



wwPDB EM Validation Summary Report ⓘ

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PDB ID : 9SMJ / pdb_00009smj
EMDB ID : EMD-55035
Title : Zuzalysin zymogen dodecahedral complex E439A
Authors : Rodriguez-Banqueri, A.; Madej, M.; Eckhard, U.; Potempa, J.
Deposited on : 2025-09-08
Resolution : 2.64 Å(reported)

This is a wwPDB EM Validation Summary 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.dev133
MolProbity : **FAILED**
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) : 2.50

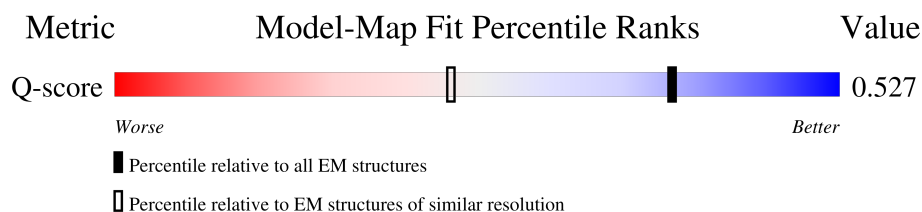
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.64 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	8968 (2.14 - 3.14)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 394860 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Zinc-dependent metalloprotease.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	A2	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	A3	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	A4	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	A5	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	B1	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	B2	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	B3	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	B4	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	B5	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	C1	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	C2	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	C3	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	C4	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	C5	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	D1	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	D2	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	D3	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	D4	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	D5	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	E1	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	E2	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	E3	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	E4	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	E5	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	F1	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	F2	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	F3	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	F4	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	F5	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	G1	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	G2	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	G3	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	G4	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	G5	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	H1	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	H2	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0
1	H3	818	Total 6578	C 4176	N 1145	O 1226	S 31	2	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	H4	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	H5	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	I1	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	I2	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	I3	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	I4	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	I5	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	J1	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	J2	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	J3	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	J4	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	J5	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	K1	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	K2	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	K3	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	K4	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	K5	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	L1	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	L2	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	L3	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		
1	L4	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	L5	818	Total	C	N	O	S	2	0
			6578	4176	1145	1226	31		

