



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:34 AM UTC

PDB ID : 8FV5 / pdb_00008fv5
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)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

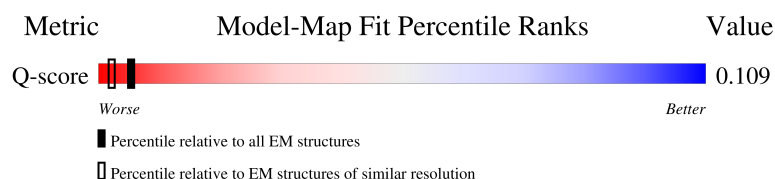
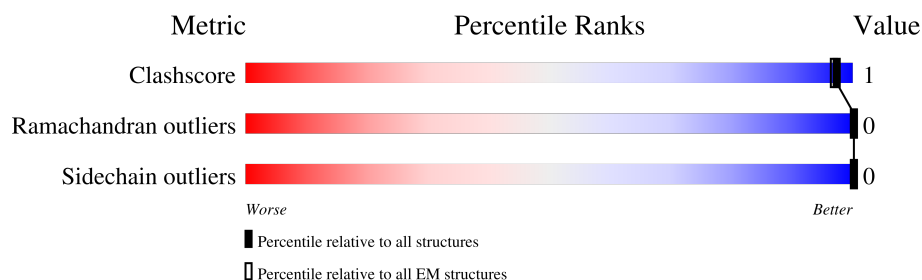
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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.



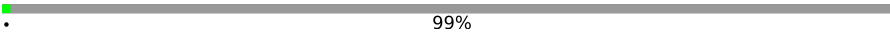
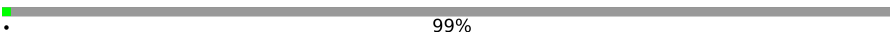
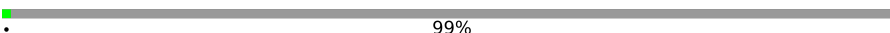
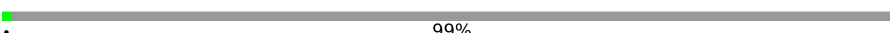
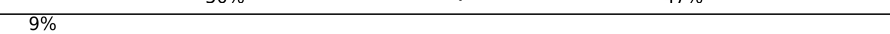
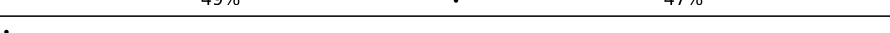
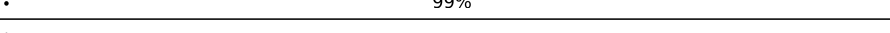
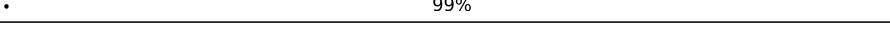
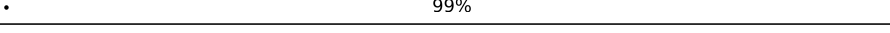
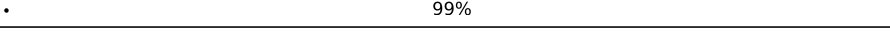
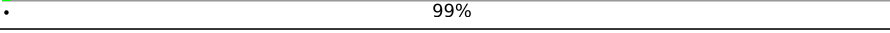
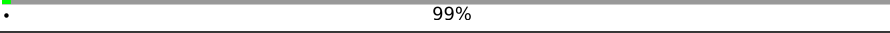
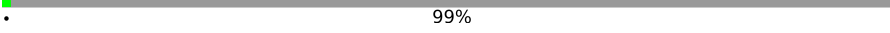
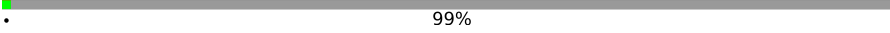
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4806 (3.71 - 4.71)

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 $\leq 5\%$. 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	
1	B	996	
1	C	996	
1	D	996	

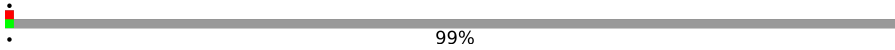
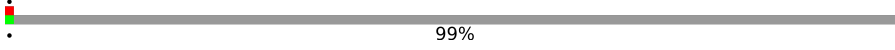
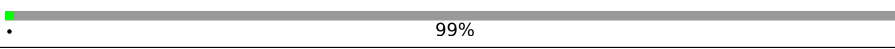
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Mol	Chain	Length	Quality of chain
1	E	996	 99%
1	F	996	 99%
1	G	996	 99%
1	H	996	 99%
1	I	996	 8% 49% 47%
1	J	996	 47% 50% 47%
1	K	996	 31% 50% 47%
1	L	996	 9% 50% 47%
1	M	996	 19% 50% 47%
1	N	996	 7% 50% 47%
1	O	996	 31% 50% 47%
1	P	996	 53% 50% 47%
1	Q	996	 36% 50% 47%
1	R	996	 39% 50% 47%
1	S	996	 52% 50% 47%
1	T	996	 9% 49% 47%
1	U	996	 99%
1	V	996	 99%
1	W	996	 99%
1	X	996	 99%
1	Y	996	 99%
1	Z	996	 99%
1	a	996	 99%
1	b	996	 99%
1	c	996	 99%

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Mol	Chain	Length	Quality of chain
1	d	996	 99%
1	e	996	 99%
1	f	996	 99%

2 Entry composition [i](#)

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

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

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

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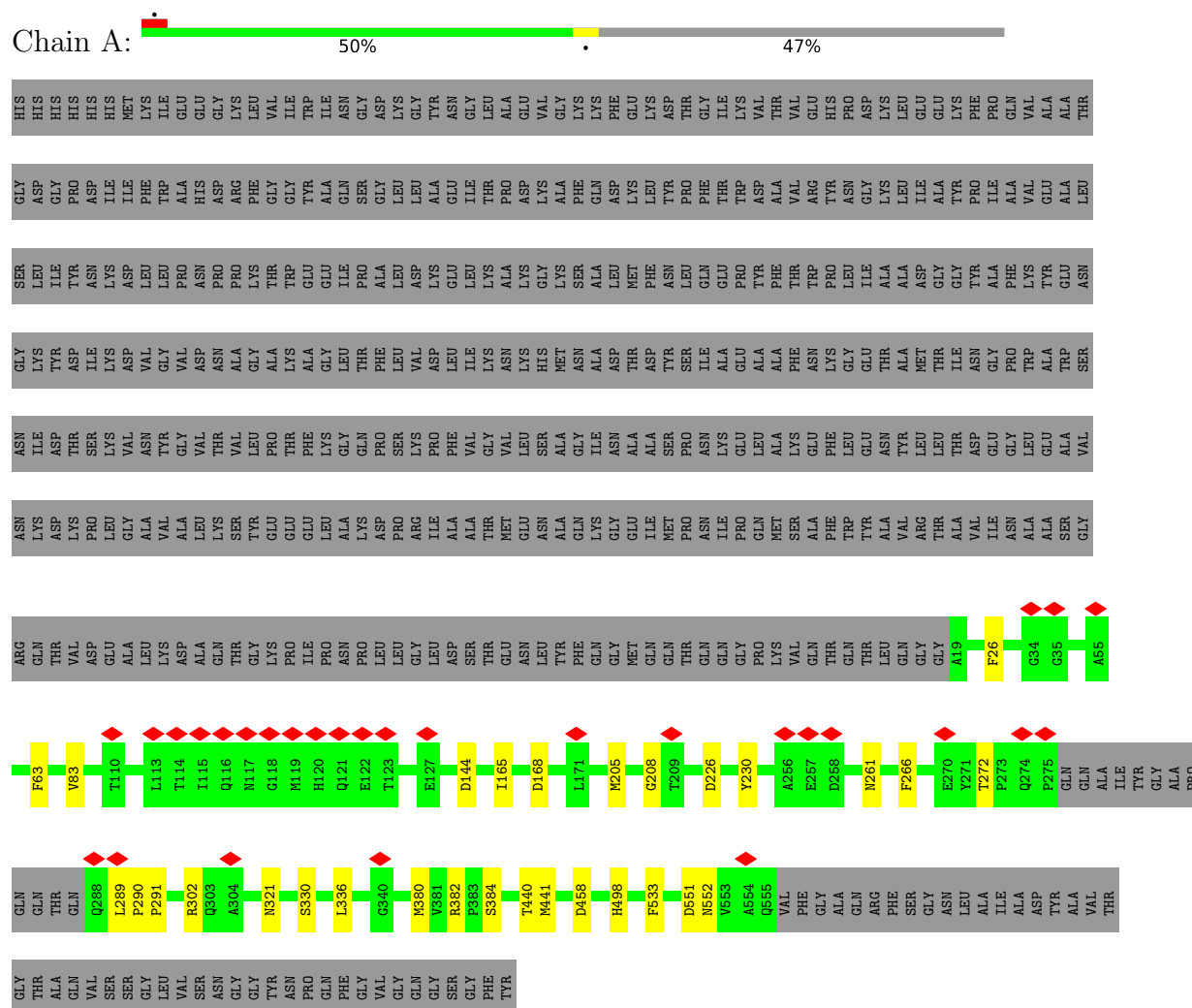
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Chain	Residue	Modelled	Actual	Comment	Reference
f	-6	GLU	-	linker	UNP P0AEX9
f	-5	ASN	-	linker	UNP P0AEX9
f	-4	LEU	-	linker	UNP P0AEX9
f	-3	TYR	-	linker	UNP P0AEX9
f	-2	PHE	-	linker	UNP P0AEX9
f	-1	GLN	-	linker	UNP P0AEX9
f	0	GLY	-	linker	UNP P0AEX9

