3	TYR	-	linker	UNP P0AEX9
H	-2	PHE	-	linker	UNP P0AEX9
H	-1	GLN	-	linker	UNP P0AEX9
H	0	GLY	-	linker	UNP P0AEX9
I	-393	HIS	-	expression tag	UNP P0AEX9
I	-392	HIS	-	expression tag	UNP P0AEX9
I	-391	HIS	-	expression tag	UNP P0AEX9
I	-390	HIS	-	expression tag	UNP P0AEX9
I	-389	HIS	-	expression tag	UNP P0AEX9
I	-388	HIS	-	expression tag	UNP P0AEX9
I	-387	MET	-	expression tag	UNP P0AEX9
I	-20	GLY	-	linker	UNP P0AEX9
I	-19	LYS	-	linker	UNP P0AEX9
I	-18	PRO	-	linker	UNP P0AEX9
I	-17	ILE	-	linker	UNP P0AEX9
I	-16	PRO	-	linker	UNP P0AEX9
I	-15	ASN	-	linker	UNP P0AEX9
I	-14	PRO	-	linker	UNP P0AEX9
I	-13	LEU	-	linker	UNP P0AEX9
I	-12	LEU	-	linker	UNP P0AEX9
I	-11	GLY	-	linker	UNP P0AEX9
I	-10	LEU	-	linker	UNP P0AEX9
I	-9	ASP	-	linker	UNP P0AEX9
I	-8	SER	-	linker	UNP P0AEX9
I	-7	THR	-	linker	UNP P0AEX9
I	-6	GLU	-	linker	UNP P0AEX9
I	-5	ASN	-	linker	UNP P0AEX9
I	-4	LEU	-	linker	UNP P0AEX9
I	-3	TYR	-	linker	UNP P0AEX9
I	-2	PHE	-	linker	UNP P0AEX9
I	-1	GLN	-	linker	UNP P0AEX9
I	0	GLY	-	linker	UNP P0AEX9
J	-393	HIS	-	expression tag	UNP P0AEX9
J	-392	HIS	-	expression tag	UNP P0AEX9
J	-391	HIS	-	expression tag	UNP P0AEX9
J	-390	HIS	-	expression tag	UNP P0AEX9
J	-389	HIS	-	expression tag	UNP P0AEX9
J	-388	HIS	-	expression tag	UNP P0AEX9
J	-387	MET	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-20	GLY	-	linker	UNP P0AEX9
J	-19	LYS	-	linker	UNP P0AEX9
J	-18	PRO	-	linker	UNP P0AEX9
J	-17	ILE	-	linker	UNP P0AEX9
J	-16	PRO	-	linker	UNP P0AEX9
J	-15	ASN	-	linker	UNP P0AEX9
J	-14	PRO	-	linker	UNP P0AEX9
J	-13	LEU	-	linker	UNP P0AEX9
J	-12	LEU	-	linker	UNP P0AEX9
J	-11	GLY	-	linker	UNP P0AEX9
J	-10	LEU	-	linker	UNP P0AEX9
J	-9	ASP	-	linker	UNP P0AEX9
J	-8	SER	-	linker	UNP P0AEX9
J	-7	THR	-	linker	UNP P0AEX9
J	-6	GLU	-	linker	UNP P0AEX9
J	-5	ASN	-	linker	UNP P0AEX9
J	-4	LEU	-	linker	UNP P0AEX9
J	-3	TYR	-	linker	UNP P0AEX9
J	-2	PHE	-	linker	UNP P0AEX9
J	-1	GLN	-	linker	UNP P0AEX9
J	0	GLY	-	linker	UNP P0AEX9
K	-393	HIS	-	expression tag	UNP P0AEX9
K	-392	HIS	-	expression tag	UNP P0AEX9
K	-391	HIS	-	expression tag	UNP P0AEX9
K	-390	HIS	-	expression tag	UNP P0AEX9
K	-389	HIS	-	expression tag	UNP P0AEX9
K	-388	HIS	-	expression tag	UNP P0AEX9
K	-387	MET	-	expression tag	UNP P0AEX9
K	-20	GLY	-	linker	UNP P0AEX9
K	-19	LYS	-	linker	UNP P0AEX9
K	-18	PRO	-	linker	UNP P0AEX9
K	-17	ILE	-	linker	UNP P0AEX9
K	-16	PRO	-	linker	UNP P0AEX9
K	-15	ASN	-	linker	UNP P0AEX9
K	-14	PRO	-	linker	UNP P0AEX9
K	-13	LEU	-	linker	UNP P0AEX9
K	-12	LEU	-	linker	UNP P0AEX9
K	-11	GLY	-	linker	UNP P0AEX9
K	-10	LEU	-	linker	UNP P0AEX9
K	-9	ASP	-	linker	UNP P0AEX9
K	-8	SER	-	linker	UNP P0AEX9
K	-7	THR	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-6	GLU	-	linker	UNP P0AEX9
K	-5	ASN	-	linker	UNP P0AEX9
K	-4	LEU	-	linker	UNP P0AEX9
K	-3	TYR	-	linker	UNP P0AEX9
K	-2	PHE	-	linker	UNP P0AEX9
K	-1	GLN	-	linker	UNP P0AEX9
K	0	GLY	-	linker	UNP P0AEX9
L	-393	HIS	-	expression tag	UNP P0AEX9
L	-392	HIS	-	expression tag	UNP P0AEX9
L	-391	HIS	-	expression tag	UNP P0AEX9
L	-390	HIS	-	expression tag	UNP P0AEX9
L	-389	HIS	-	expression tag	UNP P0AEX9
L	-388	HIS	-	expression tag	UNP P0AEX9
L	-387	MET	-	expression tag	UNP P0AEX9
L	-20	GLY	-	linker	UNP P0AEX9
L	-19	LYS	-	linker	UNP P0AEX9
L	-18	PRO	-	linker	UNP P0AEX9
L	-17	ILE	-	linker	UNP P0AEX9
L	-16	PRO	-	linker	UNP P0AEX9
L	-15	ASN	-	linker	UNP P0AEX9
L	-14	PRO	-	linker	UNP P0AEX9
L	-13	LEU	-	linker	UNP P0AEX9
L	-12	LEU	-	linker	UNP P0AEX9
L	-11	GLY	-	linker	UNP P0AEX9
L	-10	LEU	-	linker	UNP P0AEX9
L	-9	ASP	-	linker	UNP P0AEX9
L	-8	SER	-	linker	UNP P0AEX9
L	-7	THR	-	linker	UNP P0AEX9
L	-6	GLU	-	linker	UNP P0AEX9
L	-5	ASN	-	linker	UNP P0AEX9
L	-4	LEU	-	linker	UNP P0AEX9
L	-3	TYR	-	linker	UNP P0AEX9
L	-2	PHE	-	linker	UNP P0AEX9
L	-1	GLN	-	linker	UNP P0AEX9
L	0	GLY	-	linker	UNP P0AEX9
M	-393	HIS	-	expression tag	UNP P0AEX9
M	-392	HIS	-	expression tag	UNP P0AEX9
M	-391	HIS	-	expression tag	UNP P0AEX9
M	-390	HIS	-	expression tag	UNP P0AEX9
M	-389	HIS	-	expression tag	UNP P0AEX9
M	-388	HIS	-	expression tag	UNP P0AEX9
M	-387	MET	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-20	GLY	-	linker	UNP P0AEX9
M	-19	LYS	-	linker	UNP P0AEX9
M	-18	PRO	-	linker	UNP P0AEX9
M	-17	ILE	-	linker	UNP P0AEX9
M	-16	PRO	-	linker	UNP P0AEX9
M	-15	ASN	-	linker	UNP P0AEX9
M	-14	PRO	-	linker	UNP P0AEX9
M	-13	LEU	-	linker	UNP P0AEX9
M	-12	LEU	-	linker	UNP P0AEX9
M	-11	GLY	-	linker	UNP P0AEX9
M	-10	LEU	-	linker	UNP P0AEX9
M	-9	ASP	-	linker	UNP P0AEX9
M	-8	SER	-	linker	UNP P0AEX9
M	-7	THR	-	linker	UNP P0AEX9
M	-6	GLU	-	linker	UNP P0AEX9
M	-5	ASN	-	linker	UNP P0AEX9
M	-4	LEU	-	linker	UNP P0AEX9
M	-3	TYR	-	linker	UNP P0AEX9
M	-2	PHE	-	linker	UNP P0AEX9
M	-1	GLN	-	linker	UNP P0AEX9
M	0	GLY	-	linker	UNP P0AEX9
N	-393	HIS	-	expression tag	UNP P0AEX9
N	-392	HIS	-	expression tag	UNP P0AEX9
N	-391	HIS	-	expression tag	UNP P0AEX9
N	-390	HIS	-	expression tag	UNP P0AEX9
N	-389	HIS	-	expression tag	UNP P0AEX9
N	-388	HIS	-	expression tag	UNP P0AEX9
N	-387	MET	-	expression tag	UNP P0AEX9
N	-20	GLY	-	linker	UNP P0AEX9
N	-19	LYS	-	linker	UNP P0AEX9
N	-18	PRO	-	linker	UNP P0AEX9
N	-17	ILE	-	linker	UNP P0AEX9
N	-16	PRO	-	linker	UNP P0AEX9
N	-15	ASN	-	linker	UNP P0AEX9
N	-14	PRO	-	linker	UNP P0AEX9
N	-13	LEU	-	linker	UNP P0AEX9
N	-12	LEU	-	linker	UNP P0AEX9
N	-11	GLY	-	linker	UNP P0AEX9
N	-10	LEU	-	linker	UNP P0AEX9
N	-9	ASP	-	linker	UNP P0AEX9
N	-8	SER	-	linker	UNP P0AEX9
N	-7	THR	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-6	GLU	-	linker	UNP P0AEX9
N	-5	ASN	-	linker	UNP P0AEX9
N	-4	LEU	-	linker	UNP P0AEX9
N	-3	TYR	-	linker	UNP P0AEX9
N	-2	PHE	-	linker	UNP P0AEX9
N	-1	GLN	-	linker	UNP P0AEX9
N	0	GLY	-	linker	UNP P0AEX9
O	-393	HIS	-	expression tag	UNP P0AEX9
O	-392	HIS	-	expression tag	UNP P0AEX9
O	-391	HIS	-	expression tag	UNP P0AEX9
O	-390	HIS	-	expression tag	UNP P0AEX9
O	-389	HIS	-	expression tag	UNP P0AEX9
O	-388	HIS	-	expression tag	UNP P0AEX9
O	-387	MET	-	expression tag	UNP P0AEX9
O	-20	GLY	-	linker	UNP P0AEX9
O	-19	LYS	-	linker	UNP P0AEX9
O	-18	PRO	-	linker	UNP P0AEX9
O	-17	ILE	-	linker	UNP P0AEX9
O	-16	PRO	-	linker	UNP P0AEX9
O	-15	ASN	-	linker	UNP P0AEX9
O	-14	PRO	-	linker	UNP P0AEX9
O	-13	LEU	-	linker	UNP P0AEX9
O	-12	LEU	-	linker	UNP P0AEX9
O	-11	GLY	-	linker	UNP P0AEX9
O	-10	LEU	-	linker	UNP P0AEX9
O	-9	ASP	-	linker	UNP P0AEX9
O	-8	SER	-	linker	UNP P0AEX9
O	-7	THR	-	linker	UNP P0AEX9
O	-6	GLU	-	linker	UNP P0AEX9
O	-5	ASN	-	linker	UNP P0AEX9
O	-4	LEU	-	linker	UNP P0AEX9
O	-3	TYR	-	linker	UNP P0AEX9
O	-2	PHE	-	linker	UNP P0AEX9
O	-1	GLN	-	linker	UNP P0AEX9
O	0	GLY	-	linker	UNP P0AEX9
P	-393	HIS	-	expression tag	UNP P0AEX9
P	-392	HIS	-	expression tag	UNP P0AEX9
P	-391	HIS	-	expression tag	UNP P0AEX9
P	-390	HIS	-	expression tag	UNP P0AEX9
P	-389	HIS	-	expression tag	UNP P0AEX9
P	-388	HIS	-	expression tag	UNP P0AEX9
P	-387	MET	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-20	GLY	-	linker	UNP P0AEX9
P	-19	LYS	-	linker	UNP P0AEX9
P	-18	PRO	-	linker	UNP P0AEX9
P	-17	ILE	-	linker	UNP P0AEX9
P	-16	PRO	-	linker	UNP P0AEX9
P	-15	ASN	-	linker	UNP P0AEX9
P	-14	PRO	-	linker	UNP P0AEX9
P	-13	LEU	-	linker	UNP P0AEX9
P	-12	LEU	-	linker	UNP P0AEX9
P	-11	GLY	-	linker	UNP P0AEX9
P	-10	LEU	-	linker	UNP P0AEX9
P	-9	ASP	-	linker	UNP P0AEX9
P	-8	SER	-	linker	UNP P0AEX9
P	-7	THR	-	linker	UNP P0AEX9
P	-6	GLU	-	linker	UNP P0AEX9
P	-5	ASN	-	linker	UNP P0AEX9
P	-4	LEU	-	linker	UNP P0AEX9
P	-3	TYR	-	linker	UNP P0AEX9
P	-2	PHE	-	linker	UNP P0AEX9
P	-1	GLN	-	linker	UNP P0AEX9
P	0	GLY	-	linker	UNP P0AEX9
Q	-393	HIS	-	expression tag	UNP P0AEX9
Q	-392	HIS	-	expression tag	UNP P0AEX9
Q	-391	HIS	-	expression tag	UNP P0AEX9
Q	-390	HIS	-	expression tag	UNP P0AEX9
Q	-389	HIS	-	expression tag	UNP P0AEX9
Q	-388	HIS	-	expression tag	UNP P0AEX9
Q	-387	MET	-	expression tag	UNP P0AEX9
Q	-20	GLY	-	linker	UNP P0AEX9
Q	-19	LYS	-	linker	UNP P0AEX9
Q	-18	PRO	-	linker	UNP P0AEX9
Q	-17	ILE	-	linker	UNP P0AEX9
Q	-16	PRO	-	linker	UNP P0AEX9
Q	-15	ASN	-	linker	UNP P0AEX9
Q	-14	PRO	-	linker	UNP P0AEX9
Q	-13	LEU	-	linker	UNP P0AEX9
Q	-12	LEU	-	linker	UNP P0AEX9
Q	-11	GLY	-	linker	UNP P0AEX9
Q	-10	LEU	-	linker	UNP P0AEX9
Q	-9	ASP	-	linker	UNP P0AEX9
Q	-8	SER	-	linker	UNP P0AEX9
Q	-7	THR	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-6	GLU	-	linker	UNP P0AEX9
Q	-5	ASN	-	linker	UNP P0AEX9
Q	-4	LEU	-	linker	UNP P0AEX9
Q	-3	TYR	-	linker	UNP P0AEX9
Q	-2	PHE	-	linker	UNP P0AEX9
Q	-1	GLN	-	linker	UNP P0AEX9
Q	0	GLY	-	linker	UNP P0AEX9
R	-393	HIS	-	expression tag	UNP P0AEX9
R	-392	HIS	-	expression tag	UNP P0AEX9
R	-391	HIS	-	expression tag	UNP P0AEX9
R	-390	HIS	-	expression tag	UNP P0AEX9
R	-389	HIS	-	expression tag	UNP P0AEX9
R	-388	HIS	-	expression tag	UNP P0AEX9
R	-387	MET	-	expression tag	UNP P0AEX9
R	-20	GLY	-	linker	UNP P0AEX9
R	-19	LYS	-	linker	UNP P0AEX9
R	-18	PRO	-	linker	UNP P0AEX9
R	-17	ILE	-	linker	UNP P0AEX9
R	-16	PRO	-	linker	UNP P0AEX9
R	-15	ASN	-	linker	UNP P0AEX9
R	-14	PRO	-	linker	UNP P0AEX9
R	-13	LEU	-	linker	UNP P0AEX9
R	-12	LEU	-	linker	UNP P0AEX9
R	-11	GLY	-	linker	UNP P0AEX9
R	-10	LEU	-	linker	UNP P0AEX9
R	-9	ASP	-	linker	UNP P0AEX9
R	-8	SER	-	linker	UNP P0AEX9
R	-7	THR	-	linker	UNP P0AEX9
R	-6	GLU	-	linker	UNP P0AEX9
R	-5	ASN	-	linker	UNP P0AEX9
R	-4	LEU	-	linker	UNP P0AEX9
R	-3	TYR	-	linker	UNP P0AEX9
R	-2	PHE	-	linker	UNP P0AEX9
R	-1	GLN	-	linker	UNP P0AEX9
R	0	GLY	-	linker	UNP P0AEX9
S	-393	HIS	-	expression tag	UNP P0AEX9
S	-392	HIS	-	expression tag	UNP P0AEX9
S	-391	HIS	-	expression tag	UNP P0AEX9
S	-390	HIS	-	expression tag	UNP P0AEX9
S	-389	HIS	-	expression tag	UNP P0AEX9
S	-388	HIS	-	expression tag	UNP P0AEX9
S	-387	MET	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-20	GLY	-	linker	UNP P0AEX9
S	-19	LYS	-	linker	UNP P0AEX9
S	-18	PRO	-	linker	UNP P0AEX9
S	-17	ILE	-	linker	UNP P0AEX9
S	-16	PRO	-	linker	UNP P0AEX9
S	-15	ASN	-	linker	UNP P0AEX9
S	-14	PRO	-	linker	UNP P0AEX9
S	-13	LEU	-	linker	UNP P0AEX9
S	-12	LEU	-	linker	UNP P0AEX9
S	-11	GLY	-	linker	UNP P0AEX9
S	-10	LEU	-	linker	UNP P0AEX9
S	-9	ASP	-	linker	UNP P0AEX9
S	-8	SER	-	linker	UNP P0AEX9
S	-7	THR	-	linker	UNP P0AEX9
S	-6	GLU	-	linker	UNP P0AEX9
S	-5	ASN	-	linker	UNP P0AEX9
S	-4	LEU	-	linker	UNP P0AEX9
S	-3	TYR	-	linker	UNP P0AEX9
S	-2	PHE	-	linker	UNP P0AEX9
S	-1	GLN	-	linker	UNP P0AEX9
S	0	GLY	-	linker	UNP P0AEX9
T	-393	HIS	-	expression tag	UNP P0AEX9
T	-392	HIS	-	expression tag	UNP P0AEX9
T	-391	HIS	-	expression tag	UNP P0AEX9
T	-390	HIS	-	expression tag	UNP P0AEX9
T	-389	HIS	-	expression tag	UNP P0AEX9
T	-388	HIS	-	expression tag	UNP P0AEX9
T	-387	MET	-	expression tag	UNP P0AEX9
T	-20	GLY	-	linker	UNP P0AEX9
T	-19	LYS	-	linker	UNP P0AEX9
T	-18	PRO	-	linker	UNP P0AEX9
T	-17	ILE	-	linker	UNP P0AEX9
T	-16	PRO	-	linker	UNP P0AEX9
T	-15	ASN	-	linker	UNP P0AEX9
T	-14	PRO	-	linker	UNP P0AEX9
T	-13	LEU	-	linker	UNP P0AEX9
T	-12	LEU	-	linker	UNP P0AEX9
T	-11	GLY	-	linker	UNP P0AEX9
T	-10	LEU	-	linker	UNP P0AEX9
T	-9	ASP	-	linker	UNP P0AEX9
T	-8	SER	-	linker	UNP P0AEX9
T	-7	THR	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-6	GLU	-	linker	UNP P0AEX9
T	-5	ASN	-	linker	UNP P0AEX9
T	-4	LEU	-	linker	UNP P0AEX9
T	-3	TYR	-	linker	UNP P0AEX9
T	-2	PHE	-	linker	UNP P0AEX9
T	-1	GLN	-	linker	UNP P0AEX9
T	0	GLY	-	linker	UNP P0AEX9
U	-393	HIS	-	expression tag	UNP P0AEX9
U	-392	HIS	-	expression tag	UNP P0AEX9
U	-391	HIS	-	expression tag	UNP P0AEX9
U	-390	HIS	-	expression tag	UNP P0AEX9
U	-389	HIS	-	expression tag	UNP P0AEX9
U	-388	HIS	-	expression tag	UNP P0AEX9
U	-387	MET	-	expression tag	UNP P0AEX9
U	-20	GLY	-	linker	UNP P0AEX9
U	-19	LYS	-	linker	UNP P0AEX9
U	-18	PRO	-	linker	UNP P0AEX9
U	-17	ILE	-	linker	UNP P0AEX9
U	-16	PRO	-	linker	UNP P0AEX9
U	-15	ASN	-	linker	UNP P0AEX9
U	-14	PRO	-	linker	UNP P0AEX9
U	-13	LEU	-	linker	UNP P0AEX9
U	-12	LEU	-	linker	UNP P0AEX9
U	-11	GLY	-	linker	UNP P0AEX9
U	-10	LEU	-	linker	UNP P0AEX9
U	-9	ASP	-	linker	UNP P0AEX9
U	-8	SER	-	linker	UNP P0AEX9
U	-7	THR	-	linker	UNP P0AEX9
U	-6	GLU	-	linker	UNP P0AEX9
U	-5	ASN	-	linker	UNP P0AEX9
U	-4	LEU	-	linker	UNP P0AEX9
U	-3	TYR	-	linker	UNP P0AEX9
U	-2	PHE	-	linker	UNP P0AEX9
U	-1	GLN	-	linker	UNP P0AEX9
U	0	GLY	-	linker	UNP P0AEX9
V	-393	HIS	-	expression tag	UNP P0AEX9
V	-392	HIS	-	expression tag	UNP P0AEX9
V	-391	HIS	-	expression tag	UNP P0AEX9
V	-390	HIS	-	expression tag	UNP P0AEX9
V	-389	HIS	-	expression tag	UNP P0AEX9
V	-388	HIS	-	expression tag	UNP P0AEX9
V	-387	MET	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
V	-20	GLY	-	linker	UNP P0AEX9
V	-19	LYS	-	linker	UNP P0AEX9
V	-18	PRO	-	linker	UNP P0AEX9
V	-17	ILE	-	linker	UNP P0AEX9
V	-16	PRO	-	linker	UNP P0AEX9
V	-15	ASN	-	linker	UNP P0AEX9
V	-14	PRO	-	linker	UNP P0AEX9
V	-13	LEU	-	linker	UNP P0AEX9
V	-12	LEU	-	linker	UNP P0AEX9
V	-11	GLY	-	linker	UNP P0AEX9
V	-10	LEU	-	linker	UNP P0AEX9
V	-9	ASP	-	linker	UNP P0AEX9
V	-8	SER	-	linker	UNP P0AEX9
V	-7	THR	-	linker	UNP P0AEX9
V	-6	GLU	-	linker	UNP P0AEX9
V	-5	ASN	-	linker	UNP P0AEX9
V	-4	LEU	-	linker	UNP P0AEX9
V	-3	TYR	-	linker	UNP P0AEX9
V	-2	PHE	-	linker	UNP P0AEX9
V	-1	GLN	-	linker	UNP P0AEX9
V	0	GLY	-	linker	UNP P0AEX9
W	-393	HIS	-	expression tag	UNP P0AEX9
W	-392	HIS	-	expression tag	UNP P0AEX9
W	-391	HIS	-	expression tag	UNP P0AEX9
W	-390	HIS	-	expression tag	UNP P0AEX9
W	-389	HIS	-	expression tag	UNP P0AEX9
W	-388	HIS	-	expression tag	UNP P0AEX9
W	-387	MET	-	expression tag	UNP P0AEX9
W	-20	GLY	-	linker	UNP P0AEX9
W	-19	LYS	-	linker	UNP P0AEX9
W	-18	PRO	-	linker	UNP P0AEX9
W	-17	ILE	-	linker	UNP P0AEX9
W	-16	PRO	-	linker	UNP P0AEX9
W	-15	ASN	-	linker	UNP P0AEX9
W	-14	PRO	-	linker	UNP P0AEX9
W	-13	LEU	-	linker	UNP P0AEX9
W	-12	LEU	-	linker	UNP P0AEX9
W	-11	GLY	-	linker	UNP P0AEX9
W	-10	LEU	-	linker	UNP P0AEX9
W	-9	ASP	-	linker	UNP P0AEX9
W	-8	SER	-	linker	UNP P0AEX9
W	-7	THR	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
W	-6	GLU	-	linker	UNP P0AEX9
W	-5	ASN	-	linker	UNP P0AEX9
W	-4	LEU	-	linker	UNP P0AEX9
W	-3	TYR	-	linker	UNP P0AEX9
W	-2	PHE	-	linker	UNP P0AEX9
W	-1	GLN	-	linker	UNP P0AEX9
W	0	GLY	-	linker	UNP P0AEX9
X	-393	HIS	-	expression tag	UNP P0AEX9
X	-392	HIS	-	expression tag	UNP P0AEX9
X	-391	HIS	-	expression tag	UNP P0AEX9
X	-390	HIS	-	expression tag	UNP P0AEX9
X	-389	HIS	-	expression tag	UNP P0AEX9
X	-388	HIS	-	expression tag	UNP P0AEX9
X	-387	MET	-	expression tag	UNP P0AEX9
X	-20	GLY	-	linker	UNP P0AEX9
X	-19	LYS	-	linker	UNP P0AEX9
X	-18	PRO	-	linker	UNP P0AEX9
X	-17	ILE	-	linker	UNP P0AEX9
X	-16	PRO	-	linker	UNP P0AEX9
X	-15	ASN	-	linker	UNP P0AEX9
X	-14	PRO	-	linker	UNP P0AEX9
X	-13	LEU	-	linker	UNP P0AEX9
X	-12	LEU	-	linker	UNP P0AEX9
X	-11	GLY	-	linker	UNP P0AEX9
X	-10	LEU	-	linker	UNP P0AEX9
X	-9	ASP	-	linker	UNP P0AEX9
X	-8	SER	-	linker	UNP P0AEX9
X	-7	THR	-	linker	UNP P0AEX9
X	-6	GLU	-	linker	UNP P0AEX9
X	-5	ASN	-	linker	UNP P0AEX9
X	-4	LEU	-	linker	UNP P0AEX9
X	-3	TYR	-	linker	UNP P0AEX9
X	-2	PHE	-	linker	UNP P0AEX9
X	-1	GLN	-	linker	UNP P0AEX9
X	0	GLY	-	linker	UNP P0AEX9
Y	-393	HIS	-	expression tag	UNP P0AEX9
Y	-392	HIS	-	expression tag	UNP P0AEX9
Y	-391	HIS	-	expression tag	UNP P0AEX9
Y	-390	HIS	-	expression tag	UNP P0AEX9
Y	-389	HIS	-	expression tag	UNP P0AEX9
Y	-388	HIS	-	expression tag	UNP P0AEX9
Y	-387	MET	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-20	GLY	-	linker	UNP P0AEX9
Y	-19	LYS	-	linker	UNP P0AEX9
Y	-18	PRO	-	linker	UNP P0AEX9
Y	-17	ILE	-	linker	UNP P0AEX9
Y	-16	PRO	-	linker	UNP P0AEX9
Y	-15	ASN	-	linker	UNP P0AEX9
Y	-14	PRO	-	linker	UNP P0AEX9
Y	-13	LEU	-	linker	UNP P0AEX9
Y	-12	LEU	-	linker	UNP P0AEX9
Y	-11	GLY	-	linker	UNP P0AEX9
Y	-10	LEU	-	linker	UNP P0AEX9
Y	-9	ASP	-	linker	UNP P0AEX9
Y	-8	SER	-	linker	UNP P0AEX9
Y	-7	THR	-	linker	UNP P0AEX9
Y	-6	GLU	-	linker	UNP P0AEX9
Y	-5	ASN	-	linker	UNP P0AEX9
Y	-4	LEU	-	linker	UNP P0AEX9
Y	-3	TYR	-	linker	UNP P0AEX9
Y	-2	PHE	-	linker	UNP P0AEX9
Y	-1	GLN	-	linker	UNP P0AEX9
Y	0	GLY	-	linker	UNP P0AEX9
Z	-393	HIS	-	expression tag	UNP P0AEX9
Z	-392	HIS	-	expression tag	UNP P0AEX9
Z	-391	HIS	-	expression tag	UNP P0AEX9
Z	-390	HIS	-	expression tag	UNP P0AEX9
Z	-389	HIS	-	expression tag	UNP P0AEX9
Z	-388	HIS	-	expression tag	UNP P0AEX9
Z	-387	MET	-	expression tag	UNP P0AEX9
Z	-20	GLY	-	linker	UNP P0AEX9
Z	-19	LYS	-	linker	UNP P0AEX9
Z	-18	PRO	-	linker	UNP P0AEX9
Z	-17	ILE	-	linker	UNP P0AEX9
Z	-16	PRO	-	linker	UNP P0AEX9
Z	-15	ASN	-	linker	UNP P0AEX9
Z	-14	PRO	-	linker	UNP P0AEX9
Z	-13	LEU	-	linker	UNP P0AEX9
Z	-12	LEU	-	linker	UNP P0AEX9
Z	-11	GLY	-	linker	UNP P0AEX9
Z	-10	LEU	-	linker	UNP P0AEX9
Z	-9	ASP	-	linker	UNP P0AEX9
Z	-8	SER	-	linker	UNP P0AEX9
Z	-7	THR	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	-6	GLU	-	linker	UNP P0AEX9
Z	-5	ASN	-	linker	UNP P0AEX9
Z	-4	LEU	-	linker	UNP P0AEX9
Z	-3	TYR	-	linker	UNP P0AEX9
Z	-2	PHE	-	linker	UNP P0AEX9
Z	-1	GLN	-	linker	UNP P0AEX9
Z	0	GLY	-	linker	UNP P0AEX9
a	-393	HIS	-	expression tag	UNP P0AEX9
a	-392	HIS	-	expression tag	UNP P0AEX9
a	-391	HIS	-	expression tag	UNP P0AEX9
a	-390	HIS	-	expression tag	UNP P0AEX9
a	-389	HIS	-	expression tag	UNP P0AEX9
a	-388	HIS	-	expression tag	UNP P0AEX9
a	-387	MET	-	expression tag	UNP P0AEX9
a	-20	GLY	-	linker	UNP P0AEX9
a	-19	LYS	-	linker	UNP P0AEX9
a	-18	PRO	-	linker	UNP P0AEX9
a	-17	ILE	-	linker	UNP P0AEX9
a	-16	PRO	-	linker	UNP P0AEX9
a	-15	ASN	-	linker	UNP P0AEX9
a	-14	PRO	-	linker	UNP P0AEX9
a	-13	LEU	-	linker	UNP P0AEX9
a	-12	LEU	-	linker	UNP P0AEX9
a	-11	GLY	-	linker	UNP P0AEX9
a	-10	LEU	-	linker	UNP P0AEX9
a	-9	ASP	-	linker	UNP P0AEX9
a	-8	SER	-	linker	UNP P0AEX9
a	-7	THR	-	linker	UNP P0AEX9
a	-6	GLU	-	linker	UNP P0AEX9
a	-5	ASN	-	linker	UNP P0AEX9
a	-4	LEU	-	linker	UNP P0AEX9
a	-3	TYR	-	linker	UNP P0AEX9
a	-2	PHE	-	linker	UNP P0AEX9
a	-1	GLN	-	linker	UNP P0AEX9
a	0	GLY	-	linker	UNP P0AEX9
b	-393	HIS	-	expression tag	UNP P0AEX9
b	-392	HIS	-	expression tag	UNP P0AEX9
b	-391	HIS	-	expression tag	UNP P0AEX9
b	-390	HIS	-	expression tag	UNP P0AEX9
b	-389	HIS	-	expression tag	UNP P0AEX9
b	-388	HIS	-	expression tag	UNP P0AEX9
b	-387	MET	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
b	-20	GLY	-	linker	UNP P0AEX9
b	-19	LYS	-	linker	UNP P0AEX9
b	-18	PRO	-	linker	UNP P0AEX9
b	-17	ILE	-	linker	UNP P0AEX9
b	-16	PRO	-	linker	UNP P0AEX9
b	-15	ASN	-	linker	UNP P0AEX9
b	-14	PRO	-	linker	UNP P0AEX9
b	-13	LEU	-	linker	UNP P0AEX9
b	-12	LEU	-	linker	UNP P0AEX9
b	-11	GLY	-	linker	UNP P0AEX9
b	-10	LEU	-	linker	UNP P0AEX9
b	-9	ASP	-	linker	UNP P0AEX9
b	-8	SER	-	linker	UNP P0AEX9
b	-7	THR	-	linker	UNP P0AEX9
b	-6	GLU	-	linker	UNP P0AEX9
b	-5	ASN	-	linker	UNP P0AEX9
b	-4	LEU	-	linker	UNP P0AEX9
b	-3	TYR	-	linker	UNP P0AEX9
b	-2	PHE	-	linker	UNP P0AEX9
b	-1	GLN	-	linker	UNP P0AEX9
b	0	GLY	-	linker	UNP P0AEX9
c	-393	HIS	-	expression tag	UNP P0AEX9
c	-392	HIS	-	expression tag	UNP P0AEX9
c	-391	HIS	-	expression tag	UNP P0AEX9
c	-390	HIS	-	expression tag	UNP P0AEX9
c	-389	HIS	-	expression tag	UNP P0AEX9
c	-388	HIS	-	expression tag	UNP P0AEX9
c	-387	MET	-	expression tag	UNP P0AEX9
c	-20	GLY	-	linker	UNP P0AEX9
c	-19	LYS	-	linker	UNP P0AEX9
c	-18	PRO	-	linker	UNP P0AEX9
c	-17	ILE	-	linker	UNP P0AEX9
c	-16	PRO	-	linker	UNP P0AEX9
c	-15	ASN	-	linker	UNP P0AEX9
c	-14	PRO	-	linker	UNP P0AEX9
c	-13	LEU	-	linker	UNP P0AEX9
c	-12	LEU	-	linker	UNP P0AEX9
c	-11	GLY	-	linker	UNP P0AEX9
c	-10	LEU	-	linker	UNP P0AEX9
c	-9	ASP	-	linker	UNP P0AEX9
c	-8	SER	-	linker	UNP P0AEX9
c	-7	THR	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
c	-6	GLU	-	linker	UNP P0AEX9
c	-5	ASN	-	linker	UNP P0AEX9
c	-4	LEU	-	linker	UNP P0AEX9
c	-3	TYR	-	linker	UNP P0AEX9
c	-2	PHE	-	linker	UNP P0AEX9
c	-1	GLN	-	linker	UNP P0AEX9
c	0	GLY	-	linker	UNP P0AEX9
d	-393	HIS	-	expression tag	UNP P0AEX9
d	-392	HIS	-	expression tag	UNP P0AEX9
d	-391	HIS	-	expression tag	UNP P0AEX9
d	-390	HIS	-	expression tag	UNP P0AEX9
d	-389	HIS	-	expression tag	UNP P0AEX9
d	-388	HIS	-	expression tag	UNP P0AEX9
d	-387	MET	-	expression tag	UNP P0AEX9
d	-20	GLY	-	linker	UNP P0AEX9
d	-19	LYS	-	linker	UNP P0AEX9
d	-18	PRO	-	linker	UNP P0AEX9
d	-17	ILE	-	linker	UNP P0AEX9
d	-16	PRO	-	linker	UNP P0AEX9
d	-15	ASN	-	linker	UNP P0AEX9
d	-14	PRO	-	linker	UNP P0AEX9
d	-13	LEU	-	linker	UNP P0AEX9
d	-12	LEU	-	linker	UNP P0AEX9
d	-11	GLY	-	linker	UNP P0AEX9
d	-10	LEU	-	linker	UNP P0AEX9
d	-9	ASP	-	linker	UNP P0AEX9
d	-8	SER	-	linker	UNP P0AEX9
d	-7	THR	-	linker	UNP P0AEX9
d	-6	GLU	-	linker	UNP P0AEX9
d	-5	ASN	-	linker	UNP P0AEX9
d	-4	LEU	-	linker	UNP P0AEX9
d	-3	TYR	-	linker	UNP P0AEX9
d	-2	PHE	-	linker	UNP P0AEX9
d	-1	GLN	-	linker	UNP P0AEX9
d	0	GLY	-	linker	UNP P0AEX9
e	-393	HIS	-	expression tag	UNP P0AEX9
e	-392	HIS	-	expression tag	UNP P0AEX9
e	-391	HIS	-	expression tag	UNP P0AEX9
e	-390	HIS	-	expression tag	UNP P0AEX9
e	-389	HIS	-	expression tag	UNP P0AEX9
e	-388	HIS	-	expression tag	UNP P0AEX9
e	-387	MET	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
e	-20	GLY	-	linker	UNP P0AEX9
e	-19	LYS	-	linker	UNP P0AEX9
e	-18	PRO	-	linker	UNP P0AEX9
e	-17	ILE	-	linker	UNP P0AEX9
e	-16	PRO	-	linker	UNP P0AEX9
e	-15	ASN	-	linker	UNP P0AEX9
e	-14	PRO	-	linker	UNP P0AEX9
e	-13	LEU	-	linker	UNP P0AEX9
e	-12	LEU	-	linker	UNP P0AEX9
e	-11	GLY	-	linker	UNP P0AEX9
e	-10	LEU	-	linker	UNP P0AEX9
e	-9	ASP	-	linker	UNP P0AEX9
e	-8	SER	-	linker	UNP P0AEX9
e	-7	THR	-	linker	UNP P0AEX9
e	-6	GLU	-	linker	UNP P0AEX9
e	-5	ASN	-	linker	UNP P0AEX9
e	-4	LEU	-	linker	UNP P0AEX9
e	-3	TYR	-	linker	UNP P0AEX9
e	-2	PHE	-	linker	UNP P0AEX9
e	-1	GLN	-	linker	UNP P0AEX9
e	0	GLY	-	linker	UNP P0AEX9
f	-393	HIS	-	expression tag	UNP P0AEX9
f	-392	HIS	-	expression tag	UNP P0AEX9
f	-391	HIS	-	expression tag	UNP P0AEX9
f	-390	HIS	-	expression tag	UNP P0AEX9
f	-389	HIS	-	expression tag	UNP P0AEX9
f	-388	HIS	-	expression tag	UNP P0AEX9
f	-387	MET	-	expression tag	UNP P0AEX9
f	-20	GLY	-	linker	UNP P0AEX9
f	-19	LYS	-	linker	UNP P0AEX9
f	-18	PRO	-	linker	UNP P0AEX9
f	-17	ILE	-	linker	UNP P0AEX9
f	-16	PRO	-	linker	UNP P0AEX9
f	-15	ASN	-	linker	UNP P0AEX9
f	-14	PRO	-	linker	UNP P0AEX9
f	-13	LEU	-	linker	UNP P0AEX9
f	-12	LEU	-	linker	UNP P0AEX9
f	-11	GLY	-	linker	UNP P0AEX9
f	-10	LEU	-	linker	UNP P0AEX9
f	-9	ASP	-	linker	UNP P0AEX9
f	-8	SER	-	linker	UNP P0AEX9
f	-7	THR	-	linker	UNP P0AEX9