There are 1380 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	14	MET	-	initiating methionine	UNP A0AAF0BD41
A1	15	ALA	-	expression tag	UNP A0AAF0BD41
A1	16	SER	-	expression tag	UNP A0AAF0BD41
A1	17	MET	-	expression tag	UNP A0AAF0BD41
A1	18	THR	-	expression tag	UNP A0AAF0BD41
A1	19	GLY	-	expression tag	UNP A0AAF0BD41
A1	20	GLY	-	expression tag	UNP A0AAF0BD41
A1	21	GLN	-	expression tag	UNP A0AAF0BD41
A1	22	MET	-	expression tag	UNP A0AAF0BD41
A1	23	GLY	ALA	conflict	UNP A0AAF0BD41
A1	197	MET	VAL	conflict	UNP A0AAF0BD41
A1	298	PRO	LEU	conflict	UNP A0AAF0BD41
A1	306	VAL	ILE	conflict	UNP A0AAF0BD41
A1	439	ALA	GLU	conflict	UNP A0AAF0BD41
A1	751	HIS	TYR	conflict	UNP A0AAF0BD41
A1	774	HIS	TYR	conflict	UNP A0AAF0BD41
A1	805	ALA	SER	conflict	UNP A0AAF0BD41
A1	901	HIS	-	expression tag	UNP A0AAF0BD41
A1	902	HIS	-	expression tag	UNP A0AAF0BD41
A1	903	HIS	-	expression tag	UNP A0AAF0BD41
A1	904	HIS	-	expression tag	UNP A0AAF0BD41
A1	905	HIS	-	expression tag	UNP A0AAF0BD41
A1	906	HIS	-	expression tag	UNP A0AAF0BD41
A2	14	MET	-	initiating methionine	UNP A0AAF0BD41
A2	15	ALA	-	expression tag	UNP A0AAF0BD41
A2	16	SER	-	expression tag	UNP A0AAF0BD41
A2	17	MET	-	expression tag	UNP A0AAF0BD41
A2	18	THR	-	expression tag	UNP A0AAF0BD41
A2	19	GLY	-	expression tag	UNP A0AAF0BD41
A2	20	GLY	-	expression tag	UNP A0AAF0BD41
A2	21	GLN	-	expression tag	UNP A0AAF0BD41
A2	22	MET	-	expression tag	UNP A0AAF0BD41
A2	23	GLY	ALA	conflict	UNP A0AAF0BD41
A2	197	MET	VAL	conflict	UNP A0AAF0BD41
A2	298	PRO	LEU	conflict	UNP A0AAF0BD41
A2	306	VAL	ILE	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
A2	439	ALA	GLU	conflict	UNP A0AAF0BD41
A2	751	HIS	TYR	conflict	UNP A0AAF0BD41
A2	774	HIS	TYR	conflict	UNP A0AAF0BD41
A2	805	ALA	SER	conflict	UNP A0AAF0BD41
A2	901	HIS	-	expression tag	UNP A0AAF0BD41
A2	902	HIS	-	expression tag	UNP A0AAF0BD41
A2	903	HIS	-	expression tag	UNP A0AAF0BD41
A2	904	HIS	-	expression tag	UNP A0AAF0BD41
A2	905	HIS	-	expression tag	UNP A0AAF0BD41
A2	906	HIS	-	expression tag	UNP A0AAF0BD41
A3	14	MET	-	initiating methionine	UNP A0AAF0BD41
A3	15	ALA	-	expression tag	UNP A0AAF0BD41
A3	16	SER	-	expression tag	UNP A0AAF0BD41
A3	17	MET	-	expression tag	UNP A0AAF0BD41
A3	18	THR	-	expression tag	UNP A0AAF0BD41
A3	19	GLY	-	expression tag	UNP A0AAF0BD41
A3	20	GLY	-	expression tag	UNP A0AAF0BD41
A3	21	GLN	-	expression tag	UNP A0AAF0BD41
A3	22	MET	-	expression tag	UNP A0AAF0BD41
A3	23	GLY	ALA	conflict	UNP A0AAF0BD41
A3	197	MET	VAL	conflict	UNP A0AAF0BD41
A3	298	PRO	LEU	conflict	UNP A0AAF0BD41
A3	306	VAL	ILE	conflict	UNP A0AAF0BD41
A3	439	ALA	GLU	conflict	UNP A0AAF0BD41
A3	751	HIS	TYR	conflict	UNP A0AAF0BD41
A3	774	HIS	TYR	conflict	UNP A0AAF0BD41
A3	805	ALA	SER	conflict	UNP A0AAF0BD41
A3	901	HIS	-	expression tag	UNP A0AAF0BD41
A3	902	HIS	-	expression tag	UNP A0AAF0BD41
A3	903	HIS	-	expression tag	UNP A0AAF0BD41
A3	904	HIS	-	expression tag	UNP A0AAF0BD41
A3	905	HIS	-	expression tag	UNP A0AAF0BD41
A3	906	HIS	-	expression tag	UNP A0AAF0BD41
A4	14	MET	-	initiating methionine	UNP A0AAF0BD41
A4	15	ALA	-	expression tag	UNP A0AAF0BD41
A4	16	SER	-	expression tag	UNP A0AAF0BD41
A4	17	MET	-	expression tag	UNP A0AAF0BD41
A4	18	THR	-	expression tag	UNP A0AAF0BD41
A4	19	GLY	-	expression tag	UNP A0AAF0BD41
A4	20	GLY	-	expression tag	UNP A0AAF0BD41
A4	21	GLN	-	expression tag	UNP A0AAF0BD41
A4	22	MET	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
A4	23	GLY	ALA	conflict	UNP A0AAF0BD41
A4	197	MET	VAL	conflict	UNP A0AAF0BD41
A4	298	PRO	LEU	conflict	UNP A0AAF0BD41
A4	306	VAL	ILE	conflict	UNP A0AAF0BD41
A4	439	ALA	GLU	conflict	UNP A0AAF0BD41
A4	751	HIS	TYR	conflict	UNP A0AAF0BD41
A4	774	HIS	TYR	conflict	UNP A0AAF0BD41
A4	805	ALA	SER	conflict	UNP A0AAF0BD41
A4	901	HIS	-	expression tag	UNP A0AAF0BD41
A4	902	HIS	-	expression tag	UNP A0AAF0BD41
A4	903	HIS	-	expression tag	UNP A0AAF0BD41
A4	904	HIS	-	expression tag	UNP A0AAF0BD41
A4	905	HIS	-	expression tag	UNP A0AAF0BD41
A4	906	HIS	-	expression tag	UNP A0AAF0BD41
A5	14	MET	-	initiating methionine	UNP A0AAF0BD41
A5	15	ALA	-	expression tag	UNP A0AAF0BD41
A5	16	SER	-	expression tag	UNP A0AAF0BD41
A5	17	MET	-	expression tag	UNP A0AAF0BD41
A5	18	THR	-	expression tag	UNP A0AAF0BD41
A5	19	GLY	-	expression tag	UNP A0AAF0BD41
A5	20	GLY	-	expression tag	UNP A0AAF0BD41
A5	21	GLN	-	expression tag	UNP A0AAF0BD41
A5	22	MET	-	expression tag	UNP A0AAF0BD41
A5	23	GLY	ALA	conflict	UNP A0AAF0BD41
A5	197	MET	VAL	conflict	UNP A0AAF0BD41
A5	298	PRO	LEU	conflict	UNP A0AAF0BD41
A5	306	VAL	ILE	conflict	UNP A0AAF0BD41
A5	439	ALA	GLU	conflict	UNP A0AAF0BD41
A5	751	HIS	TYR	conflict	UNP A0AAF0BD41
A5	774	HIS	TYR	conflict	UNP A0AAF0BD41
A5	805	ALA	SER	conflict	UNP A0AAF0BD41
A5	901	HIS	-	expression tag	UNP A0AAF0BD41
A5	902	HIS	-	expression tag	UNP A0AAF0BD41
A5	903	HIS	-	expression tag	UNP A0AAF0BD41
A5	904	HIS	-	expression tag	UNP A0AAF0BD41
A5	905	HIS	-	expression tag	UNP A0AAF0BD41
A5	906	HIS	-	expression tag	UNP A0AAF0BD41
B1	14	MET	-	initiating methionine	UNP A0AAF0BD41
B1	15	ALA	-	expression tag	UNP A0AAF0BD41
B1	16	SER	-	expression tag	UNP A0AAF0BD41
B1	17	MET	-	expression tag	UNP A0AAF0BD41
B1	18	THR	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
B1	19	GLY	-	expression tag	UNP A0AAF0BD41
B1	20	GLY	-	expression tag	UNP A0AAF0BD41
B1	21	GLN	-	expression tag	UNP A0AAF0BD41
B1	22	MET	-	expression tag	UNP A0AAF0BD41
B1	23	GLY	ALA	conflict	UNP A0AAF0BD41
B1	197	MET	VAL	conflict	UNP A0AAF0BD41
B1	298	PRO	LEU	conflict	UNP A0AAF0BD41
B1	306	VAL	ILE	conflict	UNP A0AAF0BD41
B1	439	ALA	GLU	conflict	UNP A0AAF0BD41
B1	751	HIS	TYR	conflict	UNP A0AAF0BD41
B1	774	HIS	TYR	conflict	UNP A0AAF0BD41
B1	805	ALA	SER	conflict	UNP A0AAF0BD41
B1	901	HIS	-	expression tag	UNP A0AAF0BD41
B1	902	HIS	-	expression tag	UNP A0AAF0BD41
B1	903	HIS	-	expression tag	UNP A0AAF0BD41
B1	904	HIS	-	expression tag	UNP A0AAF0BD41
B1	905	HIS	-	expression tag	UNP A0AAF0BD41
B1	906	HIS	-	expression tag	UNP A0AAF0BD41
B2	14	MET	-	initiating methionine	UNP A0AAF0BD41
B2	15	ALA	-	expression tag	UNP A0AAF0BD41
B2	16	SER	-	expression tag	UNP A0AAF0BD41
B2	17	MET	-	expression tag	UNP A0AAF0BD41
B2	18	THR	-	expression tag	UNP A0AAF0BD41
B2	19	GLY	-	expression tag	UNP A0AAF0BD41
B2	20	GLY	-	expression tag	UNP A0AAF0BD41
B2	21	GLN	-	expression tag	UNP A0AAF0BD41
B2	22	MET	-	expression tag	UNP A0AAF0BD41
B2	23	GLY	ALA	conflict	UNP A0AAF0BD41
B2	197	MET	VAL	conflict	UNP A0AAF0BD41
B2	298	PRO	LEU	conflict	UNP A0AAF0BD41
B2	306	VAL	ILE	conflict	UNP A0AAF0BD41
B2	439	ALA	GLU	conflict	UNP A0AAF0BD41
B2	751	HIS	TYR	conflict	UNP A0AAF0BD41
B2	774	HIS	TYR	conflict	UNP A0AAF0BD41
B2	805	ALA	SER	conflict	UNP A0AAF0BD41
B2	901	HIS	-	expression tag	UNP A0AAF0BD41
B2	902	HIS	-	expression tag	UNP A0AAF0BD41
B2	903	HIS	-	expression tag	UNP A0AAF0BD41
B2	904	HIS	-	expression tag	UNP A0AAF0BD41
B2	905	HIS	-	expression tag	UNP A0AAF0BD41
B2	906	HIS	-	expression tag	UNP A0AAF0BD41
B3	14	MET	-	initiating methionine	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
B3	15	ALA	-	expression tag	UNP A0AAF0BD41
B3	16	SER	-	expression tag	UNP A0AAF0BD41
B3	17	MET	-	expression tag	UNP A0AAF0BD41
B3	18	THR	-	expression tag	UNP A0AAF0BD41
B3	19	GLY	-	expression tag	UNP A0AAF0BD41
B3	20	GLY	-	expression tag	UNP A0AAF0BD41
B3	21	GLN	-	expression tag	UNP A0AAF0BD41
B3	22	MET	-	expression tag	UNP A0AAF0BD41
B3	23	GLY	ALA	conflict	UNP A0AAF0BD41
B3	197	MET	VAL	conflict	UNP A0AAF0BD41
B3	298	PRO	LEU	conflict	UNP A0AAF0BD41
B3	306	VAL	ILE	conflict	UNP A0AAF0BD41
B3	439	ALA	GLU	conflict	UNP A0AAF0BD41
B3	751	HIS	TYR	conflict	UNP A0AAF0BD41
B3	774	HIS	TYR	conflict	UNP A0AAF0BD41
B3	805	ALA	SER	conflict	UNP A0AAF0BD41
B3	901	HIS	-	expression tag	UNP A0AAF0BD41
B3	902	HIS	-	expression tag	UNP A0AAF0BD41
B3	903	HIS	-	expression tag	UNP A0AAF0BD41
B3	904	HIS	-	expression tag	UNP A0AAF0BD41
B3	905	HIS	-	expression tag	UNP A0AAF0BD41
B3	906	HIS	-	expression tag	UNP A0AAF0BD41
B4	14	MET	-	initiating methionine	UNP A0AAF0BD41
B4	15	ALA	-	expression tag	UNP A0AAF0BD41
B4	16	SER	-	expression tag	UNP A0AAF0BD41
B4	17	MET	-	expression tag	UNP A0AAF0BD41
B4	18	THR	-	expression tag	UNP A0AAF0BD41
B4	19	GLY	-	expression tag	UNP A0AAF0BD41
B4	20	GLY	-	expression tag	UNP A0AAF0BD41
B4	21	GLN	-	expression tag	UNP A0AAF0BD41
B4	22	MET	-	expression tag	UNP A0AAF0BD41
B4	23	GLY	ALA	conflict	UNP A0AAF0BD41
B4	197	MET	VAL	conflict	UNP A0AAF0BD41
B4	298	PRO	LEU	conflict	UNP A0AAF0BD41
B4	306	VAL	ILE	conflict	UNP A0AAF0BD41
B4	439	ALA	GLU	conflict	UNP A0AAF0BD41
B4	751	HIS	TYR	conflict	UNP A0AAF0BD41
B4	774	HIS	TYR	conflict	UNP A0AAF0BD41
B4	805	ALA	SER	conflict	UNP A0AAF0BD41
B4	901	HIS	-	expression tag	UNP A0AAF0BD41
B4	902	HIS	-	expression tag	UNP A0AAF0BD41
B4	903	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
B4	904	HIS	-	expression tag	UNP A0AAF0BD41
B4	905	HIS	-	expression tag	UNP A0AAF0BD41
B4	906	HIS	-	expression tag	UNP A0AAF0BD41
B5	14	MET	-	initiating methionine	UNP A0AAF0BD41
B5	15	ALA	-	expression tag	UNP A0AAF0BD41
B5	16	SER	-	expression tag	UNP A0AAF0BD41
B5	17	MET	-	expression tag	UNP A0AAF0BD41
B5	18	THR	-	expression tag	UNP A0AAF0BD41
B5	19	GLY	-	expression tag	UNP A0AAF0BD41
B5	20	GLY	-	expression tag	UNP A0AAF0BD41
B5	21	GLN	-	expression tag	UNP A0AAF0BD41
B5	22	MET	-	expression tag	UNP A0AAF0BD41
B5	23	GLY	ALA	conflict	UNP A0AAF0BD41
B5	197	MET	VAL	conflict	UNP A0AAF0BD41
B5	298	PRO	LEU	conflict	UNP A0AAF0BD41
B5	306	VAL	ILE	conflict	UNP A0AAF0BD41
B5	439	ALA	GLU	conflict	UNP A0AAF0BD41
B5	751	HIS	TYR	conflict	UNP A0AAF0BD41
B5	774	HIS	TYR	conflict	UNP A0AAF0BD41
B5	805	ALA	SER	conflict	UNP A0AAF0BD41
B5	901	HIS	-	expression tag	UNP A0AAF0BD41
B5	902	HIS	-	expression tag	UNP A0AAF0BD41
B5	903	HIS	-	expression tag	UNP A0AAF0BD41
B5	904	HIS	-	expression tag	UNP A0AAF0BD41
B5	905	HIS	-	expression tag	UNP A0AAF0BD41
B5	906	HIS	-	expression tag	UNP A0AAF0BD41
C1	14	MET	-	initiating methionine	UNP A0AAF0BD41
C1	15	ALA	-	expression tag	UNP A0AAF0BD41
C1	16	SER	-	expression tag	UNP A0AAF0BD41
C1	17	MET	-	expression tag	UNP A0AAF0BD41
C1	18	THR	-	expression tag	UNP A0AAF0BD41
C1	19	GLY	-	expression tag	UNP A0AAF0BD41
C1	20	GLY	-	expression tag	UNP A0AAF0BD41
C1	21	GLN	-	expression tag	UNP A0AAF0BD41
C1	22	MET	-	expression tag	UNP A0AAF0BD41
C1	23	GLY	ALA	conflict	UNP A0AAF0BD41
C1	197	MET	VAL	conflict	UNP A0AAF0BD41
C1	298	PRO	LEU	conflict	UNP A0AAF0BD41
C1	306	VAL	ILE	conflict	UNP A0AAF0BD41
C1	439	ALA	GLU	conflict	UNP A0AAF0BD41
C1	751	HIS	TYR	conflict	UNP A0AAF0BD41
C1	774	HIS	TYR	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
C1	805	ALA	SER	conflict	UNP A0AAF0BD41
C1	901	HIS	-	expression tag	UNP A0AAF0BD41
C1	902	HIS	-	expression tag	UNP A0AAF0BD41
C1	903	HIS	-	expression tag	UNP A0AAF0BD41
C1	904	HIS	-	expression tag	UNP A0AAF0BD41
C1	905	HIS	-	expression tag	UNP A0AAF0BD41
C1	906	HIS	-	expression tag	UNP A0AAF0BD41
C2	14	MET	-	initiating methionine	UNP A0AAF0BD41
C2	15	ALA	-	expression tag	UNP A0AAF0BD41
C2	16	SER	-	expression tag	UNP A0AAF0BD41
C2	17	MET	-	expression tag	UNP A0AAF0BD41
C2	18	THR	-	expression tag	UNP A0AAF0BD41
C2	19	GLY	-	expression tag	UNP A0AAF0BD41
C2	20	GLY	-	expression tag	UNP A0AAF0BD41
C2	21	GLN	-	expression tag	UNP A0AAF0BD41
C2	22	MET	-	expression tag	UNP A0AAF0BD41
C2	23	GLY	ALA	conflict	UNP A0AAF0BD41
C2	197	MET	VAL	conflict	UNP A0AAF0BD41
C2	298	PRO	LEU	conflict	UNP A0AAF0BD41
C2	306	VAL	ILE	conflict	UNP A0AAF0BD41
C2	439	ALA	GLU	conflict	UNP A0AAF0BD41
C2	751	HIS	TYR	conflict	UNP A0AAF0BD41
C2	774	HIS	TYR	conflict	UNP A0AAF0BD41
C2	805	ALA	SER	conflict	UNP A0AAF0BD41
C2	901	HIS	-	expression tag	UNP A0AAF0BD41
C2	902	HIS	-	expression tag	UNP A0AAF0BD41
C2	903	HIS	-	expression tag	UNP A0AAF0BD41
C2	904	HIS	-	expression tag	UNP A0AAF0BD41
C2	905	HIS	-	expression tag	UNP A0AAF0BD41
C2	906	HIS	-	expression tag	UNP A0AAF0BD41
C3	14	MET	-	initiating methionine	UNP A0AAF0BD41
C3	15	ALA	-	expression tag	UNP A0AAF0BD41
C3	16	SER	-	expression tag	UNP A0AAF0BD41
C3	17	MET	-	expression tag	UNP A0AAF0BD41
C3	18	THR	-	expression tag	UNP A0AAF0BD41
C3	19	GLY	-	expression tag	UNP A0AAF0BD41
C3	20	GLY	-	expression tag	UNP A0AAF0BD41
C3	21	GLN	-	expression tag	UNP A0AAF0BD41
C3	22	MET	-	expression tag	UNP A0AAF0BD41
C3	23	GLY	ALA	conflict	UNP A0AAF0BD41
C3	197	MET	VAL	conflict	UNP A0AAF0BD41
C3	298	PRO	LEU	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
C3	306	VAL	ILE	conflict	UNP A0AAF0BD41
C3	439	ALA	GLU	conflict	UNP A0AAF0BD41
C3	751	HIS	TYR	conflict	UNP A0AAF0BD41
C3	774	HIS	TYR	conflict	UNP A0AAF0BD41
C3	805	ALA	SER	conflict	UNP A0AAF0BD41
C3	901	HIS	-	expression tag	UNP A0AAF0BD41
C3	902	HIS	-	expression tag	UNP A0AAF0BD41
C3	903	HIS	-	expression tag	UNP A0AAF0BD41
C3	904	HIS	-	expression tag	UNP A0AAF0BD41
C3	905	HIS	-	expression tag	UNP A0AAF0BD41
C3	906	HIS	-	expression tag	UNP A0AAF0BD41
C4	14	MET	-	initiating methionine	UNP A0AAF0BD41
C4	15	ALA	-	expression tag	UNP A0AAF0BD41
C4	16	SER	-	expression tag	UNP A0AAF0BD41
C4	17	MET	-	expression tag	UNP A0AAF0BD41
C4	18	THR	-	expression tag	UNP A0AAF0BD41
C4	19	GLY	-	expression tag	UNP A0AAF0BD41
C4	20	GLY	-	expression tag	UNP A0AAF0BD41
C4	21	GLN	-	expression tag	UNP A0AAF0BD41
C4	22	MET	-	expression tag	UNP A0AAF0BD41
C4	23	GLY	ALA	conflict	UNP A0AAF0BD41
C4	197	MET	VAL	conflict	UNP A0AAF0BD41
C4	298	PRO	LEU	conflict	UNP A0AAF0BD41
C4	306	VAL	ILE	conflict	UNP A0AAF0BD41
C4	439	ALA	GLU	conflict	UNP A0AAF0BD41
C4	751	HIS	TYR	conflict	UNP A0AAF0BD41
C4	774	HIS	TYR	conflict	UNP A0AAF0BD41
C4	805	ALA	SER	conflict	UNP A0AAF0BD41
C4	901	HIS	-	expression tag	UNP A0AAF0BD41
C4	902	HIS	-	expression tag	UNP A0AAF0BD41
C4	903	HIS	-	expression tag	UNP A0AAF0BD41
C4	904	HIS	-	expression tag	UNP A0AAF0BD41
C4	905	HIS	-	expression tag	UNP A0AAF0BD41
C4	906	HIS	-	expression tag	UNP A0AAF0BD41
C5	14	MET	-	initiating methionine	UNP A0AAF0BD41
C5	15	ALA	-	expression tag	UNP A0AAF0BD41
C5	16	SER	-	expression tag	UNP A0AAF0BD41
C5	17	MET	-	expression tag	UNP A0AAF0BD41
C5	18	THR	-	expression tag	UNP A0AAF0BD41
C5	19	GLY	-	expression tag	UNP A0AAF0BD41
C5	20	GLY	-	expression tag	UNP A0AAF0BD41
C5	21	GLN	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
C5	22	MET	-	expression tag	UNP A0AAF0BD41
C5	23	GLY	ALA	conflict	UNP A0AAF0BD41
C5	197	MET	VAL	conflict	UNP A0AAF0BD41
C5	298	PRO	LEU	conflict	UNP A0AAF0BD41
C5	306	VAL	ILE	conflict	UNP A0AAF0BD41
C5	439	ALA	GLU	conflict	UNP A0AAF0BD41
C5	751	HIS	TYR	conflict	UNP A0AAF0BD41
C5	774	HIS	TYR	conflict	UNP A0AAF0BD41
C5	805	ALA	SER	conflict	UNP A0AAF0BD41
C5	901	HIS	-	expression tag	UNP A0AAF0BD41
C5	902	HIS	-	expression tag	UNP A0AAF0BD41
C5	903	HIS	-	expression tag	UNP A0AAF0BD41
C5	904	HIS	-	expression tag	UNP A0AAF0BD41
C5	905	HIS	-	expression tag	UNP A0AAF0BD41
C5	906	HIS	-	expression tag	UNP A0AAF0BD41
D1	14	MET	-	initiating methionine	UNP A0AAF0BD41
D1	15	ALA	-	expression tag	UNP A0AAF0BD41
D1	16	SER	-	expression tag	UNP A0AAF0BD41
D1	17	MET	-	expression tag	UNP A0AAF0BD41
D1	18	THR	-	expression tag	UNP A0AAF0BD41
D1	19	GLY	-	expression tag	UNP A0AAF0BD41
D1	20	GLY	-	expression tag	UNP A0AAF0BD41
D1	21	GLN	-	expression tag	UNP A0AAF0BD41
D1	22	MET	-	expression tag	UNP A0AAF0BD41
D1	23	GLY	ALA	conflict	UNP A0AAF0BD41
D1	197	MET	VAL	conflict	UNP A0AAF0BD41
D1	298	PRO	LEU	conflict	UNP A0AAF0BD41
D1	306	VAL	ILE	conflict	UNP A0AAF0BD41
D1	439	ALA	GLU	conflict	UNP A0AAF0BD41
D1	751	HIS	TYR	conflict	UNP A0AAF0BD41
D1	774	HIS	TYR	conflict	UNP A0AAF0BD41
D1	805	ALA	SER	conflict	UNP A0AAF0BD41
D1	901	HIS	-	expression tag	UNP A0AAF0BD41
D1	902	HIS	-	expression tag	UNP A0AAF0BD41
D1	903	HIS	-	expression tag	UNP A0AAF0BD41
D1	904	HIS	-	expression tag	UNP A0AAF0BD41
D1	905	HIS	-	expression tag	UNP A0AAF0BD41
D1	906	HIS	-	expression tag	UNP A0AAF0BD41
D2	14	MET	-	initiating methionine	UNP A0AAF0BD41
D2	15	ALA	-	expression tag	UNP A0AAF0BD41
D2	16	SER	-	expression tag	UNP A0AAF0BD41
D2	17	MET	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
D2	18	THR	-	expression tag	UNP A0AAF0BD41
D2	19	GLY	-	expression tag	UNP A0AAF0BD41
D2	20	GLY	-	expression tag	UNP A0AAF0BD41
D2	21	GLN	-	expression tag	UNP A0AAF0BD41
D2	22	MET	-	expression tag	UNP A0AAF0BD41
D2	23	GLY	ALA	conflict	UNP A0AAF0BD41
D2	197	MET	VAL	conflict	UNP A0AAF0BD41
D2	298	PRO	LEU	conflict	UNP A0AAF0BD41
D2	306	VAL	ILE	conflict	UNP A0AAF0BD41
D2	439	ALA	GLU	conflict	UNP A0AAF0BD41
D2	751	HIS	TYR	conflict	UNP A0AAF0BD41
D2	774	HIS	TYR	conflict	UNP A0AAF0BD41
D2	805	ALA	SER	conflict	UNP A0AAF0BD41
D2	901	HIS	-	expression tag	UNP A0AAF0BD41
D2	902	HIS	-	expression tag	UNP A0AAF0BD41
D2	903	HIS	-	expression tag	UNP A0AAF0BD41
D2	904	HIS	-	expression tag	UNP A0AAF0BD41
D2	905	HIS	-	expression tag	UNP A0AAF0BD41
D2	906	HIS	-	expression tag	UNP A0AAF0BD41
D3	14	MET	-	initiating methionine	UNP A0AAF0BD41
D3	15	ALA	-	expression tag	UNP A0AAF0BD41
D3	16	SER	-	expression tag	UNP A0AAF0BD41
D3	17	MET	-	expression tag	UNP A0AAF0BD41
D3	18	THR	-	expression tag	UNP A0AAF0BD41
D3	19	GLY	-	expression tag	UNP A0AAF0BD41
D3	20	GLY	-	expression tag	UNP A0AAF0BD41
D3	21	GLN	-	expression tag	UNP A0AAF0BD41
D3	22	MET	-	expression tag	UNP A0AAF0BD41
D3	23	GLY	ALA	conflict	UNP A0AAF0BD41
D3	197	MET	VAL	conflict	UNP A0AAF0BD41
D3	298	PRO	LEU	conflict	UNP A0AAF0BD41
D3	306	VAL	ILE	conflict	UNP A0AAF0BD41
D3	439	ALA	GLU	conflict	UNP A0AAF0BD41
D3	751	HIS	TYR	conflict	UNP A0AAF0BD41
D3	774	HIS	TYR	conflict	UNP A0AAF0BD41
D3	805	ALA	SER	conflict	UNP A0AAF0BD41
D3	901	HIS	-	expression tag	UNP A0AAF0BD41
D3	902	HIS	-	expression tag	UNP A0AAF0BD41
D3	903	HIS	-	expression tag	UNP A0AAF0BD41
D3	904	HIS	-	expression tag	UNP A0AAF0BD41
D3	905	HIS	-	expression tag	UNP A0AAF0BD41
D3	906	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
D4	14	MET	-	initiating methionine	UNP A0AAF0BD41
D4	15	ALA	-	expression tag	UNP A0AAF0BD41
D4	16	SER	-	expression tag	UNP A0AAF0BD41
D4	17	MET	-	expression tag	UNP A0AAF0BD41
D4	18	THR	-	expression tag	UNP A0AAF0BD41
D4	19	GLY	-	expression tag	UNP A0AAF0BD41
D4	20	GLY	-	expression tag	UNP A0AAF0BD41
D4	21	GLN	-	expression tag	UNP A0AAF0BD41
D4	22	MET	-	expression tag	UNP A0AAF0BD41
D4	23	GLY	ALA	conflict	UNP A0AAF0BD41
D4	197	MET	VAL	conflict	UNP A0AAF0BD41
D4	298	PRO	LEU	conflict	UNP A0AAF0BD41
D4	306	VAL	ILE	conflict	UNP A0AAF0BD41
D4	439	ALA	GLU	conflict	UNP A0AAF0BD41
D4	751	HIS	TYR	conflict	UNP A0AAF0BD41
D4	774	HIS	TYR	conflict	UNP A0AAF0BD41
D4	805	ALA	SER	conflict	UNP A0AAF0BD41
D4	901	HIS	-	expression tag	UNP A0AAF0BD41
D4	902	HIS	-	expression tag	UNP A0AAF0BD41
D4	903	HIS	-	expression tag	UNP A0AAF0BD41
D4	904	HIS	-	expression tag	UNP A0AAF0BD41
D4	905	HIS	-	expression tag	UNP A0AAF0BD41
D4	906	HIS	-	expression tag	UNP A0AAF0BD41
D5	14	MET	-	initiating methionine	UNP A0AAF0BD41
D5	15	ALA	-	expression tag	UNP A0AAF0BD41
D5	16	SER	-	expression tag	UNP A0AAF0BD41
D5	17	MET	-	expression tag	UNP A0AAF0BD41
D5	18	THR	-	expression tag	UNP A0AAF0BD41
D5	19	GLY	-	expression tag	UNP A0AAF0BD41
D5	20	GLY	-	expression tag	UNP A0AAF0BD41
D5	21	GLN	-	expression tag	UNP A0AAF0BD41
D5	22	MET	-	expression tag	UNP A0AAF0BD41
D5	23	GLY	ALA	conflict	UNP A0AAF0BD41
D5	197	MET	VAL	conflict	UNP A0AAF0BD41
D5	298	PRO	LEU	conflict	UNP A0AAF0BD41
D5	306	VAL	ILE	conflict	UNP A0AAF0BD41
D5	439	ALA	GLU	conflict	UNP A0AAF0BD41
D5	751	HIS	TYR	conflict	UNP A0AAF0BD41
D5	774	HIS	TYR	conflict	UNP A0AAF0BD41
D5	805	ALA	SER	conflict	UNP A0AAF0BD41
D5	901	HIS	-	expression tag	UNP A0AAF0BD41
D5	902	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
D5	903	HIS	-	expression tag	UNP A0AAF0BD41
D5	904	HIS	-	expression tag	UNP A0AAF0BD41
D5	905	HIS	-	expression tag	UNP A0AAF0BD41