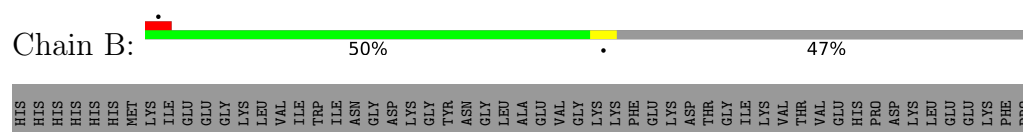
3 Residue-property plots

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

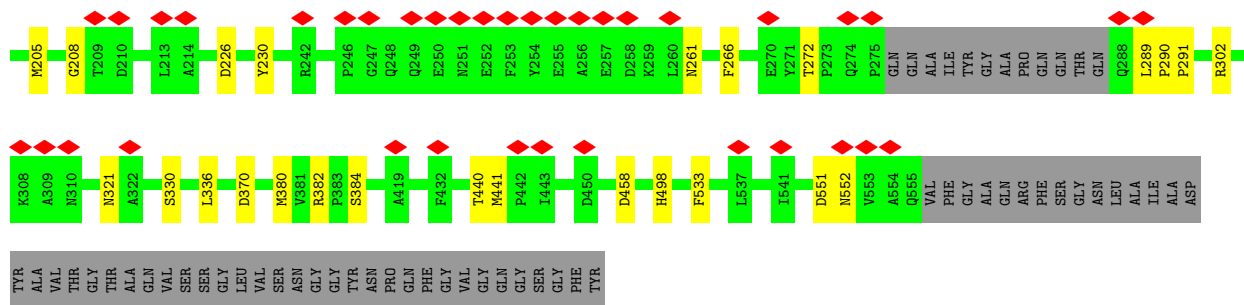


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN

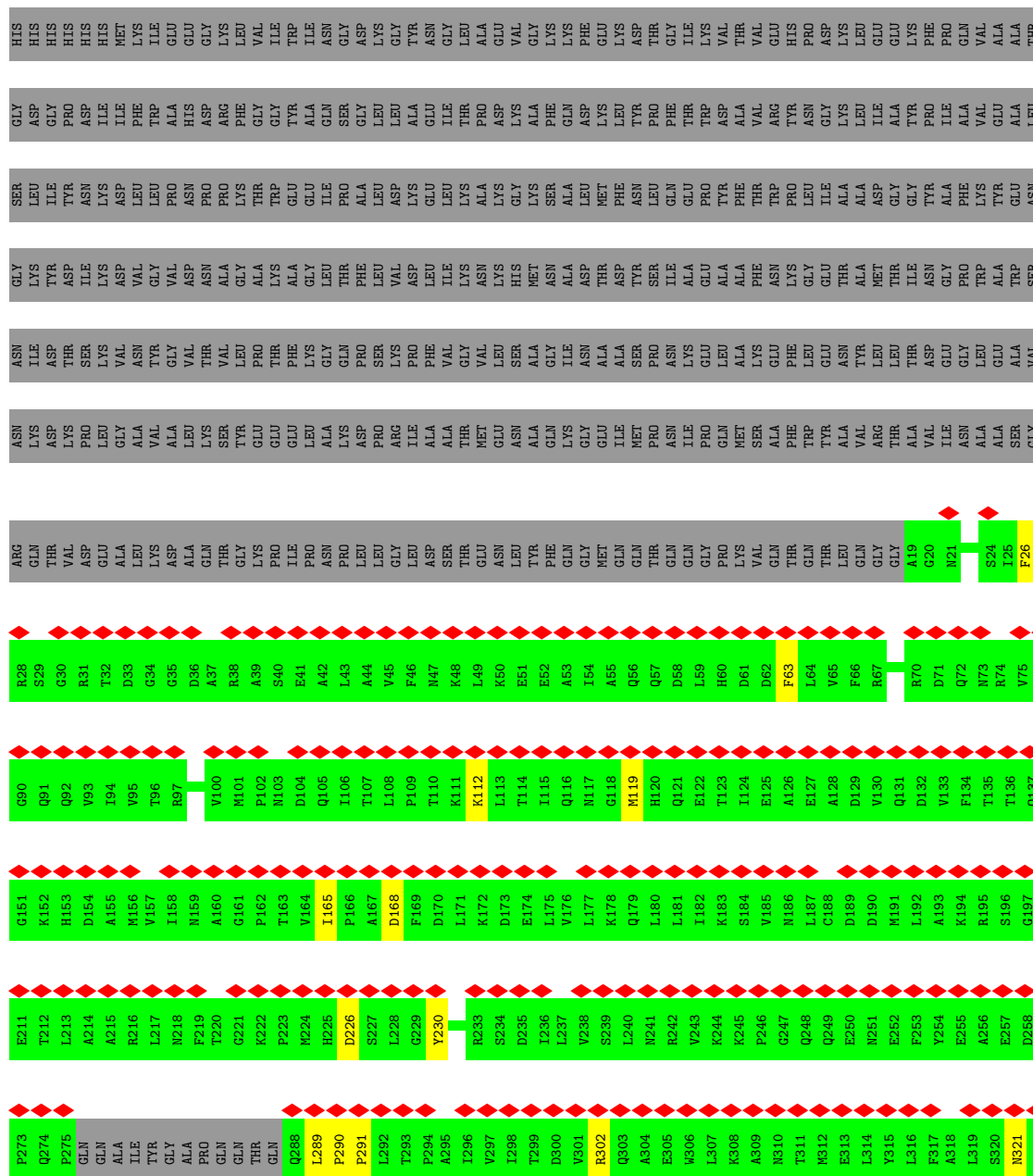


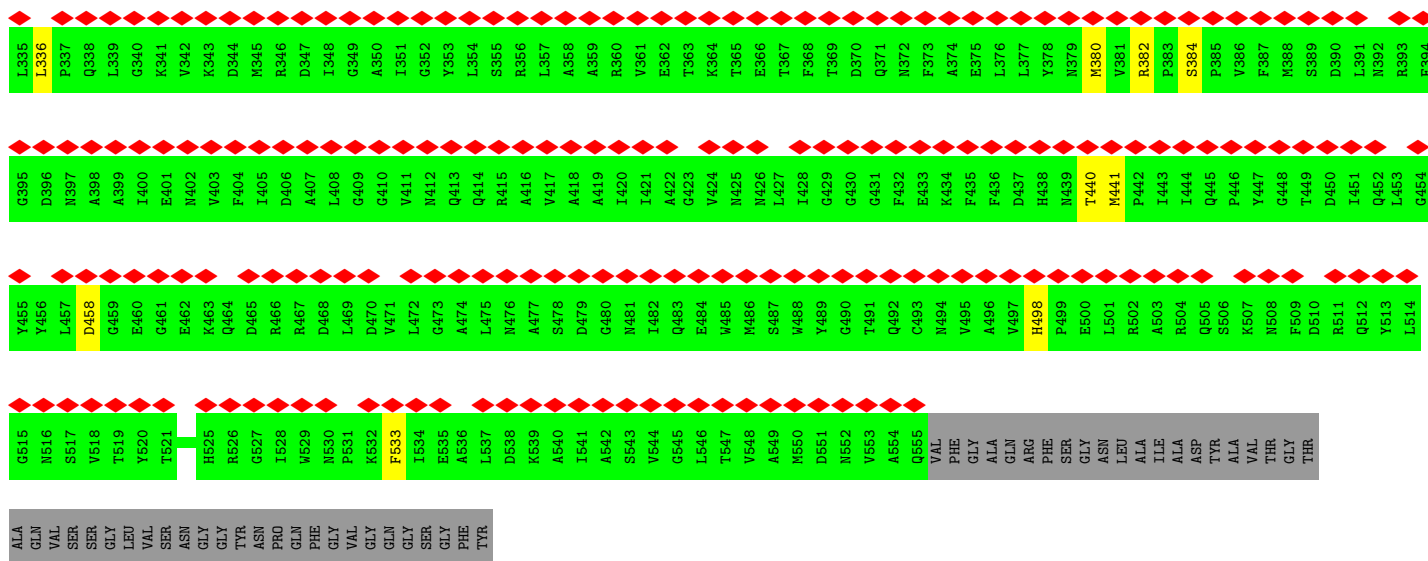




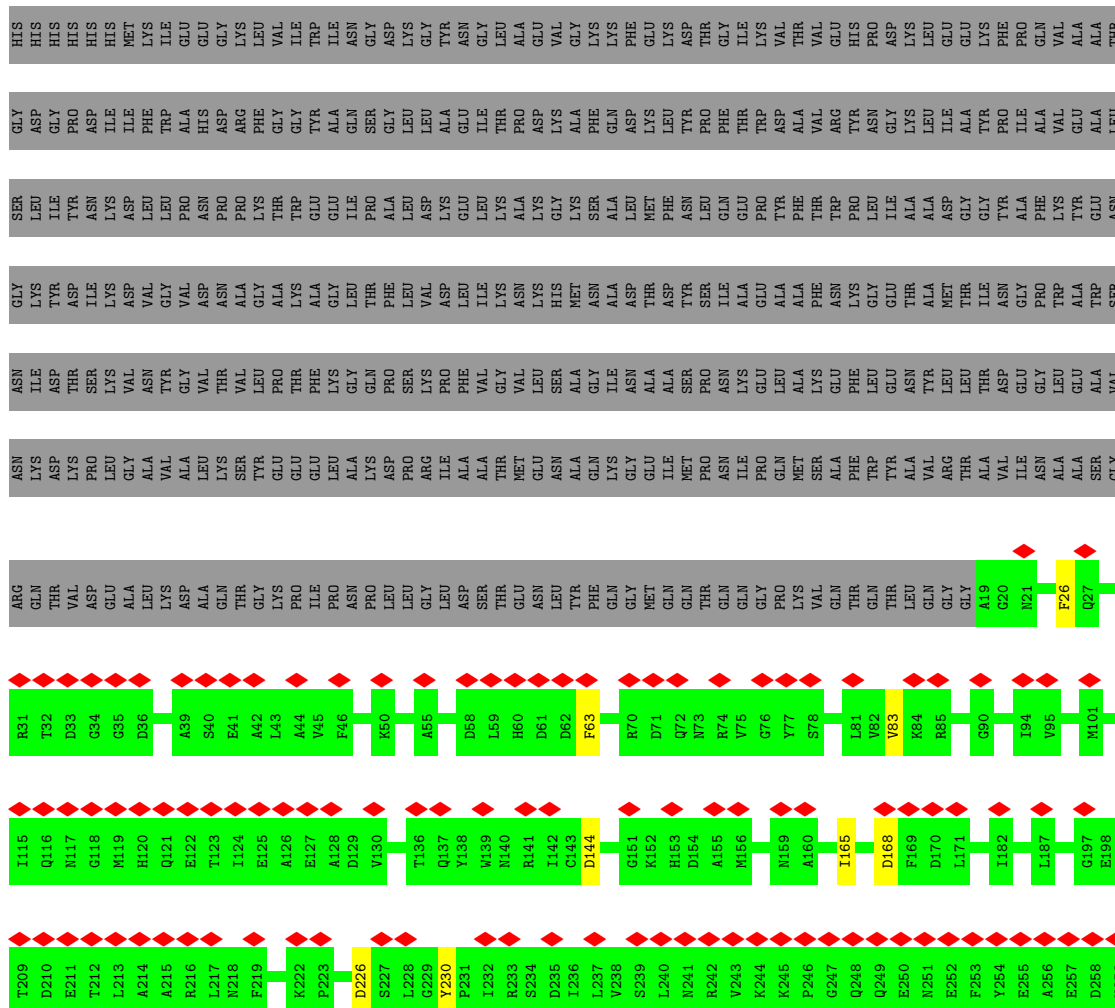


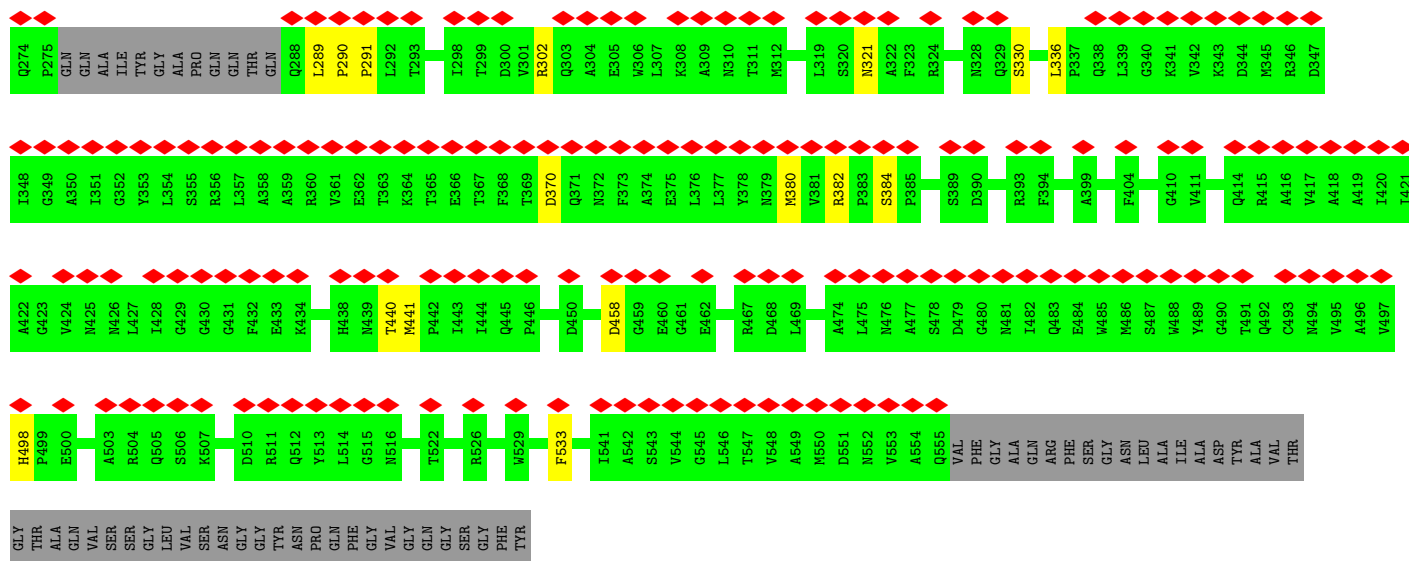
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN



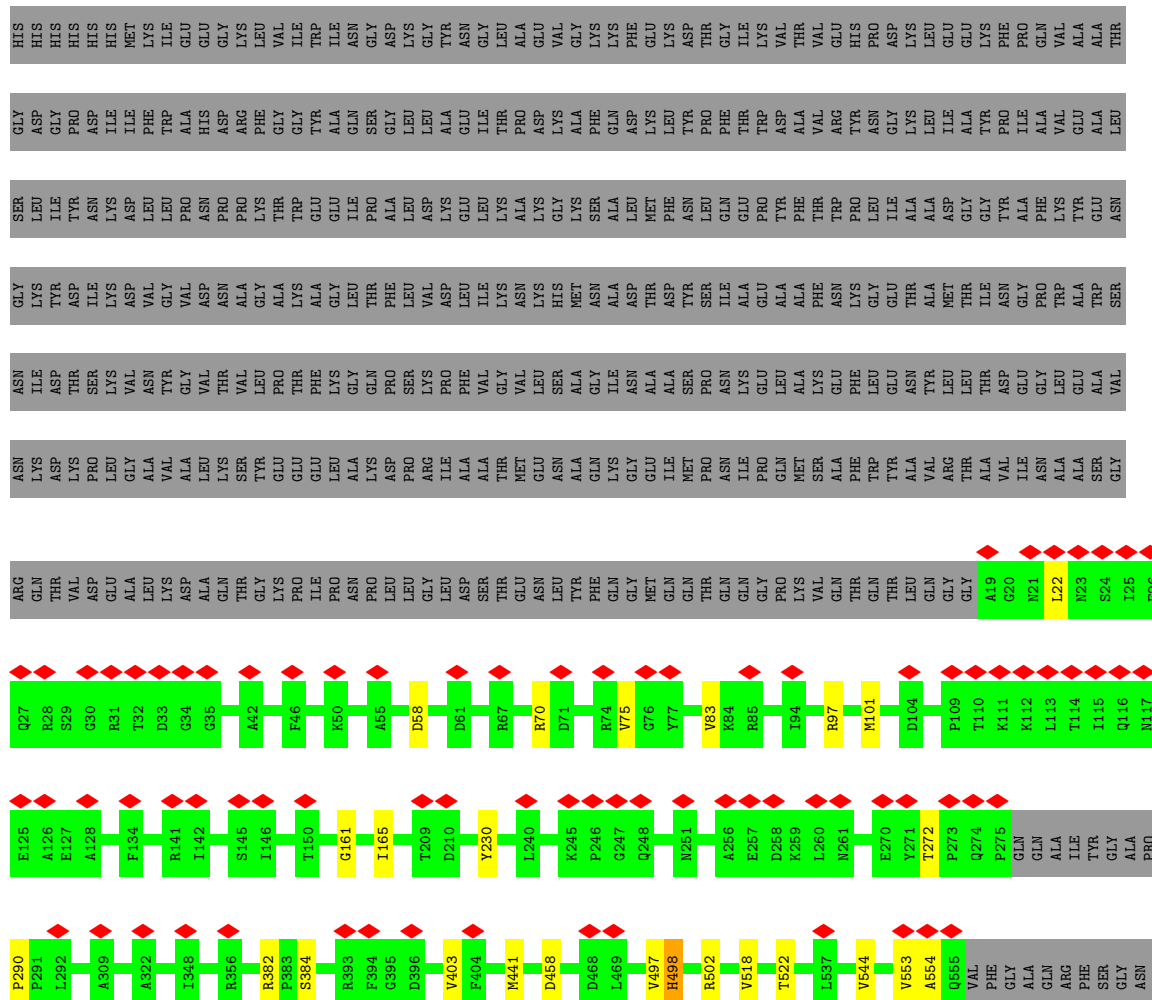


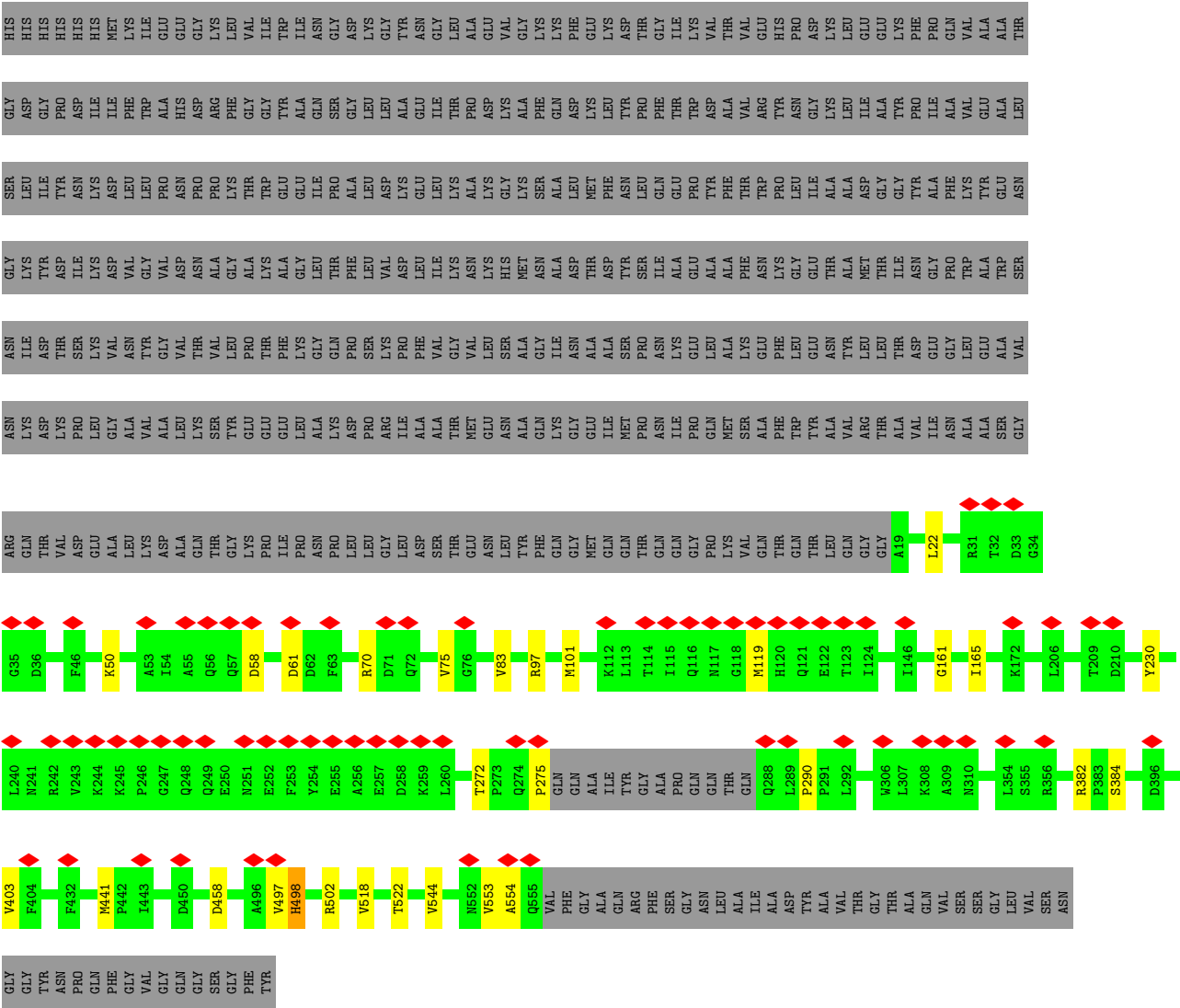
● Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN



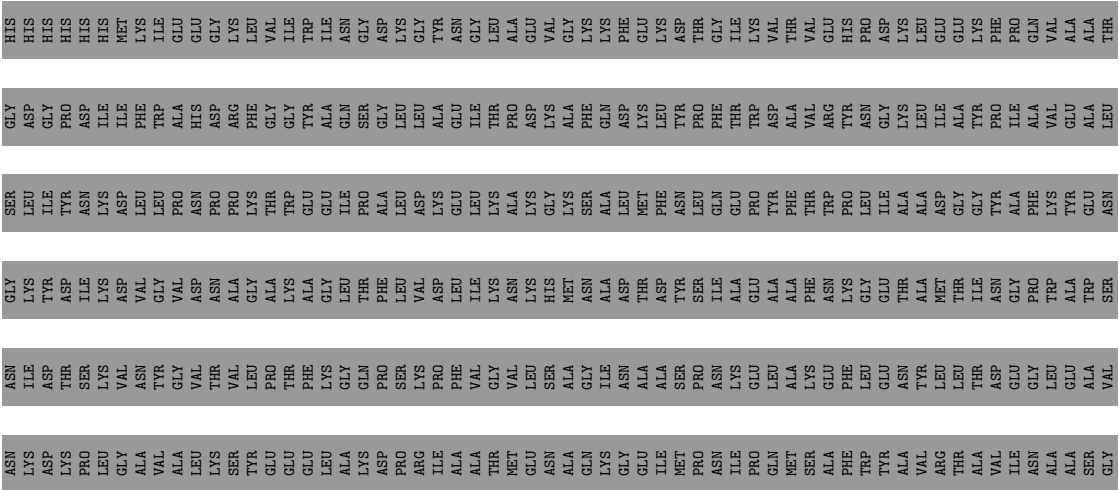


• Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN





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

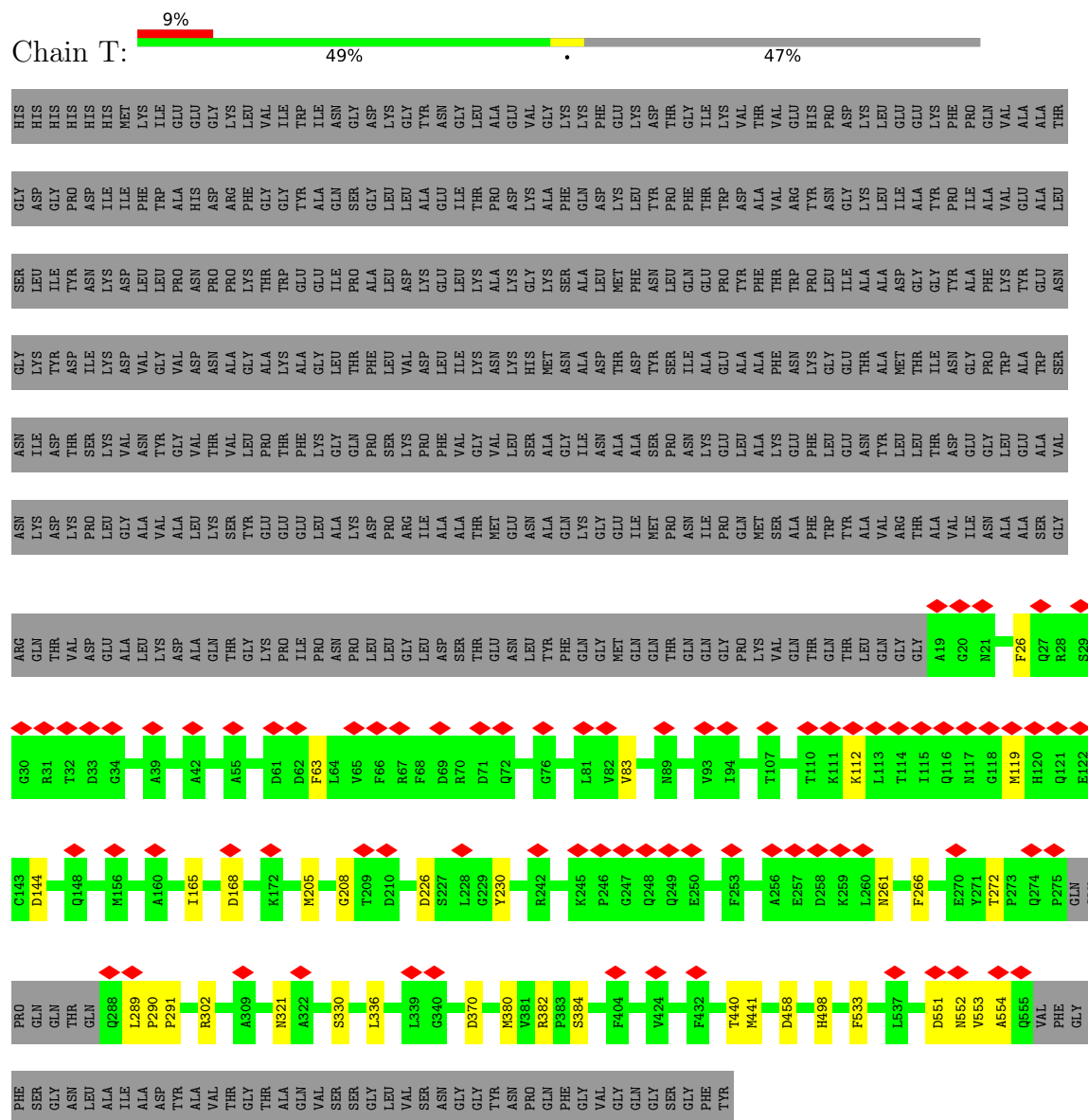




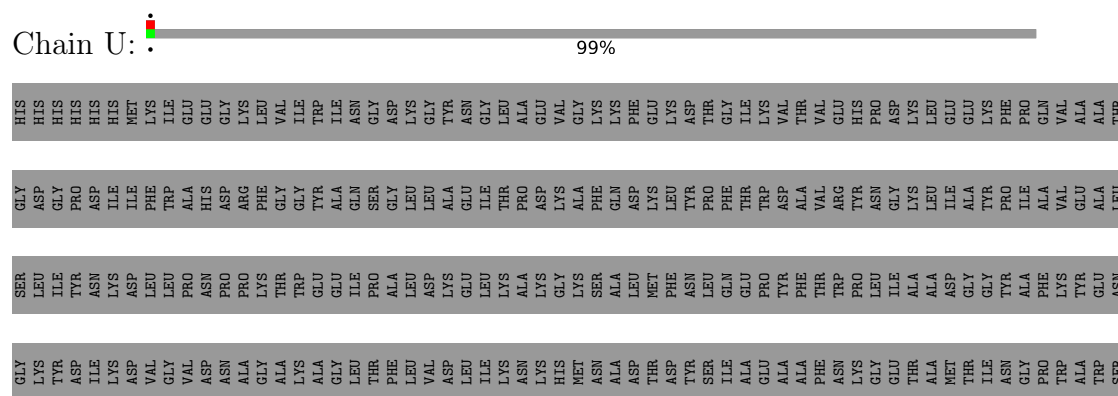


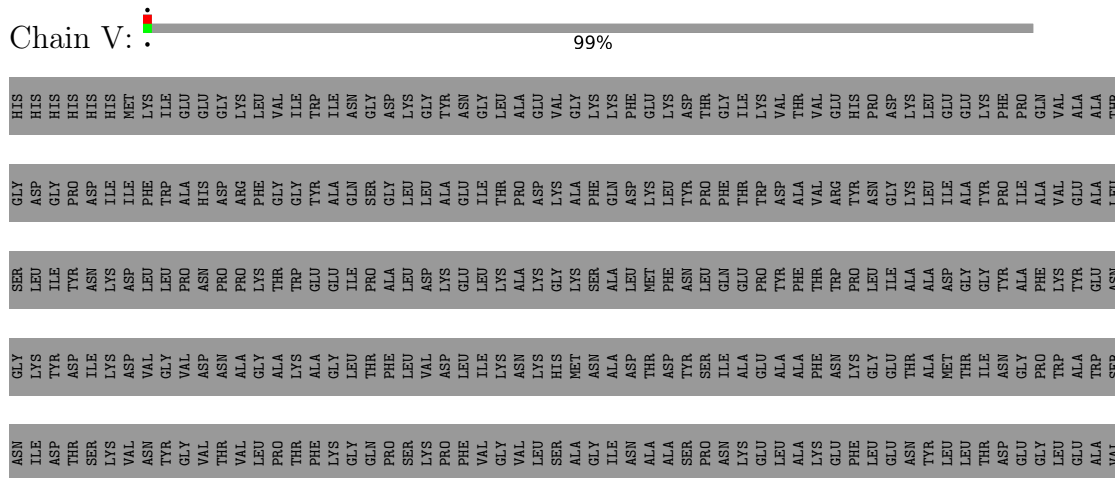


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, phiPA3 PhuN



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

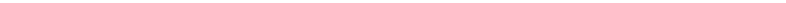






[illegible]

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

Chain b:  99%

[illegible]

[illegible]

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

[illegible]



LYS
ASN
PHE
ASP
ARG
GLN
TYR
LEU
GLY
ASN
SER
VAL
THR
TYR
THR
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
GLY
LEU
VAL
SER
ASN
GLY
GLY
TYR
ASN
P591
G594
Y595
G596
Y602

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	427.008, 427.008, 427.008	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.95	0/4203	1.33	39/5697 (0.7%)
1	B	0.93	1/4203 (0.0%)	1.27	36/5697 (0.6%)
1	C	0.92	0/4203	1.27	36/5697 (0.6%)
1	D	0.95	0/4203	1.33	39/5697 (0.7%)
1	E	0.85	0/91	1.25	1/120 (0.8%)
1	F	0.77	0/91	1.14	0/120
1	G	0.78	0/91	1.14	0/120
1	H	0.86	0/91	1.25	1/120 (0.8%)
1	I	0.95	0/4203	1.33	40/5697 (0.7%)
1	J	0.95	0/4203	1.33	39/5697 (0.7%)
1	K	0.95	0/4203	1.33	40/5697 (0.7%)
1	L	0.93	0/4203	1.27	36/5697 (0.6%)
1	M	0.93	0/4203	1.28	36/5697 (0.6%)
1	N	0.93	1/4203 (0.0%)	1.27	36/5697 (0.6%)
1	O	0.92	0/4203	1.27	36/5697 (0.6%)
1	P	0.92	0/4203	1.27	36/5697 (0.6%)
1	Q	0.92	0/4203	1.27	36/5697 (0.6%)
1	R	0.95	0/4203	1.33	40/5697 (0.7%)
1	S	0.95	0/4203	1.33	39/5697 (0.7%)
1	T	0.95	0/4203	1.33	40/5697 (0.7%)
1	U	0.86	0/91	1.25	1/120 (0.8%)
1	V	0.86	0/91	1.25	1/120 (0.8%)
1	W	0.86	0/91	1.25	1/120 (0.8%)
1	X	0.77	0/91	1.13	0/120
1	Y	0.78	0/91	1.13	0/120
1	Z	0.77	0/91	1.14	0/120
1	a	0.78	0/91	1.14	0/120
1	b	0.78	0/91	1.14	0/120
1	c	0.78	0/91	1.14	0/120
1	d	0.86	0/91	1.25	1/120 (0.8%)
1	e	0.85	0/91	1.25	1/120 (0.8%)
1	f	0.86	0/91	1.25	1/120 (0.8%)
All	All	0.93	2/68704 (0.0%)	1.30	612/93072 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	PRO	N-CD	5.01	1.54	1.47
1	N	275	PRO	N-CD	5.00	1.54	1.47