Continued on next page...

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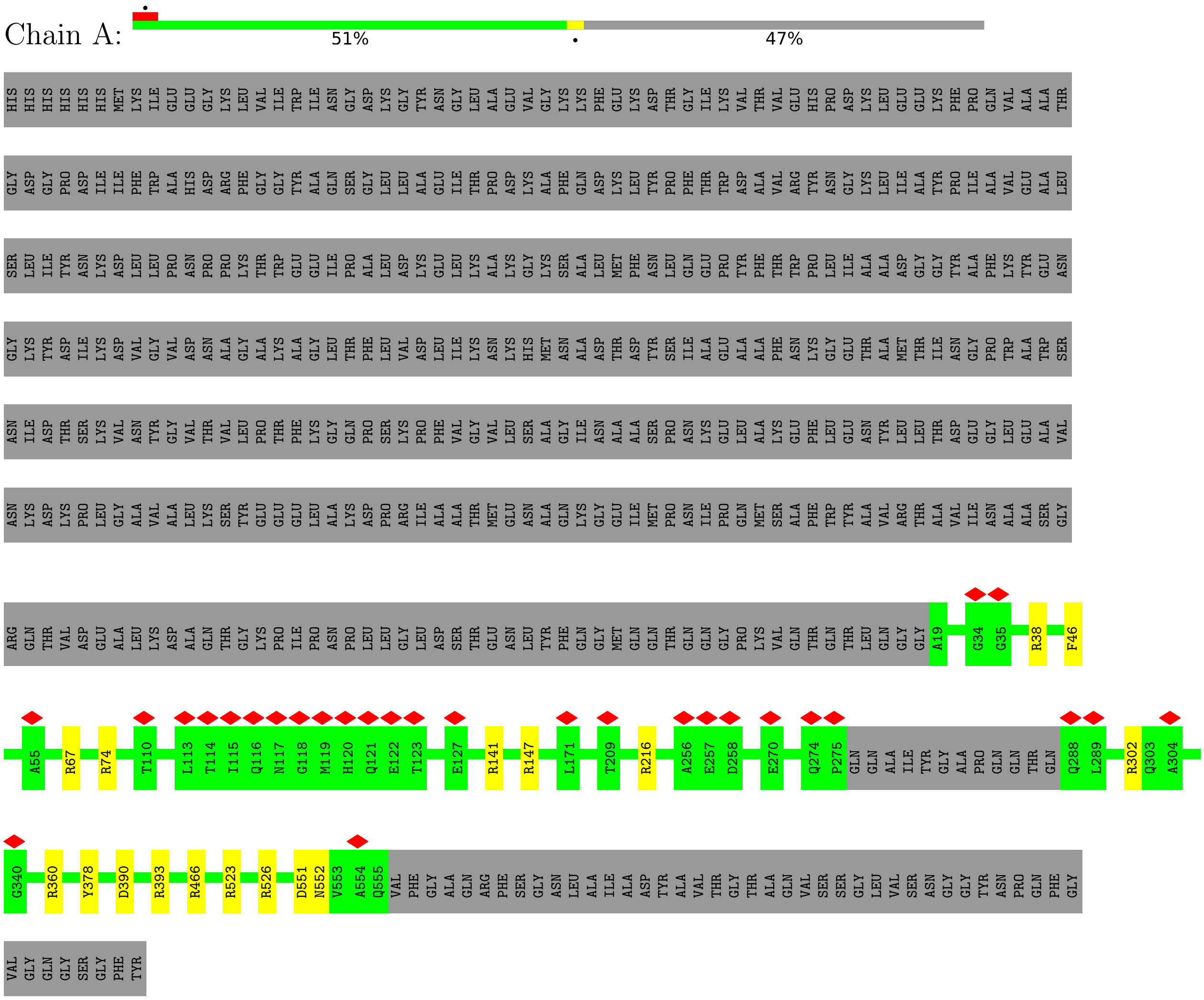
Chain	Residue	Modelled	Actual	Comment	Reference
f	-6	GLU	-	linker	UNP P0AEX9
f	-5	ASN	-	linker	UNP P0AEX9
f	-4	LEU	-	linker	UNP P0AEX9
f	-3	TYR	-	linker	UNP P0AEX9
f	-2	PHE	-	linker	UNP P0AEX9
f	-1	GLN	-	linker	UNP P0AEX9
f	0	GLY	-	linker	UNP P0AEX9

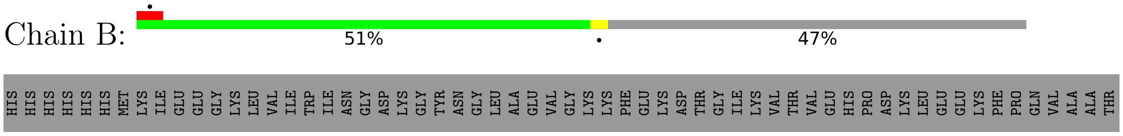
3 Residue-property plots ⓘ

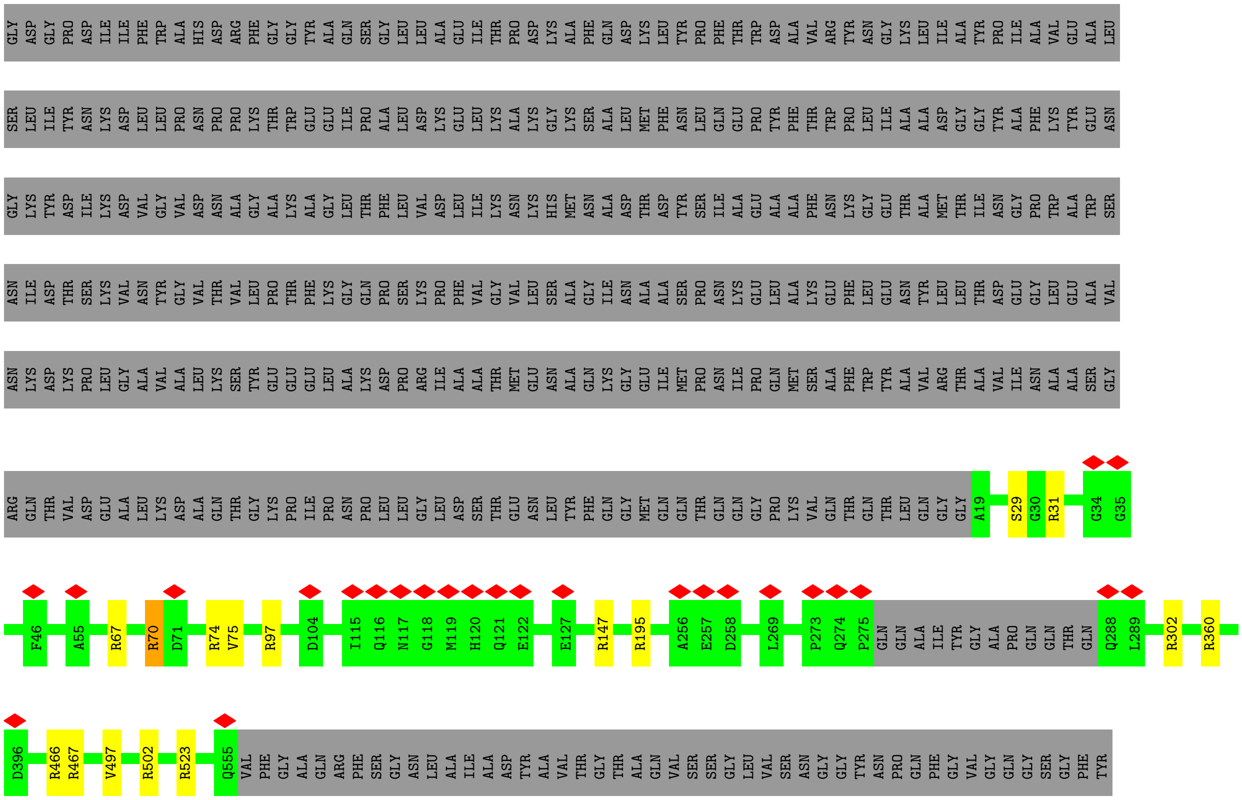
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN



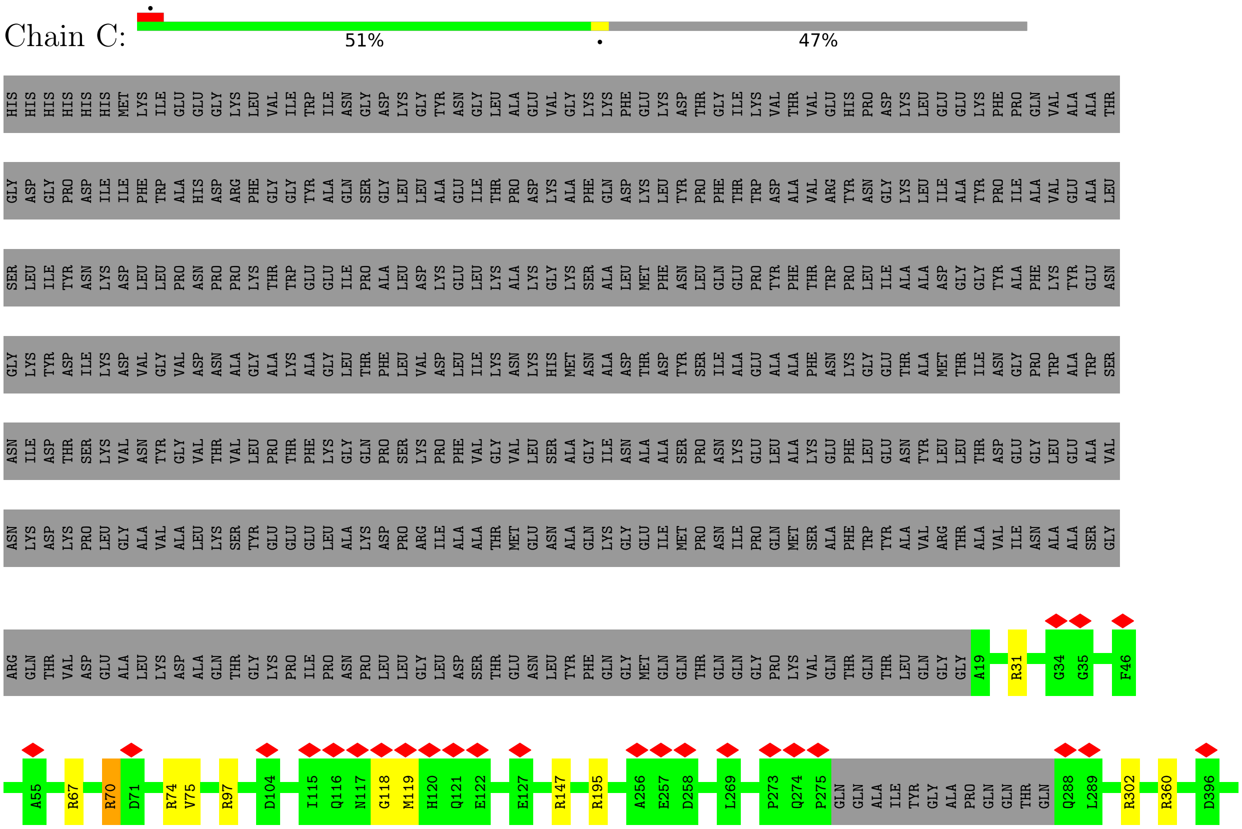
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

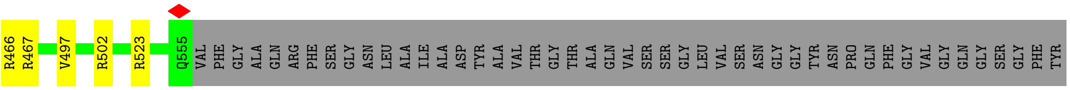




- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

Chain C:





- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

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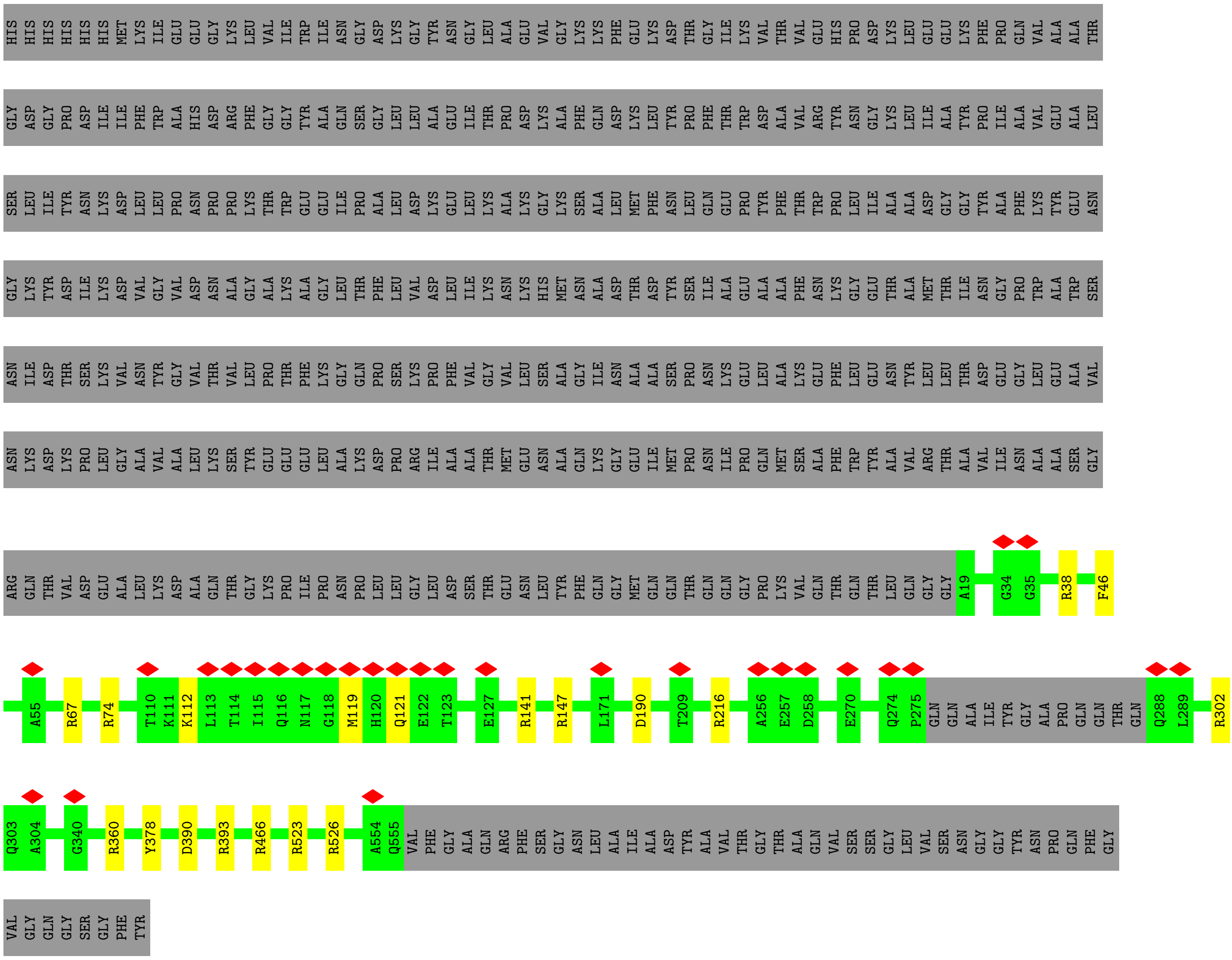

- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

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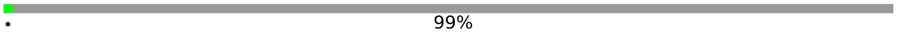
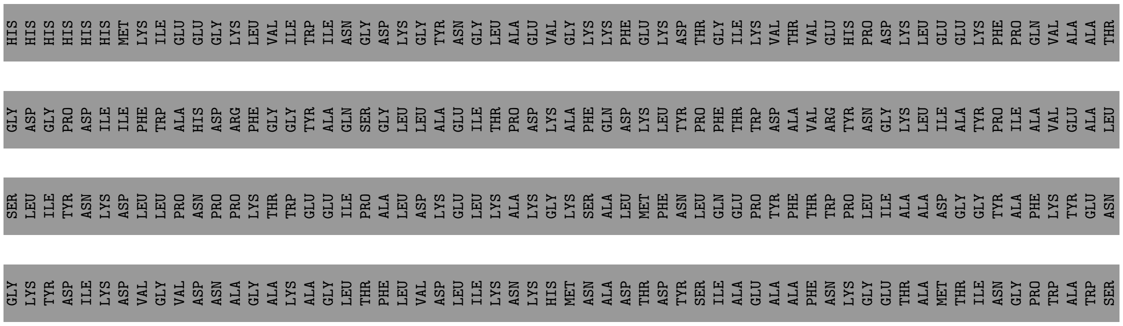
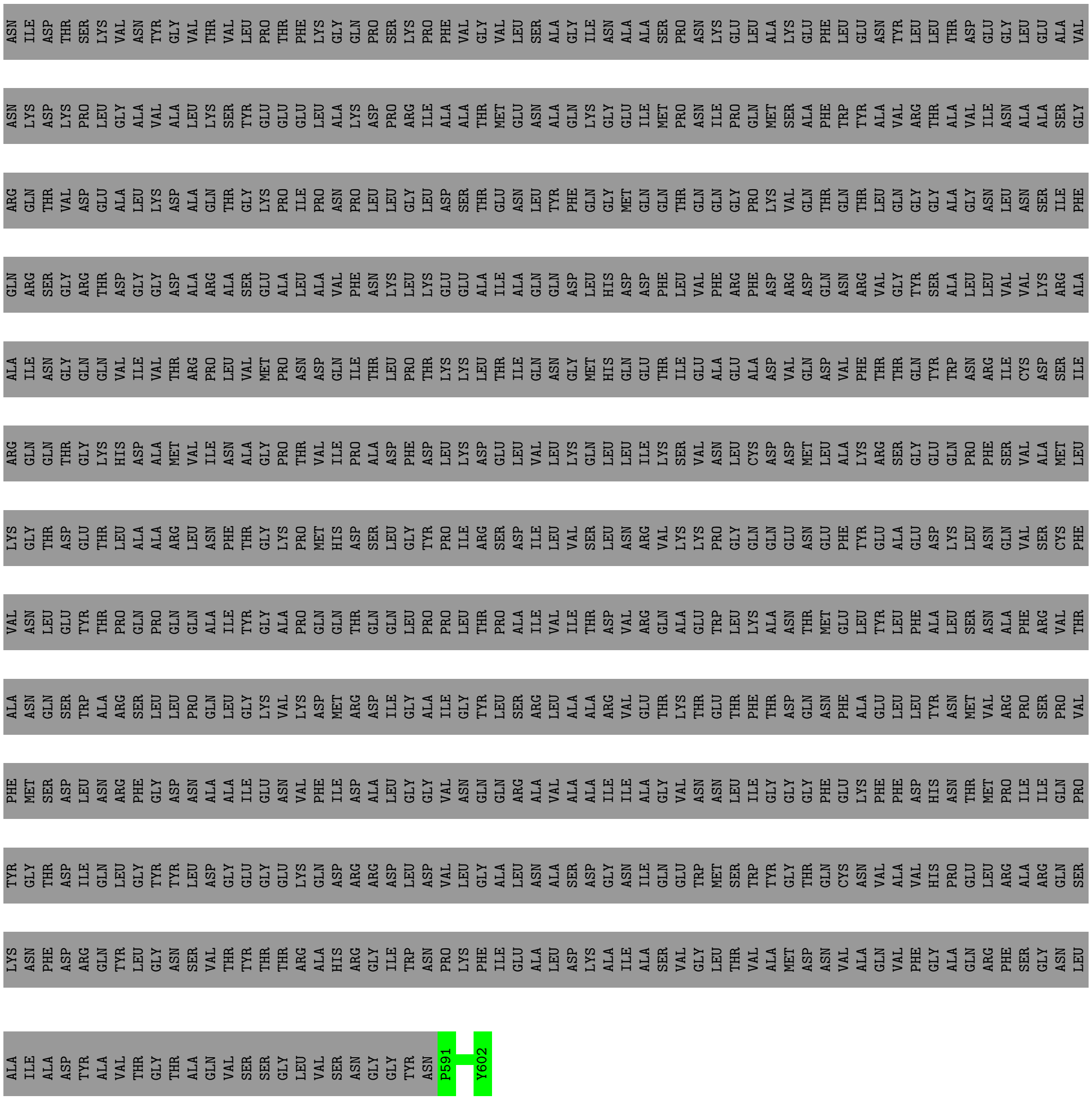
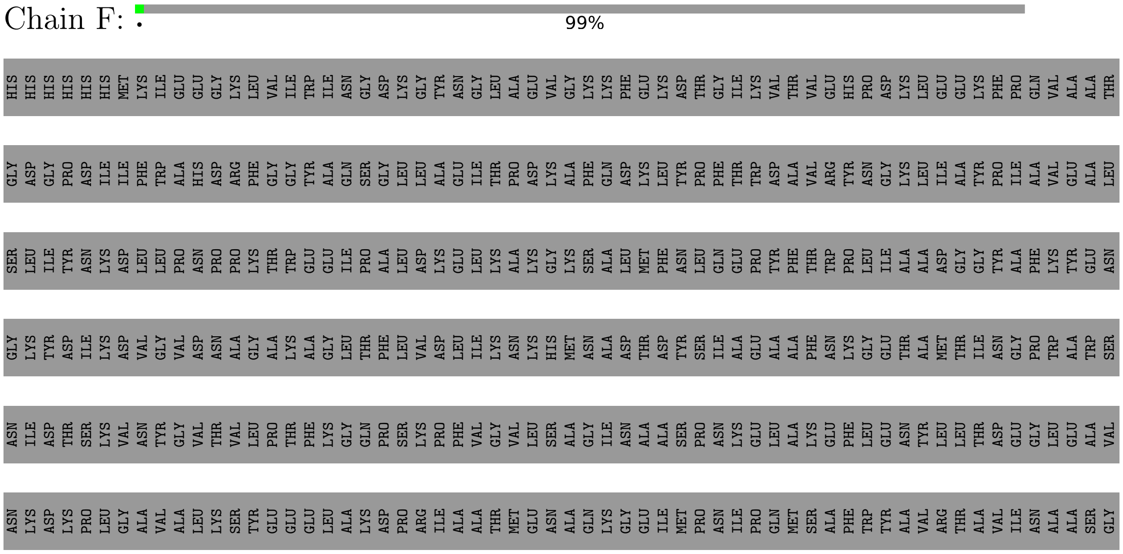






- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN



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

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

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

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

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

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

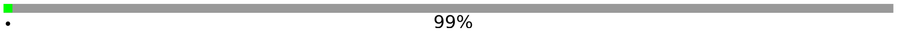
TYR GLY THR ASP ILE GLN LEU GLY TYR TYR LEU ASP GLY GLU GLY GLU LYS GLN ASP ARG ARG ASP LEU ASP VAL LEU GLY ALA LEU ASN ALA SER ASP GLY ASN ILE GLN GLU TRP MET SER TRP TYR GLY THR GLN CYS ASN VAL ALA VAL HIS PRO GLU LEU ARG ALA ARG GLN SER

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

ALA ILE ALA ASP TYR ALA VAL THR GLY THR ALA GLN VAL SER SER GLY LEU VAL SER ASN GLY GLY TYR ASN P591 Y602

- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

Chain G:



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

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

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

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

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

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

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

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

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

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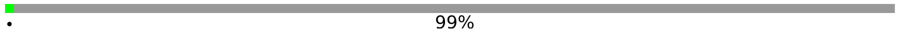
ALA ILE ALA ASP TYR ALA VAL THR GLY THR ALA GLN VAL SER SER GLY LEU VAL SER ASN GLY GLY TYR ASN P591 Y602

• Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

Chain H:



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

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

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

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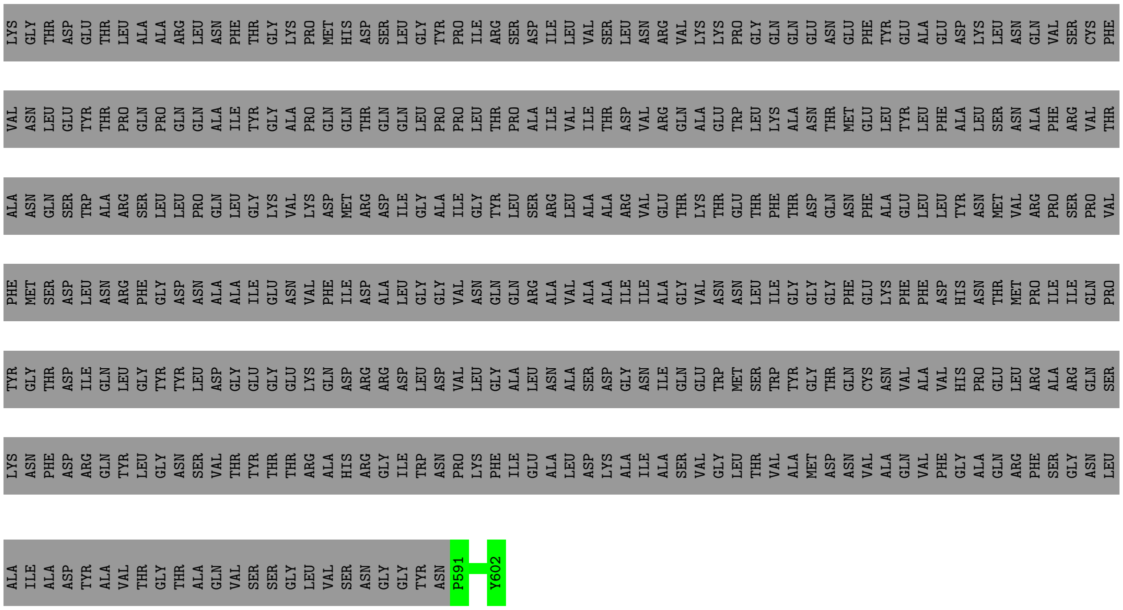
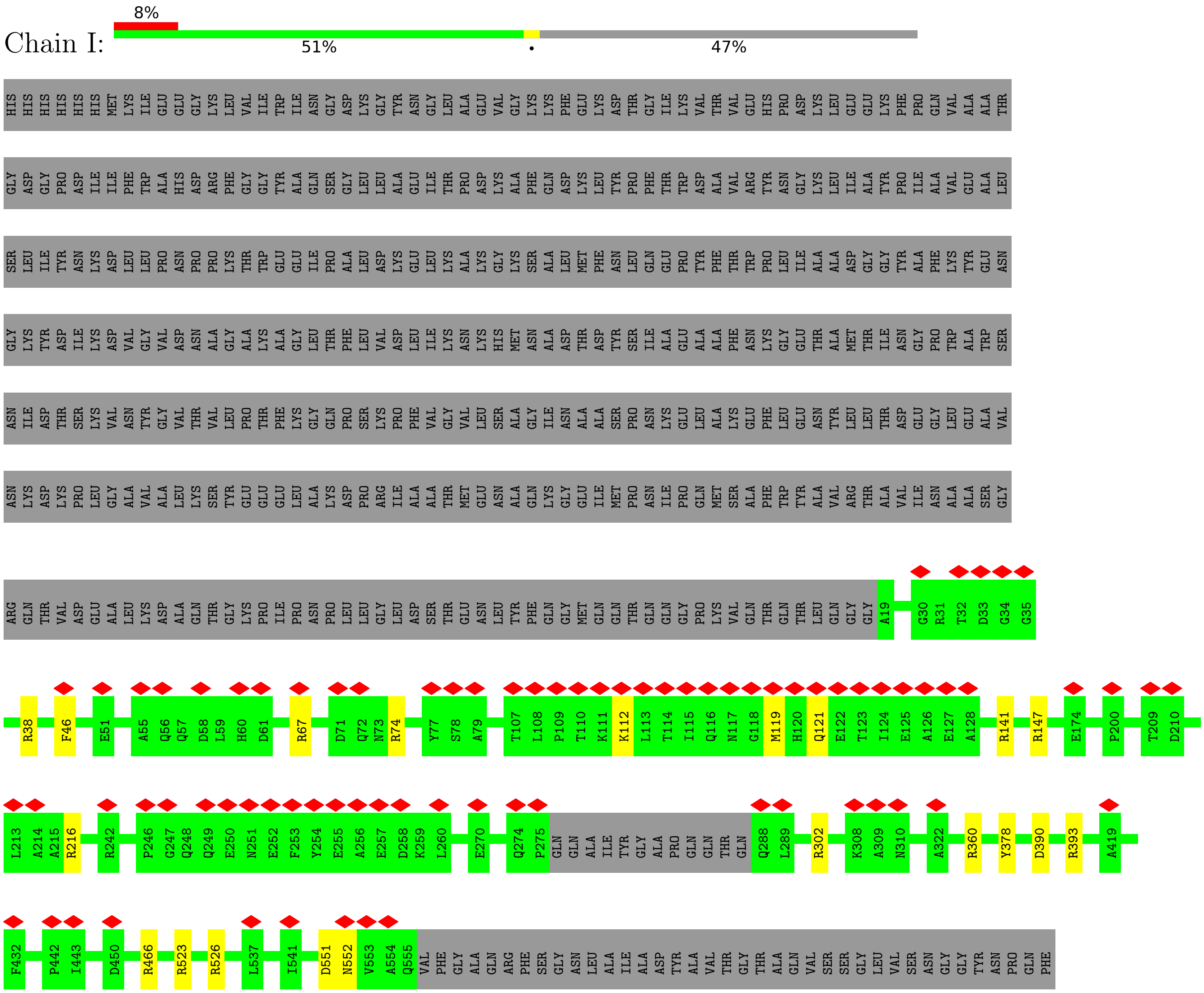
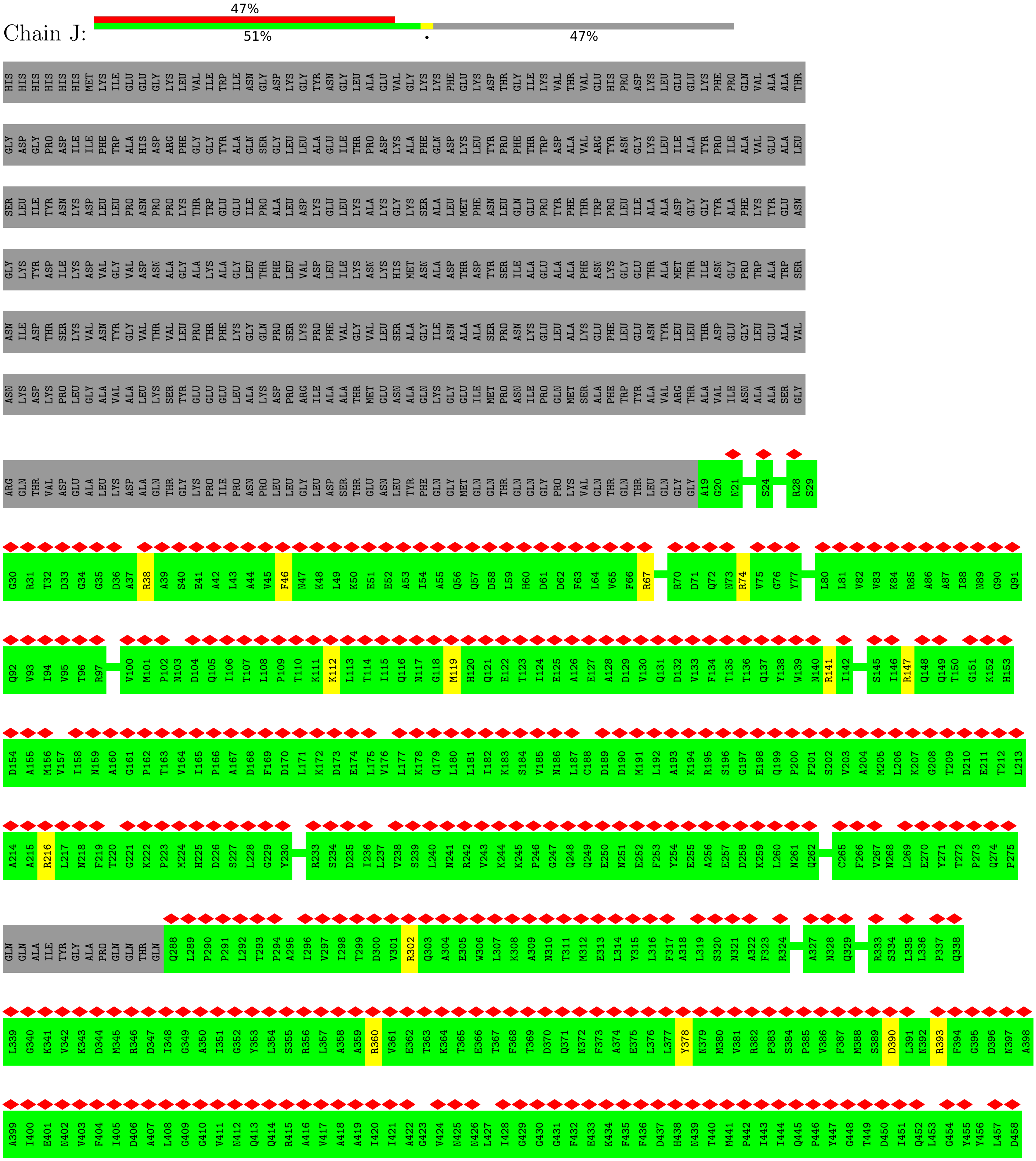
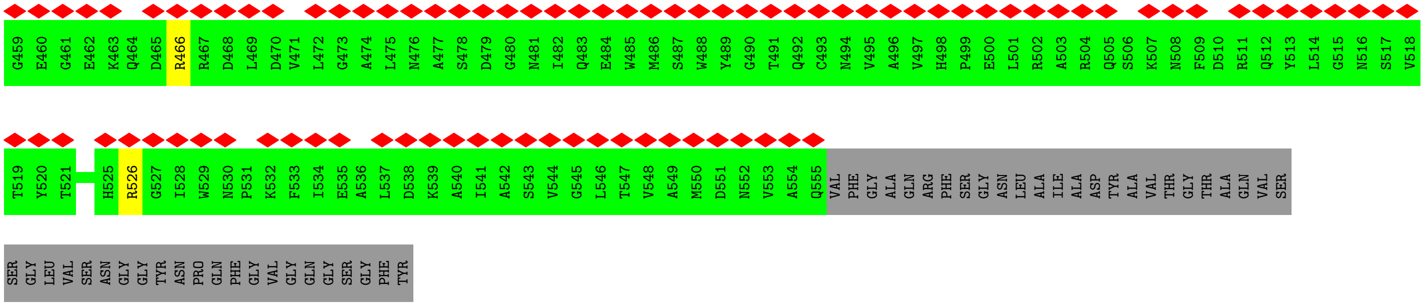


• Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN



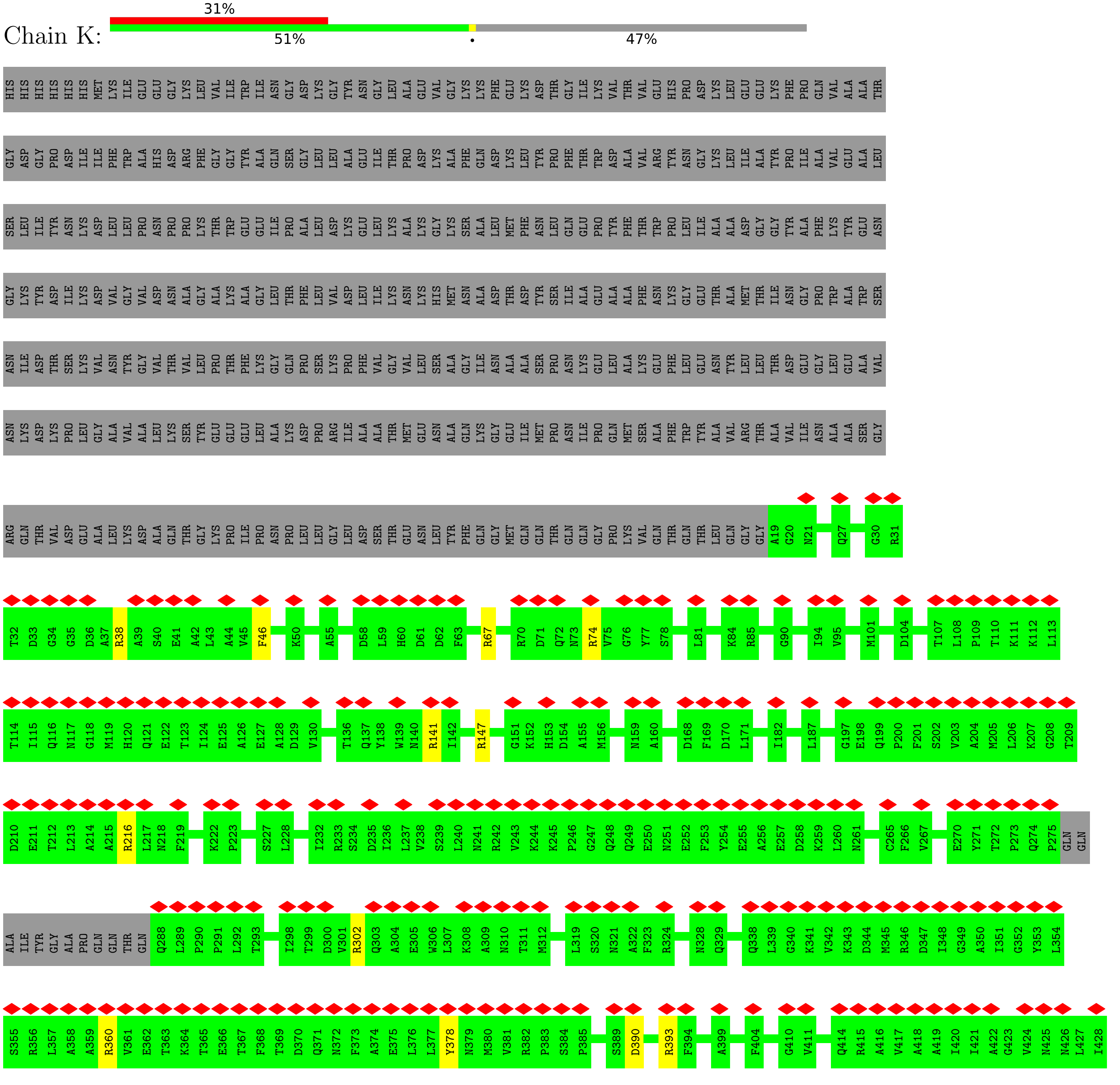
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

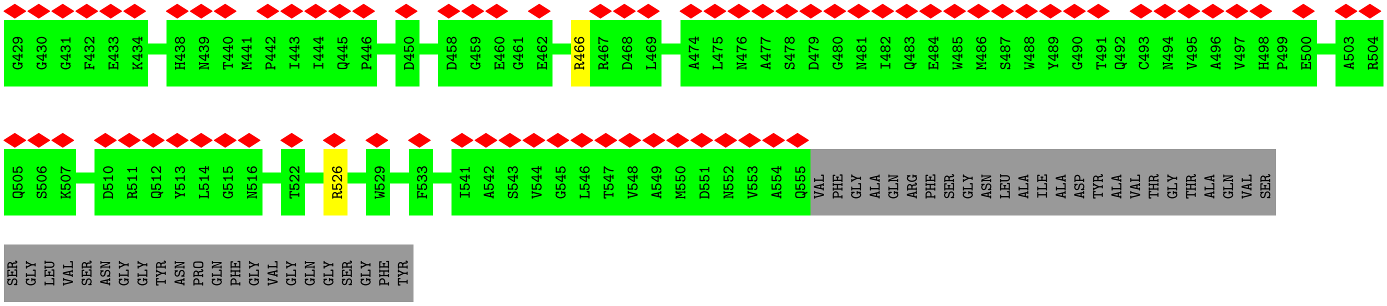




• Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

Chain K:





- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

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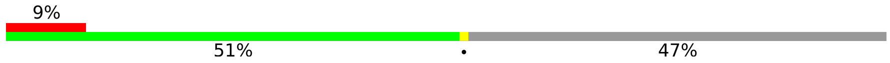
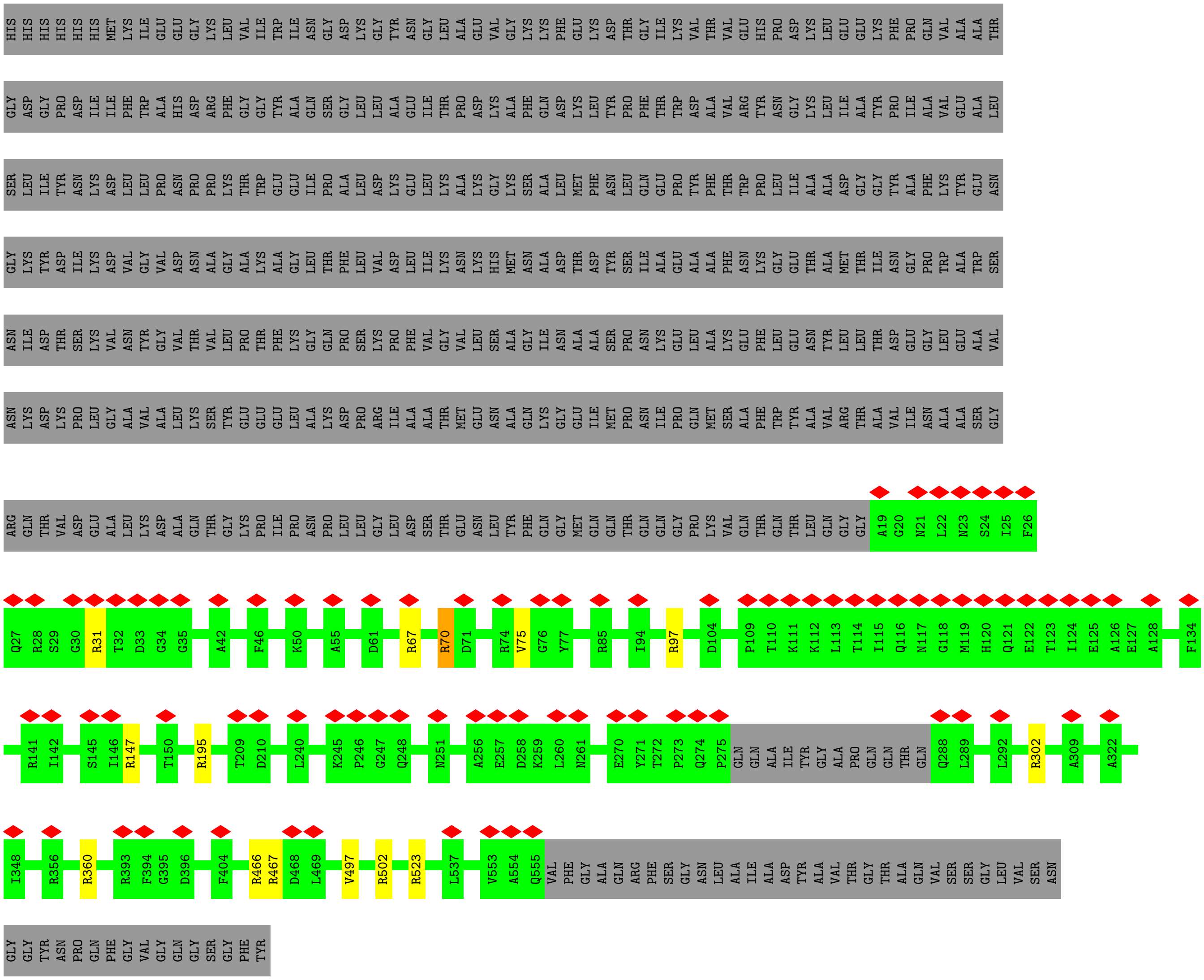
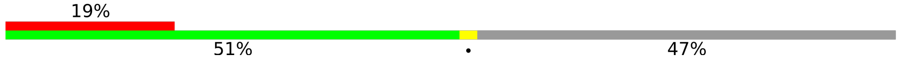
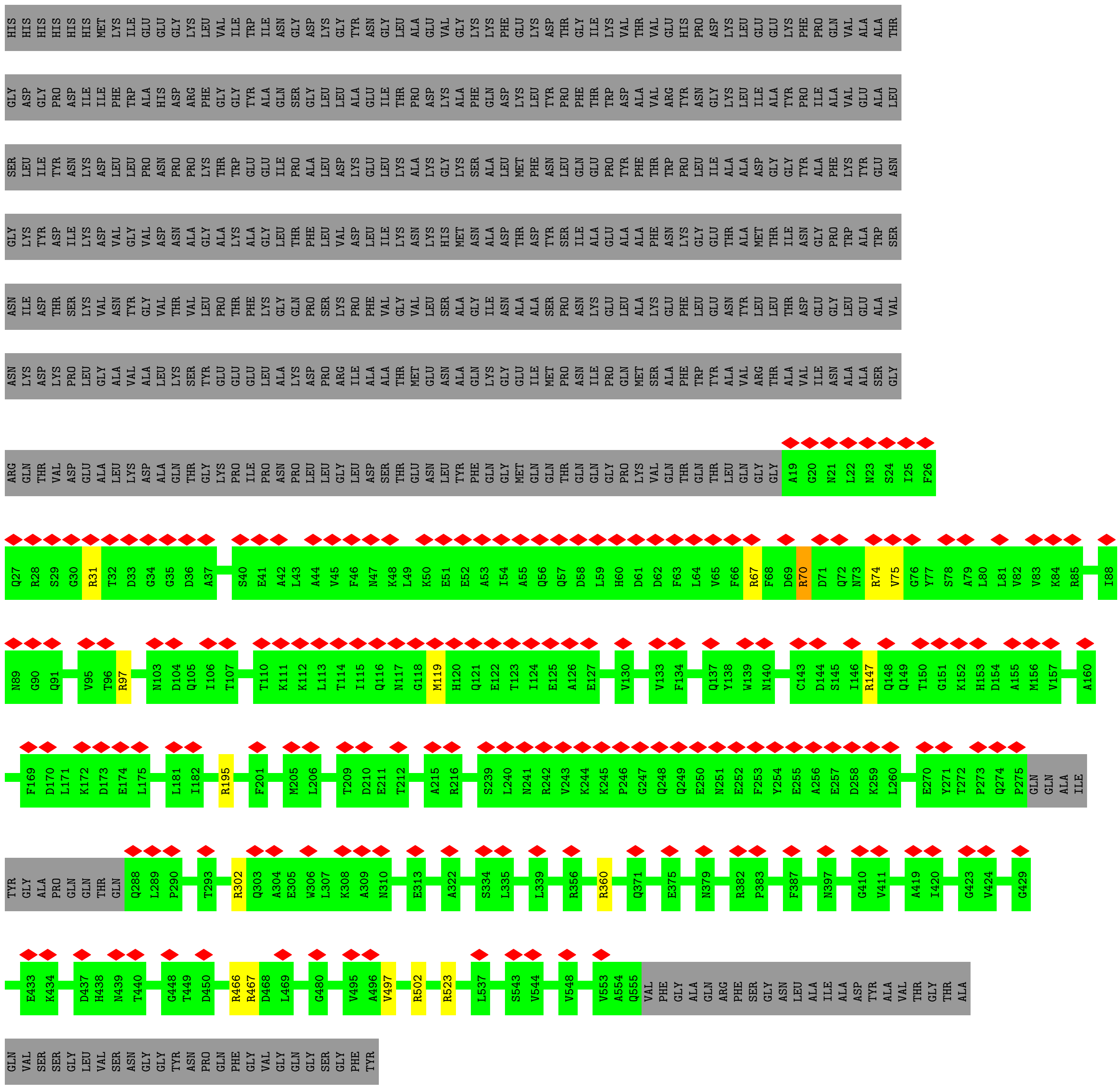




- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

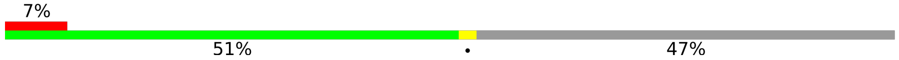
Chain M:

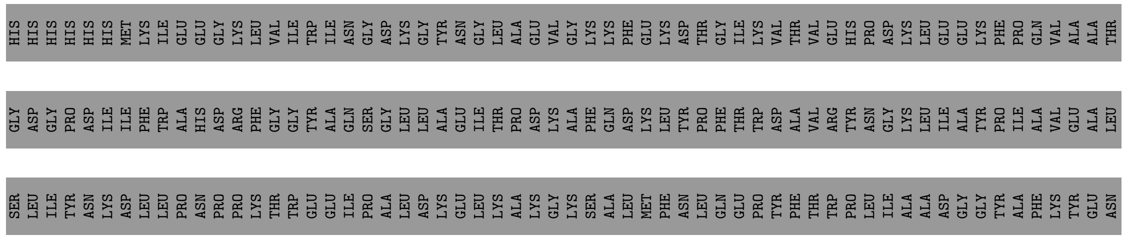


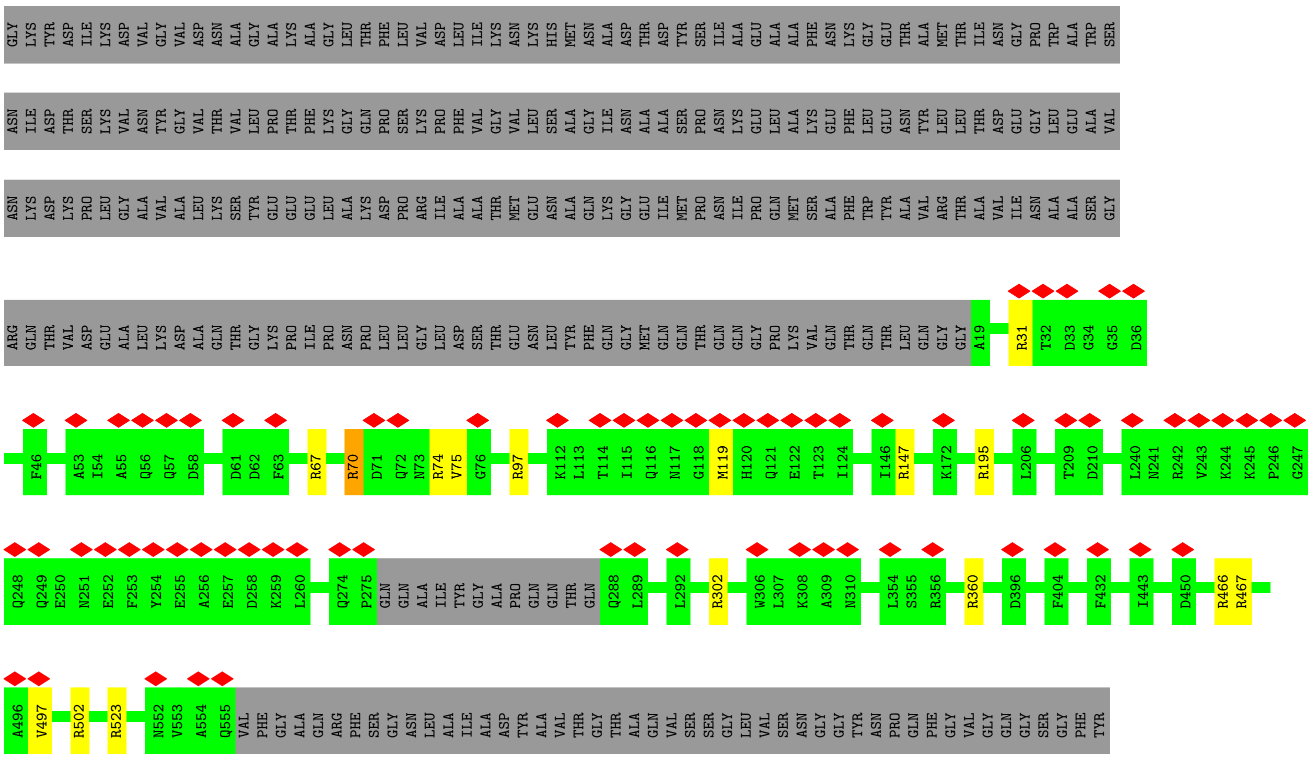


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

Chain N:

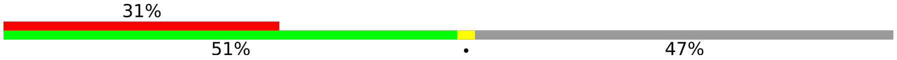


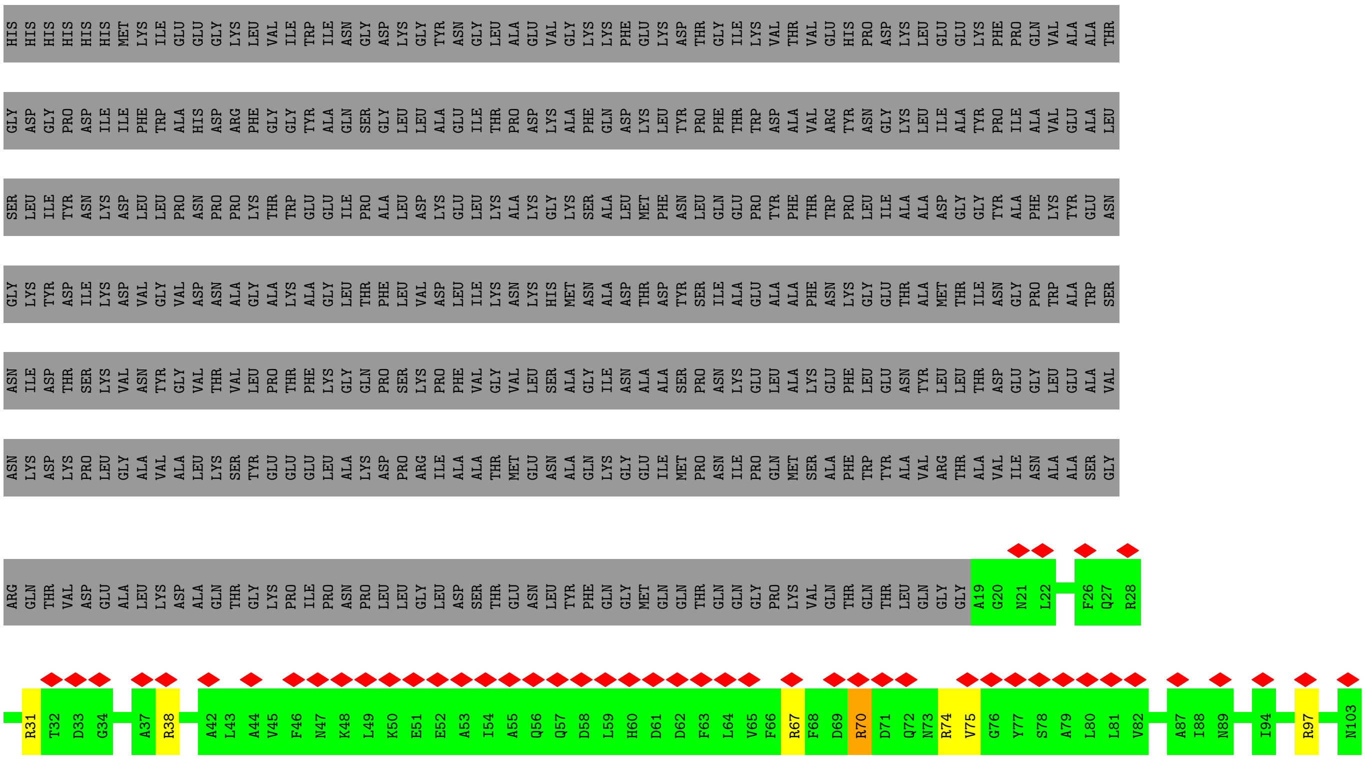


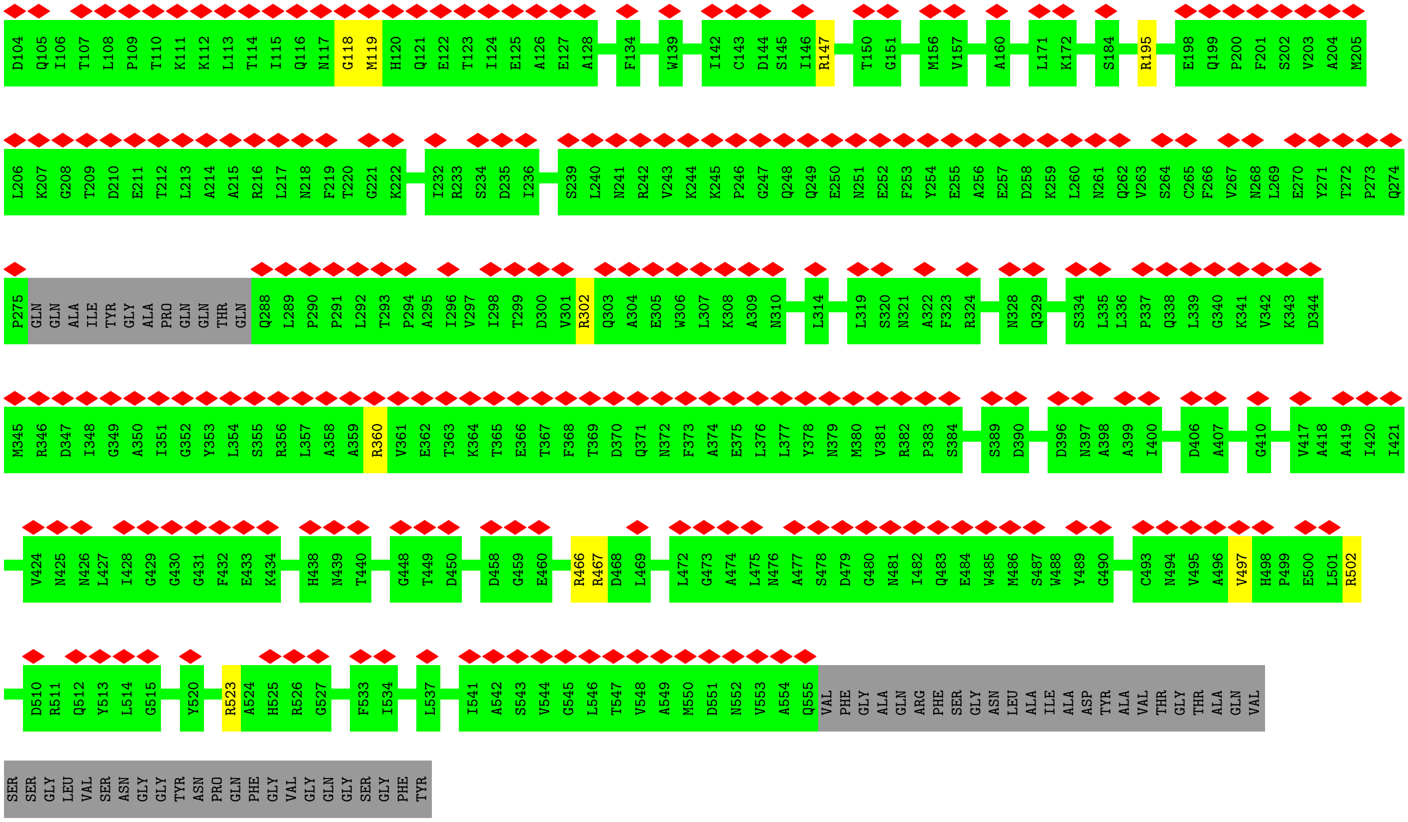


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

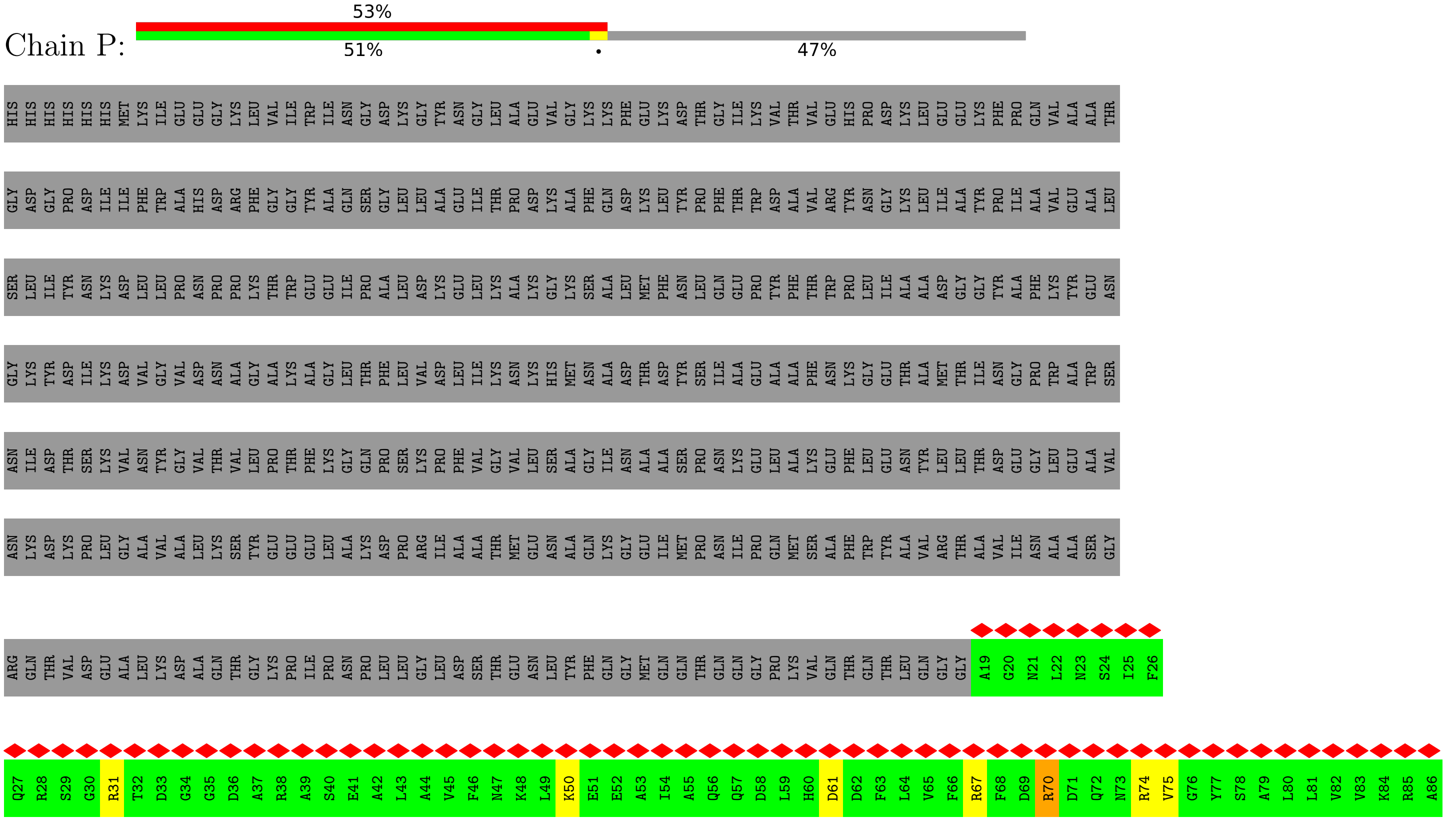
Chain O:

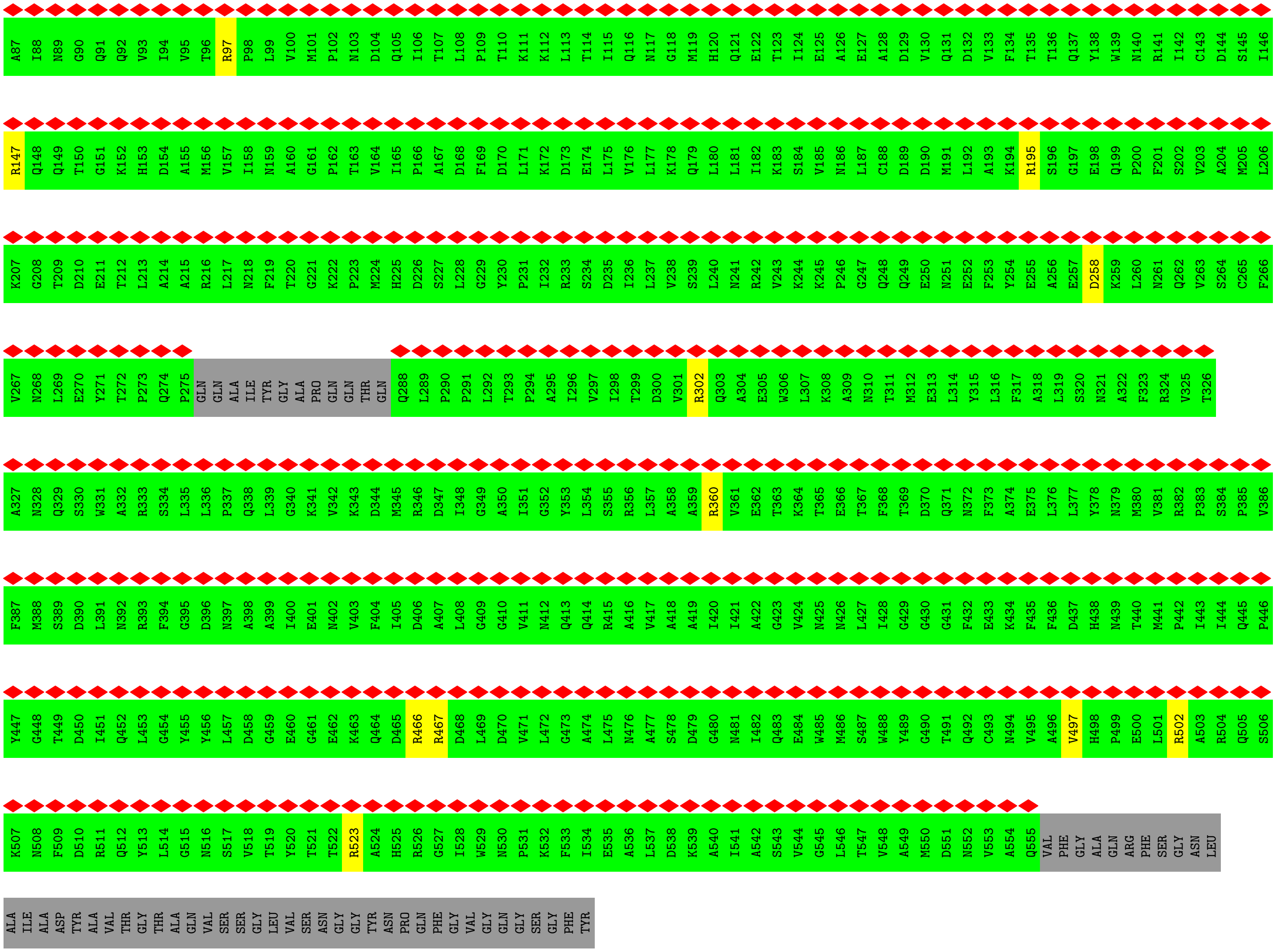




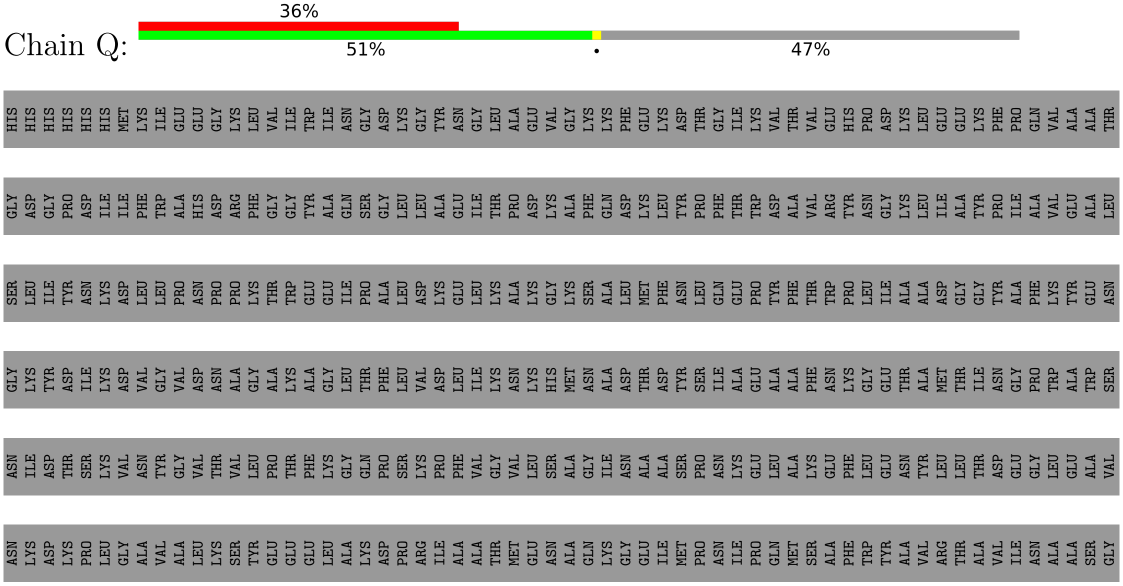


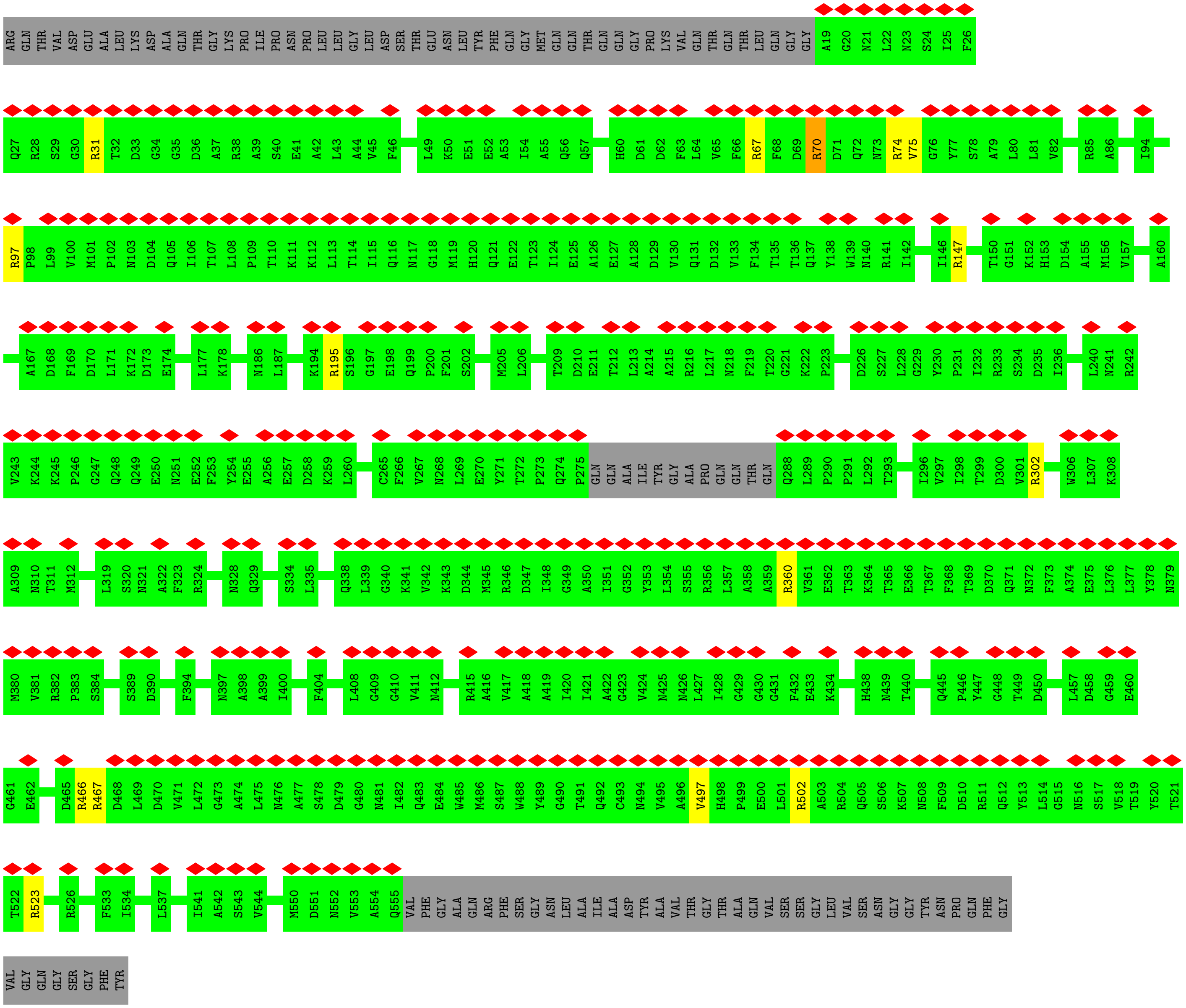
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN



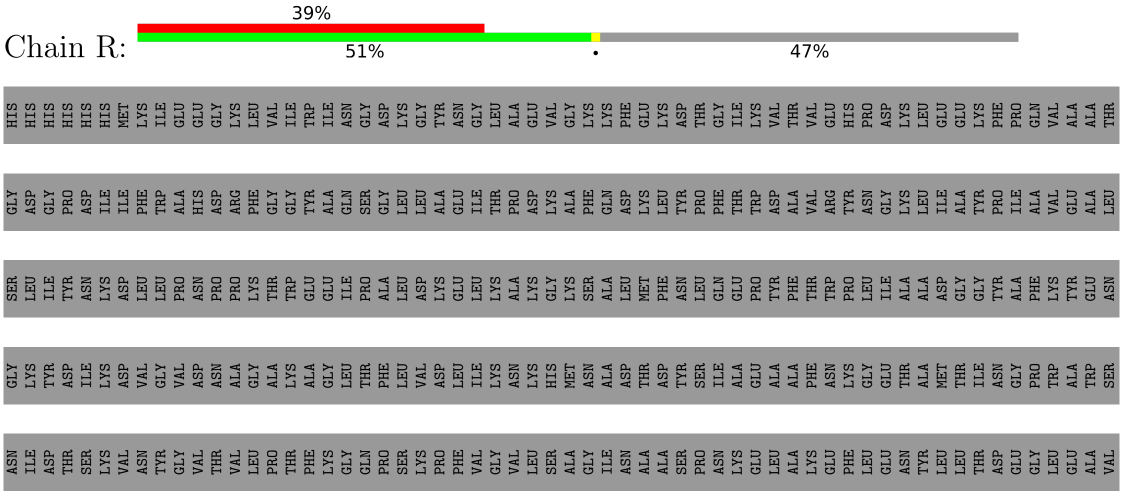


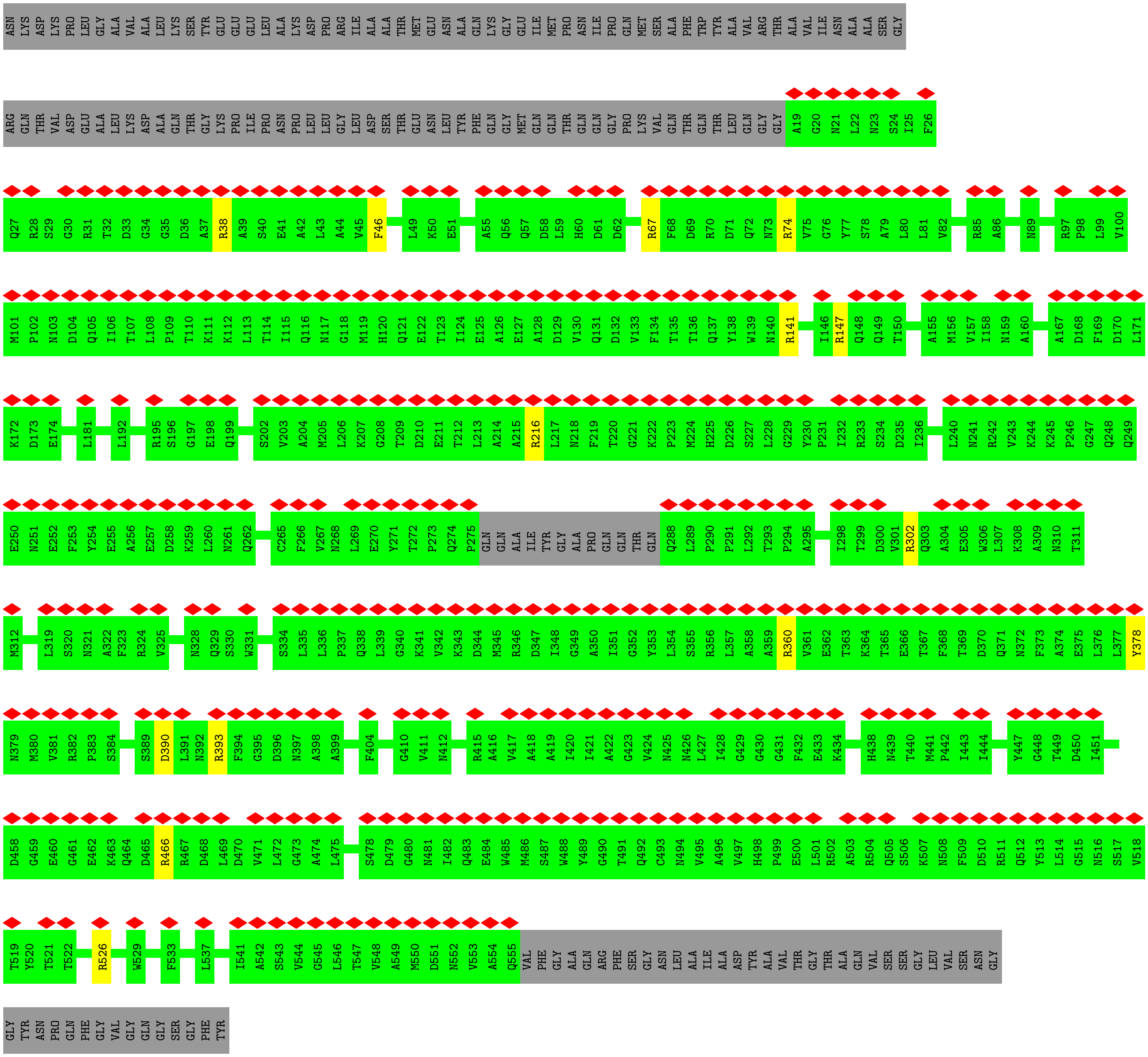
• Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN





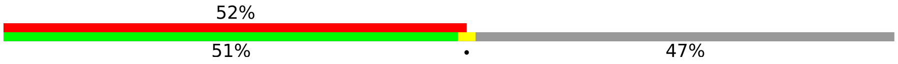
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

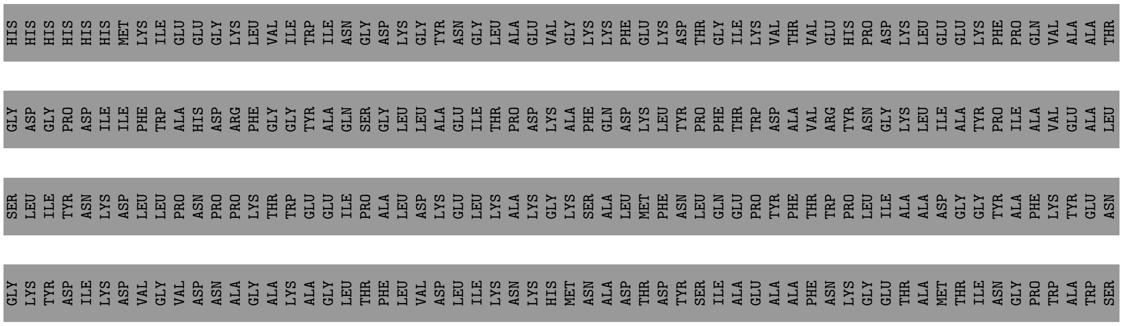


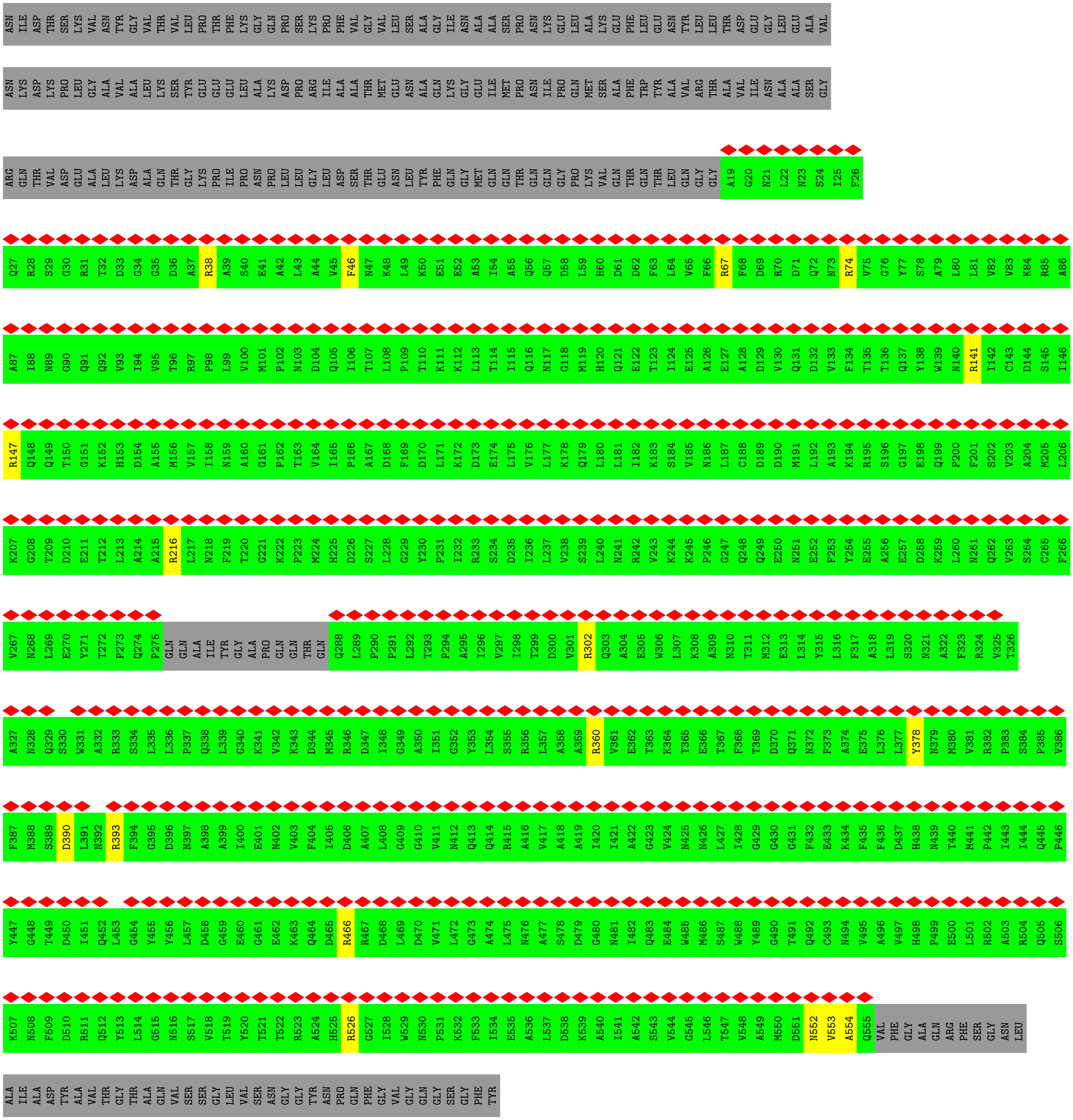


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

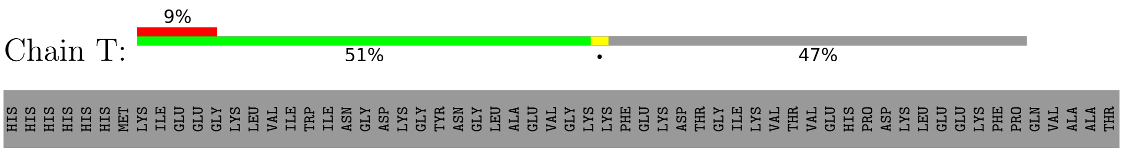
Chain S:

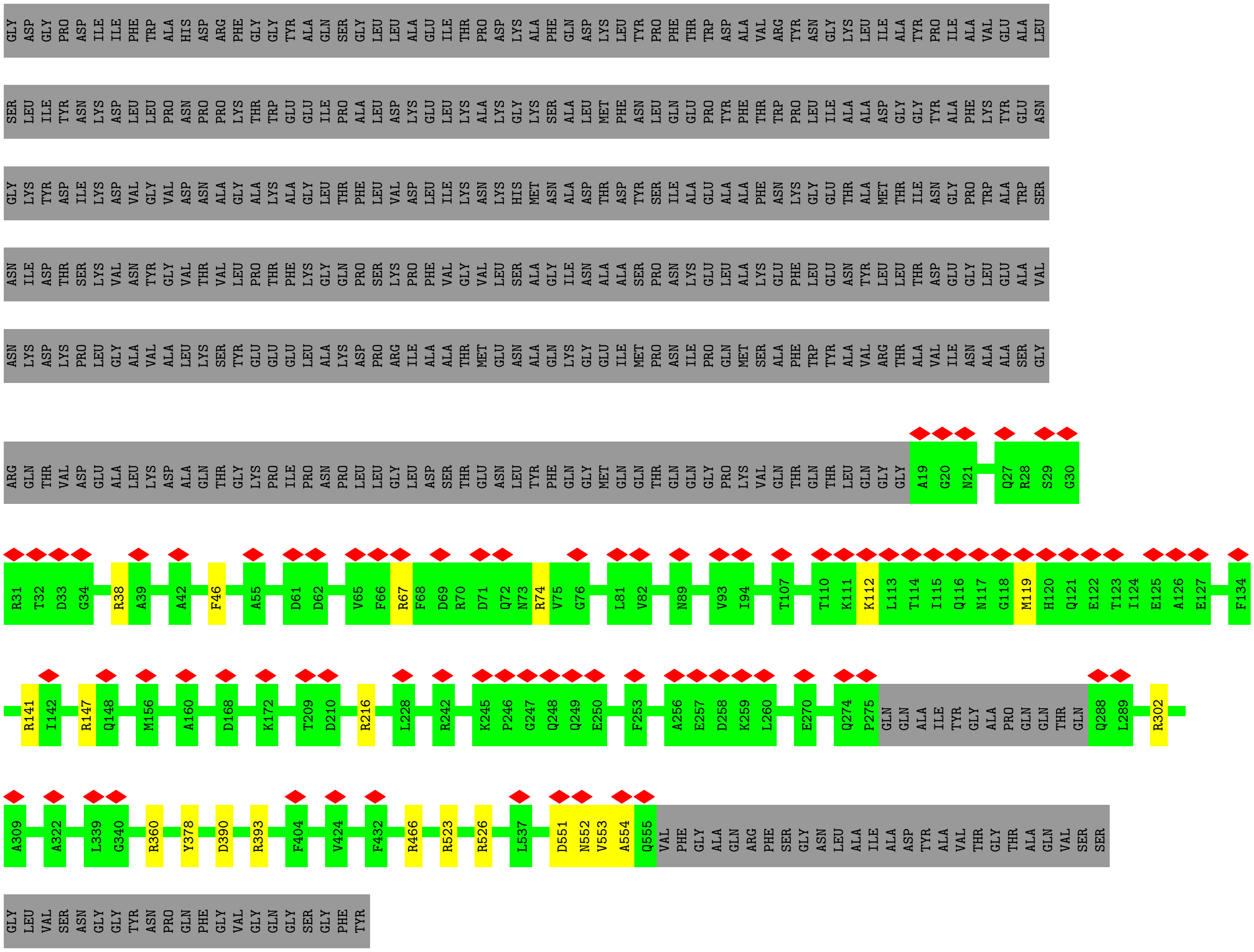






- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN





- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

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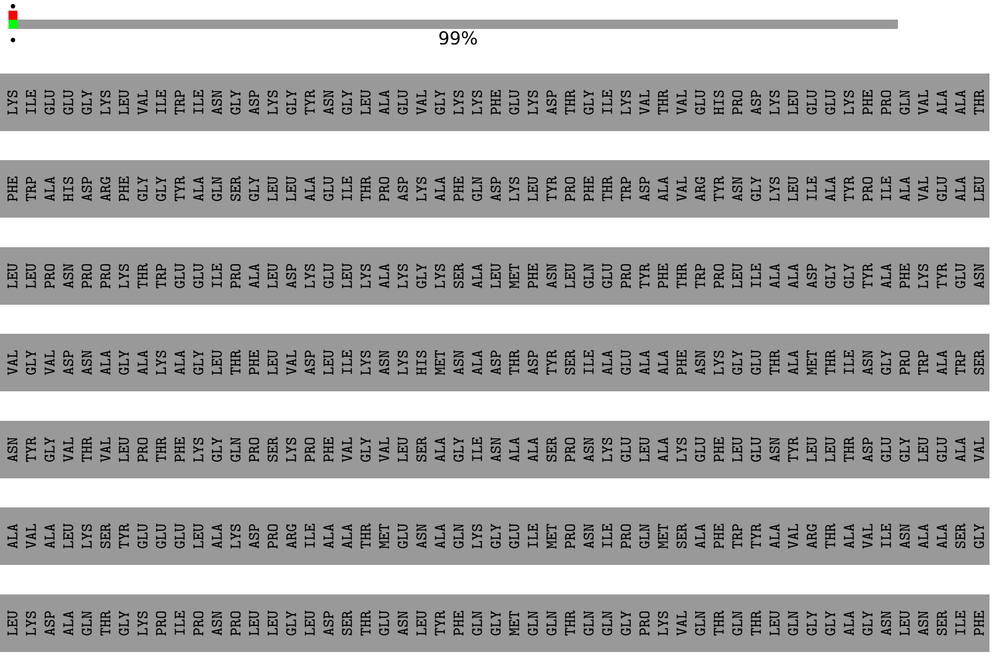

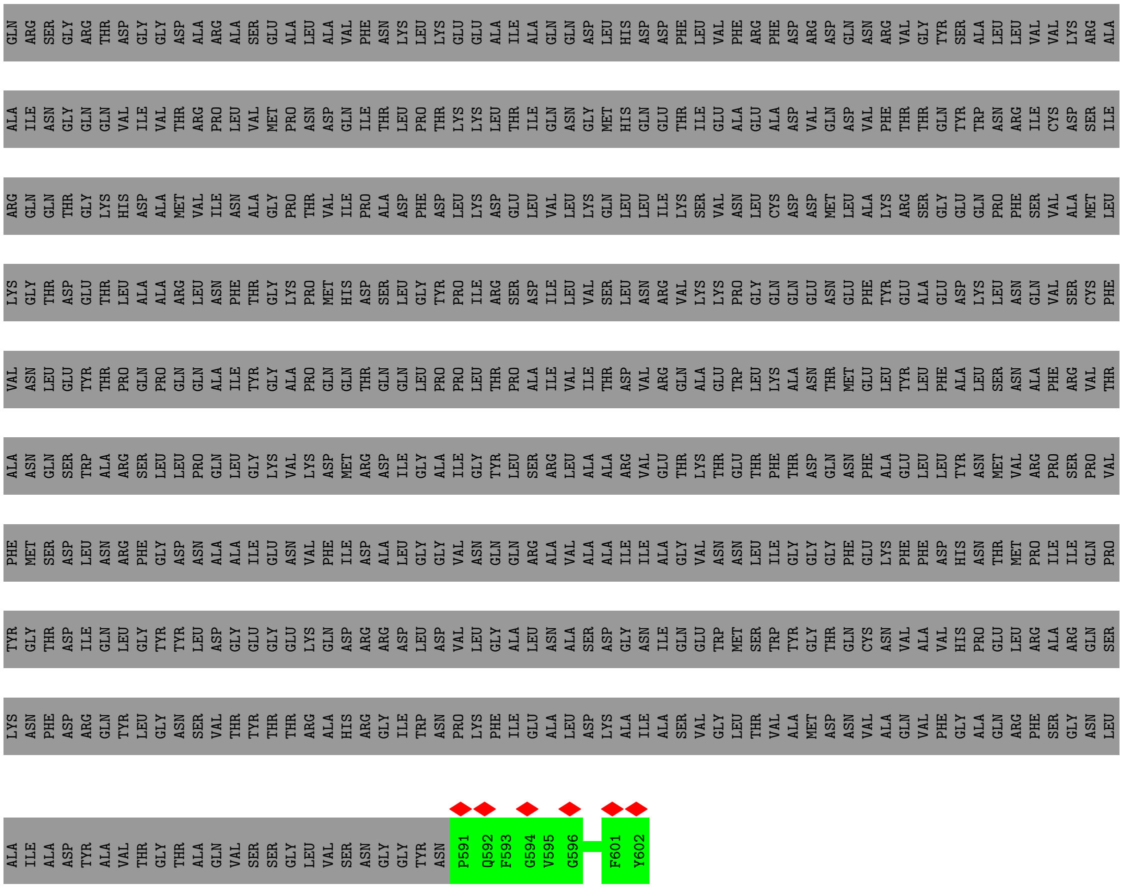

• Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

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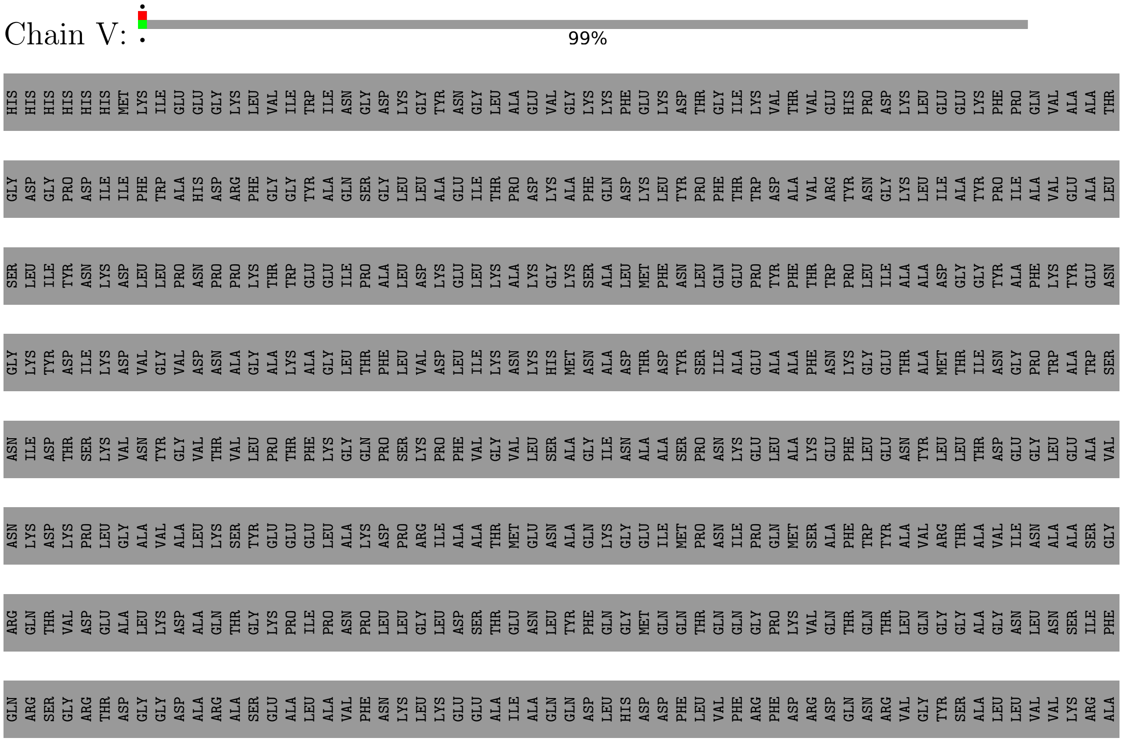
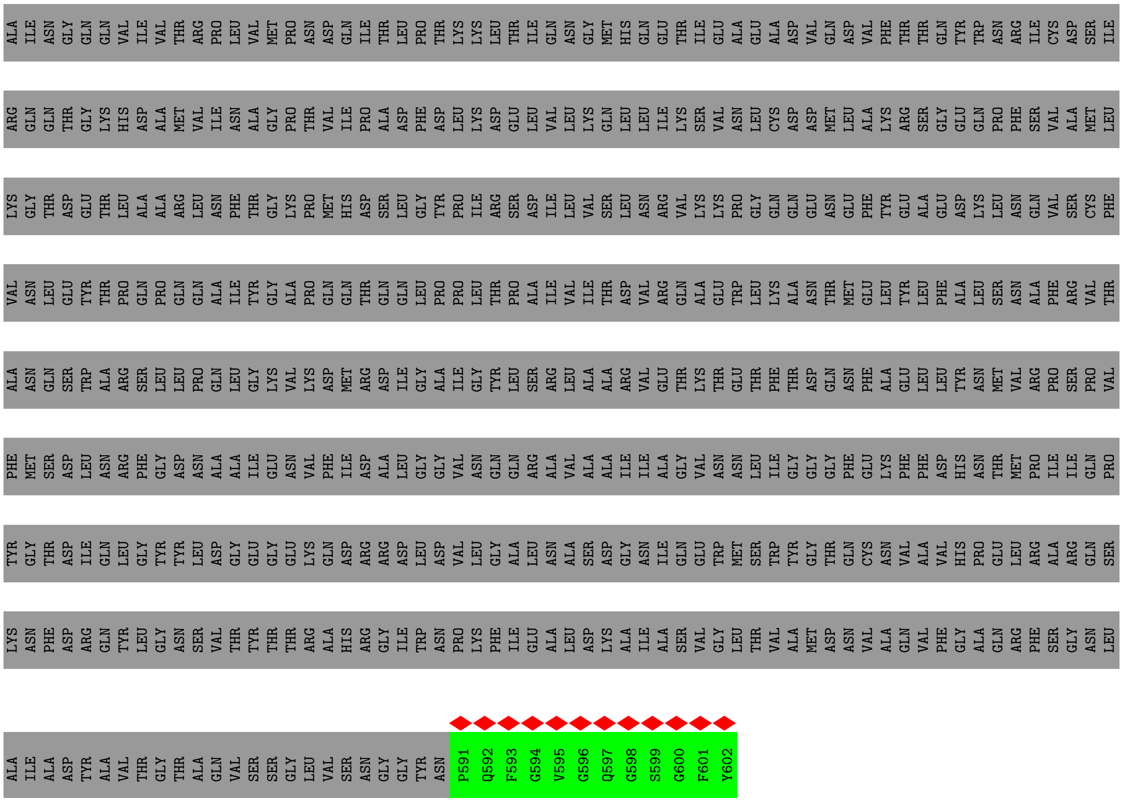
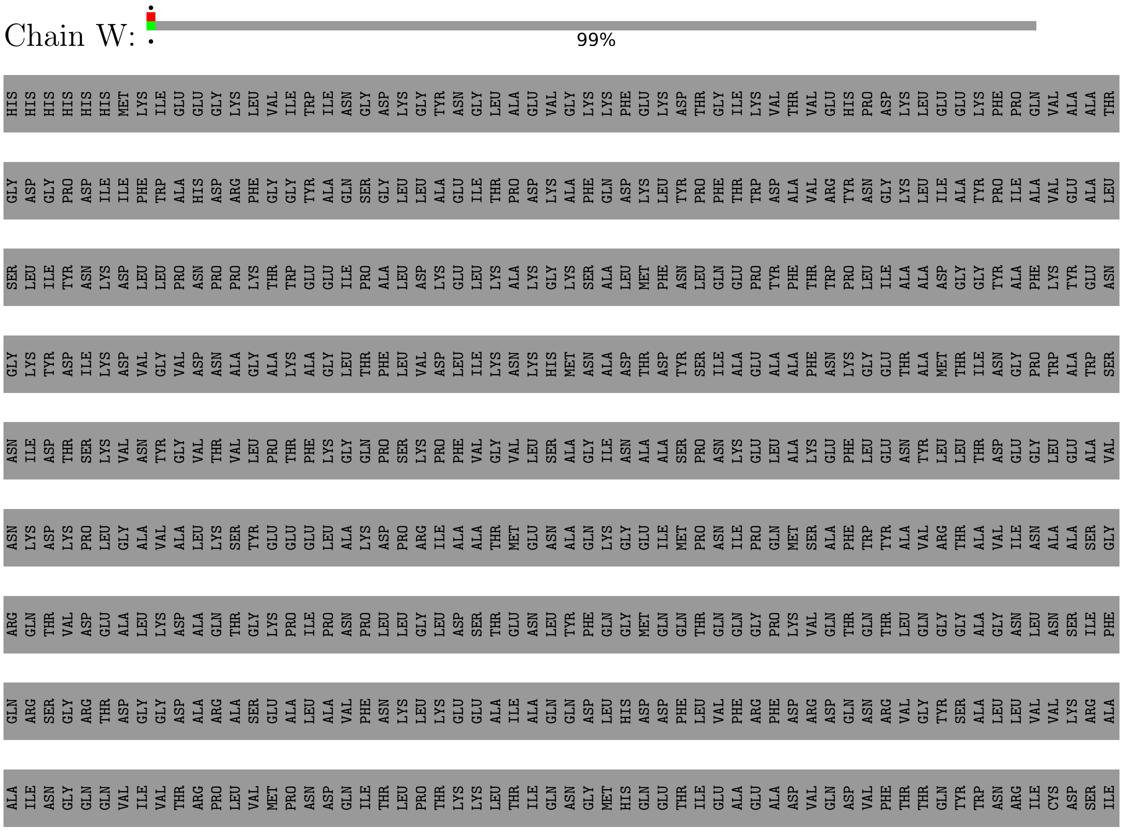
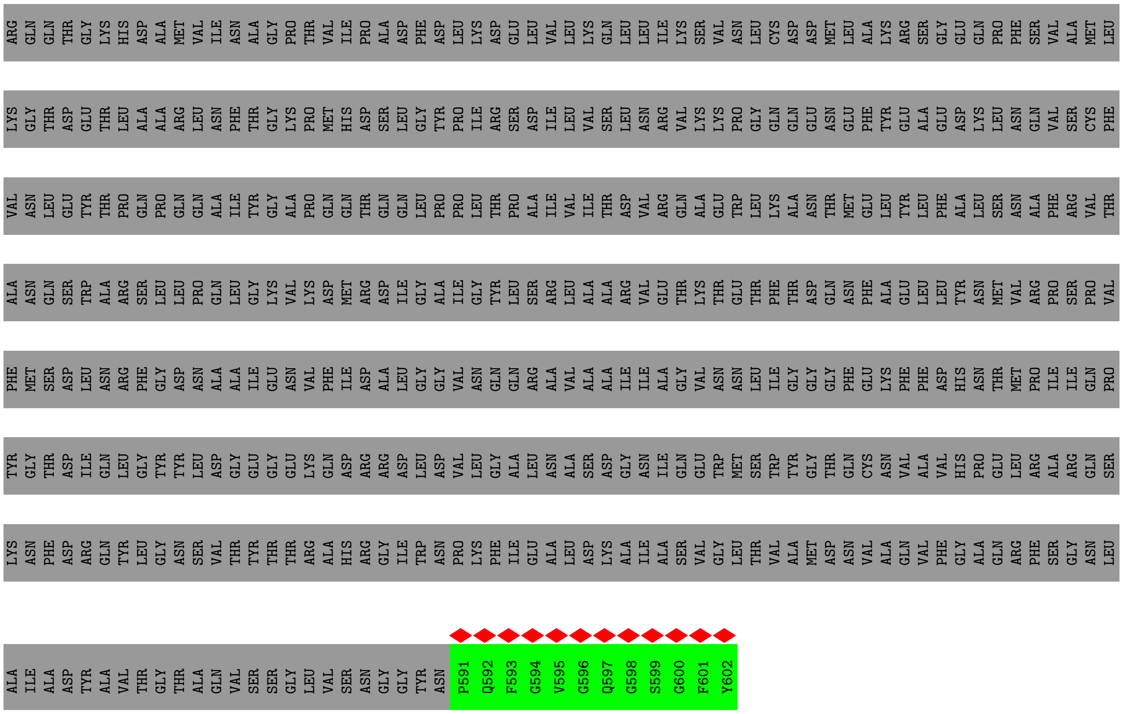


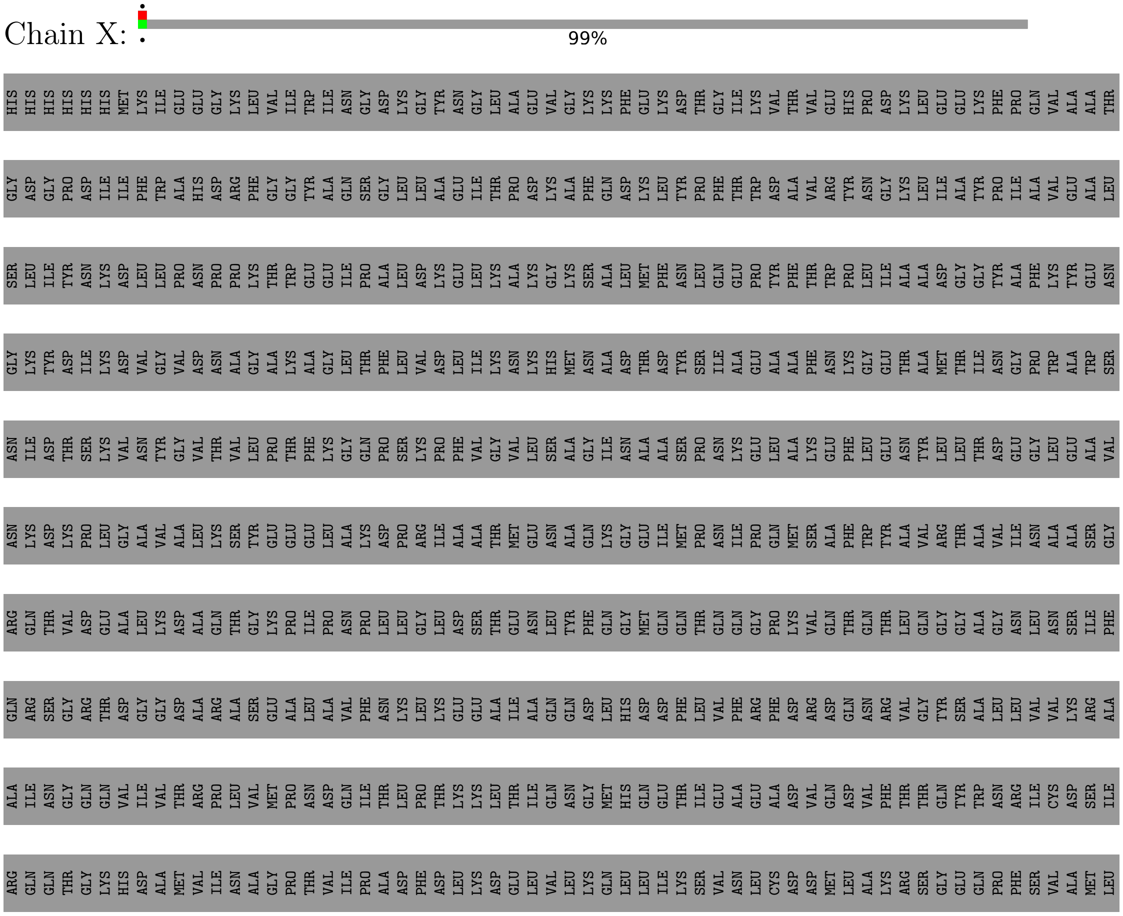


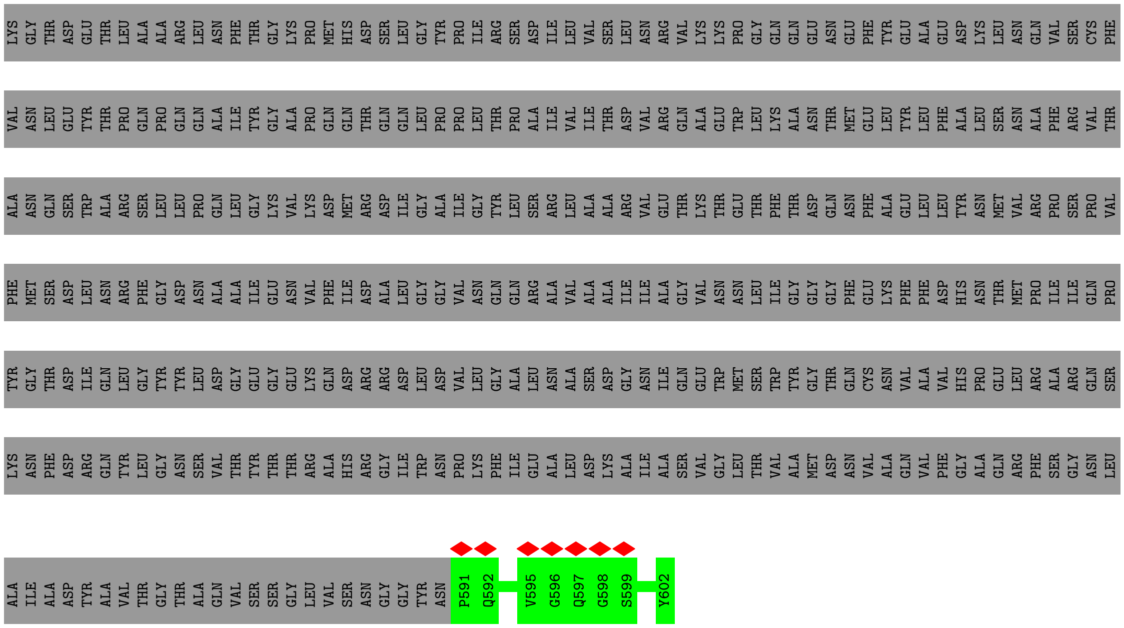
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN





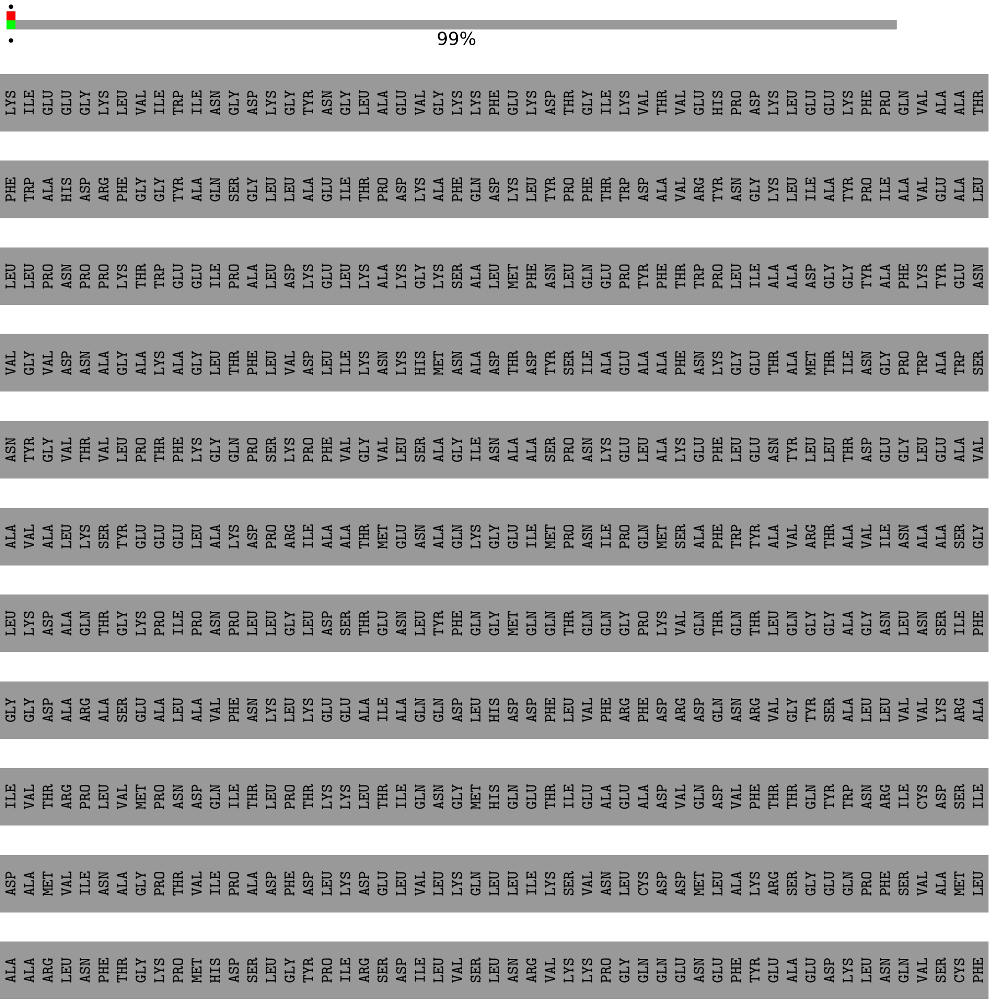
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