D5	906	HIS	-	expression tag	UNP A0AAF0BD41
E1	14	MET	-	initiating methionine	UNP A0AAF0BD41
E1	15	ALA	-	expression tag	UNP A0AAF0BD41
E1	16	SER	-	expression tag	UNP A0AAF0BD41
E1	17	MET	-	expression tag	UNP A0AAF0BD41
E1	18	THR	-	expression tag	UNP A0AAF0BD41
E1	19	GLY	-	expression tag	UNP A0AAF0BD41
E1	20	GLY	-	expression tag	UNP A0AAF0BD41
E1	21	GLN	-	expression tag	UNP A0AAF0BD41
E1	22	MET	-	expression tag	UNP A0AAF0BD41
E1	23	GLY	ALA	conflict	UNP A0AAF0BD41
E1	197	MET	VAL	conflict	UNP A0AAF0BD41
E1	298	PRO	LEU	conflict	UNP A0AAF0BD41
E1	306	VAL	ILE	conflict	UNP A0AAF0BD41
E1	439	ALA	GLU	conflict	UNP A0AAF0BD41
E1	751	HIS	TYR	conflict	UNP A0AAF0BD41
E1	774	HIS	TYR	conflict	UNP A0AAF0BD41
E1	805	ALA	SER	conflict	UNP A0AAF0BD41
E1	901	HIS	-	expression tag	UNP A0AAF0BD41
E1	902	HIS	-	expression tag	UNP A0AAF0BD41
E1	903	HIS	-	expression tag	UNP A0AAF0BD41
E1	904	HIS	-	expression tag	UNP A0AAF0BD41
E1	905	HIS	-	expression tag	UNP A0AAF0BD41
E1	906	HIS	-	expression tag	UNP A0AAF0BD41
E2	14	MET	-	initiating methionine	UNP A0AAF0BD41
E2	15	ALA	-	expression tag	UNP A0AAF0BD41
E2	16	SER	-	expression tag	UNP A0AAF0BD41
E2	17	MET	-	expression tag	UNP A0AAF0BD41
E2	18	THR	-	expression tag	UNP A0AAF0BD41
E2	19	GLY	-	expression tag	UNP A0AAF0BD41
E2	20	GLY	-	expression tag	UNP A0AAF0BD41
E2	21	GLN	-	expression tag	UNP A0AAF0BD41
E2	22	MET	-	expression tag	UNP A0AAF0BD41
E2	23	GLY	ALA	conflict	UNP A0AAF0BD41
E2	197	MET	VAL	conflict	UNP A0AAF0BD41
E2	298	PRO	LEU	conflict	UNP A0AAF0BD41
E2	306	VAL	ILE	conflict	UNP A0AAF0BD41
E2	439	ALA	GLU	conflict	UNP A0AAF0BD41
E2	751	HIS	TYR	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
E2	774	HIS	TYR	conflict	UNP A0AAF0BD41
E2	805	ALA	SER	conflict	UNP A0AAF0BD41
E2	901	HIS	-	expression tag	UNP A0AAF0BD41
E2	902	HIS	-	expression tag	UNP A0AAF0BD41
E2	903	HIS	-	expression tag	UNP A0AAF0BD41
E2	904	HIS	-	expression tag	UNP A0AAF0BD41
E2	905	HIS	-	expression tag	UNP A0AAF0BD41
E2	906	HIS	-	expression tag	UNP A0AAF0BD41
E3	14	MET	-	initiating methionine	UNP A0AAF0BD41
E3	15	ALA	-	expression tag	UNP A0AAF0BD41
E3	16	SER	-	expression tag	UNP A0AAF0BD41
E3	17	MET	-	expression tag	UNP A0AAF0BD41
E3	18	THR	-	expression tag	UNP A0AAF0BD41
E3	19	GLY	-	expression tag	UNP A0AAF0BD41
E3	20	GLY	-	expression tag	UNP A0AAF0BD41
E3	21	GLN	-	expression tag	UNP A0AAF0BD41
E3	22	MET	-	expression tag	UNP A0AAF0BD41
E3	23	GLY	ALA	conflict	UNP A0AAF0BD41
E3	197	MET	VAL	conflict	UNP A0AAF0BD41
E3	298	PRO	LEU	conflict	UNP A0AAF0BD41
E3	306	VAL	ILE	conflict	UNP A0AAF0BD41
E3	439	ALA	GLU	conflict	UNP A0AAF0BD41
E3	751	HIS	TYR	conflict	UNP A0AAF0BD41
E3	774	HIS	TYR	conflict	UNP A0AAF0BD41
E3	805	ALA	SER	conflict	UNP A0AAF0BD41
E3	901	HIS	-	expression tag	UNP A0AAF0BD41
E3	902	HIS	-	expression tag	UNP A0AAF0BD41
E3	903	HIS	-	expression tag	UNP A0AAF0BD41
E3	904	HIS	-	expression tag	UNP A0AAF0BD41
E3	905	HIS	-	expression tag	UNP A0AAF0BD41
E3	906	HIS	-	expression tag	UNP A0AAF0BD41
E4	14	MET	-	initiating methionine	UNP A0AAF0BD41
E4	15	ALA	-	expression tag	UNP A0AAF0BD41
E4	16	SER	-	expression tag	UNP A0AAF0BD41
E4	17	MET	-	expression tag	UNP A0AAF0BD41
E4	18	THR	-	expression tag	UNP A0AAF0BD41
E4	19	GLY	-	expression tag	UNP A0AAF0BD41
E4	20	GLY	-	expression tag	UNP A0AAF0BD41
E4	21	GLN	-	expression tag	UNP A0AAF0BD41
E4	22	MET	-	expression tag	UNP A0AAF0BD41
E4	23	GLY	ALA	conflict	UNP A0AAF0BD41
E4	197	MET	VAL	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
E4	298	PRO	LEU	conflict	UNP A0AAF0BD41
E4	306	VAL	ILE	conflict	UNP A0AAF0BD41
E4	439	ALA	GLU	conflict	UNP A0AAF0BD41
E4	751	HIS	TYR	conflict	UNP A0AAF0BD41
E4	774	HIS	TYR	conflict	UNP A0AAF0BD41
E4	805	ALA	SER	conflict	UNP A0AAF0BD41
E4	901	HIS	-	expression tag	UNP A0AAF0BD41
E4	902	HIS	-	expression tag	UNP A0AAF0BD41
E4	903	HIS	-	expression tag	UNP A0AAF0BD41
E4	904	HIS	-	expression tag	UNP A0AAF0BD41
E4	905	HIS	-	expression tag	UNP A0AAF0BD41
E4	906	HIS	-	expression tag	UNP A0AAF0BD41
E5	14	MET	-	initiating methionine	UNP A0AAF0BD41
E5	15	ALA	-	expression tag	UNP A0AAF0BD41
E5	16	SER	-	expression tag	UNP A0AAF0BD41
E5	17	MET	-	expression tag	UNP A0AAF0BD41
E5	18	THR	-	expression tag	UNP A0AAF0BD41
E5	19	GLY	-	expression tag	UNP A0AAF0BD41
E5	20	GLY	-	expression tag	UNP A0AAF0BD41
E5	21	GLN	-	expression tag	UNP A0AAF0BD41
E5	22	MET	-	expression tag	UNP A0AAF0BD41
E5	23	GLY	ALA	conflict	UNP A0AAF0BD41
E5	197	MET	VAL	conflict	UNP A0AAF0BD41
E5	298	PRO	LEU	conflict	UNP A0AAF0BD41
E5	306	VAL	ILE	conflict	UNP A0AAF0BD41
E5	439	ALA	GLU	conflict	UNP A0AAF0BD41
E5	751	HIS	TYR	conflict	UNP A0AAF0BD41
E5	774	HIS	TYR	conflict	UNP A0AAF0BD41
E5	805	ALA	SER	conflict	UNP A0AAF0BD41
E5	901	HIS	-	expression tag	UNP A0AAF0BD41
E5	902	HIS	-	expression tag	UNP A0AAF0BD41
E5	903	HIS	-	expression tag	UNP A0AAF0BD41
E5	904	HIS	-	expression tag	UNP A0AAF0BD41
E5	905	HIS	-	expression tag	UNP A0AAF0BD41
E5	906	HIS	-	expression tag	UNP A0AAF0BD41
F1	14	MET	-	initiating methionine	UNP A0AAF0BD41
F1	15	ALA	-	expression tag	UNP A0AAF0BD41
F1	16	SER	-	expression tag	UNP A0AAF0BD41
F1	17	MET	-	expression tag	UNP A0AAF0BD41
F1	18	THR	-	expression tag	UNP A0AAF0BD41
F1	19	GLY	-	expression tag	UNP A0AAF0BD41
F1	20	GLY	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
F1	21	GLN	-	expression tag	UNP A0AAF0BD41
F1	22	MET	-	expression tag	UNP A0AAF0BD41
F1	23	GLY	ALA	conflict	UNP A0AAF0BD41
F1	197	MET	VAL	conflict	UNP A0AAF0BD41
F1	298	PRO	LEU	conflict	UNP A0AAF0BD41
F1	306	VAL	ILE	conflict	UNP A0AAF0BD41
F1	439	ALA	GLU	conflict	UNP A0AAF0BD41
F1	751	HIS	TYR	conflict	UNP A0AAF0BD41
F1	774	HIS	TYR	conflict	UNP A0AAF0BD41
F1	805	ALA	SER	conflict	UNP A0AAF0BD41
F1	901	HIS	-	expression tag	UNP A0AAF0BD41
F1	902	HIS	-	expression tag	UNP A0AAF0BD41
F1	903	HIS	-	expression tag	UNP A0AAF0BD41
F1	904	HIS	-	expression tag	UNP A0AAF0BD41
F1	905	HIS	-	expression tag	UNP A0AAF0BD41
F1	906	HIS	-	expression tag	UNP A0AAF0BD41
F2	14	MET	-	initiating methionine	UNP A0AAF0BD41
F2	15	ALA	-	expression tag	UNP A0AAF0BD41
F2	16	SER	-	expression tag	UNP A0AAF0BD41
F2	17	MET	-	expression tag	UNP A0AAF0BD41
F2	18	THR	-	expression tag	UNP A0AAF0BD41
F2	19	GLY	-	expression tag	UNP A0AAF0BD41
F2	20	GLY	-	expression tag	UNP A0AAF0BD41
F2	21	GLN	-	expression tag	UNP A0AAF0BD41
F2	22	MET	-	expression tag	UNP A0AAF0BD41
F2	23	GLY	ALA	conflict	UNP A0AAF0BD41
F2	197	MET	VAL	conflict	UNP A0AAF0BD41
F2	298	PRO	LEU	conflict	UNP A0AAF0BD41
F2	306	VAL	ILE	conflict	UNP A0AAF0BD41
F2	439	ALA	GLU	conflict	UNP A0AAF0BD41
F2	751	HIS	TYR	conflict	UNP A0AAF0BD41
F2	774	HIS	TYR	conflict	UNP A0AAF0BD41
F2	805	ALA	SER	conflict	UNP A0AAF0BD41
F2	901	HIS	-	expression tag	UNP A0AAF0BD41
F2	902	HIS	-	expression tag	UNP A0AAF0BD41
F2	903	HIS	-	expression tag	UNP A0AAF0BD41
F2	904	HIS	-	expression tag	UNP A0AAF0BD41
F2	905	HIS	-	expression tag	UNP A0AAF0BD41
F2	906	HIS	-	expression tag	UNP A0AAF0BD41
F3	14	MET	-	initiating methionine	UNP A0AAF0BD41
F3	15	ALA	-	expression tag	UNP A0AAF0BD41
F3	16	SER	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
F3	17	MET	-	expression tag	UNP A0AAF0BD41
F3	18	THR	-	expression tag	UNP A0AAF0BD41
F3	19	GLY	-	expression tag	UNP A0AAF0BD41
F3	20	GLY	-	expression tag	UNP A0AAF0BD41
F3	21	GLN	-	expression tag	UNP A0AAF0BD41
F3	22	MET	-	expression tag	UNP A0AAF0BD41
F3	23	GLY	ALA	conflict	UNP A0AAF0BD41
F3	197	MET	VAL	conflict	UNP A0AAF0BD41
F3	298	PRO	LEU	conflict	UNP A0AAF0BD41
F3	306	VAL	ILE	conflict	UNP A0AAF0BD41
F3	439	ALA	GLU	conflict	UNP A0AAF0BD41
F3	751	HIS	TYR	conflict	UNP A0AAF0BD41
F3	774	HIS	TYR	conflict	UNP A0AAF0BD41
F3	805	ALA	SER	conflict	UNP A0AAF0BD41
F3	901	HIS	-	expression tag	UNP A0AAF0BD41
F3	902	HIS	-	expression tag	UNP A0AAF0BD41
F3	903	HIS	-	expression tag	UNP A0AAF0BD41
F3	904	HIS	-	expression tag	UNP A0AAF0BD41
F3	905	HIS	-	expression tag	UNP A0AAF0BD41
F3	906	HIS	-	expression tag	UNP A0AAF0BD41
F4	14	MET	-	initiating methionine	UNP A0AAF0BD41
F4	15	ALA	-	expression tag	UNP A0AAF0BD41
F4	16	SER	-	expression tag	UNP A0AAF0BD41
F4	17	MET	-	expression tag	UNP A0AAF0BD41
F4	18	THR	-	expression tag	UNP A0AAF0BD41
F4	19	GLY	-	expression tag	UNP A0AAF0BD41
F4	20	GLY	-	expression tag	UNP A0AAF0BD41
F4	21	GLN	-	expression tag	UNP A0AAF0BD41
F4	22	MET	-	expression tag	UNP A0AAF0BD41
F4	23	GLY	ALA	conflict	UNP A0AAF0BD41
F4	197	MET	VAL	conflict	UNP A0AAF0BD41
F4	298	PRO	LEU	conflict	UNP A0AAF0BD41
F4	306	VAL	ILE	conflict	UNP A0AAF0BD41
F4	439	ALA	GLU	conflict	UNP A0AAF0BD41
F4	751	HIS	TYR	conflict	UNP A0AAF0BD41
F4	774	HIS	TYR	conflict	UNP A0AAF0BD41
F4	805	ALA	SER	conflict	UNP A0AAF0BD41
F4	901	HIS	-	expression tag	UNP A0AAF0BD41
F4	902	HIS	-	expression tag	UNP A0AAF0BD41
F4	903	HIS	-	expression tag	UNP A0AAF0BD41
F4	904	HIS	-	expression tag	UNP A0AAF0BD41
F4	905	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
F4	906	HIS	-	expression tag	UNP A0AAF0BD41
F5	14	MET	-	initiating methionine	UNP A0AAF0BD41
F5	15	ALA	-	expression tag	UNP A0AAF0BD41
F5	16	SER	-	expression tag	UNP A0AAF0BD41
F5	17	MET	-	expression tag	UNP A0AAF0BD41
F5	18	THR	-	expression tag	UNP A0AAF0BD41
F5	19	GLY	-	expression tag	UNP A0AAF0BD41
F5	20	GLY	-	expression tag	UNP A0AAF0BD41
F5	21	GLN	-	expression tag	UNP A0AAF0BD41
F5	22	MET	-	expression tag	UNP A0AAF0BD41
F5	23	GLY	ALA	conflict	UNP A0AAF0BD41
F5	197	MET	VAL	conflict	UNP A0AAF0BD41
F5	298	PRO	LEU	conflict	UNP A0AAF0BD41
F5	306	VAL	ILE	conflict	UNP A0AAF0BD41
F5	439	ALA	GLU	conflict	UNP A0AAF0BD41
F5	751	HIS	TYR	conflict	UNP A0AAF0BD41
F5	774	HIS	TYR	conflict	UNP A0AAF0BD41
F5	805	ALA	SER	conflict	UNP A0AAF0BD41
F5	901	HIS	-	expression tag	UNP A0AAF0BD41
F5	902	HIS	-	expression tag	UNP A0AAF0BD41
F5	903	HIS	-	expression tag	UNP A0AAF0BD41
F5	904	HIS	-	expression tag	UNP A0AAF0BD41
F5	905	HIS	-	expression tag	UNP A0AAF0BD41
F5	906	HIS	-	expression tag	UNP A0AAF0BD41
G1	14	MET	-	initiating methionine	UNP A0AAF0BD41
G1	15	ALA	-	expression tag	UNP A0AAF0BD41
G1	16	SER	-	expression tag	UNP A0AAF0BD41
G1	17	MET	-	expression tag	UNP A0AAF0BD41
G1	18	THR	-	expression tag	UNP A0AAF0BD41
G1	19	GLY	-	expression tag	UNP A0AAF0BD41
G1	20	GLY	-	expression tag	UNP A0AAF0BD41
G1	21	GLN	-	expression tag	UNP A0AAF0BD41
G1	22	MET	-	expression tag	UNP A0AAF0BD41
G1	23	GLY	ALA	conflict	UNP A0AAF0BD41
G1	197	MET	VAL	conflict	UNP A0AAF0BD41
G1	298	PRO	LEU	conflict	UNP A0AAF0BD41
G1	306	VAL	ILE	conflict	UNP A0AAF0BD41
G1	439	ALA	GLU	conflict	UNP A0AAF0BD41
G1	751	HIS	TYR	conflict	UNP A0AAF0BD41
G1	774	HIS	TYR	conflict	UNP A0AAF0BD41
G1	805	ALA	SER	conflict	UNP A0AAF0BD41
G1	901	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
G1	902	HIS	-	expression tag	UNP A0AAF0BD41
G1	903	HIS	-	expression tag	UNP A0AAF0BD41
G1	904	HIS	-	expression tag	UNP A0AAF0BD41
G1	905	HIS	-	expression tag	UNP A0AAF0BD41
G1	906	HIS	-	expression tag	UNP A0AAF0BD41
G2	14	MET	-	initiating methionine	UNP A0AAF0BD41
G2	15	ALA	-	expression tag	UNP A0AAF0BD41
G2	16	SER	-	expression tag	UNP A0AAF0BD41
G2	17	MET	-	expression tag	UNP A0AAF0BD41
G2	18	THR	-	expression tag	UNP A0AAF0BD41
G2	19	GLY	-	expression tag	UNP A0AAF0BD41
G2	20	GLY	-	expression tag	UNP A0AAF0BD41
G2	21	GLN	-	expression tag	UNP A0AAF0BD41
G2	22	MET	-	expression tag	UNP A0AAF0BD41
G2	23	GLY	ALA	conflict	UNP A0AAF0BD41
G2	197	MET	VAL	conflict	UNP A0AAF0BD41
G2	298	PRO	LEU	conflict	UNP A0AAF0BD41
G2	306	VAL	ILE	conflict	UNP A0AAF0BD41
G2	439	ALA	GLU	conflict	UNP A0AAF0BD41
G2	751	HIS	TYR	conflict	UNP A0AAF0BD41
G2	774	HIS	TYR	conflict	UNP A0AAF0BD41
G2	805	ALA	SER	conflict	UNP A0AAF0BD41
G2	901	HIS	-	expression tag	UNP A0AAF0BD41
G2	902	HIS	-	expression tag	UNP A0AAF0BD41
G2	903	HIS	-	expression tag	UNP A0AAF0BD41
G2	904	HIS	-	expression tag	UNP A0AAF0BD41
G2	905	HIS	-	expression tag	UNP A0AAF0BD41
G2	906	HIS	-	expression tag	UNP A0AAF0BD41
G3	14	MET	-	initiating methionine	UNP A0AAF0BD41
G3	15	ALA	-	expression tag	UNP A0AAF0BD41
G3	16	SER	-	expression tag	UNP A0AAF0BD41
G3	17	MET	-	expression tag	UNP A0AAF0BD41
G3	18	THR	-	expression tag	UNP A0AAF0BD41
G3	19	GLY	-	expression tag	UNP A0AAF0BD41
G3	20	GLY	-	expression tag	UNP A0AAF0BD41
G3	21	GLN	-	expression tag	UNP A0AAF0BD41
G3	22	MET	-	expression tag	UNP A0AAF0BD41
G3	23	GLY	ALA	conflict	UNP A0AAF0BD41
G3	197	MET	VAL	conflict	UNP A0AAF0BD41
G3	298	PRO	LEU	conflict	UNP A0AAF0BD41
G3	306	VAL	ILE	conflict	UNP A0AAF0BD41
G3	439	ALA	GLU	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
G3	751	HIS	TYR	conflict	UNP A0AAF0BD41
G3	774	HIS	TYR	conflict	UNP A0AAF0BD41
G3	805	ALA	SER	conflict	UNP A0AAF0BD41
G3	901	HIS	-	expression tag	UNP A0AAF0BD41
G3	902	HIS	-	expression tag	UNP A0AAF0BD41
G3	903	HIS	-	expression tag	UNP A0AAF0BD41
G3	904	HIS	-	expression tag	UNP A0AAF0BD41
G3	905	HIS	-	expression tag	UNP A0AAF0BD41
G3	906	HIS	-	expression tag	UNP A0AAF0BD41
G4	14	MET	-	initiating methionine	UNP A0AAF0BD41
G4	15	ALA	-	expression tag	UNP A0AAF0BD41
G4	16	SER	-	expression tag	UNP A0AAF0BD41
G4	17	MET	-	expression tag	UNP A0AAF0BD41
G4	18	THR	-	expression tag	UNP A0AAF0BD41
G4	19	GLY	-	expression tag	UNP A0AAF0BD41
G4	20	GLY	-	expression tag	UNP A0AAF0BD41
G4	21	GLN	-	expression tag	UNP A0AAF0BD41
G4	22	MET	-	expression tag	UNP A0AAF0BD41
G4	23	GLY	ALA	conflict	UNP A0AAF0BD41
G4	197	MET	VAL	conflict	UNP A0AAF0BD41
G4	298	PRO	LEU	conflict	UNP A0AAF0BD41
G4	306	VAL	ILE	conflict	UNP A0AAF0BD41
G4	439	ALA	GLU	conflict	UNP A0AAF0BD41
G4	751	HIS	TYR	conflict	UNP A0AAF0BD41
G4	774	HIS	TYR	conflict	UNP A0AAF0BD41
G4	805	ALA	SER	conflict	UNP A0AAF0BD41
G4	901	HIS	-	expression tag	UNP A0AAF0BD41
G4	902	HIS	-	expression tag	UNP A0AAF0BD41
G4	903	HIS	-	expression tag	UNP A0AAF0BD41
G4	904	HIS	-	expression tag	UNP A0AAF0BD41
G4	905	HIS	-	expression tag	UNP A0AAF0BD41
G4	906	HIS	-	expression tag	UNP A0AAF0BD41
G5	14	MET	-	initiating methionine	UNP A0AAF0BD41
G5	15	ALA	-	expression tag	UNP A0AAF0BD41
G5	16	SER	-	expression tag	UNP A0AAF0BD41
G5	17	MET	-	expression tag	UNP A0AAF0BD41
G5	18	THR	-	expression tag	UNP A0AAF0BD41
G5	19	GLY	-	expression tag	UNP A0AAF0BD41
G5	20	GLY	-	expression tag	UNP A0AAF0BD41
G5	21	GLN	-	expression tag	UNP A0AAF0BD41
G5	22	MET	-	expression tag	UNP A0AAF0BD41
G5	23	GLY	ALA	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
G5	197	MET	VAL	conflict	UNP A0AAF0BD41
G5	298	PRO	LEU	conflict	UNP A0AAF0BD41
G5	306	VAL	ILE	conflict	UNP A0AAF0BD41
G5	439	ALA	GLU	conflict	UNP A0AAF0BD41
G5	751	HIS	TYR	conflict	UNP A0AAF0BD41
G5	774	HIS	TYR	conflict	UNP A0AAF0BD41
G5	805	ALA	SER	conflict	UNP A0AAF0BD41
G5	901	HIS	-	expression tag	UNP A0AAF0BD41
G5	902	HIS	-	expression tag	UNP A0AAF0BD41
G5	903	HIS	-	expression tag	UNP A0AAF0BD41
G5	904	HIS	-	expression tag	UNP A0AAF0BD41
G5	905	HIS	-	expression tag	UNP A0AAF0BD41
G5	906	HIS	-	expression tag	UNP A0AAF0BD41
H1	14	MET	-	initiating methionine	UNP A0AAF0BD41
H1	15	ALA	-	expression tag	UNP A0AAF0BD41
H1	16	SER	-	expression tag	UNP A0AAF0BD41
H1	17	MET	-	expression tag	UNP A0AAF0BD41
H1	18	THR	-	expression tag	UNP A0AAF0BD41
H1	19	GLY	-	expression tag	UNP A0AAF0BD41
H1	20	GLY	-	expression tag	UNP A0AAF0BD41
H1	21	GLN	-	expression tag	UNP A0AAF0BD41
H1	22	MET	-	expression tag	UNP A0AAF0BD41
H1	23	GLY	ALA	conflict	UNP A0AAF0BD41
H1	197	MET	VAL	conflict	UNP A0AAF0BD41
H1	298	PRO	LEU	conflict	UNP A0AAF0BD41
H1	306	VAL	ILE	conflict	UNP A0AAF0BD41
H1	439	ALA	GLU	conflict	UNP A0AAF0BD41
H1	751	HIS	TYR	conflict	UNP A0AAF0BD41
H1	774	HIS	TYR	conflict	UNP A0AAF0BD41
H1	805	ALA	SER	conflict	UNP A0AAF0BD41
H1	901	HIS	-	expression tag	UNP A0AAF0BD41
H1	902	HIS	-	expression tag	UNP A0AAF0BD41
H1	903	HIS	-	expression tag	UNP A0AAF0BD41
H1	904	HIS	-	expression tag	UNP A0AAF0BD41
H1	905	HIS	-	expression tag	UNP A0AAF0BD41
H1	906	HIS	-	expression tag	UNP A0AAF0BD41
H2	14	MET	-	initiating methionine	UNP A0AAF0BD41
H2	15	ALA	-	expression tag	UNP A0AAF0BD41
H2	16	SER	-	expression tag	UNP A0AAF0BD41
H2	17	MET	-	expression tag	UNP A0AAF0BD41
H2	18	THR	-	expression tag	UNP A0AAF0BD41
H2	19	GLY	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
H2	20	GLY	-	expression tag	UNP A0AAF0BD41
H2	21	GLN	-	expression tag	UNP A0AAF0BD41
H2	22	MET	-	expression tag	UNP A0AAF0BD41
H2	23	GLY	ALA	conflict	UNP A0AAF0BD41
H2	197	MET	VAL	conflict	UNP A0AAF0BD41
H2	298	PRO	LEU	conflict	UNP A0AAF0BD41
H2	306	VAL	ILE	conflict	UNP A0AAF0BD41
H2	439	ALA	GLU	conflict	UNP A0AAF0BD41
H2	751	HIS	TYR	conflict	UNP A0AAF0BD41
H2	774	HIS	TYR	conflict	UNP A0AAF0BD41
H2	805	ALA	SER	conflict	UNP A0AAF0BD41
H2	901	HIS	-	expression tag	UNP A0AAF0BD41
H2	902	HIS	-	expression tag	UNP A0AAF0BD41
H2	903	HIS	-	expression tag	UNP A0AAF0BD41
H2	904	HIS	-	expression tag	UNP A0AAF0BD41
H2	905	HIS	-	expression tag	UNP A0AAF0BD41
H2	906	HIS	-	expression tag	UNP A0AAF0BD41
H3	14	MET	-	initiating methionine	UNP A0AAF0BD41
H3	15	ALA	-	expression tag	UNP A0AAF0BD41
H3	16	SER	-	expression tag	UNP A0AAF0BD41
H3	17	MET	-	expression tag	UNP A0AAF0BD41
H3	18	THR	-	expression tag	UNP A0AAF0BD41
H3	19	GLY	-	expression tag	UNP A0AAF0BD41
H3	20	GLY	-	expression tag	UNP A0AAF0BD41
H3	21	GLN	-	expression tag	UNP A0AAF0BD41
H3	22	MET	-	expression tag	UNP A0AAF0BD41
H3	23	GLY	ALA	conflict	UNP A0AAF0BD41
H3	197	MET	VAL	conflict	UNP A0AAF0BD41
H3	298	PRO	LEU	conflict	UNP A0AAF0BD41
H3	306	VAL	ILE	conflict	UNP A0AAF0BD41
H3	439	ALA	GLU	conflict	UNP A0AAF0BD41
H3	751	HIS	TYR	conflict	UNP A0AAF0BD41
H3	774	HIS	TYR	conflict	UNP A0AAF0BD41
H3	805	ALA	SER	conflict	UNP A0AAF0BD41
H3	901	HIS	-	expression tag	UNP A0AAF0BD41
H3	902	HIS	-	expression tag	UNP A0AAF0BD41
H3	903	HIS	-	expression tag	UNP A0AAF0BD41
H3	904	HIS	-	expression tag	UNP A0AAF0BD41
H3	905	HIS	-	expression tag	UNP A0AAF0BD41
H3	906	HIS	-	expression tag	UNP A0AAF0BD41
H4	14	MET	-	initiating methionine	UNP A0AAF0BD41
H4	15	ALA	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
H4	16	SER	-	expression tag	UNP A0AAF0BD41
H4	17	MET	-	expression tag	UNP A0AAF0BD41
H4	18	THR	-	expression tag	UNP A0AAF0BD41
H4	19	GLY	-	expression tag	UNP A0AAF0BD41
H4	20	GLY	-	expression tag	UNP A0AAF0BD41
H4	21	GLN	-	expression tag	UNP A0AAF0BD41
H4	22	MET	-	expression tag	UNP A0AAF0BD41
H4	23	GLY	ALA	conflict	UNP A0AAF0BD41
H4	197	MET	VAL	conflict	UNP A0AAF0BD41
H4	298	PRO	LEU	conflict	UNP A0AAF0BD41
H4	306	VAL	ILE	conflict	UNP A0AAF0BD41
H4	439	ALA	GLU	conflict	UNP A0AAF0BD41
H4	751	HIS	TYR	conflict	UNP A0AAF0BD41
H4	774	HIS	TYR	conflict	UNP A0AAF0BD41
H4	805	ALA	SER	conflict	UNP A0AAF0BD41
H4	901	HIS	-	expression tag	UNP A0AAF0BD41
H4	902	HIS	-	expression tag	UNP A0AAF0BD41
H4	903	HIS	-	expression tag	UNP A0AAF0BD41
H4	904	HIS	-	expression tag	UNP A0AAF0BD41
H4	905	HIS	-	expression tag	UNP A0AAF0BD41
H4	906	HIS	-	expression tag	UNP A0AAF0BD41
H5	14	MET	-	initiating methionine	UNP A0AAF0BD41
H5	15	ALA	-	expression tag	UNP A0AAF0BD41
H5	16	SER	-	expression tag	UNP A0AAF0BD41
H5	17	MET	-	expression tag	UNP A0AAF0BD41
H5	18	THR	-	expression tag	UNP A0AAF0BD41
H5	19	GLY	-	expression tag	UNP A0AAF0BD41
H5	20	GLY	-	expression tag	UNP A0AAF0BD41
H5	21	GLN	-	expression tag	UNP A0AAF0BD41
H5	22	MET	-	expression tag	UNP A0AAF0BD41
H5	23	GLY	ALA	conflict	UNP A0AAF0BD41
H5	197	MET	VAL	conflict	UNP A0AAF0BD41
H5	298	PRO	LEU	conflict	UNP A0AAF0BD41
H5	306	VAL	ILE	conflict	UNP A0AAF0BD41
H5	439	ALA	GLU	conflict	UNP A0AAF0BD41
H5	751	HIS	TYR	conflict	UNP A0AAF0BD41
H5	774	HIS	TYR	conflict	UNP A0AAF0BD41
H5	805	ALA	SER	conflict	UNP A0AAF0BD41
H5	901	HIS	-	expression tag	UNP A0AAF0BD41
H5	902	HIS	-	expression tag	UNP A0AAF0BD41
H5	903	HIS	-	expression tag	UNP A0AAF0BD41
H5	904	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
H5	905	HIS	-	expression tag	UNP A0AAF0BD41