All (612) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	165	ILE	CA-C-N	8.58	128.64	119.89
1	I	165	ILE	C-N-CA	8.58	128.64	119.89
1	D	165	ILE	CA-C-N	8.54	128.60	119.89
1	D	165	ILE	C-N-CA	8.54	128.60	119.89
1	S	165	ILE	CA-C-N	8.53	128.59	119.89
1	S	165	ILE	C-N-CA	8.53	128.59	119.89
1	R	165	ILE	CA-C-N	8.53	128.59	119.89
1	R	165	ILE	C-N-CA	8.53	128.59	119.89
1	J	165	ILE	CA-C-N	8.52	128.58	119.89
1	J	165	ILE	C-N-CA	8.52	128.58	119.89
1	T	165	ILE	CA-C-N	8.51	128.57	119.89
1	T	165	ILE	C-N-CA	8.51	128.57	119.89
1	K	165	ILE	CA-C-N	8.50	128.56	119.89
1	K	165	ILE	C-N-CA	8.50	128.56	119.89
1	A	165	ILE	CA-C-N	8.49	128.55	119.89
1	A	165	ILE	C-N-CA	8.49	128.55	119.89
1	L	83	VAL	N-CA-C	8.44	120.27	108.12
1	O	83	VAL	N-CA-C	8.44	120.27	108.12
1	C	83	VAL	N-CA-C	8.41	120.23	108.12
1	Q	83	VAL	N-CA-C	8.41	120.23	108.12
1	N	83	VAL	N-CA-C	8.40	120.22	108.12
1	P	83	VAL	N-CA-C	8.40	120.21	108.12
1	M	83	VAL	N-CA-C	8.39	120.20	108.12
1	B	83	VAL	N-CA-C	8.38	120.19	108.12
1	M	165	ILE	CA-C-N	8.09	128.57	119.92
1	M	165	ILE	C-N-CA	8.09	128.57	119.92
1	C	165	ILE	CA-C-N	8.07	128.56	119.92
1	C	165	ILE	C-N-CA	8.07	128.56	119.92
1	B	165	ILE	CA-C-N	8.06	128.54	119.92
1	B	165	ILE	C-N-CA	8.06	128.54	119.92
1	L	165	ILE	CA-C-N	8.04	128.52	119.92
1	L	165	ILE	C-N-CA	8.04	128.52	119.92
1	N	165	ILE	CA-C-N	8.04	128.52	119.92
1	N	165	ILE	C-N-CA	8.04	128.52	119.92
1	P	165	ILE	CA-C-N	8.01	128.49	119.92
1	P	165	ILE	C-N-CA	8.01	128.49	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	165	ILE	CA-C-N	8.01	128.49	119.92
1	O	165	ILE	C-N-CA	8.01	128.49	119.92
1	Q	165	ILE	CA-C-N	7.99	128.47	119.92
1	Q	165	ILE	C-N-CA	7.99	128.47	119.92
1	S	290	PRO	CA-C-N	7.92	127.56	119.56
1	S	290	PRO	C-N-CA	7.92	127.56	119.56
1	R	290	PRO	CA-C-N	7.92	127.56	119.56
1	R	290	PRO	C-N-CA	7.92	127.56	119.56
1	J	290	PRO	CA-C-N	7.92	127.56	119.56
1	J	290	PRO	C-N-CA	7.92	127.56	119.56
1	T	290	PRO	CA-C-N	7.90	127.54	119.56
1	T	290	PRO	C-N-CA	7.90	127.54	119.56
1	I	290	PRO	CA-C-N	7.89	127.53	119.56
1	I	290	PRO	C-N-CA	7.89	127.53	119.56
1	K	290	PRO	CA-C-N	7.89	127.53	119.56
1	K	290	PRO	C-N-CA	7.89	127.53	119.56
1	D	290	PRO	CA-C-N	7.88	127.52	119.56
1	D	290	PRO	C-N-CA	7.88	127.52	119.56
1	A	290	PRO	CA-C-N	7.86	127.50	119.56
1	A	290	PRO	C-N-CA	7.86	127.50	119.56
1	S	440	THR	N-CA-C	-7.66	104.54	114.04
1	D	440	THR	N-CA-C	-7.65	104.56	114.04
1	J	440	THR	N-CA-C	-7.64	104.56	114.04
1	A	440	THR	N-CA-C	-7.62	104.59	114.04
1	R	440	THR	N-CA-C	-7.62	104.59	114.04
1	T	440	THR	N-CA-C	-7.62	104.59	114.04
1	I	440	THR	N-CA-C	-7.62	104.60	114.04
1	K	440	THR	N-CA-C	-7.60	104.61	114.04
1	I	208	GLY	N-CA-C	-7.32	103.17	112.54
1	R	208	GLY	N-CA-C	-7.31	103.18	112.54
1	J	208	GLY	N-CA-C	-7.31	103.18	112.54
1	K	208	GLY	N-CA-C	-7.31	103.19	112.54
1	D	208	GLY	N-CA-C	-7.29	103.20	112.54
1	A	208	GLY	N-CA-C	-7.29	103.21	112.54
1	S	208	GLY	N-CA-C	-7.29	103.22	112.54
1	T	208	GLY	N-CA-C	-7.26	103.24	112.54
1	T	291	PRO	N-CA-C	7.04	122.66	113.86
1	R	291	PRO	N-CA-C	7.03	122.64	113.86
1	D	291	PRO	N-CA-C	7.01	122.63	113.86
1	J	291	PRO	N-CA-C	7.00	122.61	113.86
1	K	291	PRO	N-CA-C	7.00	122.61	113.86
1	I	291	PRO	N-CA-C	7.00	122.60	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	PRO	N-CA-C	6.99	122.60	113.86
1	S	291	PRO	N-CA-C	6.99	122.59	113.86
1	K	168	ASP	N-CA-C	6.88	118.43	111.07
1	R	261	ASN	CA-CB-CG	6.87	119.47	112.60
1	S	261	ASN	CA-CB-CG	6.87	119.47	112.60
1	K	261	ASN	CA-CB-CG	6.87	119.47	112.60
1	T	261	ASN	CA-CB-CG	6.86	119.46	112.60
1	T	168	ASP	N-CA-C	6.86	118.41	111.07
1	I	261	ASN	CA-CB-CG	6.85	119.45	112.60
1	R	168	ASP	N-CA-C	6.84	118.39	111.07
1	D	261	ASN	CA-CB-CG	6.84	119.44	112.60
1	I	168	ASP	N-CA-C	6.84	118.39	111.07
1	S	168	ASP	N-CA-C	6.84	118.39	111.07
1	A	168	ASP	N-CA-C	6.84	118.38	111.07
1	J	168	ASP	N-CA-C	6.84	118.39	111.07
1	A	261	ASN	CA-CB-CG	6.82	119.42	112.60
1	J	261	ASN	CA-CB-CG	6.81	119.41	112.60
1	D	168	ASP	N-CA-C	6.79	118.33	111.07
1	M	522	THR	N-CA-C	6.77	117.52	108.38
1	O	522	THR	N-CA-C	6.75	117.50	108.38
1	B	522	THR	N-CA-C	6.74	117.48	108.38
1	P	522	THR	N-CA-C	6.73	117.46	108.38
1	Q	522	THR	N-CA-C	6.73	117.46	108.38
1	L	522	THR	N-CA-C	6.72	117.46	108.38
1	N	522	THR	N-CA-C	6.72	117.46	108.38
1	C	522	THR	N-CA-C	6.72	117.45	108.38
1	P	382	ARG	CA-C-N	6.71	126.33	119.56
1	P	382	ARG	C-N-CA	6.71	126.33	119.56
1	L	97	ARG	CA-C-N	6.70	126.62	119.85
1	L	97	ARG	C-N-CA	6.70	126.62	119.85
1	R	272	THR	CA-C-N	6.67	126.64	120.03
1	R	272	THR	C-N-CA	6.67	126.64	120.03
1	L	382	ARG	CA-C-N	6.67	126.30	119.56
1	L	382	ARG	C-N-CA	6.67	126.30	119.56
1	B	382	ARG	CA-C-N	6.67	126.29	119.56
1	B	382	ARG	C-N-CA	6.67	126.29	119.56
1	Q	97	ARG	CA-C-N	6.66	126.58	119.85
1	Q	97	ARG	C-N-CA	6.66	126.58	119.85
1	C	97	ARG	CA-C-N	6.66	126.57	119.85
1	C	97	ARG	C-N-CA	6.66	126.57	119.85
1	P	97	ARG	CA-C-N	6.65	126.57	119.85
1	P	97	ARG	C-N-CA	6.65	126.57	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	382	ARG	CA-C-N	6.65	126.27	119.56
1	N	382	ARG	C-N-CA	6.65	126.27	119.56
1	D	272	THR	CA-C-N	6.64	126.61	120.03
1	D	272	THR	C-N-CA	6.64	126.61	120.03
1	T	272	THR	CA-C-N	6.64	126.60	120.03
1	T	272	THR	C-N-CA	6.64	126.60	120.03
1	K	272	THR	CA-C-N	6.64	126.60	120.03
1	K	272	THR	C-N-CA	6.64	126.60	120.03
1	M	97	ARG	CA-C-N	6.64	126.55	119.85
1	M	97	ARG	C-N-CA	6.64	126.55	119.85
1	B	97	ARG	CA-C-N	6.63	126.55	119.85
1	B	97	ARG	C-N-CA	6.63	126.55	119.85
1	C	382	ARG	CA-C-N	6.63	126.26	119.56
1	C	382	ARG	C-N-CA	6.63	126.26	119.56
1	I	272	THR	CA-C-N	6.63	126.59	120.03
1	I	272	THR	C-N-CA	6.63	126.59	120.03
1	S	272	THR	CA-C-N	6.63	126.59	120.03
1	S	272	THR	C-N-CA	6.63	126.59	120.03
1	Q	382	ARG	CA-C-N	6.62	126.24	119.56
1	Q	382	ARG	C-N-CA	6.62	126.24	119.56
1	M	382	ARG	CA-C-N	6.61	126.24	119.56
1	M	382	ARG	C-N-CA	6.61	126.24	119.56
1	N	97	ARG	CA-C-N	6.61	126.53	119.85
1	N	97	ARG	C-N-CA	6.61	126.53	119.85
1	O	97	ARG	CA-C-N	6.61	126.53	119.85
1	O	97	ARG	C-N-CA	6.61	126.53	119.85
1	O	382	ARG	CA-C-N	6.61	126.24	119.56
1	O	382	ARG	C-N-CA	6.61	126.24	119.56
1	M	290	PRO	CA-C-N	6.60	126.29	119.56
1	M	290	PRO	C-N-CA	6.60	126.29	119.56
1	O	290	PRO	CA-C-N	6.60	126.29	119.56
1	O	290	PRO	C-N-CA	6.60	126.29	119.56
1	C	290	PRO	CA-C-N	6.59	126.28	119.56
1	C	290	PRO	C-N-CA	6.59	126.28	119.56
1	A	272	THR	CA-C-N	6.59	126.55	120.03
1	A	272	THR	C-N-CA	6.59	126.55	120.03
1	J	272	THR	CA-C-N	6.59	126.55	120.03
1	J	272	THR	C-N-CA	6.59	126.55	120.03
1	P	290	PRO	CA-C-N	6.58	126.28	119.56
1	P	290	PRO	C-N-CA	6.58	126.28	119.56
1	L	290	PRO	CA-C-N	6.57	126.26	119.56
1	L	290	PRO	C-N-CA	6.57	126.26	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	PRO	CA-C-N	6.56	126.25	119.56
1	B	290	PRO	C-N-CA	6.56	126.25	119.56
1	N	290	PRO	CA-C-N	6.55	126.24	119.56
1	N	290	PRO	C-N-CA	6.55	126.24	119.56
1	Q	290	PRO	CA-C-N	6.55	126.24	119.56
1	Q	290	PRO	C-N-CA	6.55	126.24	119.56
1	N	101	MET	CA-C-N	6.47	126.39	119.85
1	N	101	MET	C-N-CA	6.47	126.39	119.85
1	B	101	MET	CA-C-N	6.46	126.37	119.85
1	B	101	MET	C-N-CA	6.46	126.37	119.85
1	Q	441	MET	CA-C-N	6.45	126.36	119.85
1	Q	441	MET	C-N-CA	6.45	126.36	119.85
1	N	441	MET	CA-C-N	6.43	126.35	119.85
1	N	441	MET	C-N-CA	6.43	126.35	119.85
1	C	101	MET	CA-C-N	6.42	126.34	119.85
1	C	101	MET	C-N-CA	6.42	126.34	119.85
1	L	441	MET	CA-C-N	6.41	126.32	119.85
1	L	441	MET	C-N-CA	6.41	126.32	119.85
1	M	101	MET	CA-C-N	6.41	126.32	119.85
1	M	101	MET	C-N-CA	6.41	126.32	119.85
1	M	441	MET	CA-C-N	6.41	126.32	119.85
1	M	441	MET	C-N-CA	6.41	126.32	119.85
1	P	101	MET	CA-C-N	6.40	126.31	119.85
1	P	101	MET	C-N-CA	6.40	126.31	119.85
1	Q	101	MET	CA-C-N	6.40	126.31	119.85
1	Q	101	MET	C-N-CA	6.40	126.31	119.85
1	O	101	MET	CA-C-N	6.40	126.31	119.85
1	O	101	MET	C-N-CA	6.40	126.31	119.85
1	L	101	MET	CA-C-N	6.39	126.31	119.85
1	L	101	MET	C-N-CA	6.39	126.31	119.85
1	N	544	VAL	O-C-N	-6.39	115.95	123.04
1	C	441	MET	CA-C-N	6.38	126.30	119.85
1	C	441	MET	C-N-CA	6.38	126.30	119.85
1	O	441	MET	CA-C-N	6.36	126.27	119.85
1	O	441	MET	C-N-CA	6.36	126.27	119.85
1	P	553	VAL	CA-C-N	6.36	131.16	122.07
1	P	553	VAL	C-N-CA	6.36	131.16	122.07
1	B	441	MET	CA-C-N	6.35	126.27	119.85
1	B	441	MET	C-N-CA	6.35	126.27	119.85
1	P	441	MET	CA-C-N	6.35	126.26	119.85
1	P	441	MET	C-N-CA	6.35	126.26	119.85
1	B	544	VAL	O-C-N	-6.34	116.00	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	544	VAL	O-C-N	-6.33	116.01	123.04
1	P	544	VAL	O-C-N	-6.33	116.02	123.04
1	B	553	VAL	CA-C-N	6.32	131.11	122.07
1	B	553	VAL	C-N-CA	6.32	131.11	122.07
1	M	553	VAL	CA-C-N	6.32	131.10	122.07
1	M	553	VAL	C-N-CA	6.32	131.10	122.07
1	N	553	VAL	CA-C-N	6.32	131.10	122.07
1	N	553	VAL	C-N-CA	6.32	131.10	122.07
1	C	544	VAL	O-C-N	-6.31	116.03	123.04
1	O	553	VAL	CA-C-N	6.31	131.09	122.07
1	O	553	VAL	C-N-CA	6.31	131.09	122.07
1	Q	553	VAL	CA-C-N	6.31	131.09	122.07
1	Q	553	VAL	C-N-CA	6.31	131.09	122.07
1	L	544	VAL	O-C-N	-6.30	116.04	123.04
1	C	553	VAL	CA-C-N	6.30	131.08	122.07
1	C	553	VAL	C-N-CA	6.30	131.08	122.07
1	L	553	VAL	CA-C-N	6.29	131.07	122.07
1	L	553	VAL	C-N-CA	6.29	131.07	122.07
1	O	544	VAL	O-C-N	-6.29	116.06	123.04
1	M	544	VAL	O-C-N	-6.27	116.08	123.04
1	J	226	ASP	CA-CB-CG	6.19	118.79	112.60
1	T	226	ASP	CA-CB-CG	6.19	118.79	112.60
1	D	226	ASP	CA-CB-CG	6.18	118.78	112.60
1	R	226	ASP	CA-CB-CG	6.18	118.78	112.60
1	I	226	ASP	CA-CB-CG	6.17	118.78	112.60
1	A	226	ASP	CA-CB-CG	6.16	118.75	112.60
1	M	161	GLY	CA-C-N	6.14	126.33	120.31
1	M	161	GLY	C-N-CA	6.14	126.33	120.31
1	K	226	ASP	CA-CB-CG	6.14	118.74	112.60
1	N	161	GLY	CA-C-N	6.14	126.33	120.31
1	N	161	GLY	C-N-CA	6.14	126.33	120.31
1	C	522	THR	CA-C-N	6.13	132.19	122.62
1	C	522	THR	C-N-CA	6.13	132.19	122.62
1	B	522	THR	CA-C-N	6.13	132.18	122.62
1	B	522	THR	C-N-CA	6.13	132.18	122.62
1	O	161	GLY	CA-C-N	6.13	126.32	120.31
1	O	161	GLY	C-N-CA	6.13	126.32	120.31
1	S	226	ASP	CA-CB-CG	6.13	118.73	112.60
1	C	161	GLY	CA-C-N	6.12	126.31	120.31
1	C	161	GLY	C-N-CA	6.12	126.31	120.31
1	L	522	THR	CA-C-N	6.12	132.17	122.62
1	L	522	THR	C-N-CA	6.12	132.17	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	522	THR	CA-C-N	6.12	132.17	122.62
1	M	522	THR	C-N-CA	6.12	132.17	122.62
1	B	161	GLY	CA-C-N	6.12	126.31	120.31
1	B	161	GLY	C-N-CA	6.12	126.31	120.31
1	O	522	THR	CA-C-N	6.11	132.15	122.62
1	O	522	THR	C-N-CA	6.11	132.15	122.62
1	Q	522	THR	CA-C-N	6.11	132.15	122.62
1	Q	522	THR	C-N-CA	6.11	132.15	122.62
1	N	522	THR	CA-C-N	6.10	132.14	122.62
1	N	522	THR	C-N-CA	6.10	132.14	122.62
1	P	522	THR	CA-C-N	6.09	132.12	122.62
1	P	522	THR	C-N-CA	6.09	132.12	122.62
1	Q	384	SER	CA-C-N	6.09	126.28	120.31
1	Q	384	SER	C-N-CA	6.09	126.28	120.31
1	L	161	GLY	CA-C-N	6.07	126.25	120.31
1	L	161	GLY	C-N-CA	6.07	126.25	120.31
1	Q	161	GLY	CA-C-N	6.06	126.25	120.31
1	Q	161	GLY	C-N-CA	6.06	126.25	120.31
1	I	382	ARG	CA-C-N	6.05	125.67	119.56
1	I	382	ARG	C-N-CA	6.05	125.67	119.56
1	P	384	SER	CA-C-N	6.05	126.24	120.31
1	P	384	SER	C-N-CA	6.05	126.24	120.31
1	R	382	ARG	CA-C-N	6.05	125.67	119.56
1	R	382	ARG	C-N-CA	6.05	125.67	119.56
1	C	384	SER	CA-C-N	6.04	126.23	120.31
1	C	384	SER	C-N-CA	6.04	126.23	120.31
1	M	384	SER	CA-C-N	6.04	126.23	120.31
1	M	384	SER	C-N-CA	6.04	126.23	120.31
1	S	498	HIS	CA-C-N	6.04	125.72	119.56
1	S	498	HIS	C-N-CA	6.04	125.72	119.56
1	J	382	ARG	CA-C-N	6.04	125.66	119.56
1	J	382	ARG	C-N-CA	6.04	125.66	119.56
1	N	384	SER	CA-C-N	6.03	126.22	120.31
1	N	384	SER	C-N-CA	6.03	126.22	120.31
1	P	161	GLY	CA-C-N	6.03	126.22	120.31
1	P	161	GLY	C-N-CA	6.03	126.22	120.31
1	T	498	HIS	CA-C-N	6.03	125.71	119.56
1	T	498	HIS	C-N-CA	6.03	125.71	119.56
1	T	382	ARG	CA-C-N	6.02	125.64	119.56
1	T	382	ARG	C-N-CA	6.02	125.64	119.56
1	O	384	SER	CA-C-N	6.01	126.20	120.31
1	O	384	SER	C-N-CA	6.01	126.20	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	382	ARG	CA-C-N	6.01	125.63	119.56
1	K	382	ARG	C-N-CA	6.01	125.63	119.56
1	I	498	HIS	CA-C-N	6.01	125.69	119.56
1	I	498	HIS	C-N-CA	6.01	125.69	119.56
1	J	498	HIS	CA-C-N	6.01	125.69	119.56
1	J	498	HIS	C-N-CA	6.01	125.69	119.56
1	K	498	HIS	CA-C-N	6.01	125.69	119.56
1	K	498	HIS	C-N-CA	6.01	125.69	119.56
1	A	382	ARG	CA-C-N	6.00	125.62	119.56
1	A	382	ARG	C-N-CA	6.00	125.62	119.56
1	A	498	HIS	CA-C-N	6.00	125.67	119.56
1	A	498	HIS	C-N-CA	6.00	125.67	119.56
1	D	498	HIS	CA-C-N	6.00	125.67	119.56
1	D	498	HIS	C-N-CA	6.00	125.67	119.56
1	S	382	ARG	CA-C-N	5.99	125.61	119.56
1	S	382	ARG	C-N-CA	5.99	125.61	119.56
1	L	384	SER	CA-C-N	5.99	126.18	120.31
1	L	384	SER	C-N-CA	5.99	126.18	120.31
1	B	458	ASP	CA-CB-CG	5.98	118.58	112.60
1	B	272	THR	CA-C-N	5.98	125.94	119.78
1	B	272	THR	C-N-CA	5.98	125.94	119.78
1	P	272	THR	CA-C-N	5.98	125.94	119.78
1	P	272	THR	C-N-CA	5.98	125.94	119.78
1	B	384	SER	CA-C-N	5.97	126.17	120.31
1	B	384	SER	C-N-CA	5.97	126.17	120.31
1	R	498	HIS	CA-C-N	5.97	125.66	119.56
1	R	498	HIS	C-N-CA	5.97	125.66	119.56
1	M	58	ASP	N-CA-C	-5.97	105.08	112.90
1	Q	272	THR	CA-C-N	5.97	125.93	119.78
1	Q	272	THR	C-N-CA	5.97	125.93	119.78
1	D	382	ARG	CA-C-N	5.97	125.59	119.56
1	D	382	ARG	C-N-CA	5.97	125.59	119.56
1	C	272	THR	CA-C-N	5.96	125.92	119.78
1	C	272	THR	C-N-CA	5.96	125.92	119.78
1	M	272	THR	CA-C-N	5.96	125.92	119.78
1	M	272	THR	C-N-CA	5.96	125.92	119.78
1	R	266	PHE	CA-C-N	-5.96	115.17	123.10
1	R	266	PHE	C-N-CA	-5.96	115.17	123.10
1	B	58	ASP	N-CA-C	-5.96	105.10	112.90
1	P	458	ASP	CA-CB-CG	5.96	118.56	112.60
1	L	58	ASP	N-CA-C	-5.95	105.10	112.90
1	P	58	ASP	N-CA-C	-5.95	105.10	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	266	PHE	CA-C-N	-5.94	115.19	123.10
1	T	266	PHE	C-N-CA	-5.94	115.19	123.10
1	L	272	THR	CA-C-N	5.94	125.90	119.78
1	L	272	THR	C-N-CA	5.94	125.90	119.78
1	A	266	PHE	CA-C-N	-5.94	115.20	123.10
1	A	266	PHE	C-N-CA	-5.94	115.20	123.10
1	Q	58	ASP	N-CA-C	-5.94	105.12	112.90
1	N	58	ASP	N-CA-C	-5.94	105.12	112.90
1	S	266	PHE	CA-C-N	-5.93	115.21	123.10
1	S	266	PHE	C-N-CA	-5.93	115.21	123.10
1	D	266	PHE	CA-C-N	-5.93	115.21	123.10
1	D	266	PHE	C-N-CA	-5.93	115.21	123.10
1	N	272	THR	CA-C-N	5.93	125.89	119.78
1	N	272	THR	C-N-CA	5.93	125.89	119.78
1	C	458	ASP	CA-CB-CG	5.93	118.53	112.60
1	N	458	ASP	CA-CB-CG	5.93	118.53	112.60
1	C	58	ASP	N-CA-C	-5.93	105.14	112.90
1	O	58	ASP	N-CA-C	-5.93	105.14	112.90
1	Q	458	ASP	CA-CB-CG	5.93	118.53	112.60
1	K	266	PHE	CA-C-N	-5.92	115.23	123.10
1	K	266	PHE	C-N-CA	-5.92	115.23	123.10
1	O	458	ASP	CA-CB-CG	5.92	118.52	112.60
1	L	458	ASP	CA-CB-CG	5.92	118.52	112.60
1	M	458	ASP	CA-CB-CG	5.91	118.51	112.60
1	O	272	THR	CA-C-N	5.90	125.86	119.78
1	O	272	THR	C-N-CA	5.90	125.86	119.78
1	A	384	SER	CA-C-N	5.89	125.80	119.85
1	A	384	SER	C-N-CA	5.89	125.80	119.85
1	I	266	PHE	CA-C-N	-5.89	115.27	123.10
1	I	266	PHE	C-N-CA	-5.89	115.27	123.10
1	K	83	VAL	N-CA-C	5.89	116.35	108.11
1	J	266	PHE	CA-C-N	-5.88	115.28	123.10
1	J	266	PHE	C-N-CA	-5.88	115.28	123.10
1	J	83	VAL	N-CA-C	5.88	116.34	108.11
1	T	83	VAL	N-CA-C	5.88	116.34	108.11
1	A	83	VAL	N-CA-C	5.87	116.33	108.11
1	D	83	VAL	N-CA-C	5.87	116.33	108.11
1	J	384	SER	CA-C-N	5.87	125.78	119.85
1	J	384	SER	C-N-CA	5.87	125.78	119.85
1	T	384	SER	CA-C-N	5.87	125.78	119.85
1	T	384	SER	C-N-CA	5.87	125.78	119.85
1	S	83	VAL	N-CA-C	5.87	116.32	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	384	SER	CA-C-N	5.86	125.77	119.85
1	R	384	SER	C-N-CA	5.86	125.77	119.85
1	R	83	VAL	N-CA-C	5.86	116.31	108.11
1	K	384	SER	CA-C-N	5.83	125.74	119.85
1	K	384	SER	C-N-CA	5.83	125.74	119.85
1	S	384	SER	CA-C-N	5.83	125.74	119.85
1	S	384	SER	C-N-CA	5.83	125.74	119.85
1	I	83	VAL	N-CA-C	5.83	116.28	108.11
1	D	384	SER	CA-C-N	5.83	125.74	119.85
1	D	384	SER	C-N-CA	5.83	125.74	119.85
1	I	384	SER	CA-C-N	5.82	125.73	119.85
1	I	384	SER	C-N-CA	5.82	125.73	119.85
1	N	290	PRO	N-CA-C	-5.69	103.76	110.70
1	Q	290	PRO	N-CA-C	-5.65	103.80	110.70
1	C	290	PRO	N-CA-C	-5.65	103.81	110.70
1	L	290	PRO	N-CA-C	-5.65	103.81	110.70
1	J	380	MET	N-CA-C	5.65	120.30	113.41
1	M	290	PRO	N-CA-C	-5.64	103.81	110.70
1	B	290	PRO	N-CA-C	-5.64	103.82	110.70
1	R	380	MET	N-CA-C	5.64	120.29	113.41
1	K	380	MET	N-CA-C	5.64	120.29	113.41
1	Q	403	VAL	N-CA-C	-5.64	104.86	111.00
1	P	290	PRO	N-CA-C	-5.63	103.83	110.70
1	A	380	MET	N-CA-C	5.63	120.28	113.41
1	C	403	VAL	N-CA-C	-5.63	104.87	111.00
1	O	290	PRO	N-CA-C	-5.62	103.84	110.70
1	O	403	VAL	N-CA-C	-5.62	104.87	111.00
1	I	380	MET	N-CA-C	5.62	120.27	113.41
1	M	403	VAL	N-CA-C	-5.62	104.88	111.00
1	B	403	VAL	N-CA-C	-5.62	104.88	111.00
1	D	380	MET	N-CA-C	5.61	120.26	113.41
1	T	380	MET	N-CA-C	5.61	120.26	113.41
1	P	403	VAL	N-CA-C	-5.61	104.89	111.00
1	N	403	VAL	N-CA-C	-5.61	104.89	111.00
1	L	403	VAL	N-CA-C	-5.61	104.89	111.00
1	S	380	MET	N-CA-C	5.61	120.25	113.41
1	Q	498	HIS	CA-C-N	5.54	125.21	119.56
1	Q	498	HIS	C-N-CA	5.54	125.21	119.56
1	N	498	HIS	CA-C-N	5.53	125.20	119.56
1	N	498	HIS	C-N-CA	5.53	125.20	119.56
1	C	498	HIS	CA-C-N	5.52	125.19	119.56
1	C	498	HIS	C-N-CA	5.52	125.19	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	498	HIS	CA-C-N	5.51	125.18	119.56
1	P	498	HIS	C-N-CA	5.51	125.18	119.56
1	B	498	HIS	CA-C-N	5.50	125.17	119.56
1	B	498	HIS	C-N-CA	5.50	125.17	119.56
1	M	498	HIS	CA-C-N	5.50	125.17	119.56
1	M	498	HIS	C-N-CA	5.50	125.17	119.56
1	L	498	HIS	CA-C-N	5.50	125.17	119.56
1	L	498	HIS	C-N-CA	5.50	125.17	119.56
1	A	321	ASN	CA-CB-CG	5.49	118.09	112.60
1	J	321	ASN	CA-CB-CG	5.49	118.09	112.60
1	K	321	ASN	CA-CB-CG	5.47	118.07	112.60
1	O	498	HIS	CA-C-N	5.47	125.14	119.56
1	O	498	HIS	C-N-CA	5.47	125.14	119.56
1	T	321	ASN	CA-CB-CG	5.46	118.06	112.60
1	I	533	PHE	N-CA-C	-5.45	105.42	111.36
1	B	518	VAL	CA-C-N	5.45	131.35	123.13
1	B	518	VAL	C-N-CA	5.45	131.35	123.13
1	R	321	ASN	CA-CB-CG	5.45	118.05	112.60
1	T	533	PHE	N-CA-C	-5.45	105.42	111.36
1	A	533	PHE	N-CA-C	-5.44	105.43	111.36
1	R	533	PHE	N-CA-C	-5.44	105.43	111.36
1	M	518	VAL	CA-C-N	5.44	131.34	123.13
1	M	518	VAL	C-N-CA	5.44	131.34	123.13
1	L	518	VAL	CA-C-N	5.43	131.33	123.13
1	L	518	VAL	C-N-CA	5.43	131.33	123.13
1	D	321	ASN	CA-CB-CG	5.43	118.03	112.60
1	S	321	ASN	CA-CB-CG	5.43	118.03	112.60
1	J	533	PHE	N-CA-C	-5.43	105.44	111.36
1	N	230	TYR	CA-C-N	5.43	125.33	119.85
1	N	230	TYR	C-N-CA	5.43	125.33	119.85
1	I	321	ASN	CA-CB-CG	5.42	118.03	112.60
1	P	518	VAL	CA-C-N	5.42	131.32	123.13
1	P	518	VAL	C-N-CA	5.42	131.32	123.13
1	D	533	PHE	N-CA-C	-5.42	105.45	111.36
1	N	518	VAL	CA-C-N	5.42	131.31	123.13
1	N	518	VAL	C-N-CA	5.42	131.31	123.13
1	O	518	VAL	CA-C-N	5.41	131.30	123.13
1	O	518	VAL	C-N-CA	5.41	131.30	123.13
1	S	533	PHE	N-CA-C	-5.41	105.47	111.36
1	T	289	LEU	CA-C-N	5.41	125.95	120.38
1	T	289	LEU	C-N-CA	5.41	125.95	120.38
1	L	230	TYR	CA-C-N	5.41	125.31	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	230	TYR	C-N-CA	5.41	125.31	119.85
1	M	230	TYR	CA-C-N	5.41	125.31	119.85
1	M	230	TYR	C-N-CA	5.41	125.31	119.85
1	I	330	SER	CA-C-N	5.40	129.24	120.60
1	I	330	SER	C-N-CA	5.40	129.24	120.60
1	K	330	SER	CA-C-N	5.40	129.24	120.60
1	K	330	SER	C-N-CA	5.40	129.24	120.60
1	K	533	PHE	N-CA-C	-5.40	105.47	111.36
1	T	330	SER	CA-C-N	5.40	129.24	120.60
1	T	330	SER	C-N-CA	5.40	129.24	120.60
1	C	518	VAL	CA-C-N	5.40	131.28	123.13
1	C	518	VAL	C-N-CA	5.40	131.28	123.13
1	R	289	LEU	CA-C-N	5.39	125.94	120.38
1	R	289	LEU	C-N-CA	5.39	125.94	120.38
1	A	330	SER	CA-C-N	5.39	129.23	120.60
1	A	330	SER	C-N-CA	5.39	129.23	120.60
1	Q	518	VAL	CA-C-N	5.38	131.26	123.13
1	Q	518	VAL	C-N-CA	5.38	131.26	123.13
1	T	441	MET	CA-C-N	5.38	125.32	119.78
1	T	441	MET	C-N-CA	5.38	125.32	119.78
1	B	230	TYR	CA-C-N	5.38	125.28	119.85
1	B	230	TYR	C-N-CA	5.38	125.28	119.85
1	D	289	LEU	CA-C-N	5.38	125.92	120.38
1	D	289	LEU	C-N-CA	5.38	125.92	120.38
1	I	289	LEU	CA-C-N	5.37	125.91	120.38
1	I	289	LEU	C-N-CA	5.37	125.91	120.38
1	R	144	ASP	CA-CB-CG	5.37	117.97	112.60
1	R	330	SER	CA-C-N	5.37	129.20	120.60
1	R	330	SER	C-N-CA	5.37	129.20	120.60
1	K	289	LEU	CA-C-N	5.37	125.91	120.38
1	K	289	LEU	C-N-CA	5.37	125.91	120.38
1	A	144	ASP	CA-CB-CG	5.37	117.97	112.60
1	S	330	SER	CA-C-N	5.37	129.19	120.60
1	S	330	SER	C-N-CA	5.37	129.19	120.60
1	O	554	ALA	N-CA-C	5.37	118.84	111.54
1	S	289	LEU	CA-C-N	5.37	125.91	120.38
1	S	289	LEU	C-N-CA	5.37	125.91	120.38
1	T	144	ASP	CA-CB-CG	5.36	117.96	112.60
1	M	554	ALA	N-CA-C	5.36	118.83	111.54
1	J	330	SER	CA-C-N	5.36	129.18	120.60
1	J	330	SER	C-N-CA	5.36	129.18	120.60
1	K	26	PHE	CA-CB-CG	5.36	119.16	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	230	TYR	CA-C-N	5.36	125.27	119.85
1	P	230	TYR	C-N-CA	5.36	125.27	119.85
1	S	441	MET	CA-C-N	5.36	125.30	119.78
1	S	441	MET	C-N-CA	5.36	125.30	119.78
1	R	441	MET	CA-C-N	5.36	125.30	119.78
1	R	441	MET	C-N-CA	5.36	125.30	119.78
1	D	330	SER	CA-C-N	5.36	129.17	120.60
1	D	330	SER	C-N-CA	5.36	129.17	120.60
1	D	144	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	289	LEU	CA-C-N	5.35	125.89	120.38
1	A	289	LEU	C-N-CA	5.35	125.89	120.38
1	S	144	ASP	CA-CB-CG	5.35	117.95	112.60
1	C	230	TYR	CA-C-N	5.35	125.25	119.85
1	C	230	TYR	C-N-CA	5.35	125.25	119.85
1	I	441	MET	CA-C-N	5.35	125.29	119.78
1	I	441	MET	C-N-CA	5.35	125.29	119.78
1	O	230	TYR	CA-C-N	5.35	125.25	119.85
1	O	230	TYR	C-N-CA	5.35	125.25	119.85
1	I	144	ASP	CA-CB-CG	5.34	117.94	112.60
1	L	554	ALA	N-CA-C	5.34	118.81	111.54
1	D	441	MET	CA-C-N	5.34	125.28	119.78
1	D	441	MET	C-N-CA	5.34	125.28	119.78
1	P	554	ALA	N-CA-C	5.34	118.80	111.54
1	B	554	ALA	N-CA-C	5.34	118.80	111.54
1	Q	554	ALA	N-CA-C	5.34	118.80	111.54
1	A	441	MET	CA-C-N	5.34	125.28	119.78
1	A	441	MET	C-N-CA	5.34	125.28	119.78
1	C	554	ALA	N-CA-C	5.33	118.79	111.54
1	J	289	LEU	CA-C-N	5.33	125.87	120.38
1	J	289	LEU	C-N-CA	5.33	125.87	120.38
1	J	144	ASP	CA-CB-CG	5.33	117.93	112.60
1	S	26	PHE	CA-CB-CG	5.33	119.13	113.80
1	R	26	PHE	CA-CB-CG	5.33	119.13	113.80
1	Q	230	TYR	CA-C-N	5.32	125.23	119.85
1	Q	230	TYR	C-N-CA	5.32	125.23	119.85
1	I	26	PHE	CA-CB-CG	5.32	119.12	113.80
1	N	554	ALA	N-CA-C	5.32	118.78	111.54
1	A	26	PHE	CA-CB-CG	5.32	119.12	113.80
1	T	26	PHE	CA-CB-CG	5.32	119.12	113.80
1	K	144	ASP	CA-CB-CG	5.31	117.91	112.60
1	J	441	MET	CA-C-N	5.30	125.24	119.78
1	J	441	MET	C-N-CA	5.30	125.24	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	26	PHE	CA-CB-CG	5.30	119.10	113.80
1	K	441	MET	CA-C-N	5.30	125.24	119.78
1	K	441	MET	C-N-CA	5.30	125.24	119.78
1	D	63	PHE	N-CA-C	5.29	115.53	108.38
1	T	63	PHE	N-CA-C	5.29	115.52	108.38
1	R	63	PHE	N-CA-C	5.28	115.51	108.38
1	S	63	PHE	N-CA-C	5.28	115.50	108.38
1	D	26	PHE	CA-CB-CG	5.27	119.07	113.80
1	K	63	PHE	N-CA-C	5.26	115.49	108.38
1	J	63	PHE	N-CA-C	5.25	115.47	108.38
1	I	63	PHE	N-CA-C	5.25	115.47	108.38
1	A	63	PHE	N-CA-C	5.25	115.46	108.38
1	R	302	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	T	302	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	K	302	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	D	302	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	J	458	ASP	CA-CB-CG	5.21	117.81	112.60
1	J	302	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	I	302	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	A	302	ARG	NE-CZ-NH2	5.18	123.87	119.20
1	S	302	ARG	NE-CZ-NH2	5.18	123.87	119.20
1	K	230	TYR	CA-C-N	5.17	125.07	119.85
1	K	230	TYR	C-N-CA	5.17	125.07	119.85
1	K	458	ASP	CA-CB-CG	5.17	117.77	112.60
1	T	458	ASP	CA-CB-CG	5.15	117.75	112.60
1	I	458	ASP	CA-CB-CG	5.15	117.75	112.60
1	T	230	TYR	CA-C-N	5.15	125.05	119.85
1	T	230	TYR	C-N-CA	5.15	125.05	119.85
1	S	458	ASP	CA-CB-CG	5.14	117.74	112.60
1	D	458	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	230	TYR	CA-C-N	5.13	125.03	119.85
1	A	230	TYR	C-N-CA	5.13	125.03	119.85
1	R	458	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	458	ASP	CA-CB-CG	5.12	117.72	112.60
1	S	230	TYR	CA-C-N	5.12	125.02	119.85
1	S	230	TYR	C-N-CA	5.12	125.02	119.85
1	W	594	GLY	N-CA-C	-5.11	105.77	112.82
1	R	230	TYR	CA-C-N	5.10	125.00	119.85
1	R	230	TYR	C-N-CA	5.10	125.00	119.85
1	I	230	TYR	CA-C-N	5.10	125.00	119.85
1	I	230	TYR	C-N-CA	5.10	125.00	119.85
1	E	594	GLY	N-CA-C	-5.09	105.79	112.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	230	TYR	CA-C-N	5.09	125.00	119.85
1	J	230	TYR	C-N-CA	5.09	125.00	119.85
1	V	594	GLY	N-CA-C	-5.09	105.80	112.82
1	A	336	LEU	CA-C-N	5.09	124.99	119.85
1	A	336	LEU	C-N-CA	5.09	124.99	119.85
1	S	336	LEU	CA-C-N	5.08	124.99	119.85
1	S	336	LEU	C-N-CA	5.08	124.99	119.85
1	e	594	GLY	N-CA-C	-5.08	105.81	112.82
1	f	594	GLY	N-CA-C	-5.08	105.81	112.82
1	D	230	TYR	CA-C-N	5.07	124.97	119.85
1	D	230	TYR	C-N-CA	5.07	124.97	119.85
1	U	594	GLY	N-CA-C	-5.07	105.82	112.82
1	I	336	LEU	CA-C-N	5.07	124.97	119.85
1	I	336	LEU	C-N-CA	5.07	124.97	119.85
1	d	594	GLY	N-CA-C	-5.06	105.83	112.82
1	T	336	LEU	CA-C-N	5.06	124.96	119.85
1	T	336	LEU	C-N-CA	5.06	124.96	119.85
1	H	594	GLY	N-CA-C	-5.05	105.84	112.82
1	R	336	LEU	CA-C-N	5.04	124.95	119.85
1	R	336	LEU	C-N-CA	5.04	124.95	119.85
1	K	336	LEU	CA-C-N	5.04	124.94	119.85
1	K	336	LEU	C-N-CA	5.04	124.94	119.85
1	J	336	LEU	CA-C-N	5.03	124.93	119.85
1	J	336	LEU	C-N-CA	5.03	124.93	119.85
1	D	336	LEU	CA-C-N	5.03	124.93	119.85
1	D	336	LEU	C-N-CA	5.03	124.93	119.85
1	R	470	ASP	CA-CB-CG	5.02	117.62	112.60
1	I	370	ASP	CA-CB-CG	5.01	117.61	112.60
1	T	370	ASP	CA-CB-CG	5.01	117.61	112.60
1	K	370	ASP	CA-CB-CG	5.01	117.61	112.60