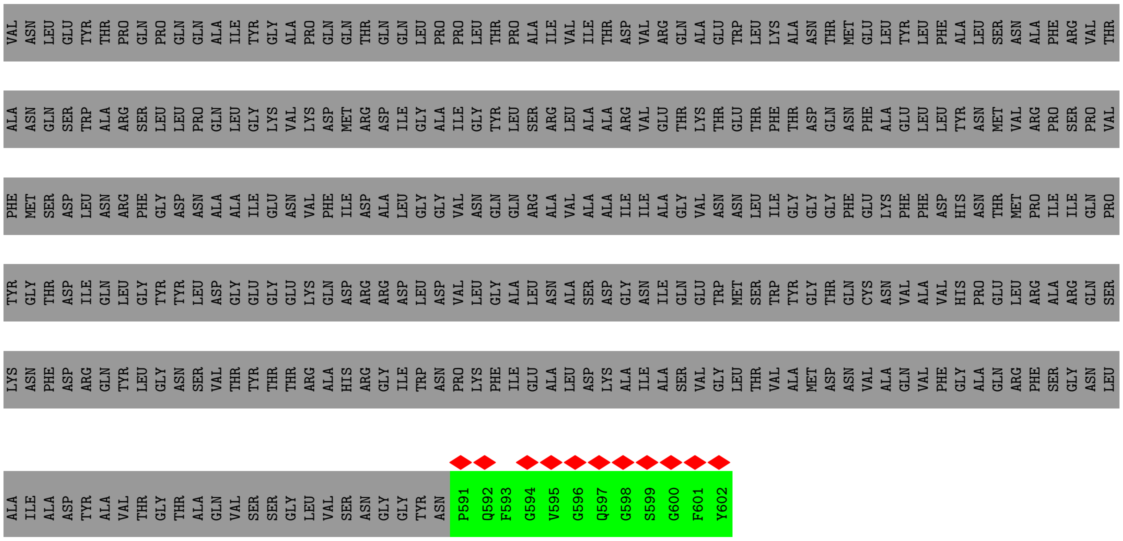




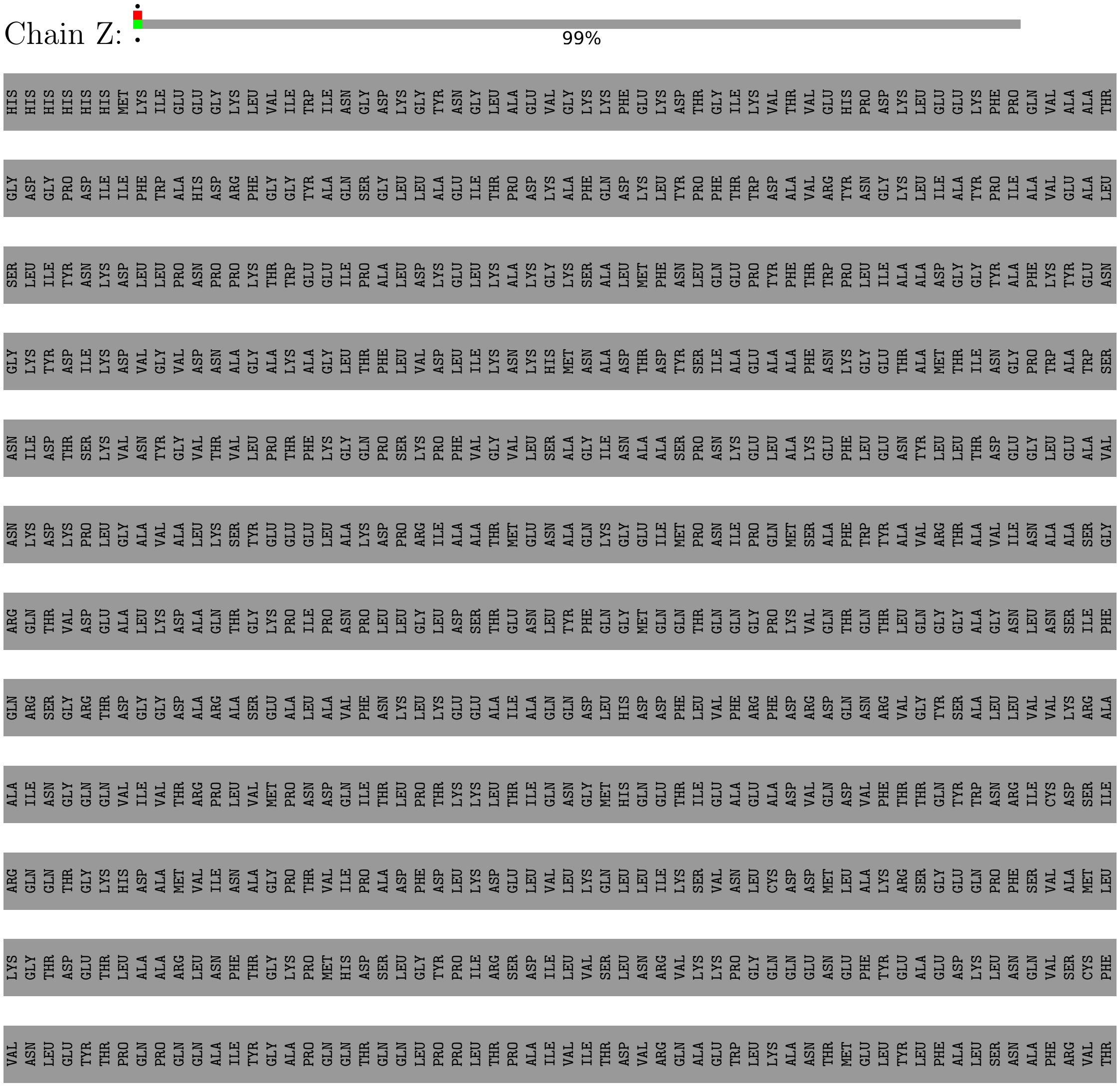
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

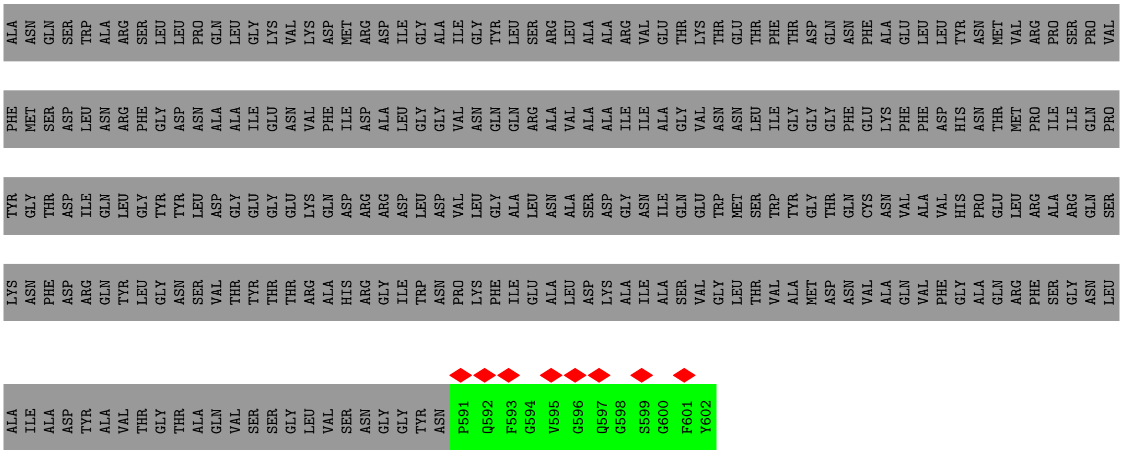
Chain Y:



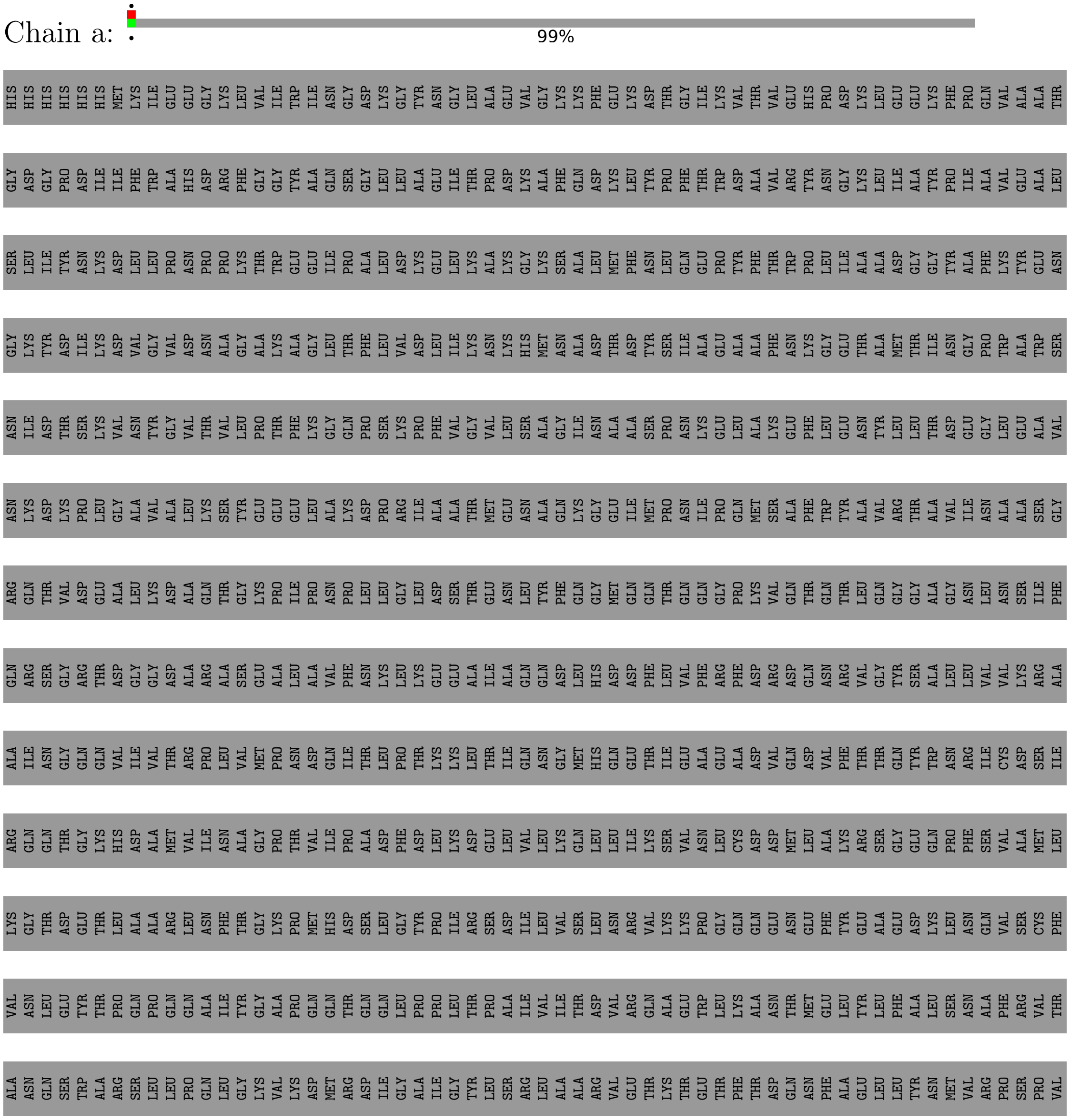


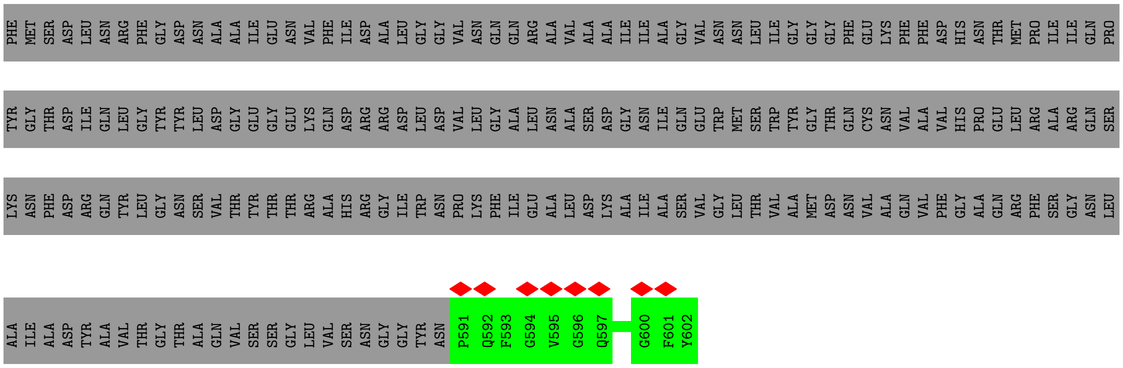
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN





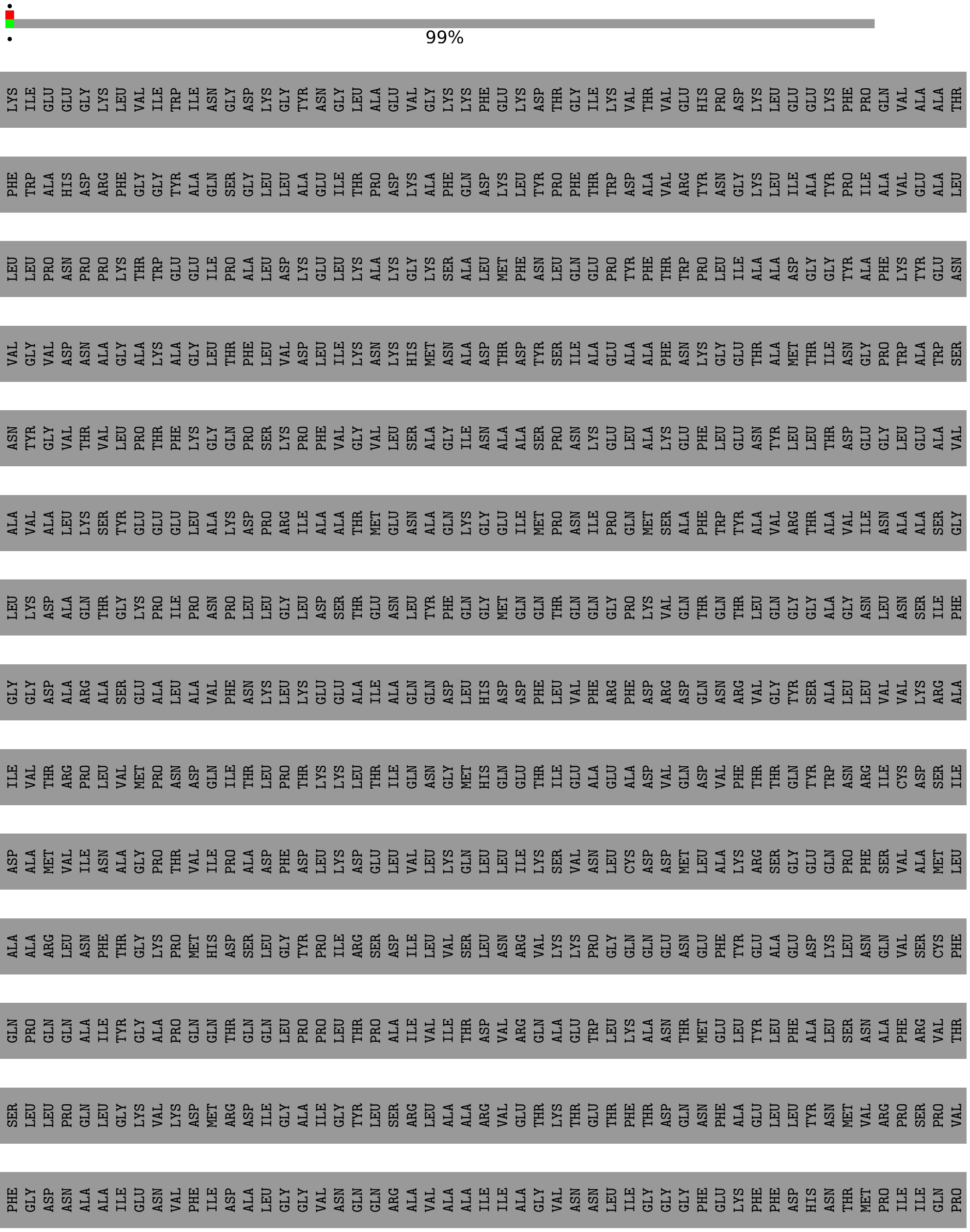
• Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

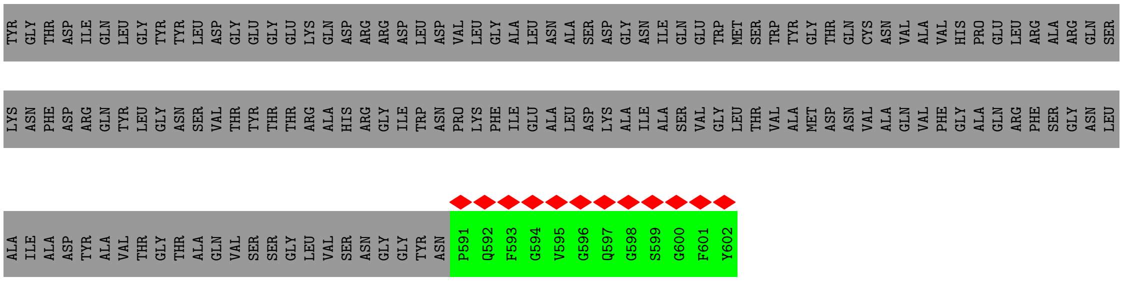




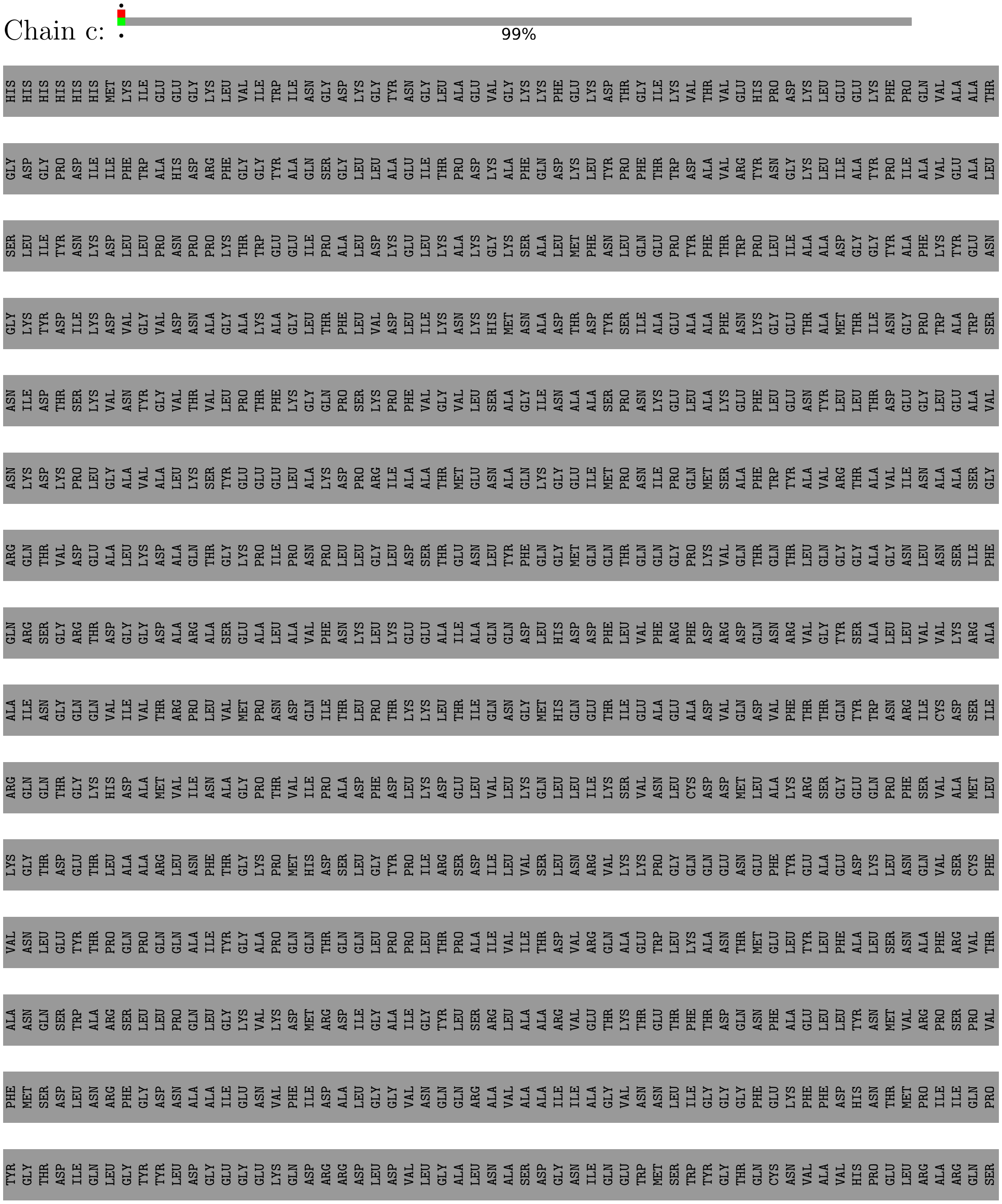
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

Chain b:





• Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

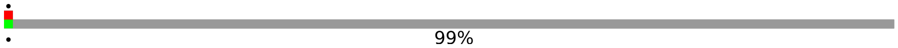


LYS ASN PHE ASP ARG GLN TYR LEU GLY ASN SER VAL THR TYR THR THR ARG ALA HIS ARG GLY ILE TRP ASN PRO LYS PHE ILE GLU ALA LEU ASP LYS ALA ILE ALA SER VAL GLY LEU THR VAL ALA MET ASP ASN VAL ALA GLN VAL PHE GLY ALA GLN ARG PHE SER GLY ASN LEU

ALA ILE ALA ASP TYR ALA VAL THR GLY THR ALA GLN VAL SER SER GLY LEU VAL SER ASN GLY GLY TYR ASN P591 Q592 F593 G594 V595 G596 Q597 G598 S599 G600 F601 Y602

- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

Chain d:



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

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

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

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

ASN ILE ASP THR SER LYS VAL ASN TYR GLY VAL THR VAL LEU PRO THR PHE LYS GLY GLN PRO SER LYS PRO PHE VAL GLY VAL LEU SER ALA GLY ILE ASN ALA ALA SER PRO ASN LYS GLU LEU ALA LYS GLU PHE LEU GLU ASN TYR LEU LEU THR ASP GLU GLY LEU GLU ALA VAL

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

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

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

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

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

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

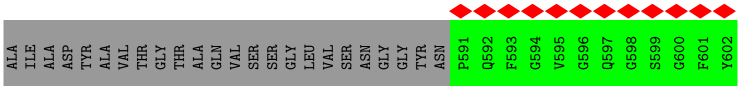
VAL ASN LEU GLU TYR THR PRO GLN PRO GLN GLN ALA ILE TYR GLY ALA PRO GLN GLN THR GLN GLN LEU PRO PRO LEU THR PRO ALA ILE VAL ILE THR ASP VAL ARG GLN ALA GLU TRP LEU LYS ALA ASN THR MET GLU LEU TYR LEU PHE ALA LEU SER ASN ALA PHE ARG VAL THR

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

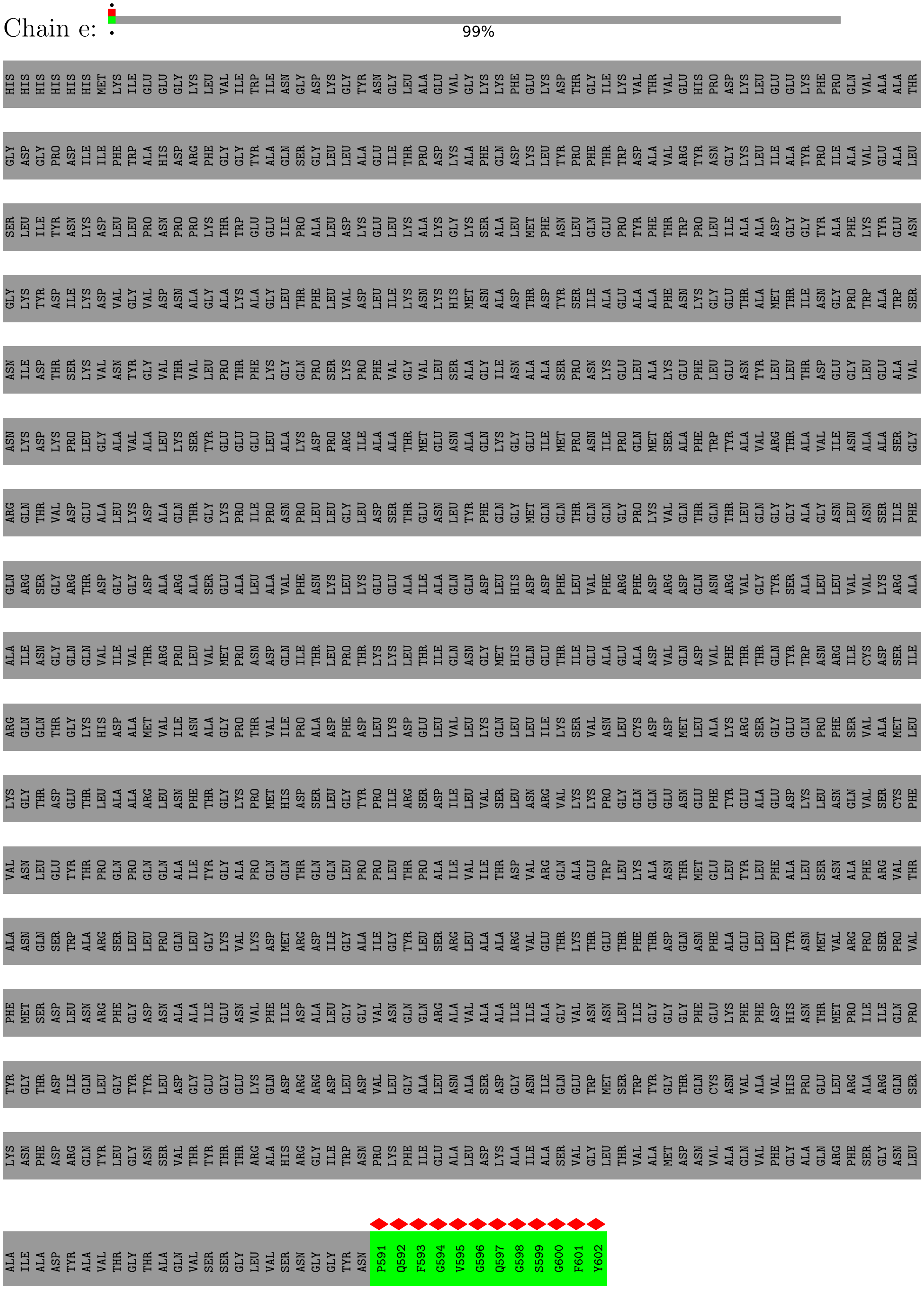
PHE MET SER ASP LEU ASN ARG PHE GLY ASP ASN ALA ALA ILE GLU ASN VAL PHE ILE ASP ALA LEU GLY GLY VAL ASN GLN GLN ARG ALA VAL ALA ALA ILE ILE ALA GLY VAL ASN ASN LEU ILE GLY GLY GLY PHE GLU LYS PHE PHE ASP HIS ASN THR MET PRO ILE ILE GLN PRO