H5	906	HIS	-	expression tag	UNP A0AAF0BD41
I1	14	MET	-	initiating methionine	UNP A0AAF0BD41
I1	15	ALA	-	expression tag	UNP A0AAF0BD41
I1	16	SER	-	expression tag	UNP A0AAF0BD41
I1	17	MET	-	expression tag	UNP A0AAF0BD41
I1	18	THR	-	expression tag	UNP A0AAF0BD41
I1	19	GLY	-	expression tag	UNP A0AAF0BD41
I1	20	GLY	-	expression tag	UNP A0AAF0BD41
I1	21	GLN	-	expression tag	UNP A0AAF0BD41
I1	22	MET	-	expression tag	UNP A0AAF0BD41
I1	23	GLY	ALA	conflict	UNP A0AAF0BD41
I1	197	MET	VAL	conflict	UNP A0AAF0BD41
I1	298	PRO	LEU	conflict	UNP A0AAF0BD41
I1	306	VAL	ILE	conflict	UNP A0AAF0BD41
I1	439	ALA	GLU	conflict	UNP A0AAF0BD41
I1	751	HIS	TYR	conflict	UNP A0AAF0BD41
I1	774	HIS	TYR	conflict	UNP A0AAF0BD41
I1	805	ALA	SER	conflict	UNP A0AAF0BD41
I1	901	HIS	-	expression tag	UNP A0AAF0BD41
I1	902	HIS	-	expression tag	UNP A0AAF0BD41
I1	903	HIS	-	expression tag	UNP A0AAF0BD41
I1	904	HIS	-	expression tag	UNP A0AAF0BD41
I1	905	HIS	-	expression tag	UNP A0AAF0BD41
I1	906	HIS	-	expression tag	UNP A0AAF0BD41
I2	14	MET	-	initiating methionine	UNP A0AAF0BD41
I2	15	ALA	-	expression tag	UNP A0AAF0BD41
I2	16	SER	-	expression tag	UNP A0AAF0BD41
I2	17	MET	-	expression tag	UNP A0AAF0BD41
I2	18	THR	-	expression tag	UNP A0AAF0BD41
I2	19	GLY	-	expression tag	UNP A0AAF0BD41
I2	20	GLY	-	expression tag	UNP A0AAF0BD41
I2	21	GLN	-	expression tag	UNP A0AAF0BD41
I2	22	MET	-	expression tag	UNP A0AAF0BD41
I2	23	GLY	ALA	conflict	UNP A0AAF0BD41
I2	197	MET	VAL	conflict	UNP A0AAF0BD41
I2	298	PRO	LEU	conflict	UNP A0AAF0BD41
I2	306	VAL	ILE	conflict	UNP A0AAF0BD41
I2	439	ALA	GLU	conflict	UNP A0AAF0BD41
I2	751	HIS	TYR	conflict	UNP A0AAF0BD41
I2	774	HIS	TYR	conflict	UNP A0AAF0BD41
I2	805	ALA	SER	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
I2	901	HIS	-	expression tag	UNP A0AAF0BD41
I2	902	HIS	-	expression tag	UNP A0AAF0BD41
I2	903	HIS	-	expression tag	UNP A0AAF0BD41
I2	904	HIS	-	expression tag	UNP A0AAF0BD41
I2	905	HIS	-	expression tag	UNP A0AAF0BD41
I2	906	HIS	-	expression tag	UNP A0AAF0BD41
I3	14	MET	-	initiating methionine	UNP A0AAF0BD41
I3	15	ALA	-	expression tag	UNP A0AAF0BD41
I3	16	SER	-	expression tag	UNP A0AAF0BD41
I3	17	MET	-	expression tag	UNP A0AAF0BD41
I3	18	THR	-	expression tag	UNP A0AAF0BD41
I3	19	GLY	-	expression tag	UNP A0AAF0BD41
I3	20	GLY	-	expression tag	UNP A0AAF0BD41
I3	21	GLN	-	expression tag	UNP A0AAF0BD41
I3	22	MET	-	expression tag	UNP A0AAF0BD41
I3	23	GLY	ALA	conflict	UNP A0AAF0BD41
I3	197	MET	VAL	conflict	UNP A0AAF0BD41
I3	298	PRO	LEU	conflict	UNP A0AAF0BD41
I3	306	VAL	ILE	conflict	UNP A0AAF0BD41
I3	439	ALA	GLU	conflict	UNP A0AAF0BD41
I3	751	HIS	TYR	conflict	UNP A0AAF0BD41
I3	774	HIS	TYR	conflict	UNP A0AAF0BD41
I3	805	ALA	SER	conflict	UNP A0AAF0BD41
I3	901	HIS	-	expression tag	UNP A0AAF0BD41
I3	902	HIS	-	expression tag	UNP A0AAF0BD41
I3	903	HIS	-	expression tag	UNP A0AAF0BD41
I3	904	HIS	-	expression tag	UNP A0AAF0BD41
I3	905	HIS	-	expression tag	UNP A0AAF0BD41
I3	906	HIS	-	expression tag	UNP A0AAF0BD41
I4	14	MET	-	initiating methionine	UNP A0AAF0BD41
I4	15	ALA	-	expression tag	UNP A0AAF0BD41
I4	16	SER	-	expression tag	UNP A0AAF0BD41
I4	17	MET	-	expression tag	UNP A0AAF0BD41
I4	18	THR	-	expression tag	UNP A0AAF0BD41
I4	19	GLY	-	expression tag	UNP A0AAF0BD41
I4	20	GLY	-	expression tag	UNP A0AAF0BD41
I4	21	GLN	-	expression tag	UNP A0AAF0BD41
I4	22	MET	-	expression tag	UNP A0AAF0BD41
I4	23	GLY	ALA	conflict	UNP A0AAF0BD41
I4	197	MET	VAL	conflict	UNP A0AAF0BD41
I4	298	PRO	LEU	conflict	UNP A0AAF0BD41
I4	306	VAL	ILE	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
I4	439	ALA	GLU	conflict	UNP A0AAF0BD41
I4	751	HIS	TYR	conflict	UNP A0AAF0BD41
I4	774	HIS	TYR	conflict	UNP A0AAF0BD41
I4	805	ALA	SER	conflict	UNP A0AAF0BD41
I4	901	HIS	-	expression tag	UNP A0AAF0BD41
I4	902	HIS	-	expression tag	UNP A0AAF0BD41
I4	903	HIS	-	expression tag	UNP A0AAF0BD41
I4	904	HIS	-	expression tag	UNP A0AAF0BD41
I4	905	HIS	-	expression tag	UNP A0AAF0BD41
I4	906	HIS	-	expression tag	UNP A0AAF0BD41
I5	14	MET	-	initiating methionine	UNP A0AAF0BD41
I5	15	ALA	-	expression tag	UNP A0AAF0BD41
I5	16	SER	-	expression tag	UNP A0AAF0BD41
I5	17	MET	-	expression tag	UNP A0AAF0BD41
I5	18	THR	-	expression tag	UNP A0AAF0BD41
I5	19	GLY	-	expression tag	UNP A0AAF0BD41
I5	20	GLY	-	expression tag	UNP A0AAF0BD41
I5	21	GLN	-	expression tag	UNP A0AAF0BD41
I5	22	MET	-	expression tag	UNP A0AAF0BD41
I5	23	GLY	ALA	conflict	UNP A0AAF0BD41
I5	197	MET	VAL	conflict	UNP A0AAF0BD41
I5	298	PRO	LEU	conflict	UNP A0AAF0BD41
I5	306	VAL	ILE	conflict	UNP A0AAF0BD41
I5	439	ALA	GLU	conflict	UNP A0AAF0BD41
I5	751	HIS	TYR	conflict	UNP A0AAF0BD41
I5	774	HIS	TYR	conflict	UNP A0AAF0BD41
I5	805	ALA	SER	conflict	UNP A0AAF0BD41
I5	901	HIS	-	expression tag	UNP A0AAF0BD41
I5	902	HIS	-	expression tag	UNP A0AAF0BD41
I5	903	HIS	-	expression tag	UNP A0AAF0BD41
I5	904	HIS	-	expression tag	UNP A0AAF0BD41
I5	905	HIS	-	expression tag	UNP A0AAF0BD41
I5	906	HIS	-	expression tag	UNP A0AAF0BD41
J1	14	MET	-	initiating methionine	UNP A0AAF0BD41
J1	15	ALA	-	expression tag	UNP A0AAF0BD41
J1	16	SER	-	expression tag	UNP A0AAF0BD41
J1	17	MET	-	expression tag	UNP A0AAF0BD41
J1	18	THR	-	expression tag	UNP A0AAF0BD41
J1	19	GLY	-	expression tag	UNP A0AAF0BD41
J1	20	GLY	-	expression tag	UNP A0AAF0BD41
J1	21	GLN	-	expression tag	UNP A0AAF0BD41
J1	22	MET	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
J1	23	GLY	ALA	conflict	UNP A0AAF0BD41
J1	197	MET	VAL	conflict	UNP A0AAF0BD41
J1	298	PRO	LEU	conflict	UNP A0AAF0BD41
J1	306	VAL	ILE	conflict	UNP A0AAF0BD41
J1	439	ALA	GLU	conflict	UNP A0AAF0BD41
J1	751	HIS	TYR	conflict	UNP A0AAF0BD41
J1	774	HIS	TYR	conflict	UNP A0AAF0BD41
J1	805	ALA	SER	conflict	UNP A0AAF0BD41
J1	901	HIS	-	expression tag	UNP A0AAF0BD41
J1	902	HIS	-	expression tag	UNP A0AAF0BD41
J1	903	HIS	-	expression tag	UNP A0AAF0BD41
J1	904	HIS	-	expression tag	UNP A0AAF0BD41
J1	905	HIS	-	expression tag	UNP A0AAF0BD41
J1	906	HIS	-	expression tag	UNP A0AAF0BD41
J2	14	MET	-	initiating methionine	UNP A0AAF0BD41
J2	15	ALA	-	expression tag	UNP A0AAF0BD41
J2	16	SER	-	expression tag	UNP A0AAF0BD41
J2	17	MET	-	expression tag	UNP A0AAF0BD41
J2	18	THR	-	expression tag	UNP A0AAF0BD41
J2	19	GLY	-	expression tag	UNP A0AAF0BD41
J2	20	GLY	-	expression tag	UNP A0AAF0BD41
J2	21	GLN	-	expression tag	UNP A0AAF0BD41
J2	22	MET	-	expression tag	UNP A0AAF0BD41
J2	23	GLY	ALA	conflict	UNP A0AAF0BD41
J2	197	MET	VAL	conflict	UNP A0AAF0BD41
J2	298	PRO	LEU	conflict	UNP A0AAF0BD41
J2	306	VAL	ILE	conflict	UNP A0AAF0BD41
J2	439	ALA	GLU	conflict	UNP A0AAF0BD41
J2	751	HIS	TYR	conflict	UNP A0AAF0BD41
J2	774	HIS	TYR	conflict	UNP A0AAF0BD41
J2	805	ALA	SER	conflict	UNP A0AAF0BD41
J2	901	HIS	-	expression tag	UNP A0AAF0BD41
J2	902	HIS	-	expression tag	UNP A0AAF0BD41
J2	903	HIS	-	expression tag	UNP A0AAF0BD41
J2	904	HIS	-	expression tag	UNP A0AAF0BD41
J2	905	HIS	-	expression tag	UNP A0AAF0BD41
J2	906	HIS	-	expression tag	UNP A0AAF0BD41
J3	14	MET	-	initiating methionine	UNP A0AAF0BD41
J3	15	ALA	-	expression tag	UNP A0AAF0BD41
J3	16	SER	-	expression tag	UNP A0AAF0BD41
J3	17	MET	-	expression tag	UNP A0AAF0BD41
J3	18	THR	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
J3	19	GLY	-	expression tag	UNP A0AAF0BD41
J3	20	GLY	-	expression tag	UNP A0AAF0BD41
J3	21	GLN	-	expression tag	UNP A0AAF0BD41
J3	22	MET	-	expression tag	UNP A0AAF0BD41
J3	23	GLY	ALA	conflict	UNP A0AAF0BD41
J3	197	MET	VAL	conflict	UNP A0AAF0BD41
J3	298	PRO	LEU	conflict	UNP A0AAF0BD41
J3	306	VAL	ILE	conflict	UNP A0AAF0BD41
J3	439	ALA	GLU	conflict	UNP A0AAF0BD41
J3	751	HIS	TYR	conflict	UNP A0AAF0BD41
J3	774	HIS	TYR	conflict	UNP A0AAF0BD41
J3	805	ALA	SER	conflict	UNP A0AAF0BD41
J3	901	HIS	-	expression tag	UNP A0AAF0BD41
J3	902	HIS	-	expression tag	UNP A0AAF0BD41
J3	903	HIS	-	expression tag	UNP A0AAF0BD41
J3	904	HIS	-	expression tag	UNP A0AAF0BD41
J3	905	HIS	-	expression tag	UNP A0AAF0BD41
J3	906	HIS	-	expression tag	UNP A0AAF0BD41
J4	14	MET	-	initiating methionine	UNP A0AAF0BD41
J4	15	ALA	-	expression tag	UNP A0AAF0BD41
J4	16	SER	-	expression tag	UNP A0AAF0BD41
J4	17	MET	-	expression tag	UNP A0AAF0BD41
J4	18	THR	-	expression tag	UNP A0AAF0BD41
J4	19	GLY	-	expression tag	UNP A0AAF0BD41
J4	20	GLY	-	expression tag	UNP A0AAF0BD41
J4	21	GLN	-	expression tag	UNP A0AAF0BD41
J4	22	MET	-	expression tag	UNP A0AAF0BD41
J4	23	GLY	ALA	conflict	UNP A0AAF0BD41
J4	197	MET	VAL	conflict	UNP A0AAF0BD41
J4	298	PRO	LEU	conflict	UNP A0AAF0BD41
J4	306	VAL	ILE	conflict	UNP A0AAF0BD41
J4	439	ALA	GLU	conflict	UNP A0AAF0BD41
J4	751	HIS	TYR	conflict	UNP A0AAF0BD41
J4	774	HIS	TYR	conflict	UNP A0AAF0BD41
J4	805	ALA	SER	conflict	UNP A0AAF0BD41
J4	901	HIS	-	expression tag	UNP A0AAF0BD41
J4	902	HIS	-	expression tag	UNP A0AAF0BD41
J4	903	HIS	-	expression tag	UNP A0AAF0BD41
J4	904	HIS	-	expression tag	UNP A0AAF0BD41
J4	905	HIS	-	expression tag	UNP A0AAF0BD41
J4	906	HIS	-	expression tag	UNP A0AAF0BD41
J5	14	MET	-	initiating methionine	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
J5	15	ALA	-	expression tag	UNP A0AAF0BD41
J5	16	SER	-	expression tag	UNP A0AAF0BD41
J5	17	MET	-	expression tag	UNP A0AAF0BD41
J5	18	THR	-	expression tag	UNP A0AAF0BD41
J5	19	GLY	-	expression tag	UNP A0AAF0BD41
J5	20	GLY	-	expression tag	UNP A0AAF0BD41
J5	21	GLN	-	expression tag	UNP A0AAF0BD41
J5	22	MET	-	expression tag	UNP A0AAF0BD41
J5	23	GLY	ALA	conflict	UNP A0AAF0BD41
J5	197	MET	VAL	conflict	UNP A0AAF0BD41
J5	298	PRO	LEU	conflict	UNP A0AAF0BD41
J5	306	VAL	ILE	conflict	UNP A0AAF0BD41
J5	439	ALA	GLU	conflict	UNP A0AAF0BD41
J5	751	HIS	TYR	conflict	UNP A0AAF0BD41
J5	774	HIS	TYR	conflict	UNP A0AAF0BD41
J5	805	ALA	SER	conflict	UNP A0AAF0BD41
J5	901	HIS	-	expression tag	UNP A0AAF0BD41
J5	902	HIS	-	expression tag	UNP A0AAF0BD41
J5	903	HIS	-	expression tag	UNP A0AAF0BD41
J5	904	HIS	-	expression tag	UNP A0AAF0BD41
J5	905	HIS	-	expression tag	UNP A0AAF0BD41
J5	906	HIS	-	expression tag	UNP A0AAF0BD41
K1	14	MET	-	initiating methionine	UNP A0AAF0BD41
K1	15	ALA	-	expression tag	UNP A0AAF0BD41
K1	16	SER	-	expression tag	UNP A0AAF0BD41
K1	17	MET	-	expression tag	UNP A0AAF0BD41
K1	18	THR	-	expression tag	UNP A0AAF0BD41
K1	19	GLY	-	expression tag	UNP A0AAF0BD41
K1	20	GLY	-	expression tag	UNP A0AAF0BD41
K1	21	GLN	-	expression tag	UNP A0AAF0BD41
K1	22	MET	-	expression tag	UNP A0AAF0BD41
K1	23	GLY	ALA	conflict	UNP A0AAF0BD41
K1	197	MET	VAL	conflict	UNP A0AAF0BD41
K1	298	PRO	LEU	conflict	UNP A0AAF0BD41
K1	306	VAL	ILE	conflict	UNP A0AAF0BD41
K1	439	ALA	GLU	conflict	UNP A0AAF0BD41
K1	751	HIS	TYR	conflict	UNP A0AAF0BD41
K1	774	HIS	TYR	conflict	UNP A0AAF0BD41
K1	805	ALA	SER	conflict	UNP A0AAF0BD41
K1	901	HIS	-	expression tag	UNP A0AAF0BD41
K1	902	HIS	-	expression tag	UNP A0AAF0BD41
K1	903	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
K1	904	HIS	-	expression tag	UNP A0AAF0BD41
K1	905	HIS	-	expression tag	UNP A0AAF0BD41
K1	906	HIS	-	expression tag	UNP A0AAF0BD41
K2	14	MET	-	initiating methionine	UNP A0AAF0BD41
K2	15	ALA	-	expression tag	UNP A0AAF0BD41
K2	16	SER	-	expression tag	UNP A0AAF0BD41
K2	17	MET	-	expression tag	UNP A0AAF0BD41
K2	18	THR	-	expression tag	UNP A0AAF0BD41
K2	19	GLY	-	expression tag	UNP A0AAF0BD41
K2	20	GLY	-	expression tag	UNP A0AAF0BD41
K2	21	GLN	-	expression tag	UNP A0AAF0BD41
K2	22	MET	-	expression tag	UNP A0AAF0BD41
K2	23	GLY	ALA	conflict	UNP A0AAF0BD41
K2	197	MET	VAL	conflict	UNP A0AAF0BD41
K2	298	PRO	LEU	conflict	UNP A0AAF0BD41
K2	306	VAL	ILE	conflict	UNP A0AAF0BD41
K2	439	ALA	GLU	conflict	UNP A0AAF0BD41
K2	751	HIS	TYR	conflict	UNP A0AAF0BD41
K2	774	HIS	TYR	conflict	UNP A0AAF0BD41
K2	805	ALA	SER	conflict	UNP A0AAF0BD41
K2	901	HIS	-	expression tag	UNP A0AAF0BD41
K2	902	HIS	-	expression tag	UNP A0AAF0BD41
K2	903	HIS	-	expression tag	UNP A0AAF0BD41
K2	904	HIS	-	expression tag	UNP A0AAF0BD41
K2	905	HIS	-	expression tag	UNP A0AAF0BD41
K2	906	HIS	-	expression tag	UNP A0AAF0BD41
K3	14	MET	-	initiating methionine	UNP A0AAF0BD41
K3	15	ALA	-	expression tag	UNP A0AAF0BD41
K3	16	SER	-	expression tag	UNP A0AAF0BD41
K3	17	MET	-	expression tag	UNP A0AAF0BD41
K3	18	THR	-	expression tag	UNP A0AAF0BD41
K3	19	GLY	-	expression tag	UNP A0AAF0BD41
K3	20	GLY	-	expression tag	UNP A0AAF0BD41
K3	21	GLN	-	expression tag	UNP A0AAF0BD41
K3	22	MET	-	expression tag	UNP A0AAF0BD41
K3	23	GLY	ALA	conflict	UNP A0AAF0BD41
K3	197	MET	VAL	conflict	UNP A0AAF0BD41
K3	298	PRO	LEU	conflict	UNP A0AAF0BD41
K3	306	VAL	ILE	conflict	UNP A0AAF0BD41
K3	439	ALA	GLU	conflict	UNP A0AAF0BD41
K3	751	HIS	TYR	conflict	UNP A0AAF0BD41
K3	774	HIS	TYR	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
K3	805	ALA	SER	conflict	UNP A0AAF0BD41
K3	901	HIS	-	expression tag	UNP A0AAF0BD41
K3	902	HIS	-	expression tag	UNP A0AAF0BD41
K3	903	HIS	-	expression tag	UNP A0AAF0BD41
K3	904	HIS	-	expression tag	UNP A0AAF0BD41
K3	905	HIS	-	expression tag	UNP A0AAF0BD41
K3	906	HIS	-	expression tag	UNP A0AAF0BD41
K4	14	MET	-	initiating methionine	UNP A0AAF0BD41
K4	15	ALA	-	expression tag	UNP A0AAF0BD41
K4	16	SER	-	expression tag	UNP A0AAF0BD41
K4	17	MET	-	expression tag	UNP A0AAF0BD41
K4	18	THR	-	expression tag	UNP A0AAF0BD41
K4	19	GLY	-	expression tag	UNP A0AAF0BD41
K4	20	GLY	-	expression tag	UNP A0AAF0BD41
K4	21	GLN	-	expression tag	UNP A0AAF0BD41
K4	22	MET	-	expression tag	UNP A0AAF0BD41
K4	23	GLY	ALA	conflict	UNP A0AAF0BD41
K4	197	MET	VAL	conflict	UNP A0AAF0BD41
K4	298	PRO	LEU	conflict	UNP A0AAF0BD41
K4	306	VAL	ILE	conflict	UNP A0AAF0BD41
K4	439	ALA	GLU	conflict	UNP A0AAF0BD41
K4	751	HIS	TYR	conflict	UNP A0AAF0BD41
K4	774	HIS	TYR	conflict	UNP A0AAF0BD41
K4	805	ALA	SER	conflict	UNP A0AAF0BD41
K4	901	HIS	-	expression tag	UNP A0AAF0BD41
K4	902	HIS	-	expression tag	UNP A0AAF0BD41
K4	903	HIS	-	expression tag	UNP A0AAF0BD41
K4	904	HIS	-	expression tag	UNP A0AAF0BD41
K4	905	HIS	-	expression tag	UNP A0AAF0BD41
K4	906	HIS	-	expression tag	UNP A0AAF0BD41
K5	14	MET	-	initiating methionine	UNP A0AAF0BD41
K5	15	ALA	-	expression tag	UNP A0AAF0BD41
K5	16	SER	-	expression tag	UNP A0AAF0BD41
K5	17	MET	-	expression tag	UNP A0AAF0BD41
K5	18	THR	-	expression tag	UNP A0AAF0BD41
K5	19	GLY	-	expression tag	UNP A0AAF0BD41
K5	20	GLY	-	expression tag	UNP A0AAF0BD41
K5	21	GLN	-	expression tag	UNP A0AAF0BD41
K5	22	MET	-	expression tag	UNP A0AAF0BD41
K5	23	GLY	ALA	conflict	UNP A0AAF0BD41
K5	197	MET	VAL	conflict	UNP A0AAF0BD41
K5	298	PRO	LEU	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
K5	306	VAL	ILE	conflict	UNP A0AAF0BD41
K5	439	ALA	GLU	conflict	UNP A0AAF0BD41
K5	751	HIS	TYR	conflict	UNP A0AAF0BD41
K5	774	HIS	TYR	conflict	UNP A0AAF0BD41
K5	805	ALA	SER	conflict	UNP A0AAF0BD41
K5	901	HIS	-	expression tag	UNP A0AAF0BD41
K5	902	HIS	-	expression tag	UNP A0AAF0BD41
K5	903	HIS	-	expression tag	UNP A0AAF0BD41
K5	904	HIS	-	expression tag	UNP A0AAF0BD41
K5	905	HIS	-	expression tag	UNP A0AAF0BD41
K5	906	HIS	-	expression tag	UNP A0AAF0BD41
L1	14	MET	-	initiating methionine	UNP A0AAF0BD41
L1	15	ALA	-	expression tag	UNP A0AAF0BD41
L1	16	SER	-	expression tag	UNP A0AAF0BD41
L1	17	MET	-	expression tag	UNP A0AAF0BD41
L1	18	THR	-	expression tag	UNP A0AAF0BD41
L1	19	GLY	-	expression tag	UNP A0AAF0BD41
L1	20	GLY	-	expression tag	UNP A0AAF0BD41
L1	21	GLN	-	expression tag	UNP A0AAF0BD41
L1	22	MET	-	expression tag	UNP A0AAF0BD41
L1	23	GLY	ALA	conflict	UNP A0AAF0BD41
L1	197	MET	VAL	conflict	UNP A0AAF0BD41
L1	298	PRO	LEU	conflict	UNP A0AAF0BD41
L1	306	VAL	ILE	conflict	UNP A0AAF0BD41
L1	439	ALA	GLU	conflict	UNP A0AAF0BD41
L1	751	HIS	TYR	conflict	UNP A0AAF0BD41
L1	774	HIS	TYR	conflict	UNP A0AAF0BD41
L1	805	ALA	SER	conflict	UNP A0AAF0BD41
L1	901	HIS	-	expression tag	UNP A0AAF0BD41
L1	902	HIS	-	expression tag	UNP A0AAF0BD41
L1	903	HIS	-	expression tag	UNP A0AAF0BD41
L1	904	HIS	-	expression tag	UNP A0AAF0BD41
L1	905	HIS	-	expression tag	UNP A0AAF0BD41
L1	906	HIS	-	expression tag	UNP A0AAF0BD41
L2	14	MET	-	initiating methionine	UNP A0AAF0BD41
L2	15	ALA	-	expression tag	UNP A0AAF0BD41
L2	16	SER	-	expression tag	UNP A0AAF0BD41
L2	17	MET	-	expression tag	UNP A0AAF0BD41
L2	18	THR	-	expression tag	UNP A0AAF0BD41
L2	19	GLY	-	expression tag	UNP A0AAF0BD41
L2	20	GLY	-	expression tag	UNP A0AAF0BD41
L2	21	GLN	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
L2	22	MET	-	expression tag	UNP A0AAF0BD41
L2	23	GLY	ALA	conflict	UNP A0AAF0BD41
L2	197	MET	VAL	conflict	UNP A0AAF0BD41
L2	298	PRO	LEU	conflict	UNP A0AAF0BD41
L2	306	VAL	ILE	conflict	UNP A0AAF0BD41
L2	439	ALA	GLU	conflict	UNP A0AAF0BD41
L2	751	HIS	TYR	conflict	UNP A0AAF0BD41
L2	774	HIS	TYR	conflict	UNP A0AAF0BD41
L2	805	ALA	SER	conflict	UNP A0AAF0BD41
L2	901	HIS	-	expression tag	UNP A0AAF0BD41
L2	902	HIS	-	expression tag	UNP A0AAF0BD41
L2	903	HIS	-	expression tag	UNP A0AAF0BD41
L2	904	HIS	-	expression tag	UNP A0AAF0BD41
L2	905	HIS	-	expression tag	UNP A0AAF0BD41
L2	906	HIS	-	expression tag	UNP A0AAF0BD41
L3	14	MET	-	initiating methionine	UNP A0AAF0BD41
L3	15	ALA	-	expression tag	UNP A0AAF0BD41
L3	16	SER	-	expression tag	UNP A0AAF0BD41
L3	17	MET	-	expression tag	UNP A0AAF0BD41
L3	18	THR	-	expression tag	UNP A0AAF0BD41
L3	19	GLY	-	expression tag	UNP A0AAF0BD41
L3	20	GLY	-	expression tag	UNP A0AAF0BD41
L3	21	GLN	-	expression tag	UNP A0AAF0BD41
L3	22	MET	-	expression tag	UNP A0AAF0BD41
L3	23	GLY	ALA	conflict	UNP A0AAF0BD41
L3	197	MET	VAL	conflict	UNP A0AAF0BD41
L3	298	PRO	LEU	conflict	UNP A0AAF0BD41
L3	306	VAL	ILE	conflict	UNP A0AAF0BD41
L3	439	ALA	GLU	conflict	UNP A0AAF0BD41
L3	751	HIS	TYR	conflict	UNP A0AAF0BD41
L3	774	HIS	TYR	conflict	UNP A0AAF0BD41
L3	805	ALA	SER	conflict	UNP A0AAF0BD41
L3	901	HIS	-	expression tag	UNP A0AAF0BD41
L3	902	HIS	-	expression tag	UNP A0AAF0BD41
L3	903	HIS	-	expression tag	UNP A0AAF0BD41
L3	904	HIS	-	expression tag	UNP A0AAF0BD41
L3	905	HIS	-	expression tag	UNP A0AAF0BD41
L3	906	HIS	-	expression tag	UNP A0AAF0BD41
L4	14	MET	-	initiating methionine	UNP A0AAF0BD41
L4	15	ALA	-	expression tag	UNP A0AAF0BD41
L4	16	SER	-	expression tag	UNP A0AAF0BD41
L4	17	MET	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
L4	18	THR	-	expression tag	UNP A0AAF0BD41
L4	19	GLY	-	expression tag	UNP A0AAF0BD41
L4	20	GLY	-	expression tag	UNP A0AAF0BD41
L4	21	GLN	-	expression tag	UNP A0AAF0BD41
L4	22	MET	-	expression tag	UNP A0AAF0BD41
L4	23	GLY	ALA	conflict	UNP A0AAF0BD41
L4	197	MET	VAL	conflict	UNP A0AAF0BD41
L4	298	PRO	LEU	conflict	UNP A0AAF0BD41
L4	306	VAL	ILE	conflict	UNP A0AAF0BD41
L4	439	ALA	GLU	conflict	UNP A0AAF0BD41
L4	751	HIS	TYR	conflict	UNP A0AAF0BD41
L4	774	HIS	TYR	conflict	UNP A0AAF0BD41
L4	805	ALA	SER	conflict	UNP A0AAF0BD41
L4	901	HIS	-	expression tag	UNP A0AAF0BD41
L4	902	HIS	-	expression tag	UNP A0AAF0BD41
L4	903	HIS	-	expression tag	UNP A0AAF0BD41
L4	904	HIS	-	expression tag	UNP A0AAF0BD41
L4	905	HIS	-	expression tag	UNP A0AAF0BD41
L4	906	HIS	-	expression tag	UNP A0AAF0BD41
L5	14	MET	-	initiating methionine	UNP A0AAF0BD41
L5	15	ALA	-	expression tag	UNP A0AAF0BD41
L5	16	SER	-	expression tag	UNP A0AAF0BD41
L5	17	MET	-	expression tag	UNP A0AAF0BD41
L5	18	THR	-	expression tag	UNP A0AAF0BD41
L5	19	GLY	-	expression tag	UNP A0AAF0BD41
L5	20	GLY	-	expression tag	UNP A0AAF0BD41
L5	21	GLN	-	expression tag	UNP A0AAF0BD41
L5	22	MET	-	expression tag	UNP A0AAF0BD41
L5	23	GLY	ALA	conflict	UNP A0AAF0BD41
L5	197	MET	VAL	conflict	UNP A0AAF0BD41
L5	298	PRO	LEU	conflict	UNP A0AAF0BD41
L5	306	VAL	ILE	conflict	UNP A0AAF0BD41
L5	439	ALA	GLU	conflict	UNP A0AAF0BD41
L5	751	HIS	TYR	conflict	UNP A0AAF0BD41
L5	774	HIS	TYR	conflict	UNP A0AAF0BD41
L5	805	ALA	SER	conflict	UNP A0AAF0BD41
L5	901	HIS	-	expression tag	UNP A0AAF0BD41
L5	902	HIS	-	expression tag	UNP A0AAF0BD41
L5	903	HIS	-	expression tag	UNP A0AAF0BD41
L5	904	HIS	-	expression tag	UNP A0AAF0BD41
L5	905	HIS	-	expression tag	UNP A0AAF0BD41
L5	906	HIS	-	expression tag	UNP A0AAF0BD41