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	4	0
1	B	4128	4085	4083	5	0
1	C	4128	4085	4083	13	0
1	D	4128	4085	4083	11	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	16	0
1	J	4128	4085	4083	13	0
1	K	4128	4085	4083	1	0
1	L	4128	4085	4083	4	0
1	M	4128	4085	4083	9	0
1	N	4128	4085	4083	8	0
1	O	4128	4085	4083	10	0
1	P	4128	4085	4083	6	0
1	Q	4128	4085	4083	4	0
1	R	4128	4085	4083	1	0
1	S	4128	4085	4083	7	0
1	T	4128	4085	4083	22	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	81	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 (81) 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:J:119:MET:HE3	1:T:112:LYS:CE	1.58	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:MET:CE	1:T:551:ASP:O	1.80	1.29
1:J:112:LYS:CE	1:T:119:MET:HE3	1.74	1.17
1:J:112:LYS:HE3	1:T:119:MET:HE3	1.20	1.15
1:O:119:MET:SD	1:S:552:ASN:CA	2.34	1.14
1:J:119:MET:HE3	1:T:112:LYS:HE3	1.18	1.11
1:C:119:MET:HE1	1:T:551:ASP:C	1.80	1.07
1:C:119:MET:SD	1:T:552:ASN:HA	1.95	1.06
1:D:112:LYS:HE3	1:I:119:MET:HE3	1.37	1.05
1:C:119:MET:HE1	1:T:551:ASP:O	0.86	1.04
1:O:118:GLY:HA2	1:S:554:ALA:HB3	1.37	1.03
1:D:112:LYS:CE	1:I:119:MET:HE3	1.90	1.01
1:D:119:MET:HE3	1:I:112:LYS:HE3	1.40	1.01
1:J:119:MET:CE	1:T:112:LYS:CE	2.40	0.98
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:O:119:MET:SD	1:S:552:ASN:C	2.51	0.94
1:A:551:ASP:O	1:N:119:MET:HE1	1.67	0.93
1:J:119:MET:HE3	1:T:112:LYS:HE2	1.49	0.92
1:J:119:MET:CE	1:T:112:LYS:HE3	1.99	0.91
1:O:119:MET:CE	1:S:552:ASN:HA	2.00	0.89
1:J:119:MET:CE	1:T:112:LYS:HE2	2.02	0.89
1:I:551:ASP:O	1:M:119:MET:HE1	1.73	0.86
1:D:119:MET:HE3	1:I:112:LYS:CE	2.04	0.86
1:I:552:ASN:HA	1:M:119:MET:SD	2.21	0.81
1:J:112:LYS:HE2	1:T:119:MET:HE3	1.62	0.79
1:N:22:LEU:HD23	1:T:205:MET:HE2	1.67	0.76
1:B:22:LEU:HD23	1:D:205:MET:HE2	1.67	0.76
1:M:22:LEU:HD23	1:S:205:MET:HE2	1.67	0.76
1:L:22:LEU:HD23	1:R:205:MET:HE2	1.67	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:CE	1:T:119:MET:CE	2.61	0.75
1:K:205:MET:HE2	1:Q:22:LEU:HD23	1.67	0.75
1:A:205:MET:HE2	1:C:22:LEU:HD23	1.67	0.75
1:J:205:MET:HE2	1:P:22:LEU:HD23	1.67	0.75
1:I:205:MET:HE2	1:O:22:LEU:HD23	1.67	0.75
1:C:118:GLY:HA2	1:T:554:ALA:HB3	1.69	0.74
1:D:112:LYS:CE	1:I:119:MET:CE	2.66	0.72
1:D:112:LYS:HE3	1:I:119:MET:CE	2.16	0.72
1:J:112:LYS:HE3	1:T:119:MET:CE	2.13	0.67
1:A:552:ASN:HA	1:N:119:MET:SD	2.35	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:112:LYS:HE2	1:T:119:MET:CE	2.23	0.66
1:C:119:MET:SD	1:T:553:VAL:N	2.71	0.64
1:C:119:MET:SD	1:T:552:ASN:C	2.87	0.58
1:D:112:LYS:HE2	1:I:119:MET:CE	2.35	0.56
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: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:P:70:ARG:HA	1:P:75:VAL:HG22	1.91	0.53
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:CE	2.45	0.47
1:D:119:MET:CE	1:I:112:LYS:CE	2.86	0.45
1:I:552:ASN:HA	1:M:119:MET:HE1	1.98	0.44
1:C:497:VAL:O	1:C:498:HIS:C	2.61	0.43
1:Q:497:VAL:O	1:Q:498:HIS:C	2.61	0.43
1:O:497:VAL:O	1:O:498:HIS:C	2.61	0.43
1:P:497:VAL:O	1:P:498:HIS:C	2.61	0.43
1:D:119:MET:HE3	1:I:112:LYS:HE2	1.98	0.42
1:B:50:LYS:NZ	1:B:61:ASP:OD1	2.45	0.42
1:N:50:LYS:NZ	1:N:61:ASP:OD1	2.45	0.42
1:L:497:VAL:O	1:L:498:HIS:C	2.61	0.42
1:M:497:VAL:O	1:M:498:HIS:C	2.61	0.42
1:N:497:VAL:O	1:N:498:HIS:C	2.61	0.41
1:B:497:VAL:O	1:B:498:HIS:C	2.61	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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 (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	117	ASN
1	A	148	GLN
1	A	149	GLN
1	A	328	ASN
1	A	492	GLN
1	A	516	ASN
1	A	552	ASN
1	B	73	ASN
1	B	116	GLN