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

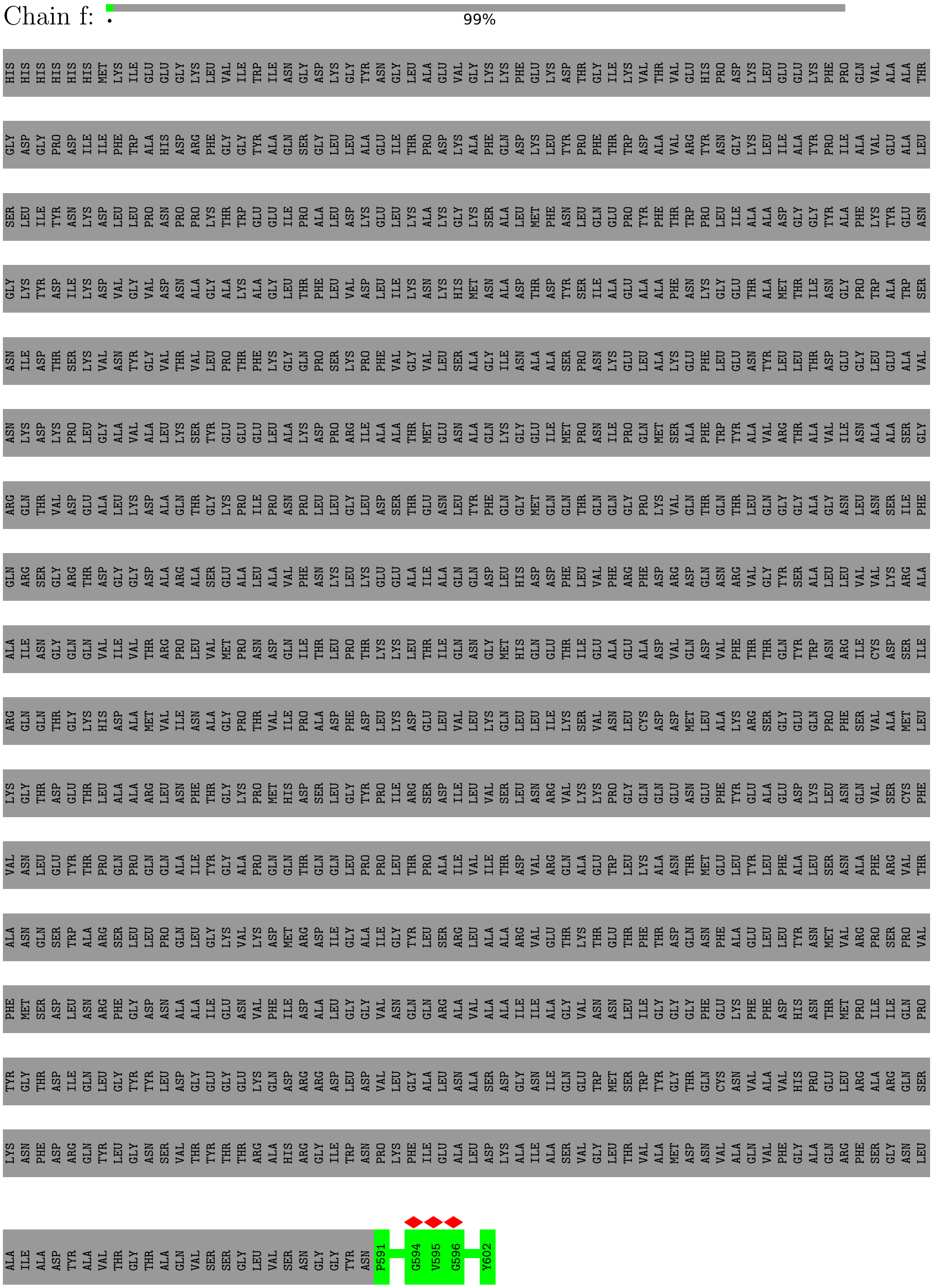
LYS ASN PHE ASP ARG GLN TYR LEU GLY ASN SER VAL THR TYR THR THR ARG ALA HIS ARG GLY ILE TRP ASN PRO LYS PHE ILE GLU ALA LEU ASP LYS ALA ILE ALA SER VAL GLY LEU THR VAL ALA MET ASP ASN VAL ALA GLN VAL PHE GLY ALA GLN ARG PHE SER GLY ASN LEU



- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN



- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	161270	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	67	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.003	Depositor
Minimum map value	-2.345	Depositor
Average map value	-0.010	Depositor
Map value standard deviation	0.157	Depositor
Recommended contour level	0.325	Depositor
Map size (Å)	427.008, 427.008, 427.008	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	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	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.91	0/4203	1.01	18/5697 (0.3%)
1	B	0.90	0/4203	0.96	16/5697 (0.3%)
1	C	0.89	0/4203	0.96	16/5697 (0.3%)
1	D	0.91	0/4203	1.01	18/5697 (0.3%)
1	E	0.85	0/91	0.81	0/120
1	F	0.83	0/91	0.85	0/120
1	G	0.83	0/91	0.85	0/120
1	H	0.85	0/91	0.80	0/120
1	I	0.91	0/4203	1.01	18/5697 (0.3%)
1	J	0.91	0/4203	1.01	17/5697 (0.3%)
1	K	0.91	0/4203	1.01	17/5697 (0.3%)
1	L	0.90	0/4203	0.96	15/5697 (0.3%)
1	M	0.90	0/4203	0.96	16/5697 (0.3%)
1	N	0.90	0/4203	0.96	16/5697 (0.3%)
1	O	0.89	0/4203	0.96	17/5697 (0.3%)
1	P	0.89	0/4203	0.96	16/5697 (0.3%)
1	Q	0.89	0/4203	0.96	16/5697 (0.3%)
1	R	0.91	0/4203	1.01	17/5697 (0.3%)
1	S	0.91	0/4203	1.01	17/5697 (0.3%)
1	T	0.91	0/4203	1.01	18/5697 (0.3%)
1	U	0.85	0/91	0.81	0/120
1	V	0.85	0/91	0.80	0/120
1	W	0.85	0/91	0.80	0/120
1	X	0.83	0/91	0.85	0/120
1	Y	0.83	0/91	0.85	0/120
1	Z	0.83	0/91	0.85	0/120
1	a	0.84	0/91	0.85	0/120
1	b	0.83	0/91	0.85	0/120
1	c	0.83	0/91	0.85	0/120
1	d	0.85	0/91	0.80	0/120
1	e	0.85	0/91	0.80	0/120
1	f	0.85	0/91	0.80	0/120
All	All	0.90	0/68704	0.98	268/93072 (0.3%)

There are no bond length outliers.

All (268) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	302	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	Q	302	ARG	NE-CZ-NH2	-10.71	114.94	120.30
1	P	302	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	C	302	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	M	302	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	L	302	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	O	302	ARG	NE-CZ-NH2	-10.55	115.02	120.30
1	B	302	ARG	NE-CZ-NH2	-10.53	115.03	120.30
1	D	216	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	T	216	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	R	216	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	S	216	ARG	NE-CZ-NH2	-9.57	115.51	120.30
1	I	216	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	A	216	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	A	466	ARG	NE-CZ-NH2	-9.49	115.55	120.30
1	K	216	ARG	NE-CZ-NH2	-9.49	115.55	120.30
1	J	216	ARG	NE-CZ-NH2	-9.43	115.59	120.30
1	K	466	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	J	466	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	S	466	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	T	466	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	I	466	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	D	466	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	I	360	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	R	466	ARG	NE-CZ-NH2	-9.25	115.68	120.30
1	K	360	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	A	360	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	D	360	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	R	360	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	J	360	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	T	360	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	S	360	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	B	466	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	J	141	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	B	147	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	N	147	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	M	147	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	L	466	ARG	NE-CZ-NH2	-9.03	115.79	120.30
1	A	141	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	P	147	ARG	NE-CZ-NH2	-9.02	115.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	141	ARG	NE-CZ-NH2	-9.01	115.79	120.30
1	L	147	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	I	141	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	O	147	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	Q	147	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	K	141	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	C	147	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	P	466	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	D	141	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	M	466	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	T	141	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	Q	466	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	R	141	ARG	NE-CZ-NH2	-8.85	115.87	120.30
1	K	67	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	N	466	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	J	67	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	C	466	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	D	67	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	O	466	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	S	67	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	I	67	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	A	67	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	R	67	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	T	67	ARG	NE-CZ-NH1	8.65	124.63	120.30
1	A	526	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	I	526	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	K	526	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	J	526	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	D	526	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	R	526	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	S	526	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	T	526	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	D	147	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	T	147	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	J	147	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	S	147	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	K	147	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	R	147	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	147	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	I	147	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	K	466	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	D	466	ARG	NE-CZ-NH1	7.61	124.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	466	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	A	466	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	T	466	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	M	67	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	L	67	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	P	67	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	S	466	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	C	67	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	J	466	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	R	466	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	O	67	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	Q	67	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	67	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	N	67	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	T	302	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	R	302	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	K	302	ARG	NE-CZ-NH2	7.21	123.90	120.30
1	D	302	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	J	302	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	I	302	ARG	NE-CZ-NH2	7.14	123.87	120.30
1	A	302	ARG	NE-CZ-NH2	7.13	123.87	120.30
1	S	302	ARG	NE-CZ-NH2	7.13	123.87	120.30
1	O	467	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	C	467	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	M	360	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	L	467	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	P	467	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	467	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	M	467	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	Q	360	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	Q	467	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	O	360	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	P	360	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	N	467	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	C	360	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	B	360	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	L	360	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	N	360	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	R	38	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	S	38	ARG	NE-CZ-NH2	6.77	123.68	120.30
1	J	38	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	D	38	ARG	NE-CZ-NH2	6.73	123.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	38	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	A	38	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	I	38	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	K	38	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	M	147	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	N	147	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	M	466	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	L	466	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	M	302	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	L	147	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	Q	466	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	466	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	466	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	P	302	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	P	466	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	N	302	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	147	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	B	302	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	L	302	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	N	466	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	Q	147	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	P	147	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	O	147	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	O	466	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	C	147	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	C	302	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	Q	302	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	O	302	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	T	393	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	K	393	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	I	393	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	R	393	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	D	302	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	A	393	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	J	393	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	T	302	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	D	393	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	S	393	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	R	302	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	S	302	ARG	NE-CZ-NH1	-5.77	117.41	120.30
1	I	302	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	J	302	ARG	NE-CZ-NH1	-5.73	117.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	K	302	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	46	PHE	CB-CG-CD1	5.69	124.78	120.80
1	T	378	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	K	46	PHE	CB-CG-CD1	5.68	124.78	120.80
1	K	378	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	J	46	PHE	CB-CG-CD1	5.67	124.77	120.80
1	T	46	PHE	CB-CG-CD1	5.67	124.77	120.80
1	D	46	PHE	CB-CG-CD1	5.66	124.76	120.80
1	S	378	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	J	378	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	I	46	PHE	CB-CG-CD1	5.63	124.74	120.80
1	R	46	PHE	CB-CG-CD1	5.62	124.73	120.80
1	D	378	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	N	70	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	I	378	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	R	378	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	A	378	TYR	CB-CG-CD2	-5.59	117.65	121.00
1	S	46	PHE	CB-CG-CD1	5.57	124.70	120.80
1	M	70	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	L	70	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	B	523	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	C	70	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	P	70	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	L	523	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	O	523	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	P	195	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	N	523	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	Q	195	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	Q	70	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	B	70	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	B	195	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	M	523	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	O	70	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	T	390	ASP	CB-CG-OD1	5.41	123.17	118.30
1	Q	523	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	97	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	O	195	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	I	360	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	D	390	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	523	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	O	97	ARG	NE-CZ-NH2	-5.38	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	ASP	CB-CG-OD1	5.38	123.14	118.30
1	I	390	ASP	CB-CG-OD1	5.36	123.13	118.30
1	L	97	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	S	390	ASP	CB-CG-OD1	5.36	123.13	118.30
1	K	390	ASP	CB-CG-OD1	5.36	123.12	118.30
1	Q	97	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	J	360	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	R	360	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	J	390	ASP	CB-CG-OD1	5.33	123.10	118.30
1	K	360	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	P	523	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	D	360	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	N	97	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	P	97	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	360	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	B	97	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	M	195	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	N	67	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	M	97	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	195	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	R	390	ASP	CB-CG-OD1	5.29	123.06	118.30
1	T	360	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	N	195	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	L	67	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	I	74	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	M	67	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	S	360	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	R	74	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	L	195	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	L	31	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	67	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	D	74	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	74	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	O	31	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	S	74	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	31	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	C	31	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	T	74	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	67	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	Q	67	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	P	31	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	M	74	ARG	NE-CZ-NH2	5.08	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	31	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	P	74	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	T	523	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	O	74	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	I	523	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	K	74	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	M	31	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	N	31	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	Q	74	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	A	523	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	O	67	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	P	67	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	523	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	J	74	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	B	74	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	N	74	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	O	38	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	C	74	ARG	NE-CZ-NH2	5.01	122.80	120.30

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	4128	4085	4083	5	0
1	B	4128	4085	4083	3	0
1	C	4128	4085	4083	13	0
1	D	4128	4085	4083	14	0
1	E	88	76	76	0	0
1	F	88	76	76	0	0
1	G	88	76	76	0	0
1	H	88	76	76	0	0
1	I	4128	4085	4083	19	0
1	J	4128	4085	4083	15	0
1	K	4128	4085	4083	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	4128	4085	4083	2	0
1	M	4128	4085	4083	8	0
1	N	4128	4085	4083	7	0
1	O	4128	4085	4083	8	0
1	P	4128	4085	4083	4	0
1	Q	4128	4085	4083	2	0
1	R	4128	4085	4083	0	0
1	S	4128	4085	4083	6	0
1	T	4128	4085	4083	26	0
1	U	88	76	76	0	0
1	V	88	76	76	0	0
1	W	88	76	76	0	0
1	X	88	76	76	0	0
1	Y	88	76	76	0	0
1	Z	88	76	76	0	0
1	a	88	76	76	0	0
1	b	88	76	76	0	0
1	c	88	76	76	0	0
1	d	88	76	76	0	0
1	e	88	76	76	0	0
1	f	88	76	76	0	0
All	All	67456	66576	66544	75	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 1.

All (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:119:MET:SD	1:S:552:ASN:HA	1.60	1.41
1:C:119:MET:CE	1:T:551:ASP:O	1.80	1.29
1:C:119:MET:HE1	1:T:551:ASP:O	1.11	1.27
1:O:119:MET:SD	1:S:552:ASN:CA	2.34	1.14
1:J:119:MET:HE1	1:T:112:LYS:HE3	1.31	1.09
1:C:119:MET:SD	1:T:552:ASN:HA	1.95	1.06
1:O:118:GLY:HA2	1:S:554:ALA:HB3	1.37	1.03
1:J:119:MET:HE1	1:T:112:LYS:CE	1.91	1.00
1:J:119:MET:CE	1:T:112:LYS:CE	2.40	0.99
1:O:119:MET:SD	1:S:553:VAL:N	2.37	0.98
1:D:121:GLN:OE1	1:I:121:GLN:OE1	1.80	0.97
1:J:119:MET:CE	1:T:112:LYS:HE3	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:LYS:HE3	1:I:119:MET:HE1	1.54	0.89
1:O:119:MET:CE	1:S:552:ASN:HA	2.00	0.89
1:O:119:MET:SD	1:S:552:ASN:C	2.51	0.89
1:J:119:MET:CE	1:T:112:LYS:HE2	2.02	0.89
1:J:112:LYS:CE	1:T:119:MET:HE2	2.09	0.81
1:I:552:ASN:HA	1:M:119:MET:SD	2.21	0.81
1:J:119:MET:HE3	1:T:112:LYS:CE	2.12	0.80
1:J:112:LYS:CE	1:T:119:MET:CE	2.61	0.78
1:J:112:LYS:HE3	1:T:119:MET:CE	2.13	0.77
1:D:112:LYS:HE3	1:I:119:MET:CE	2.16	0.76
1:C:119:MET:CE	1:T:552:ASN:HA	2.16	0.76
1:C:119:MET:SD	1:T:552:ASN:CA	2.74	0.75
1:J:112:LYS:HE2	1:T:119:MET:HE2	1.68	0.74
1:C:118:GLY:HA2	1:T:554:ALA:HB3	1.69	0.74
1:J:119:MET:HE3	1:T:112:LYS:HE2	1.70	0.73
1:D:112:LYS:CE	1:I:119:MET:CE	2.66	0.72
1:J:112:LYS:HE3	1:T:119:MET:HE3	1.71	0.72
1:D:112:LYS:CE	1:I:119:MET:HE1	2.23	0.68
1:J:112:LYS:HE2	1:T:119:MET:CE	2.23	0.66
1:A:552:ASN:HA	1:N:119:MET:SD	2.35	0.66
1:C:119:MET:SD	1:T:553:VAL:N	2.71	0.64
1:D:119:MET:CE	1:I:112:LYS:HE3	2.30	0.62
1:D:112:LYS:CE	1:I:119:MET:HE3	2.30	0.62
1:C:119:MET:HE2	1:T:552:ASN:HA	1.80	0.61
1:C:119:MET:HE2	1:T:551:ASP:O	1.93	0.59
1:D:119:MET:HE3	1:I:112:LYS:HE3	1.84	0.58
1:D:112:LYS:HE2	1:I:119:MET:CE	2.35	0.56
1:J:112:LYS:CE	1:T:119:MET:HE3	2.32	0.56
1:D:119:MET:HE2	1:I:112:LYS:CE	2.36	0.55
1:I:552:ASN:HA	1:M:119:MET:CE	2.37	0.55
1:I:552:ASN:OD1	1:M:119:MET:SD	2.65	0.55
1:D:119:MET:CE	1:I:112:LYS:CE	2.86	0.54
1:N:70:ARG:HA	1:N:75:VAL:HG22	1.90	0.54
1:B:70:ARG:HA	1:B:75:VAL:HG22	1.91	0.53
1:M:70:ARG:HA	1:M:75:VAL:HG22	1.91	0.53
1:L:70:ARG:HA	1:L:75:VAL:HG22	1.91	0.53
1:Q:70:ARG:HA	1:Q:75:VAL:HG22	1.90	0.53
1:O:70:ARG:HA	1:O:75:VAL:HG22	1.91	0.53
1:C:70:ARG:HA	1:C:75:VAL:HG22	1.91	0.53
1:C:119:MET:SD	1:T:552:ASN:C	2.87	0.53
1:P:70:ARG:HA	1:P:75:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:552:ASN:HA	1:M:119:MET:HE1	1.90	0.52
1:A:551:ASP:O	1:N:119:MET:CE	2.60	0.50
1:A:551:ASP:O	1:N:119:MET:HE3	2.12	0.50
1:O:497:VAL:O	1:O:502:ARG:NH1	2.47	0.48
1:P:497:VAL:O	1:P:502:ARG:NH1	2.47	0.48
1:B:497:VAL:O	1:B:502:ARG:NH1	2.47	0.48
1:C:497:VAL:O	1:C:502:ARG:NH1	2.47	0.48
1:L:497:VAL:O	1:L:502:ARG:NH1	2.47	0.48
1:Q:497:VAL:O	1:Q:502:ARG:NH1	2.47	0.48
1:M:497:VAL:O	1:M:502:ARG:NH1	2.47	0.48
1:N:497:VAL:O	1:N:502:ARG:NH1	2.47	0.48
1:A:552:ASN:HA	1:N:119:MET:HE1	1.96	0.48
1:C:119:MET:CE	1:T:551:ASP:C	2.73	0.47
1:A:552:ASN:HA	1:N:119:MET:CE	2.45	0.47
1:I:551:ASP:O	1:M:119:MET:CE	2.63	0.46
1:D:119:MET:HE2	1:I:112:LYS:HE3	1.98	0.44
1:J:112:LYS:HE3	1:T:119:MET:HE2	1.83	0.44
1:B:29:SER:HG	1:D:190:ASP:CG	2.23	0.42
1:D:112:LYS:HE2	1:I:119:MET:HE3	2.01	0.41
1:I:551:ASP:O	1:M:119:MET:HE3	2.21	0.41
1:P:258:ASP:OD1	1:P:258:ASP:N	2.51	0.40
1:P:50:LYS:NZ	1:P:61:ASP:OD1	2.45	0.40

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	521/996 (52%)	518 (99%)	3 (1%)	0	100	100
1	B	521/996 (52%)	514 (99%)	7 (1%)	0	100	100
1	C	521/996 (52%)	514 (99%)	7 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	521/996 (52%)	518 (99%)	3 (1%)	0	100	100
1	E	10/996 (1%)	10 (100%)	0	0	100	100
1	F	10/996 (1%)	9 (90%)	1 (10%)	0	100	100
1	G	10/996 (1%)	9 (90%)	1 (10%)	0	100	100
1	H	10/996 (1%)	10 (100%)	0	0	100	100
1	I	521/996 (52%)	518 (99%)	3 (1%)	0	100	100
1	J	521/996 (52%)	518 (99%)	3 (1%)	0	100	100
1	K	521/996 (52%)	518 (99%)	3 (1%)	0	100	100
1	L	521/996 (52%)	514 (99%)	7 (1%)	0	100	100
1	M	521/996 (52%)	514 (99%)	7 (1%)	0	100	100
1	N	521/996 (52%)	514 (99%)	7 (1%)	0	100	100
1	O	521/996 (52%)	514 (99%)	7 (1%)	0	100	100
1	P	521/996 (52%)	514 (99%)	7 (1%)	0	100	100
1	Q	521/996 (52%)	514 (99%)	7 (1%)	0	100	100
1	R	521/996 (52%)	518 (99%)	3 (1%)	0	100	100
1	S	521/996 (52%)	518 (99%)	3 (1%)	0	100	100
1	T	521/996 (52%)	518 (99%)	3 (1%)	0	100	100
1	U	10/996 (1%)	10 (100%)	0	0	100	100
1	V	10/996 (1%)	10 (100%)	0	0	100	100
1	W	10/996 (1%)	10 (100%)	0	0	100	100
1	X	10/996 (1%)	9 (90%)	1 (10%)	0	100	100
1	Y	10/996 (1%)	9 (90%)	1 (10%)	0	100	100
1	Z	10/996 (1%)	9 (90%)	1 (10%)	0	100	100
1	a	10/996 (1%)	9 (90%)	1 (10%)	0	100	100
1	b	10/996 (1%)	9 (90%)	1 (10%)	0	100	100
1	c	10/996 (1%)	9 (90%)	1 (10%)	0	100	100
1	d	10/996 (1%)	10 (100%)	0	0	100	100
1	e	10/996 (1%)	10 (100%)	0	0	100	100
1	f	10/996 (1%)	10 (100%)	0	0	100	100
All	All	8496/31872 (27%)	8408 (99%)	88 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	443/817 (54%)	443 (100%)	0	100	100
1	B	443/817 (54%)	443 (100%)	0	100	100
1	C	443/817 (54%)	443 (100%)	0	100	100
1	D	443/817 (54%)	443 (100%)	0	100	100
1	E	8/817 (1%)	8 (100%)	0	100	100
1	F	8/817 (1%)	8 (100%)	0	100	100
1	G	8/817 (1%)	8 (100%)	0	100	100
1	H	8/817 (1%)	8 (100%)	0	100	100
1	I	443/817 (54%)	443 (100%)	0	100	100
1	J	443/817 (54%)	443 (100%)	0	100	100
1	K	443/817 (54%)	443 (100%)	0	100	100
1	L	443/817 (54%)	443 (100%)	0	100	100
1	M	443/817 (54%)	443 (100%)	0	100	100
1	N	443/817 (54%)	443 (100%)	0	100	100
1	O	443/817 (54%)	443 (100%)	0	100	100
1	P	443/817 (54%)	443 (100%)	0	100	100
1	Q	443/817 (54%)	443 (100%)	0	100	100
1	R	443/817 (54%)	443 (100%)	0	100	100
1	S	443/817 (54%)	443 (100%)	0	100	100
1	T	443/817 (54%)	443 (100%)	0	100	100
1	U	8/817 (1%)	8 (100%)	0	100	100
1	V	8/817 (1%)	8 (100%)	0	100	100
1	W	8/817 (1%)	8 (100%)	0	100	100
1	X	8/817 (1%)	8 (100%)	0	100	100
1	Y	8/817 (1%)	8 (100%)	0	100	100
1	Z	8/817 (1%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	8/817 (1%)	8 (100%)	0	100	100
1	b	8/817 (1%)	8 (100%)	0	100	100
1	c	8/817 (1%)	8 (100%)	0	100	100
1	d	8/817 (1%)	8 (100%)	0	100	100
1	e	8/817 (1%)	8 (100%)	0	100	100
1	f	8/817 (1%)	8 (100%)	0	100	100
All	All	7216/26144 (28%)	7216 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	552	ASN
1	I	121	GLN
1	I	552	ASN
1	J	121	GLN
1	T	552	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

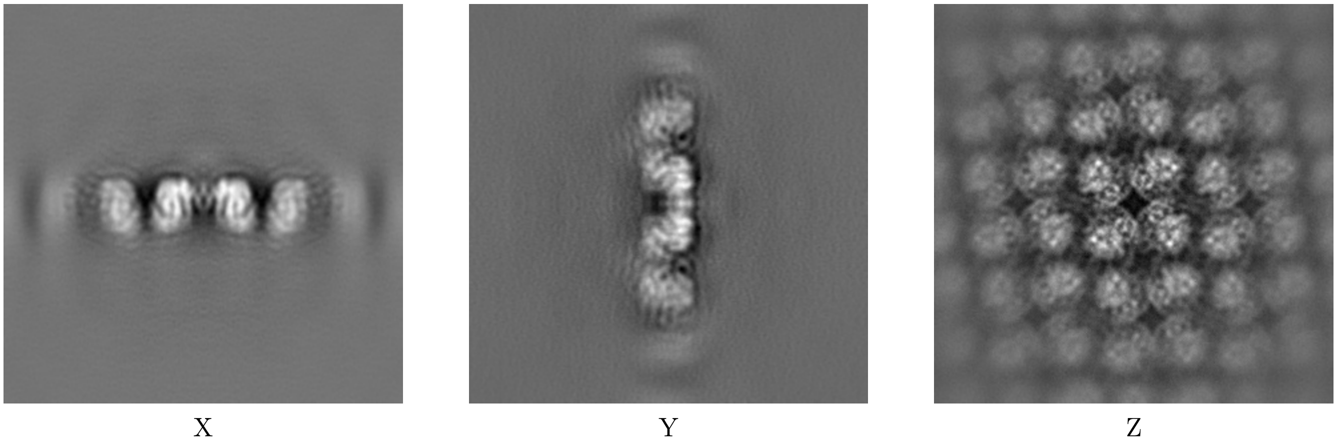
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-29451. These allow visual inspection of the internal detail of the map and identification of artifacts.

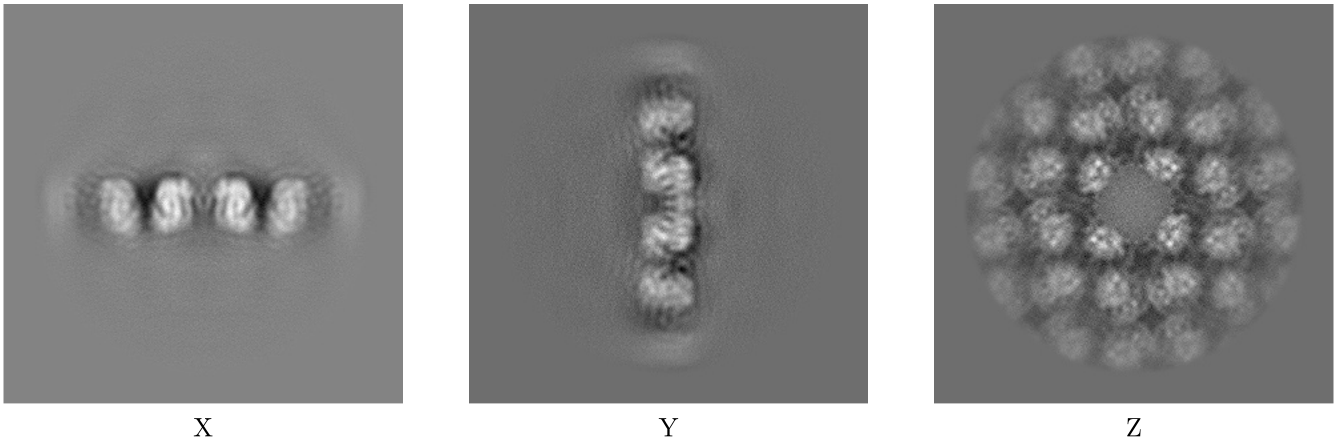
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X Y Z

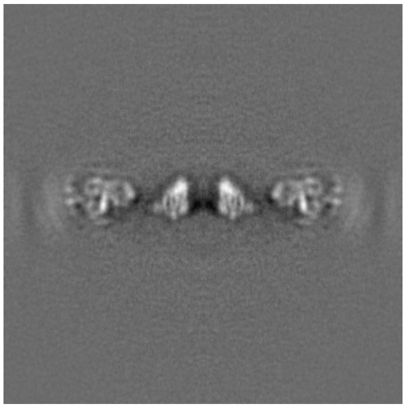
6.1.2 Raw map


X Y Z

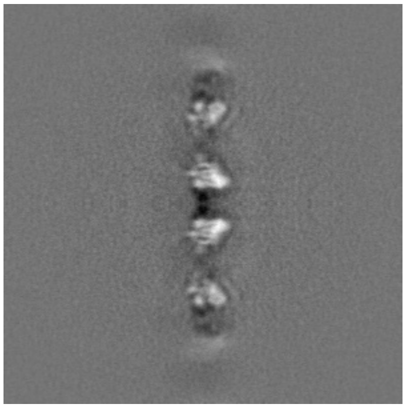
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

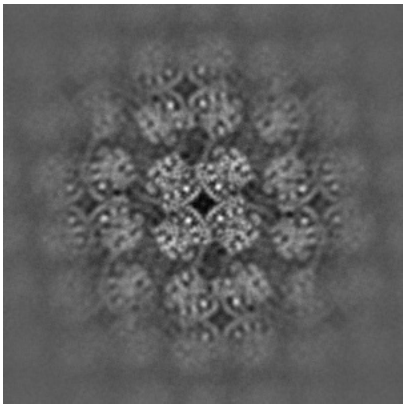
6.2.1 Primary map



X Index: 256

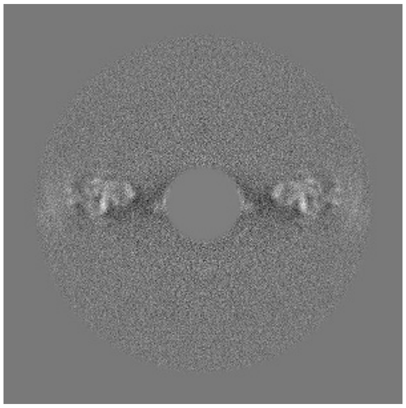


Y Index: 256

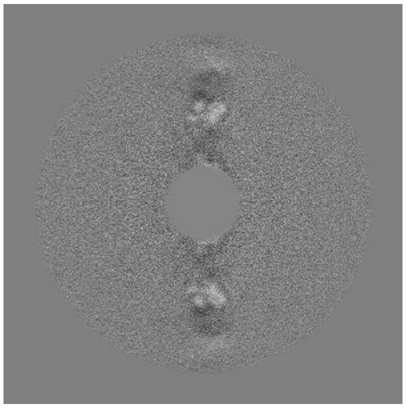


Z Index: 256

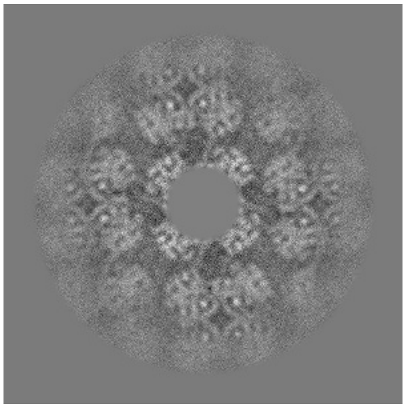
6.2.2 Raw map



X Index: 256



Y Index: 256

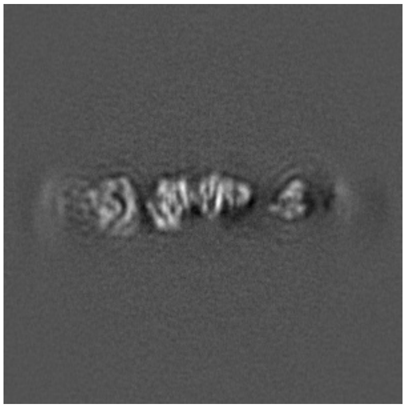


Z Index: 256

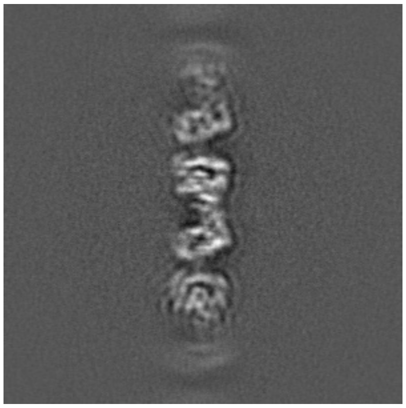
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