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	A1	2	Total Ca 2 2	0
2	A2	2	Total Ca 2 2	0
2	A3	2	Total Ca 2 2	0
2	A4	2	Total Ca 2 2	0
2	A5	2	Total Ca 2 2	0
2	B1	2	Total Ca 2 2	0
2	B2	2	Total Ca 2 2	0
2	B3	2	Total Ca 2 2	0
2	B4	2	Total Ca 2 2	0
2	B5	2	Total Ca 2 2	0
2	C1	2	Total Ca 2 2	0
2	C2	2	Total Ca 2 2	0
2	C3	2	Total Ca 2 2	0
2	C4	2	Total Ca 2 2	0
2	C5	2	Total Ca 2 2	0
2	D1	2	Total Ca 2 2	0
2	D2	2	Total Ca 2 2	0
2	D3	2	Total Ca 2 2	0
2	D4	2	Total Ca 2 2	0
2	D5	2	Total Ca 2 2	0

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Mol	Chain	Residues	Atoms		AltConf
2	E1	2	Total 2	Ca 2	0
2	E2	2	Total 2	Ca 2	0
2	E3	2	Total 2	Ca 2	0
2	E4	2	Total 2	Ca 2	0
2	E5	2	Total 2	Ca 2	0
2	F1	2	Total 2	Ca 2	0
2	F2	2	Total 2	Ca 2	0
2	F3	2	Total 2	Ca 2	0
2	F4	2	Total 2	Ca 2	0
2	F5	2	Total 2	Ca 2	0
2	G1	2	Total 2	Ca 2	0
2	G2	2	Total 2	Ca 2	0
2	G3	2	Total 2	Ca 2	0
2	G4	2	Total 2	Ca 2	0
2	G5	2	Total 2	Ca 2	0
2	H1	2	Total 2	Ca 2	0
2	H2	2	Total 2	Ca 2	0
2	H3	2	Total 2	Ca 2	0
2	H4	2	Total 2	Ca 2	0
2	H5	2	Total 2	Ca 2	0
2	I1	2	Total 2	Ca 2	0