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Mol	Chain	Res	Type
1	B	120	HIS
1	B	121	GLN
1	B	288	GLN
1	C	73	ASN
1	C	116	GLN
1	C	120	HIS
1	C	121	GLN
1	C	288	GLN
1	D	27	GLN
1	D	117	ASN
1	D	148	GLN
1	D	149	GLN
1	D	328	ASN
1	I	27	GLN
1	I	117	ASN
1	I	121	GLN
1	I	148	GLN
1	I	328	ASN
1	I	492	GLN
1	I	516	ASN
1	I	552	ASN
1	J	27	GLN
1	J	117	ASN
1	J	121	GLN
1	J	148	GLN
1	J	328	ASN
1	J	492	GLN
1	J	516	ASN
1	K	27	GLN
1	K	117	ASN
1	K	148	GLN
1	K	149	GLN
1	K	328	ASN
1	K	492	GLN
1	K	516	ASN
1	L	73	ASN
1	L	116	GLN
1	L	120	HIS
1	L	121	GLN
1	L	288	GLN
1	M	73	ASN
1	M	116	GLN

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Mol	Chain	Res	Type
1	M	120	HIS
1	M	121	GLN
1	M	288	GLN
1	N	73	ASN
1	N	116	GLN
1	N	120	HIS
1	N	121	GLN
1	N	288	GLN
1	O	73	ASN
1	O	116	GLN
1	O	120	HIS
1	O	121	GLN
1	O	288	GLN
1	P	73	ASN
1	P	116	GLN
1	P	120	HIS
1	P	121	GLN
1	P	288	GLN
1	Q	73	ASN
1	Q	116	GLN
1	Q	120	HIS
1	Q	121	GLN
1	Q	288	GLN
1	R	27	GLN
1	R	117	ASN
1	R	148	GLN
1	R	149	GLN
1	R	328	ASN
1	R	516	ASN
1	S	27	GLN
1	S	117	ASN
1	S	121	GLN
1	S	148	GLN
1	S	149	GLN
1	S	328	ASN
1	S	516	ASN
1	T	27	GLN
1	T	117	ASN
1	T	148	GLN
1	T	149	GLN
1	T	328	ASN
1	T	552	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

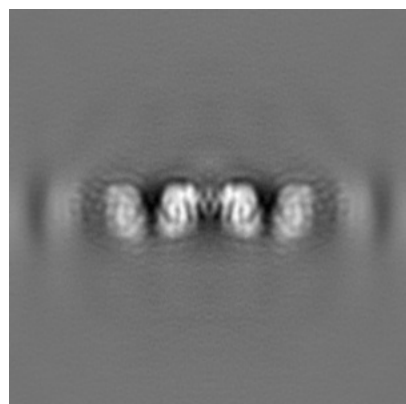
6 Map visualisation [i](#)

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.

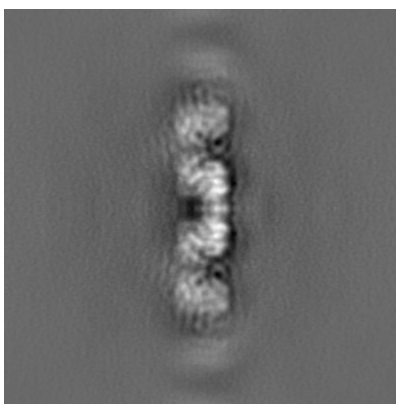
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

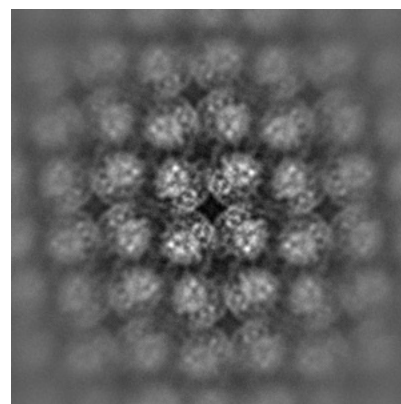
6.1.1 Primary map



X

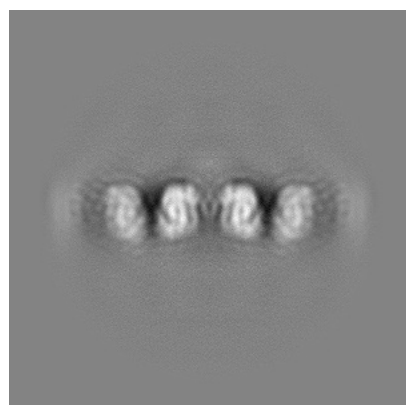


Y

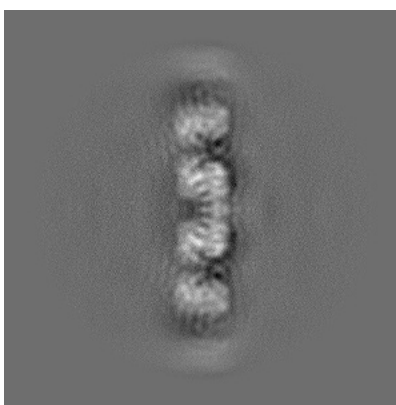


Z

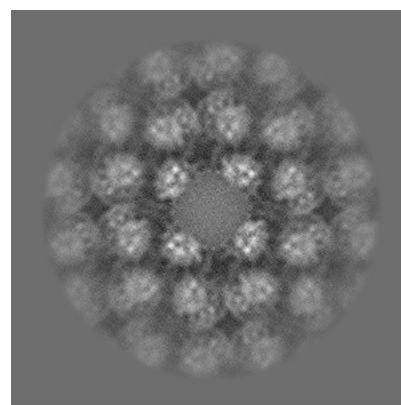
6.1.2 Raw map



X



Y

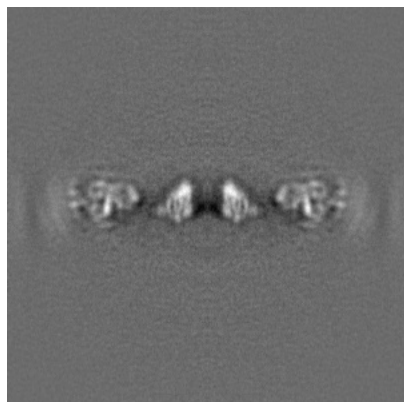


Z

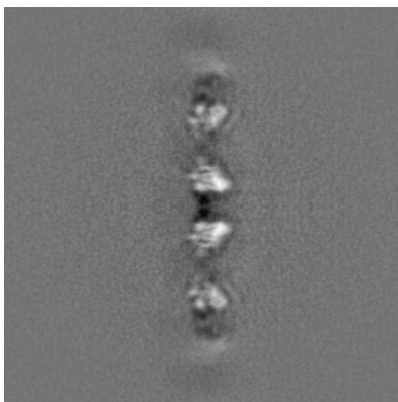
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