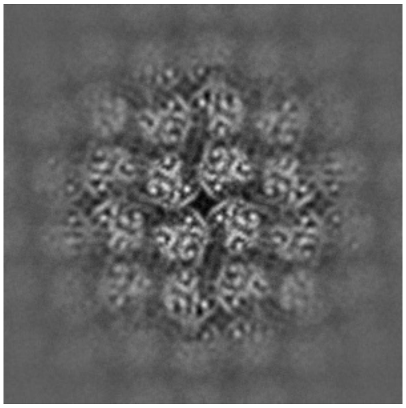
6.3.1 Primary map



X Index: 233

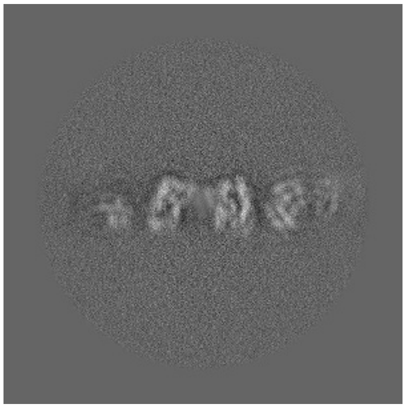


Y Index: 302

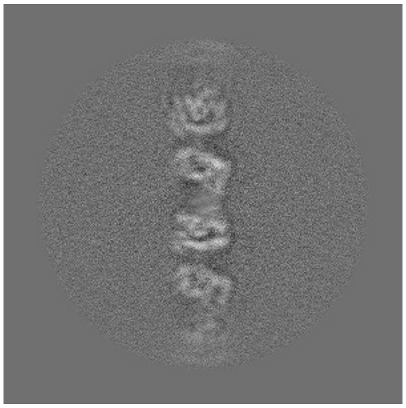


Z Index: 251

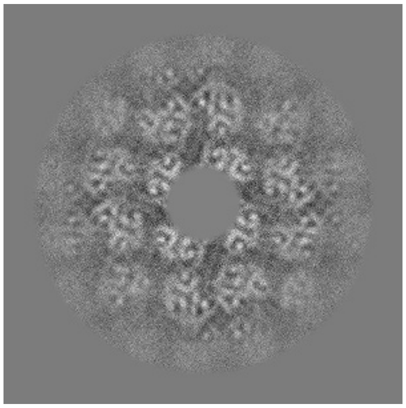
6.3.2 Raw map



X Index: 210



Y Index: 210



Z Index: 251

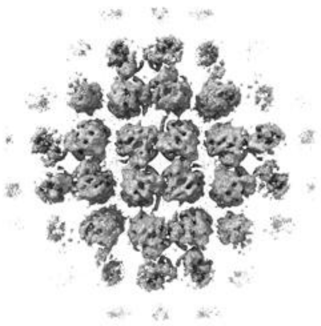
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views

6.4.1 Primary map

X

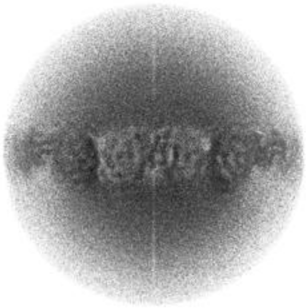
Y



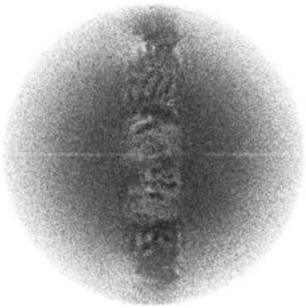
Z

The images above show the 3D surface view of the map at the recommended contour level 0.325. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

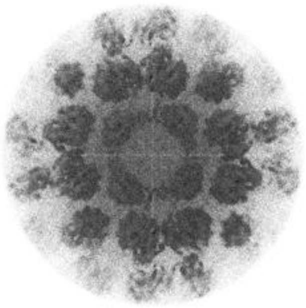
6.4.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

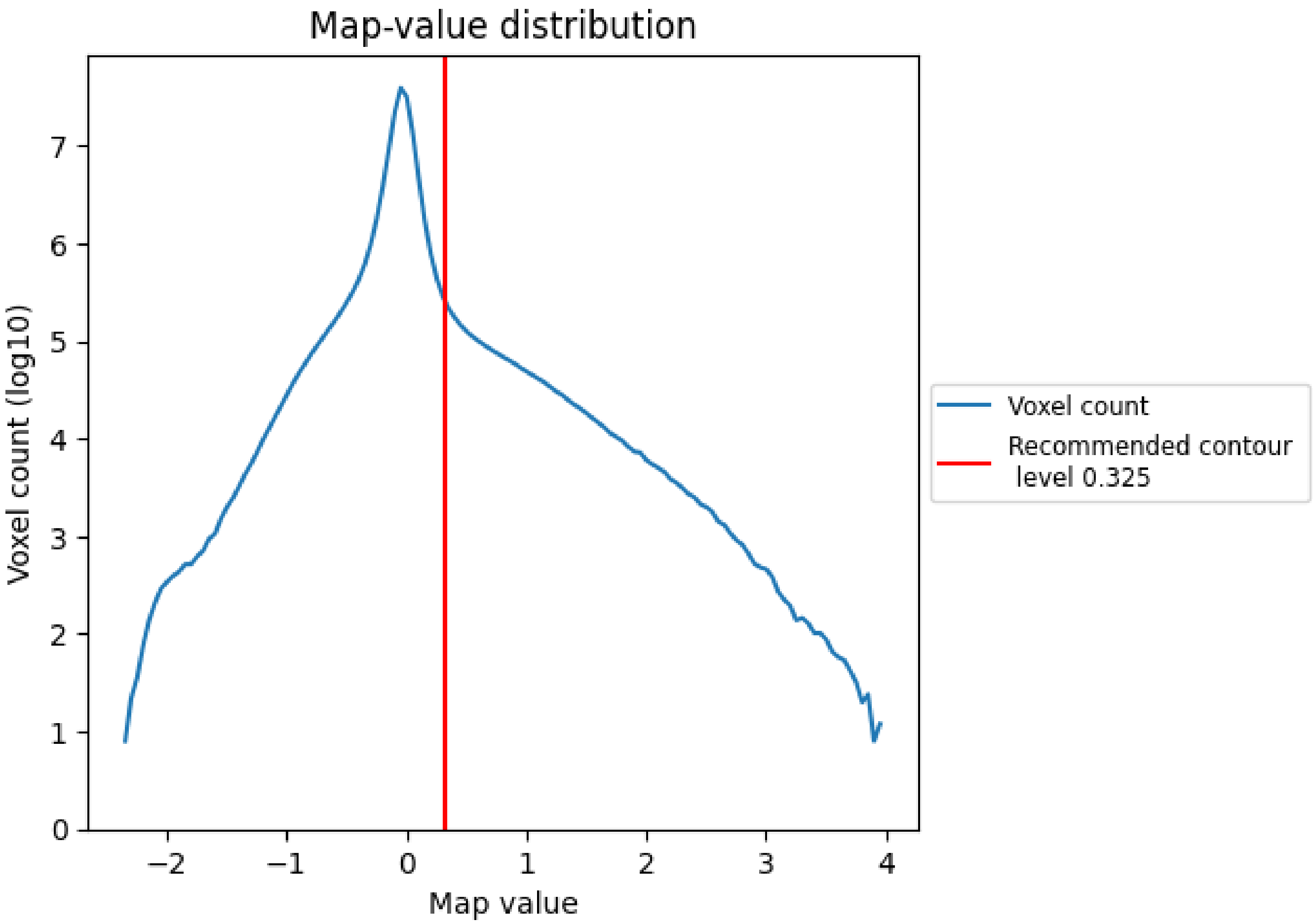
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

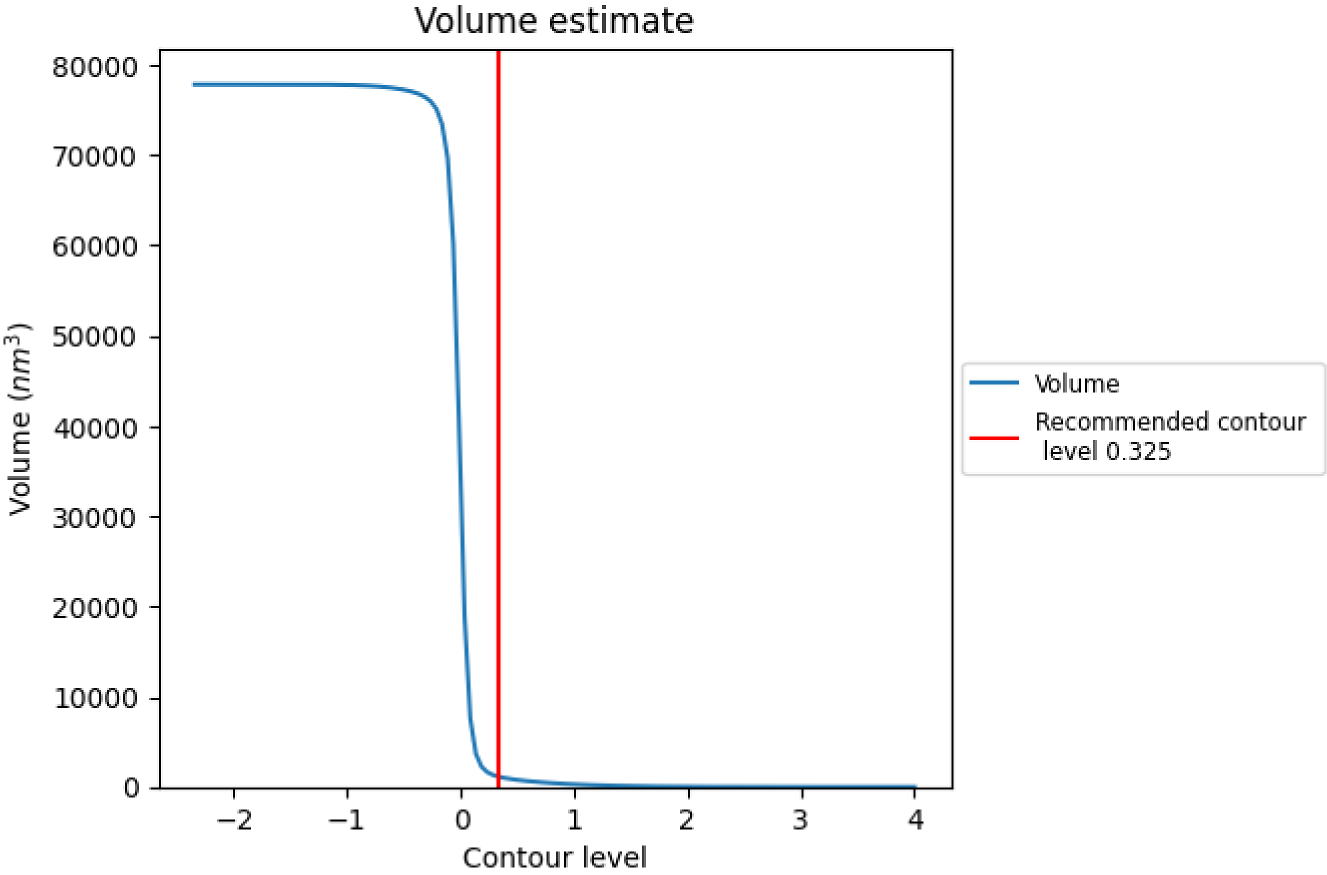
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

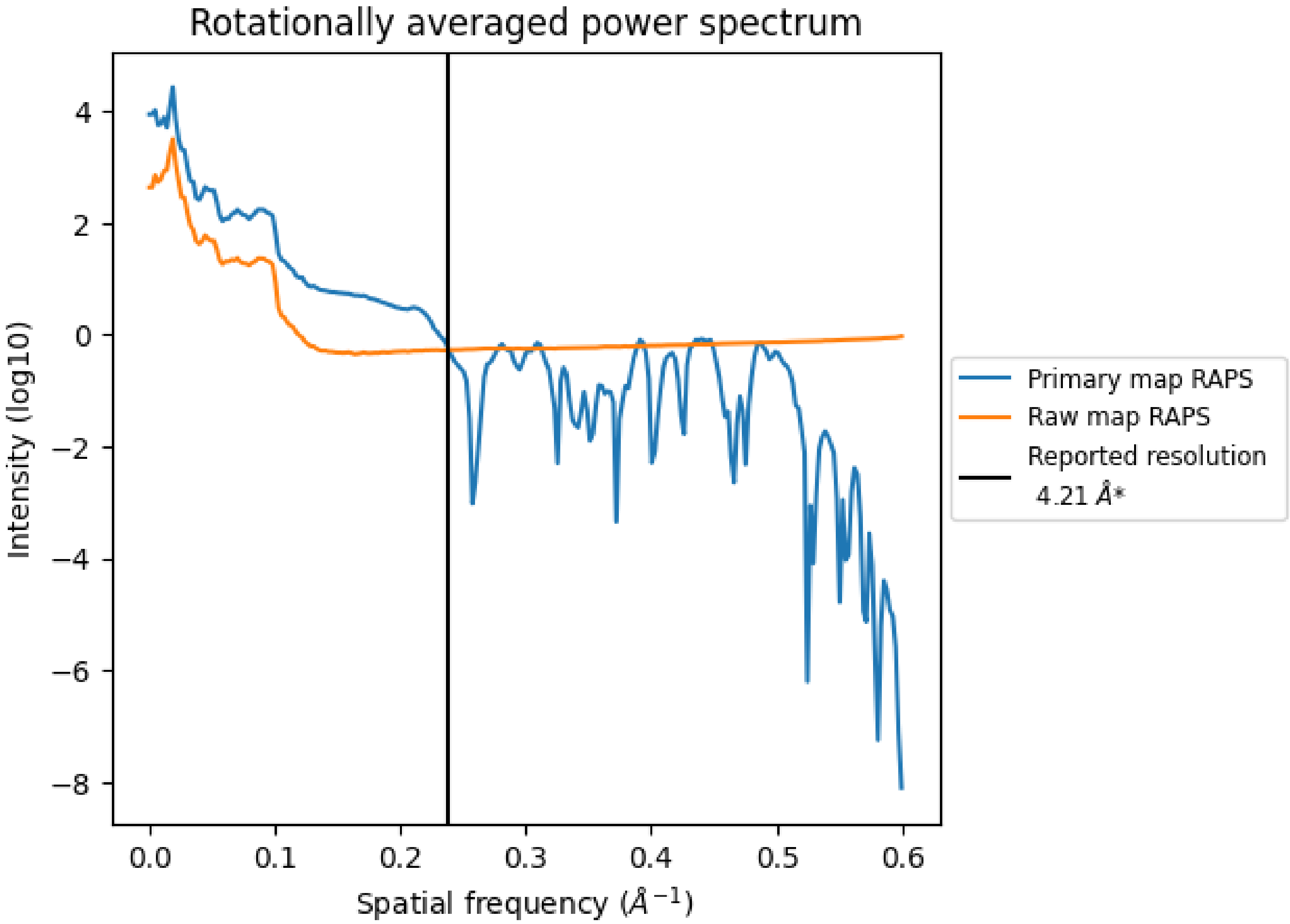
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1173 nm^3; this corresponds to an approximate mass of 1059 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

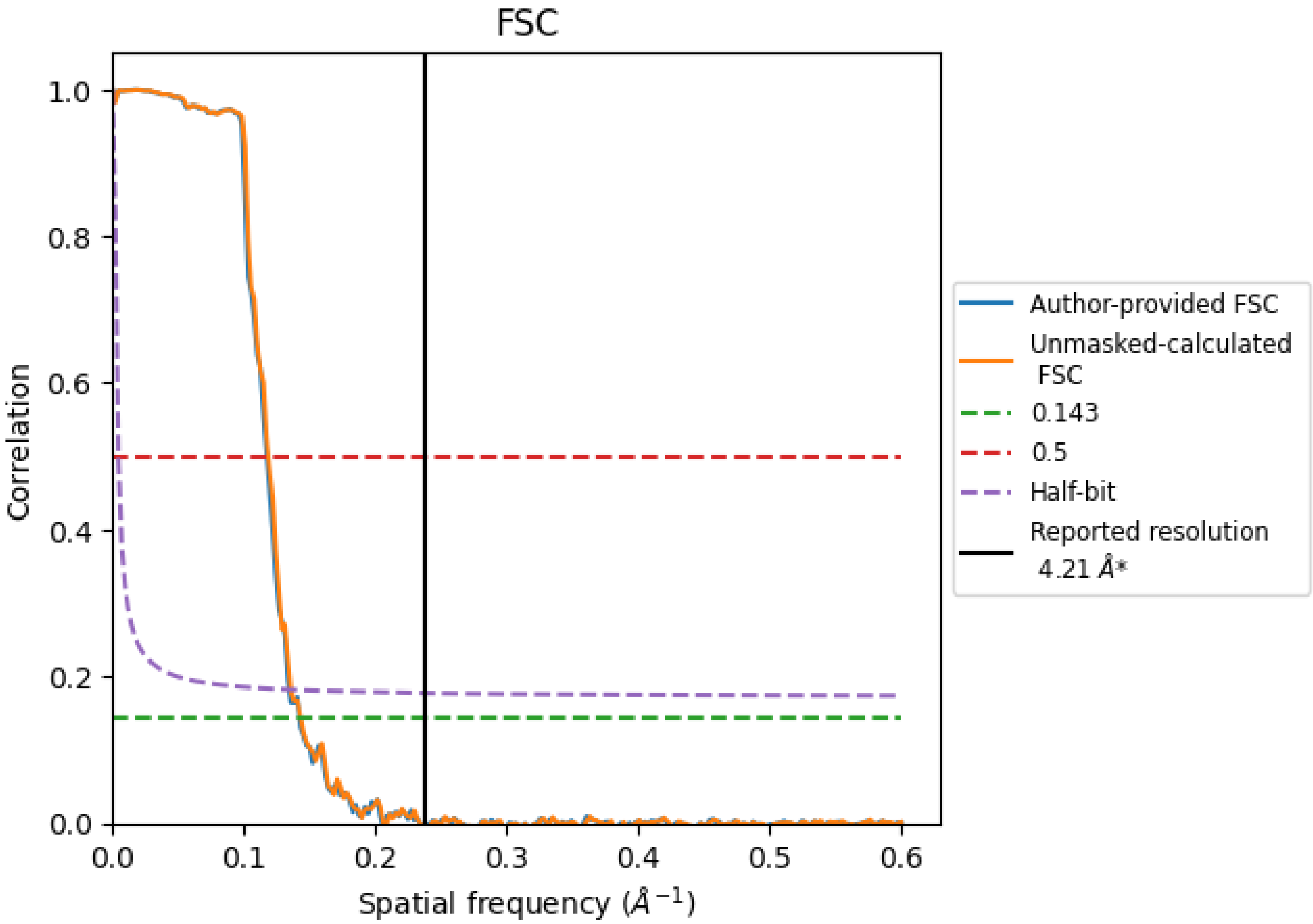


*Reported resolution corresponds to spatial frequency of 0.238 $\AA^{-1}$

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	4.21	-	-
Author-provided FSC curve	7.04	8.52	7.43
Unmasked-calculated*	6.99	8.44	7.37

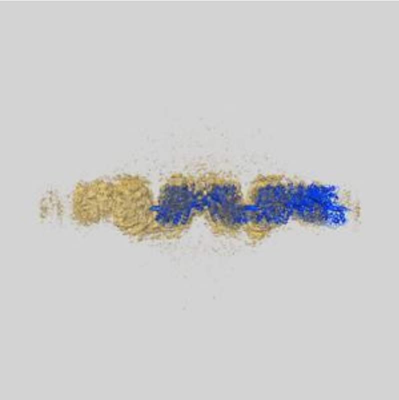
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.04 differs from the reported value 4.21 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.99 differs from the reported value 4.21 by more than 10 %

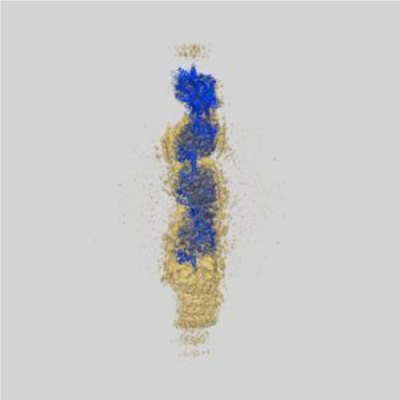
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-29451 and PDB model 8FV5. Per-residue inclusion information can be found in section 3 on page 28.

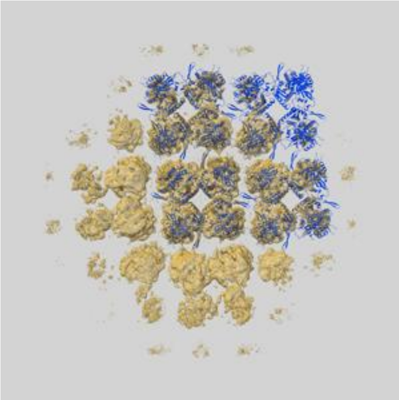
9.1 Map-model overlay ⓘ



X



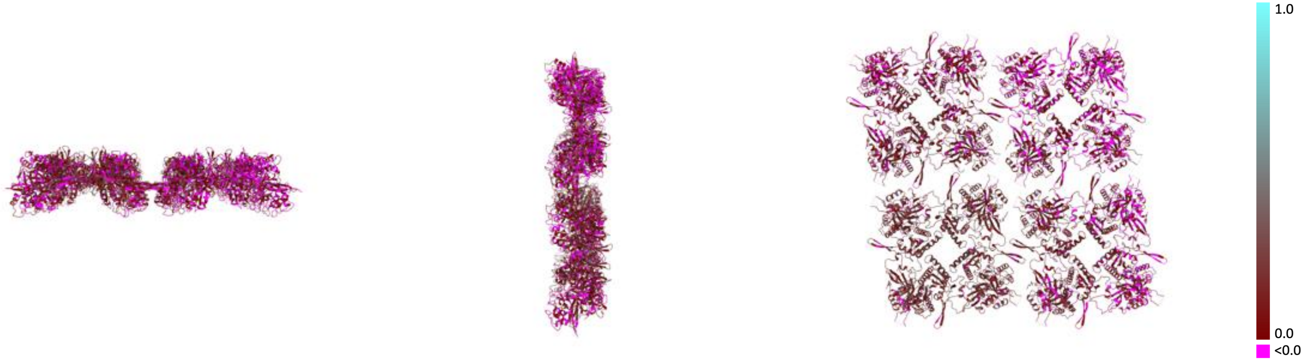
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.325 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

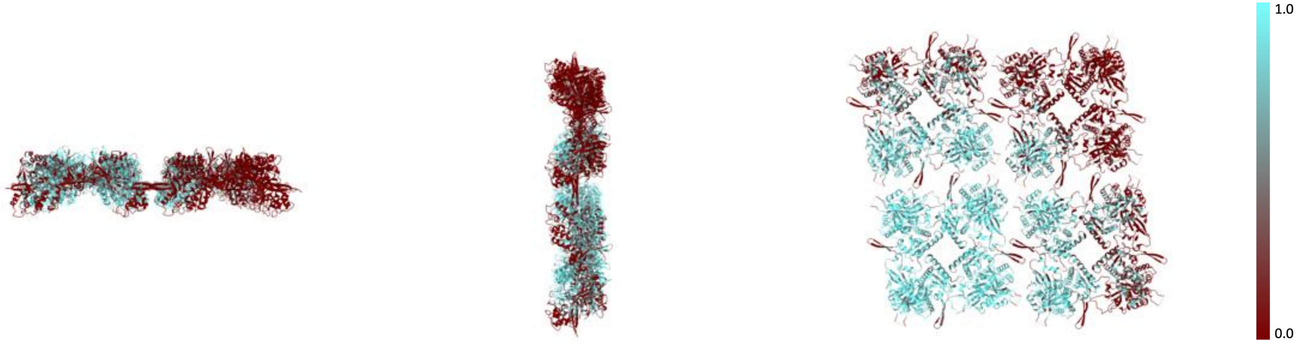
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

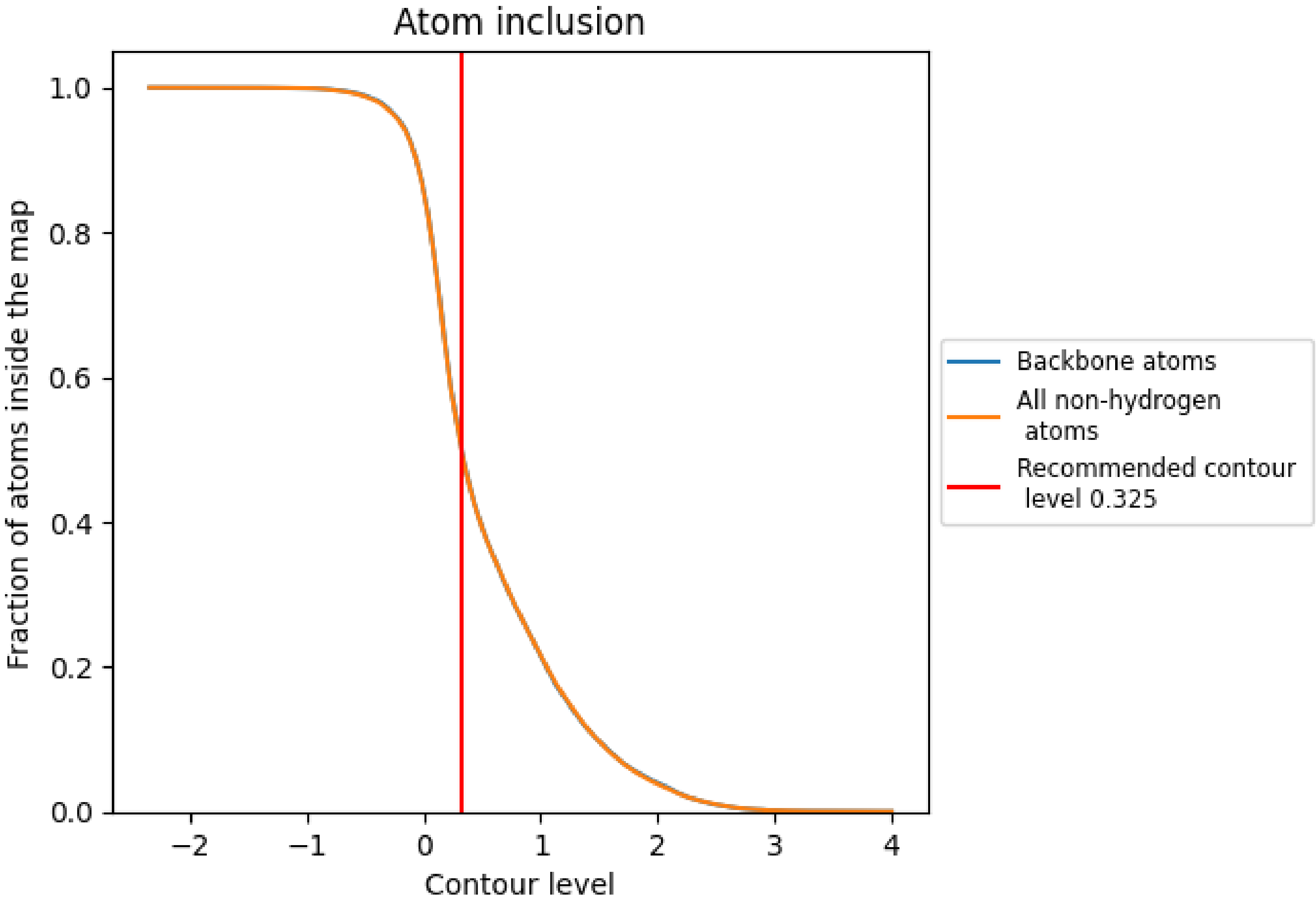
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.325).

9.4 Atom inclusion ⓘ



At the recommended contour level, 50% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.325) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4978	0.1090
A	0.8288	0.1900
B	0.8454	0.1870
C	0.8444	0.1880
D	0.8298	0.1900
E	0.9310	0.1930
F	0.8851	0.1380
G	0.8851	0.1480
H	0.9310	0.1890
I	0.7258	0.1370
J	0.1050	0.0360
K	0.3310	0.0700
L	0.7120	0.1280
M	0.5472	0.0800
N	0.7367	0.1390
O	0.3456	0.0780
P	0.0005	0.0140
Q	0.2777	0.0850
R	0.2354	0.0680
S	0.0294	0.0370
T	0.7208	0.1370
U	0.4828	0.1240
V	0.0000	-0.0990
W	0.0805	0.0220
X	0.4023	0.0670
Y	0.1839	-0.0280
Z	0.3333	0.0120
a	0.2989	0.0440
b	0.0000	0.0410
c	0.1264	0.0240
d	0.0115	0.0170
e	0.0000	0.0140
f	0.7356	0.1420