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Mol	Chain	Residues	Atoms		AltConf
2	I2	2	Total 2	Ca 2	0
2	I3	2	Total 2	Ca 2	0
2	I4	2	Total 2	Ca 2	0
2	I5	2	Total 2	Ca 2	0
2	J1	2	Total 2	Ca 2	0
2	J2	2	Total 2	Ca 2	0
2	J3	2	Total 2	Ca 2	0
2	J4	2	Total 2	Ca 2	0
2	J5	2	Total 2	Ca 2	0
2	K1	2	Total 2	Ca 2	0
2	K2	2	Total 2	Ca 2	0
2	K3	2	Total 2	Ca 2	0
2	K4	2	Total 2	Ca 2	0
2	K5	2	Total 2	Ca 2	0
2	L1	2	Total 2	Ca 2	0
2	L2	2	Total 2	Ca 2	0
2	L3	2	Total 2	Ca 2	0
2	L4	2	Total 2	Ca 2	0
2	L5	2	Total 2	Ca 2	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A1	1	Total 1	Zn 1	0
3	A2	1	Total 1	Zn 1	0
3	A3	1	Total 1	Zn 1	0
3	A4	1	Total 1	Zn 1	0
3	A5	1	Total 1	Zn 1	0
3	B1	1	Total 1	Zn 1	0
3	B2	1	Total 1	Zn 1	0
3	B3	1	Total 1	Zn 1	0
3	B4	1	Total 1	Zn 1	0
3	B5	1	Total 1	Zn 1	0
3	C1	1	Total 1	Zn 1	0
3	C2	1	Total 1	Zn 1	0
3	C3	1	Total 1	Zn 1	0
3	C4	1	Total 1	Zn 1	0
3	C5	1	Total 1	Zn 1	0
3	D1	1	Total 1	Zn 1	0
3	D2	1	Total 1	Zn 1	0
3	D3	1	Total 1	Zn 1	0
3	D4	1	Total 1	Zn 1	0
3	D5	1	Total 1	Zn 1	0
3	E1	1	Total 1	Zn 1	0
3	E2	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
3	E3	1	Total 1	Zn 1	0
3	E4	1	Total 1	Zn 1	0
3	E5	1	Total 1	Zn 1	0
3	F1	1	Total 1	Zn 1	0
3	F2	1	Total 1	Zn 1	0
3	F3	1	Total 1	Zn 1	0
3	F4	1	Total 1	Zn 1	0
3	F5	1	Total 1	Zn 1	0
3	G1	1	Total 1	Zn 1	0
3	G2	1	Total 1	Zn 1	0
3	G3	1	Total 1	Zn 1	0
3	G4	1	Total 1	Zn 1	0
3	G5	1	Total 1	Zn 1	0
3	H1	1	Total 1	Zn 1	0
3	H2	1	Total 1	Zn 1	0
3	H3	1	Total 1	Zn 1	0
3	H4	1	Total 1	Zn 1	0
3	H5	1	Total 1	Zn 1	0
3	I1	1	Total 1	Zn 1	0
3	I2	1	Total 1	Zn 1	0
3	I3	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
3	I4	1	Total 1	Zn 1	0
3	I5	1	Total 1	Zn 1	0
3	J1	1	Total 1	Zn 1	0
3	J2	1	Total 1	Zn 1	0
3	J3	1	Total 1	Zn 1	0
3	J4	1	Total 1	Zn 1	0
3	J5	1	Total 1	Zn 1	0
3	K1	1	Total 1	Zn 1	0
3	K2	1	Total 1	Zn 1	0
3	K3	1	Total 1	Zn 1	0
3	K4	1	Total 1	Zn 1	0
3	K5	1	Total 1	Zn 1	0
3	L1	1	Total 1	Zn 1	0
3	L2	1	Total 1	Zn 1	0
3	L3	1	Total 1	Zn 1	0
3	L4	1	Total 1	Zn 1	0
3	L5	1	Total 1	Zn 1	0