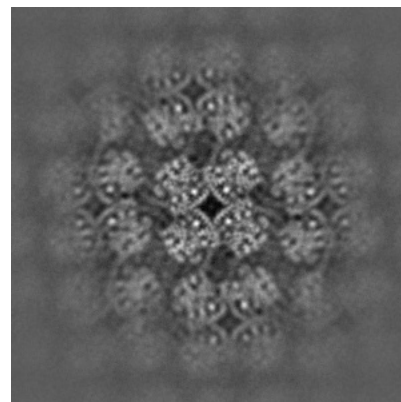
6.2.1 Primary map



X Index: 256

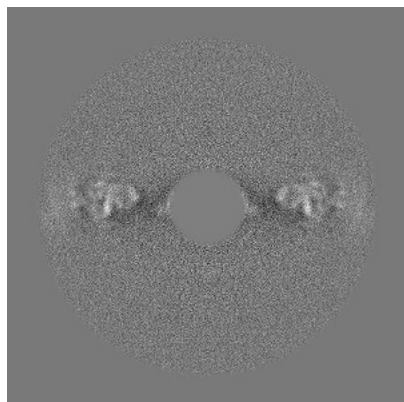


Y Index: 256

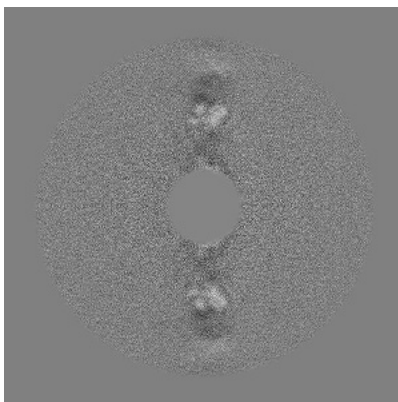


Z Index: 256

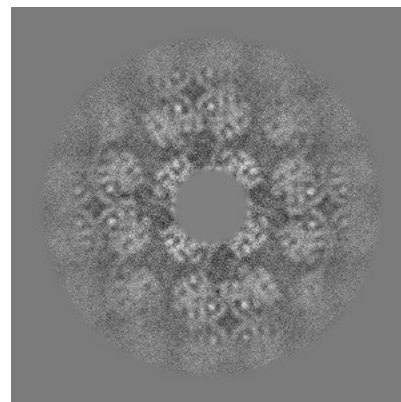
6.2.2 Raw map



X Index: 256



Y Index: 256

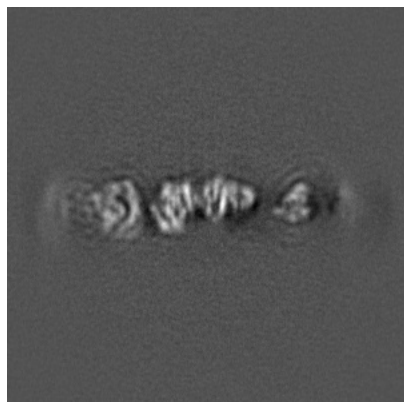


Z Index: 256

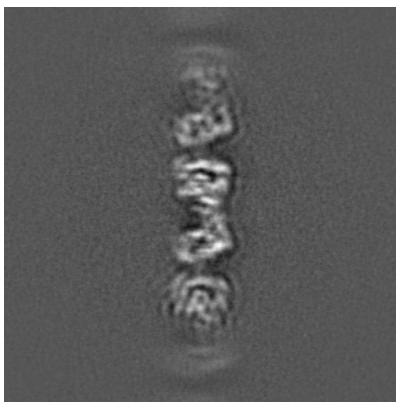
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

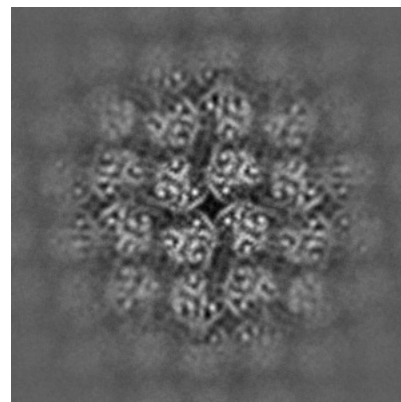
6.3.1 Primary map



X Index: 233

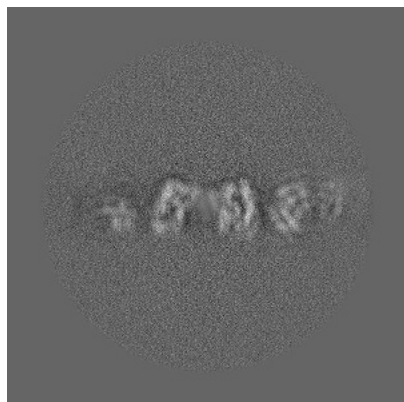


Y Index: 302

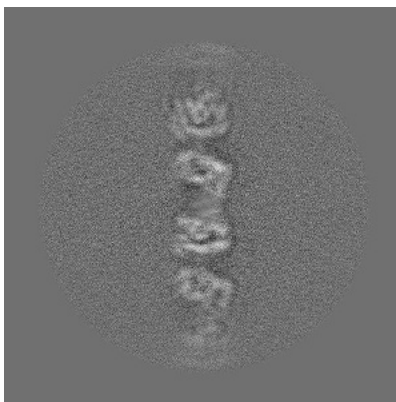


Z Index: 251

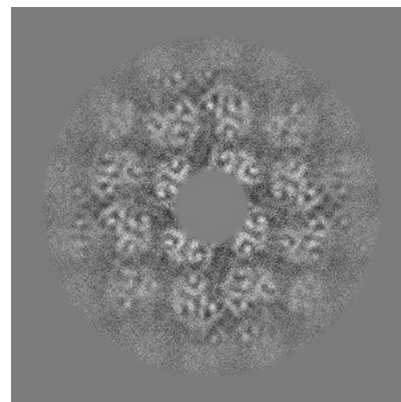
6.3.2 Raw map



X Index: 210



Y Index: 210

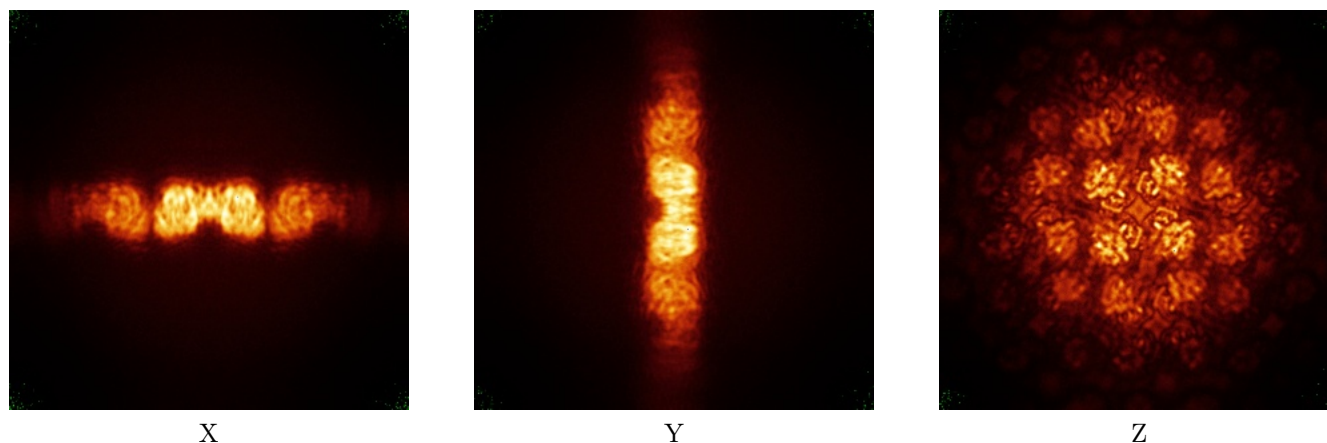


Z Index: 251

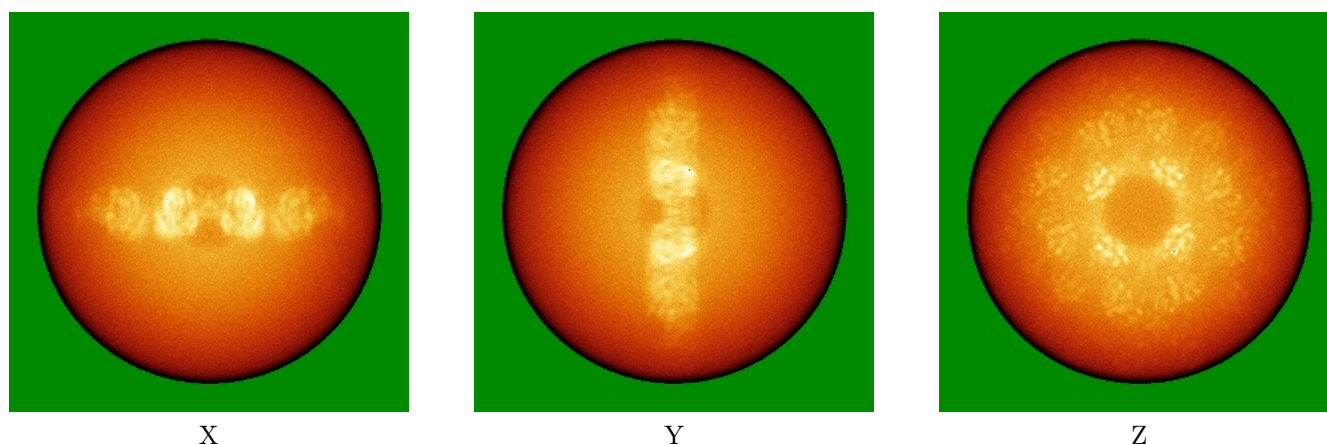
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

This section was not generated.

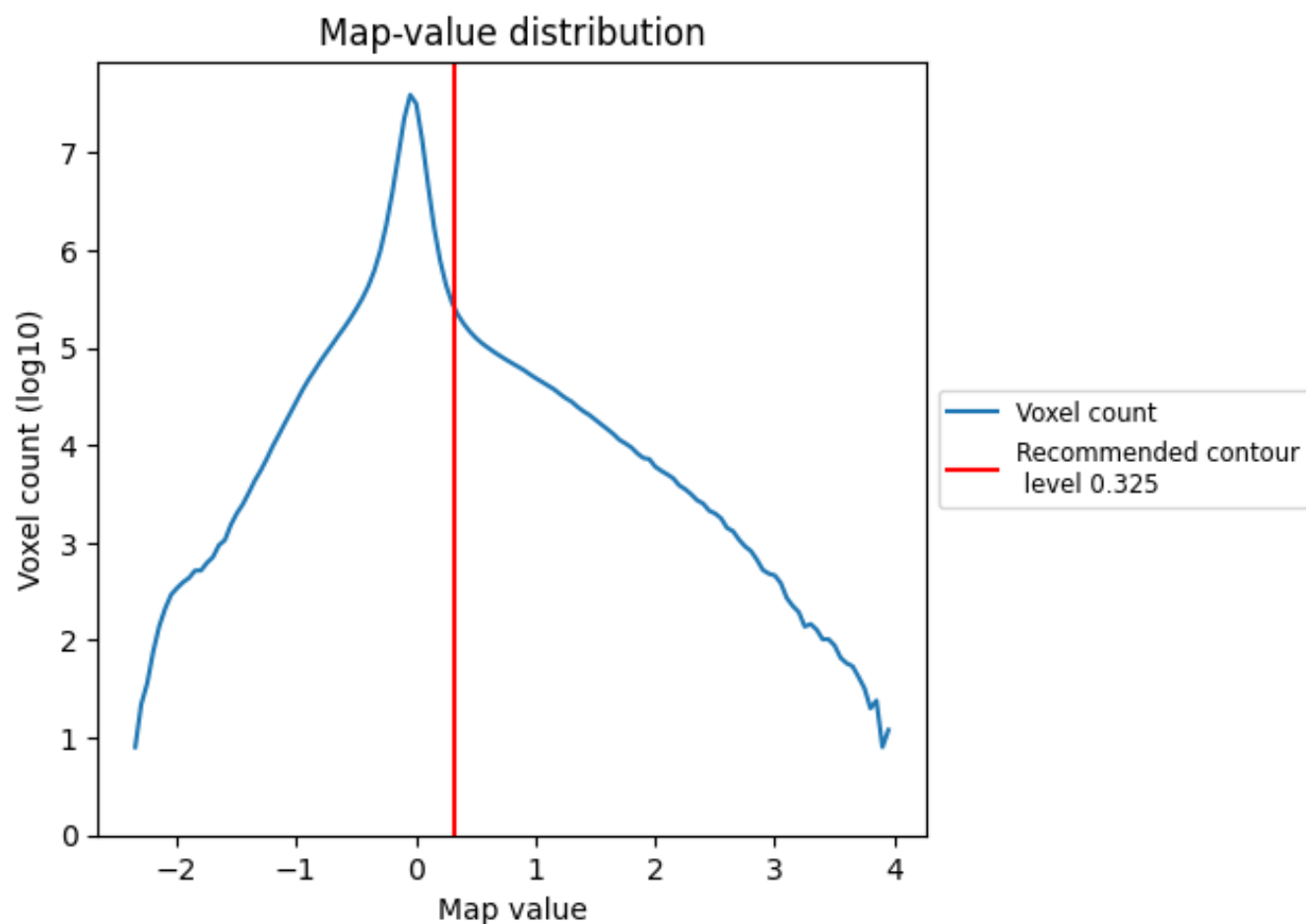
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

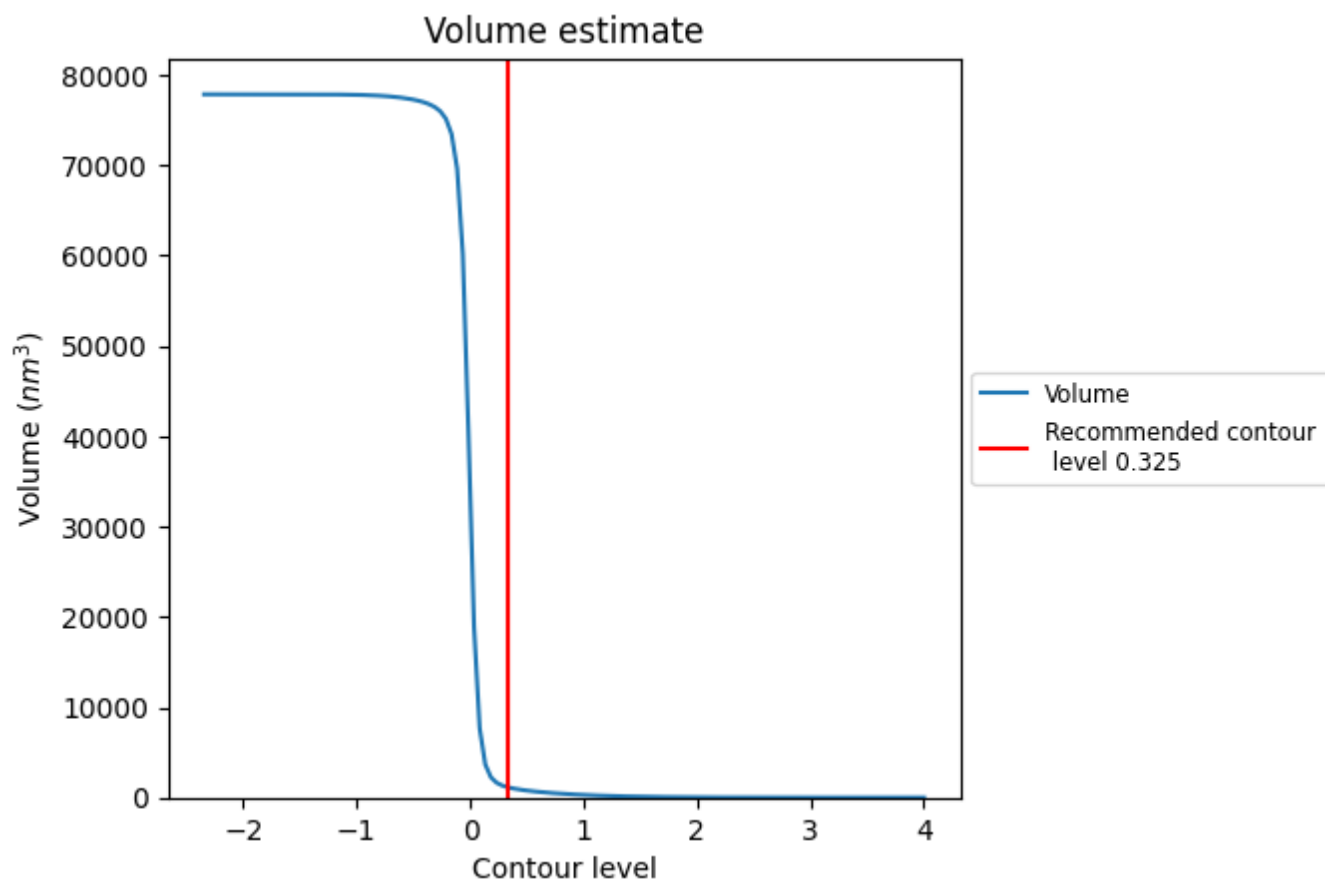
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