SEQUENCE-PLOTS INFOmissingINFO

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36983	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38.58	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.354	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	372.0, 372.0, 372.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 180 ligands modelled in this entry, 180 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

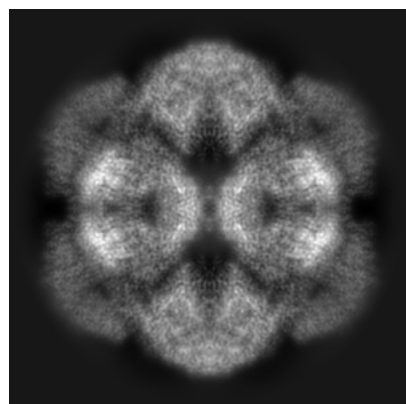
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55035. These allow visual inspection of the internal detail of the map and identification of artifacts.

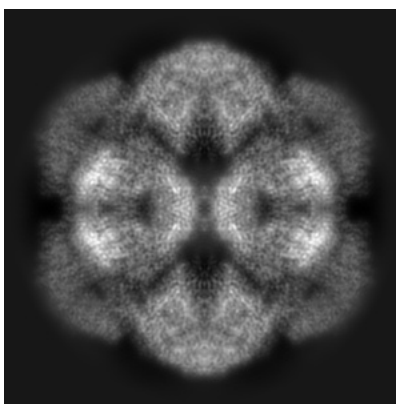
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

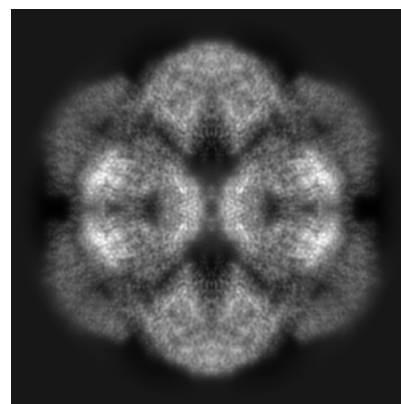
5.1.1 Primary map



X

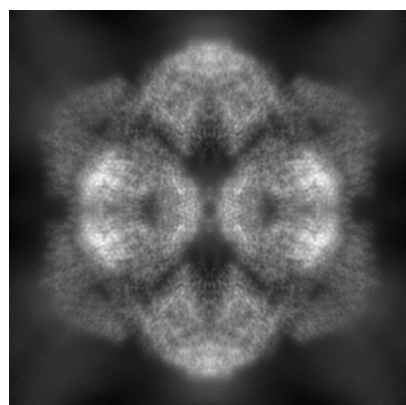


Y

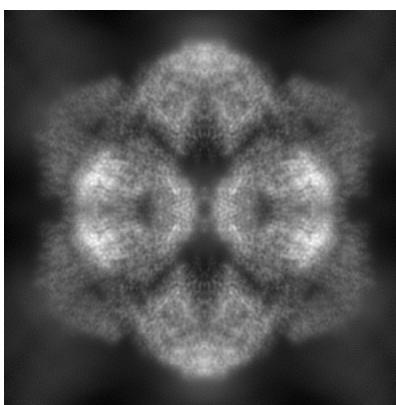


Z

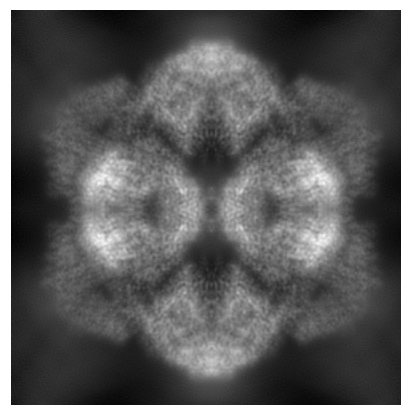
5.1.2 Raw map



X



Y

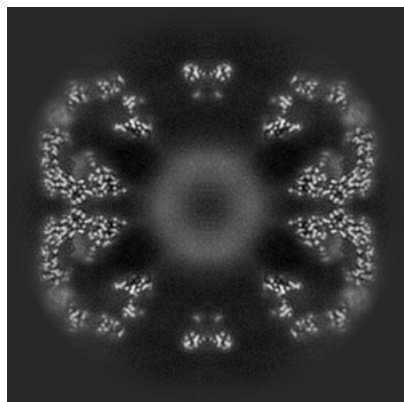


Z

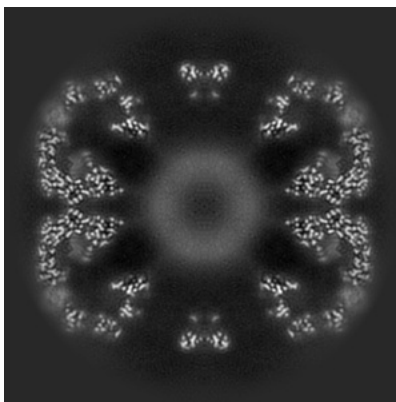
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

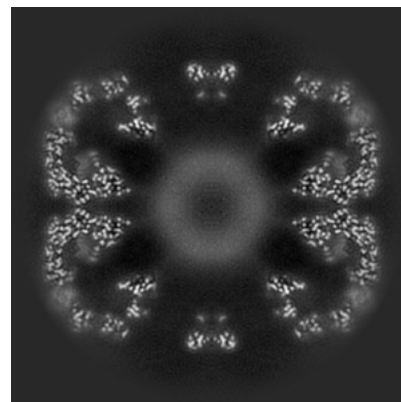
5.2.1 Primary map



X Index: 200

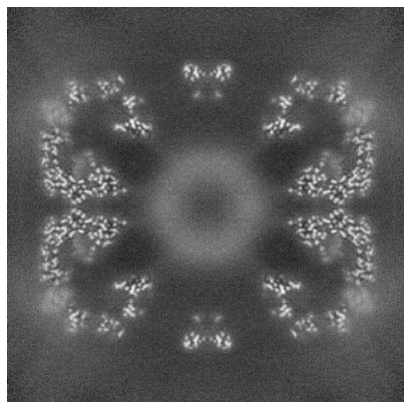


Y Index: 200

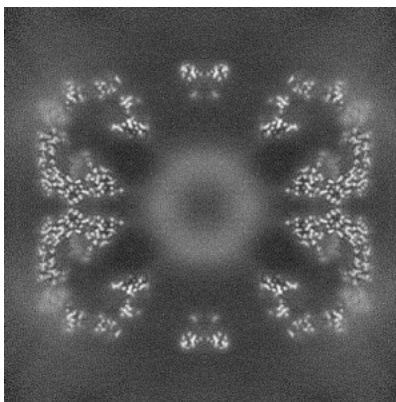


Z Index: 200

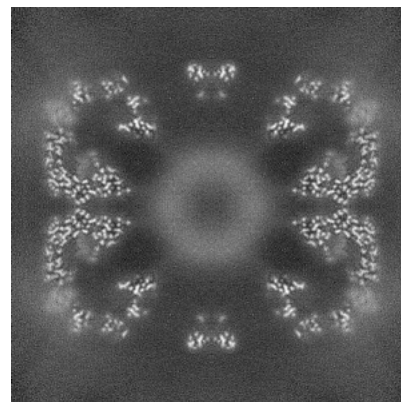
5.2.2 Raw map



X Index: 200



Y Index: 200

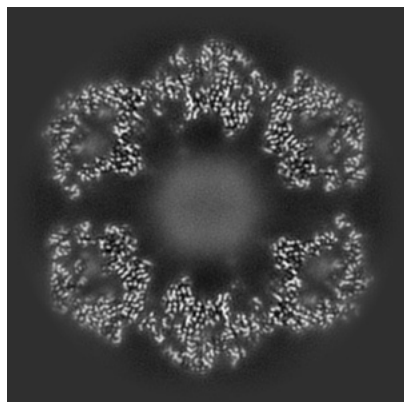


Z Index: 200

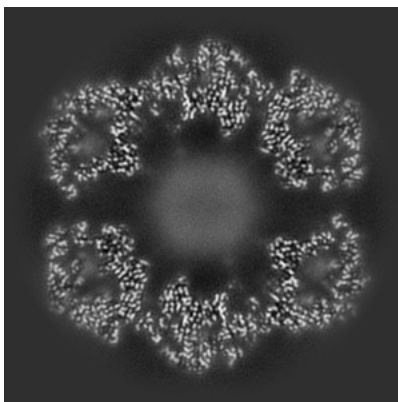
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

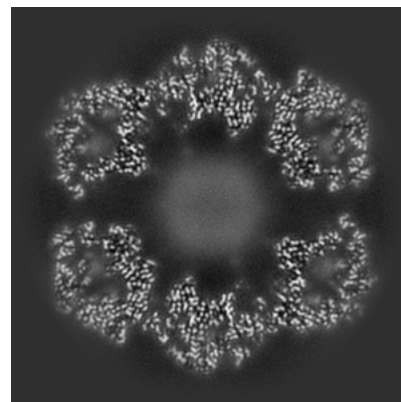
5.3.1 Primary map



X Index: 170

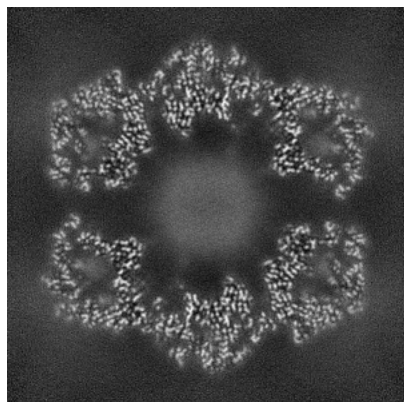


Y Index: 170

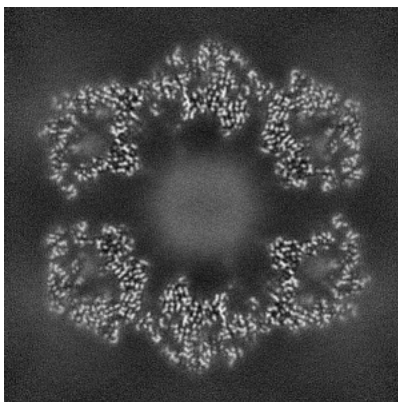


Z Index: 170

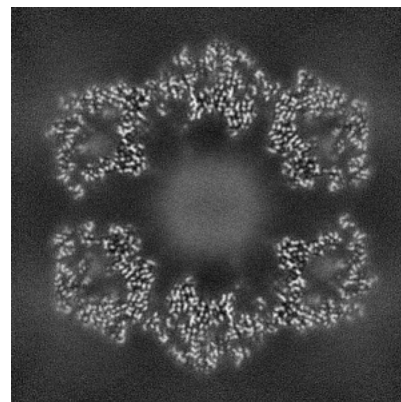
5.3.2 Raw map



X Index: 230



Y Index: 170

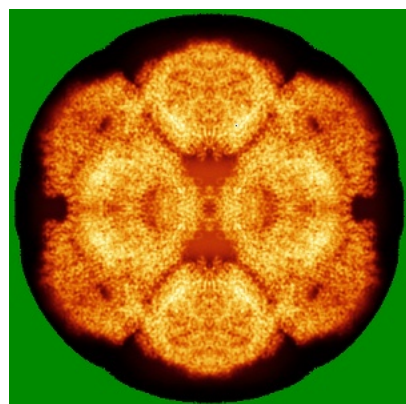


Z Index: 170

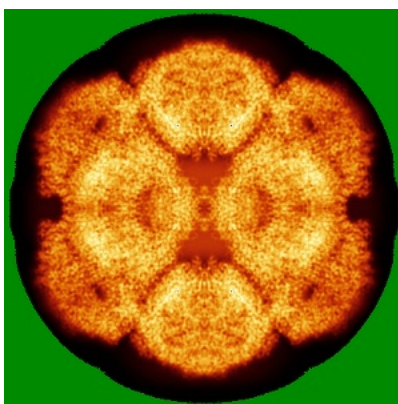
The images above show the largest variance slices of the map in three orthogonal directions.

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

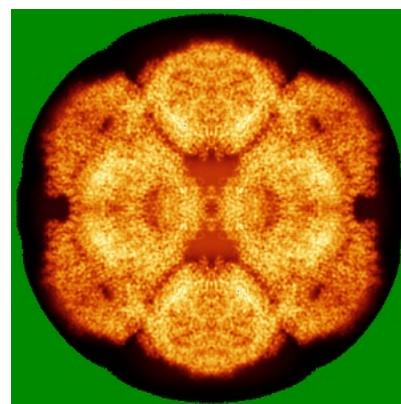
5.4.1 Primary map



X

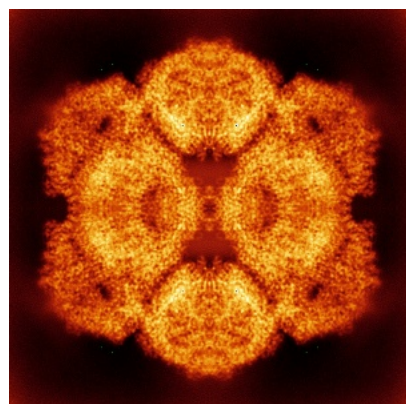


Y

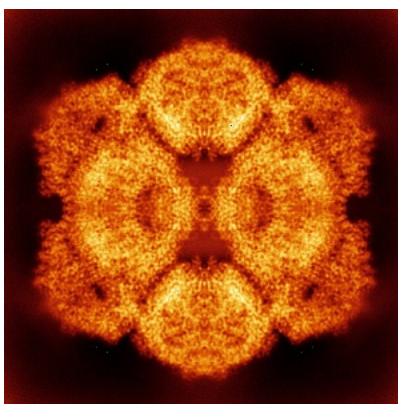


Z

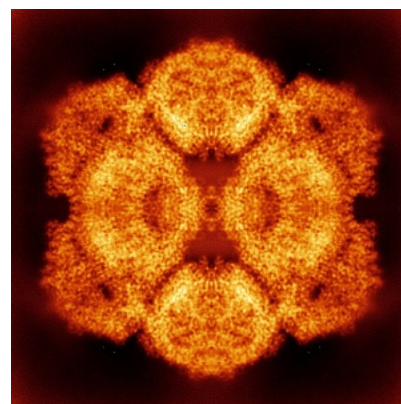
5.4.2 Raw map



X



Y



Z

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.

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



X



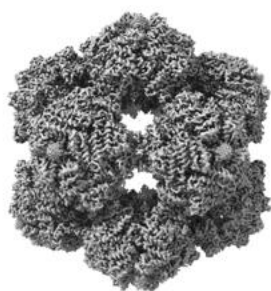
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

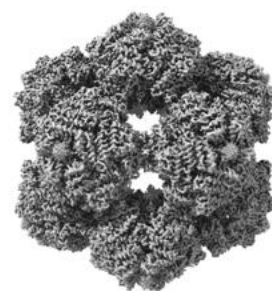
5.5.2 Raw map



X



Y



Z

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

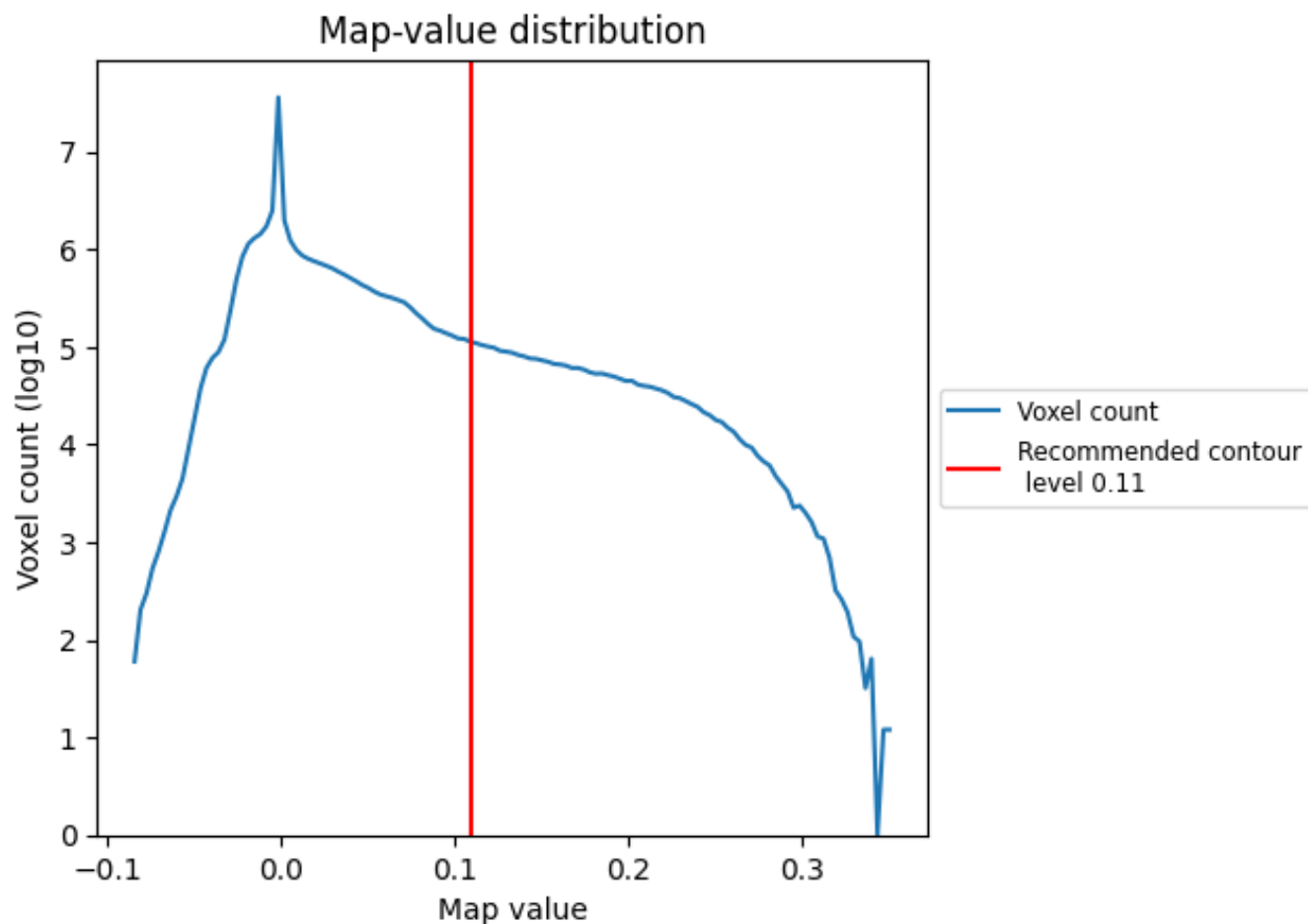
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