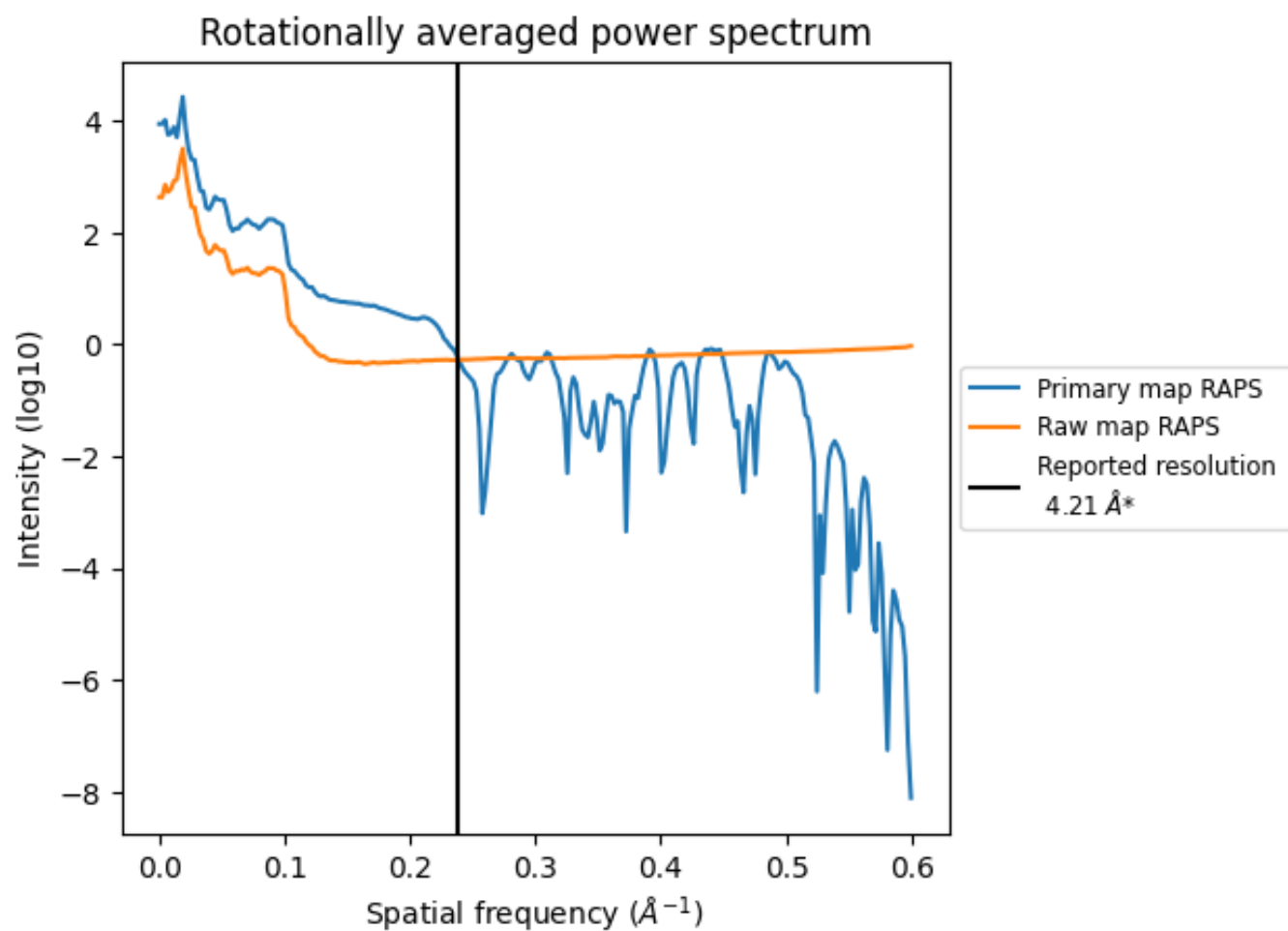
7.2 Volume estimate [i](#)



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 ⓘ

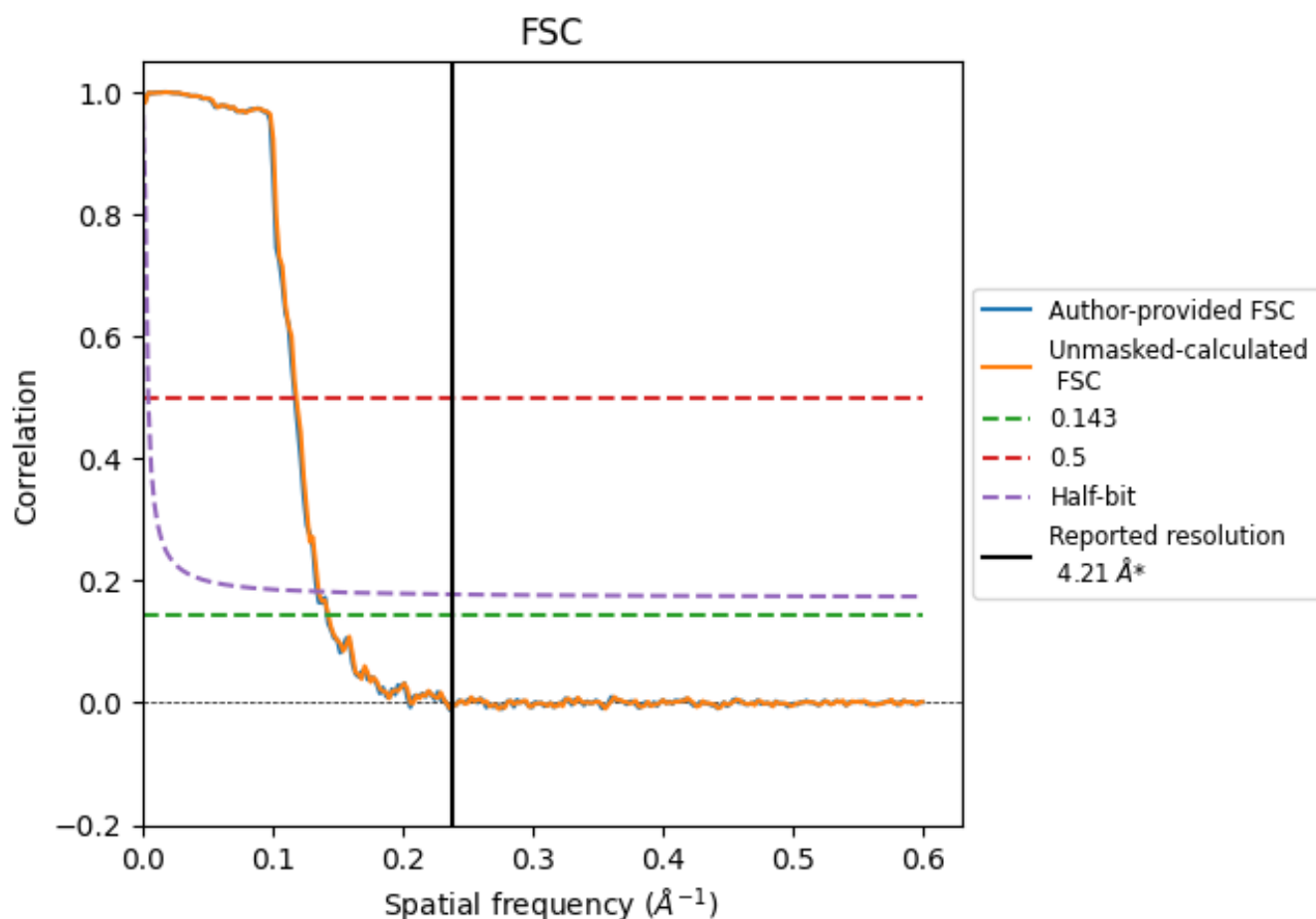


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 $0.238 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

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

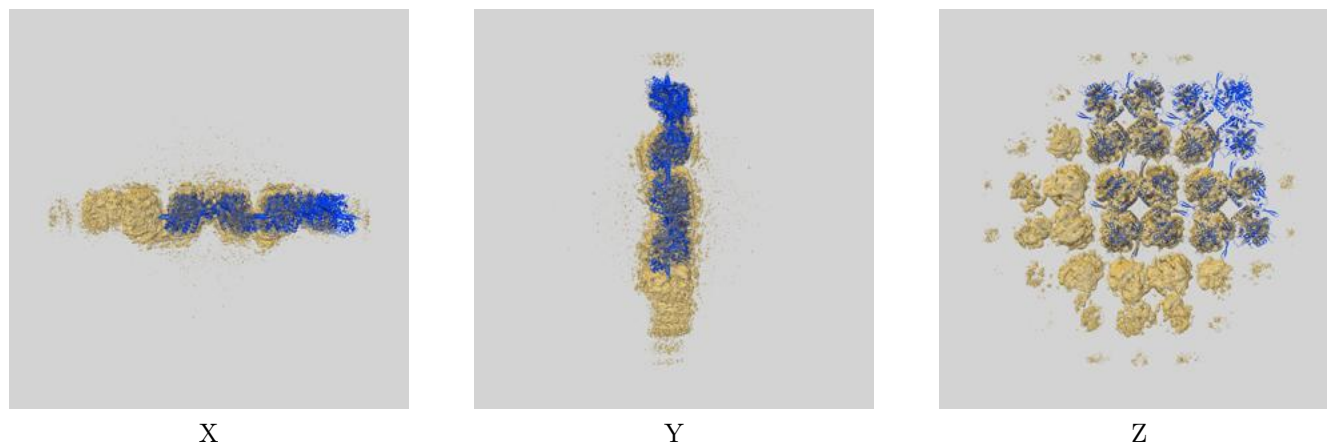
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.04 differs from the reported value 4.21 by more than 10 %

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 [i](#)

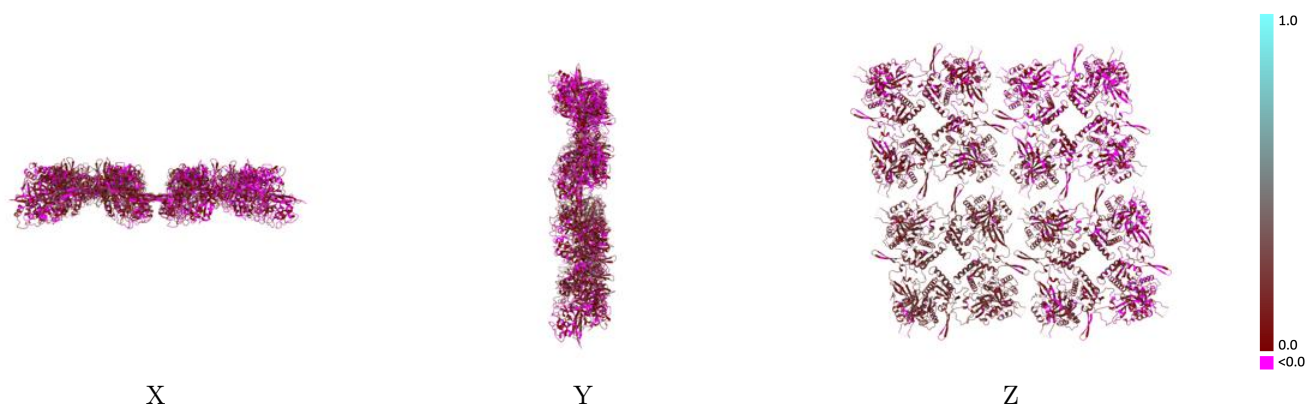
This section contains information regarding the fit between EMDB map EMD-29451 and PDB model 8FV5. Per-residue inclusion information can be found in section [3](#) on page [29](#).

9.1 Map-model overlay [i](#)



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 [i](#)

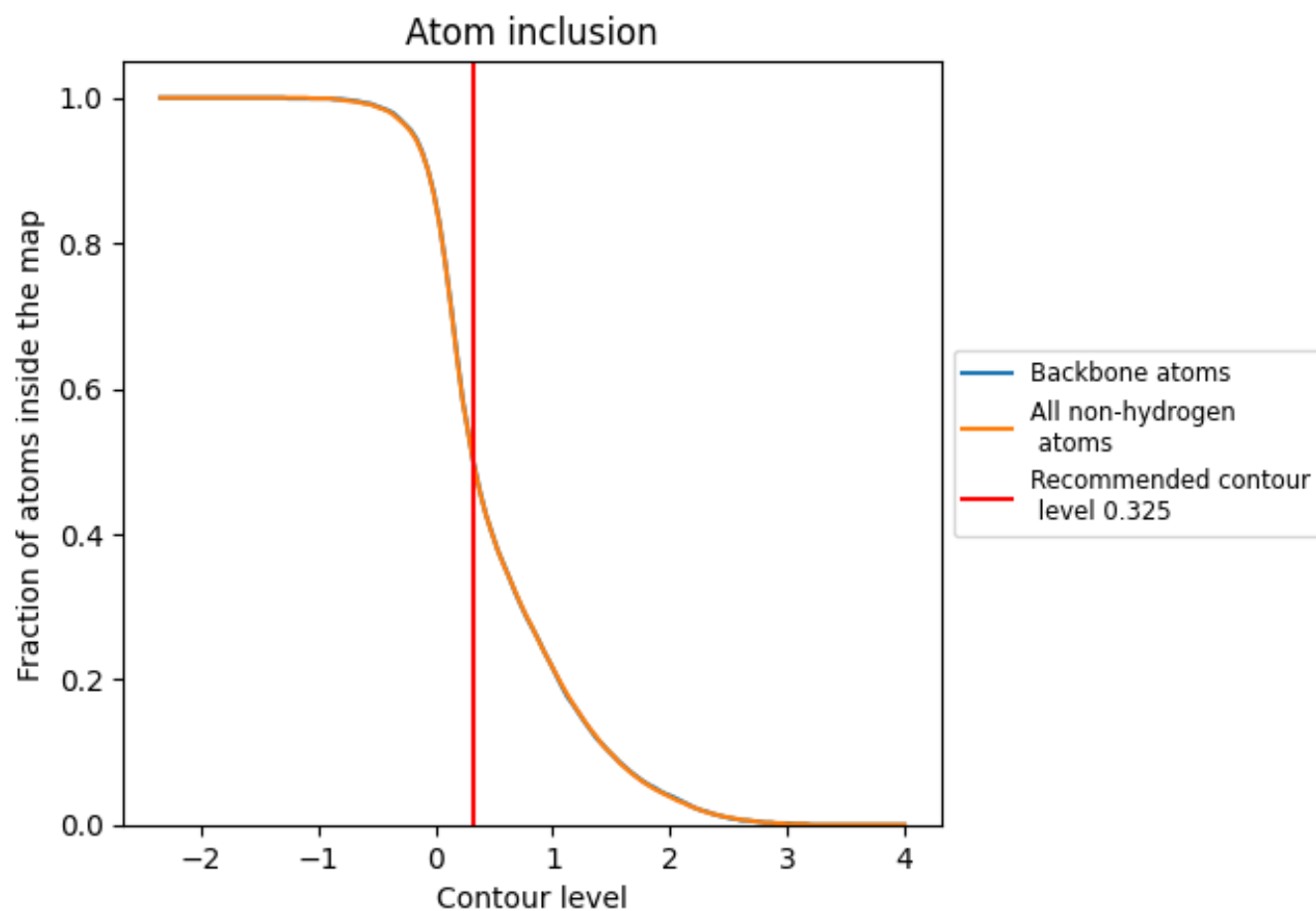


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



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	 0.4980	 0.1090
A	 0.8290	 0.1900
B	 0.8450	 0.1870
C	 0.8440	 0.1880
D	 0.8300	 0.1900
E	 0.9310	 0.1930
F	 0.8850	 0.1380
G	 0.8850	 0.1480
H	 0.9310	 0.1890
I	 0.7260	 0.1370
J	 0.1050	 0.0360
K	 0.3310	 0.0700
L	 0.7120	 0.1280
M	 0.5470	 0.0800
N	 0.7370	 0.1390
O	 0.3460	 0.0780
P	 0.0010	 0.0140
Q	 0.2780	 0.0850
R	 0.2350	 0.0680
S	 0.0290	 0.0370
T	 0.7210	 0.1370
U	 0.4830	 0.1240
V	 0.0000	 -0.0990
W	 0.0810	 0.0220
X	 0.4020	 0.0670
Y	 0.1840	 -0.0280
Z	 0.3330	 0.0120
a	 0.2990	 0.0440
b	 0.0000	 0.0410
c	 0.1260	 0.0240
d	 0.0110	 0.0170
e	 0.0000	 0.0140
f	 0.7360	 0.1420