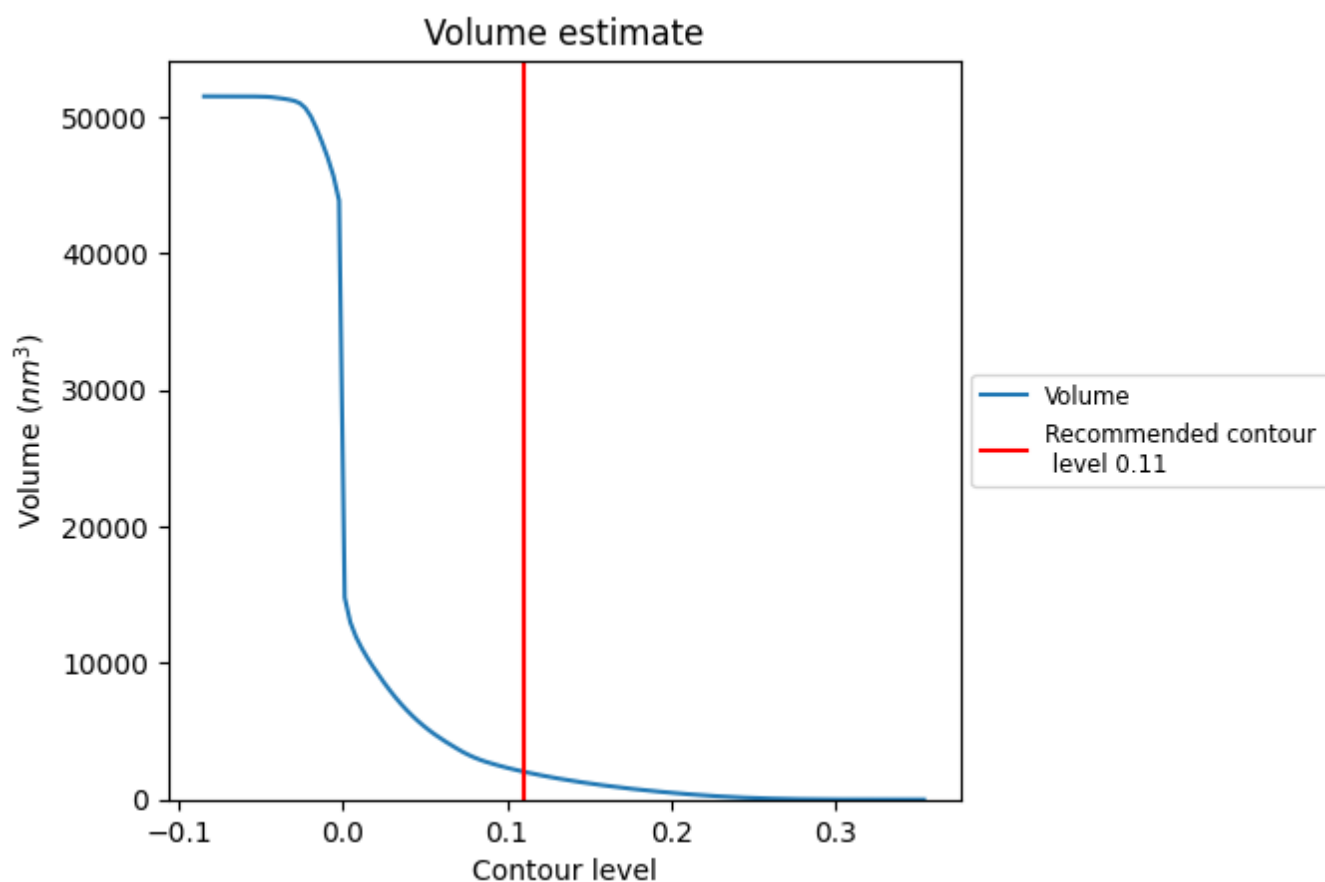
This section contains the results of statistical analysis of the map.

6.1 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.

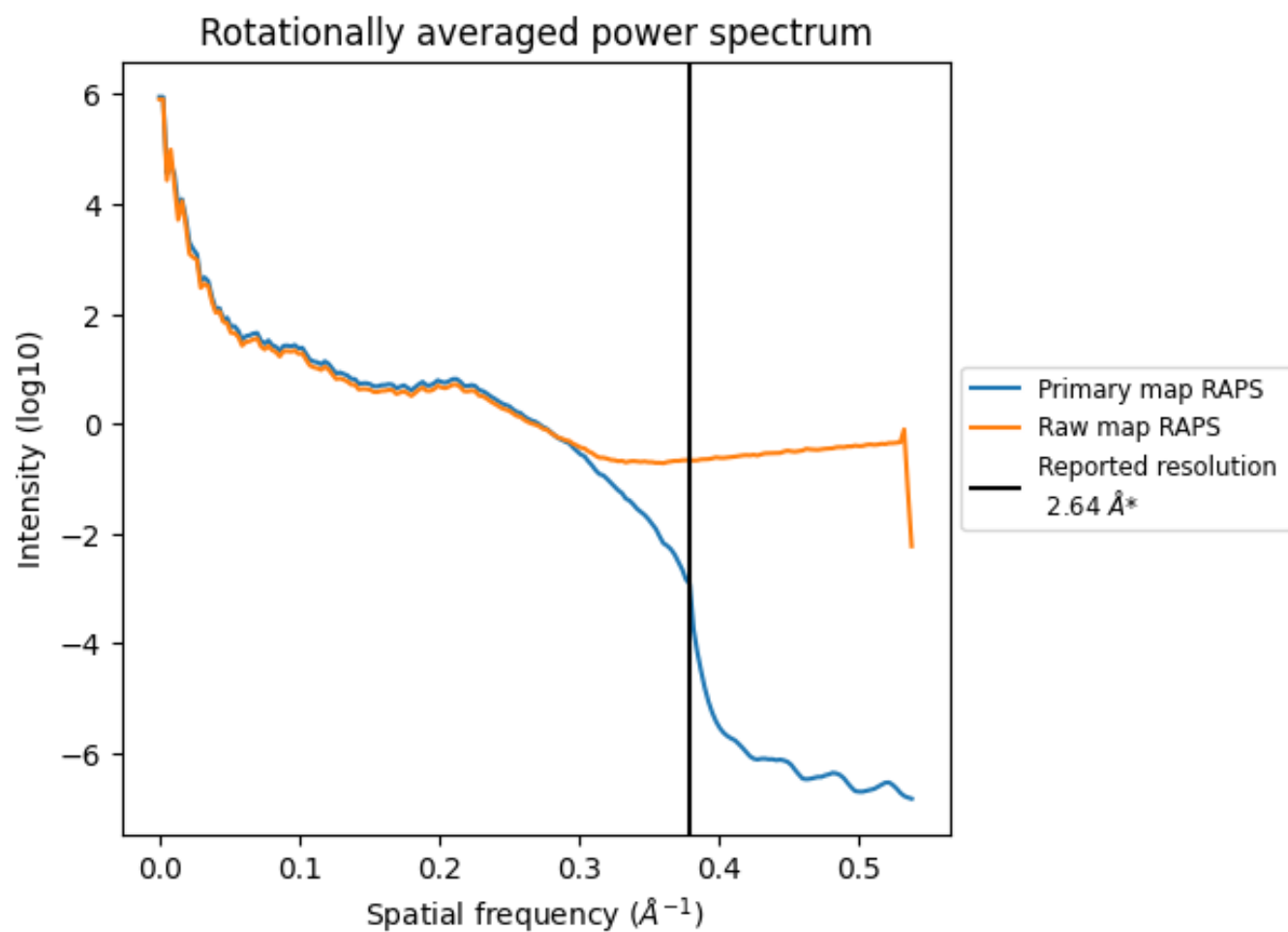
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 2044 nm³; this corresponds to an approximate mass of 1847 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.

6.3 Rotationally averaged power spectrum ⓘ

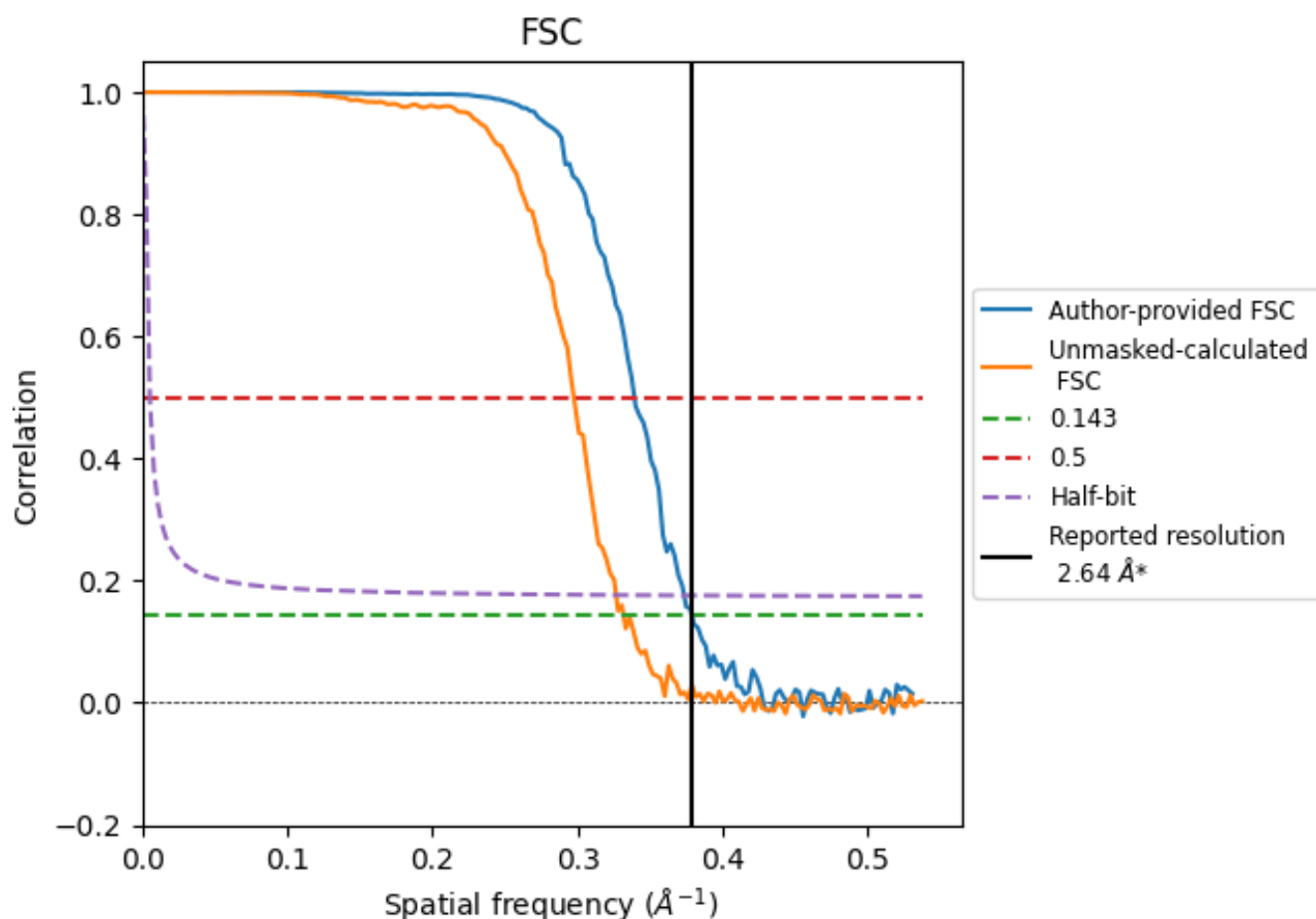


*Reported resolution corresponds to spatial frequency of 0.379 $\text{\AA}^{-1}$

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.379 \text{ \AA}^{-1}$

7.2 Resolution estimates [i](#)

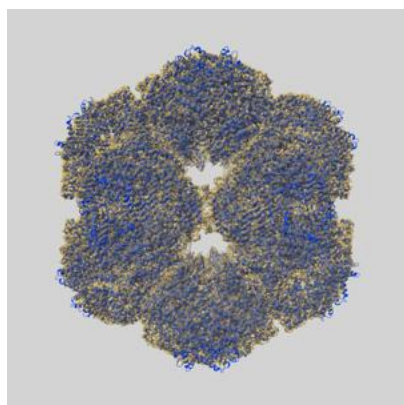
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.64	-	-
Author-provided FSC curve	2.64	2.95	2.68
Unmasked-calculated*	3.01	3.36	3.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.01 differs from the reported value 2.64 by more than 10 %

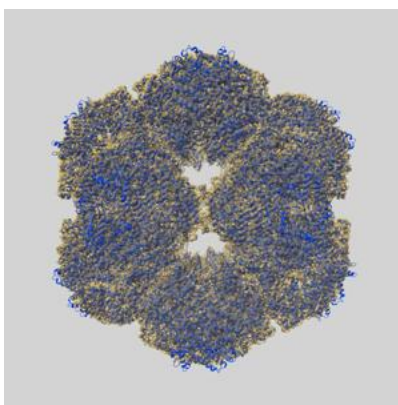
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55035 and PDB model 9SMJ. Per-residue inclusion information can be found in section ?? on page ??.

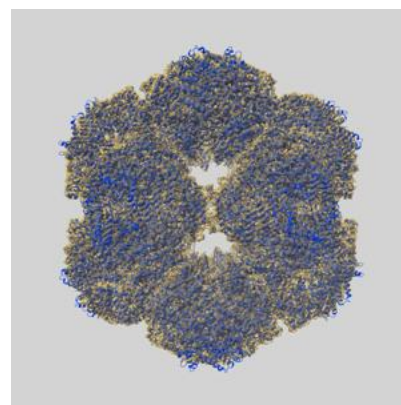
8.1 Map-model overlay [i](#)



X



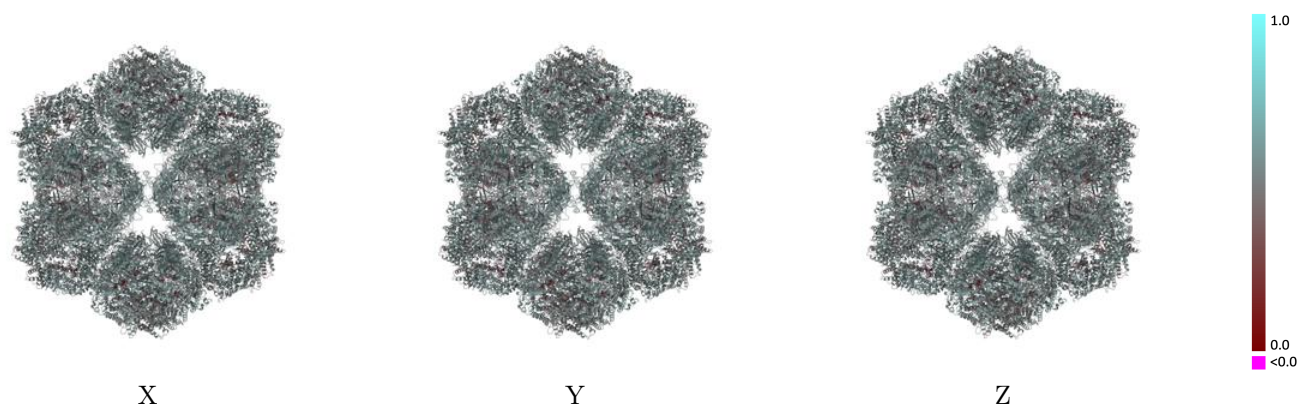
Y



Z

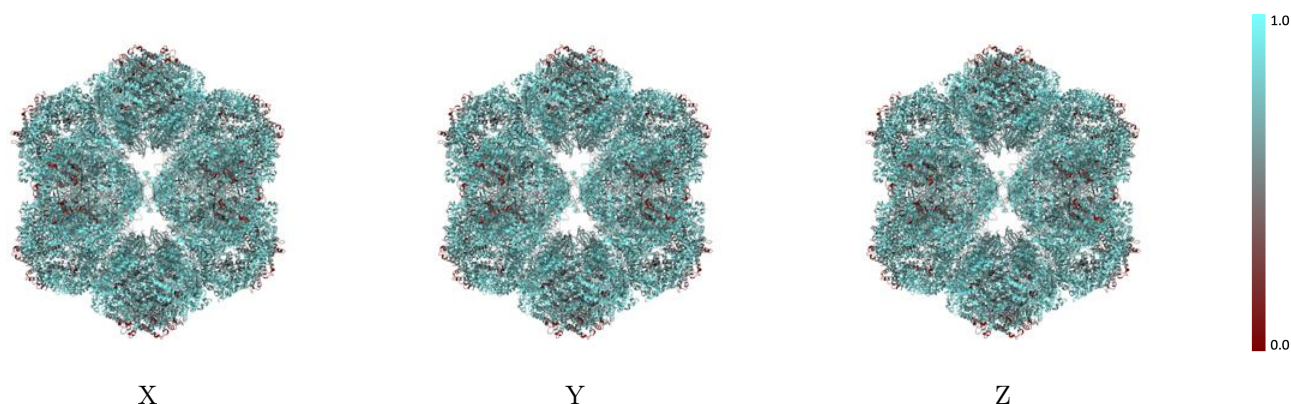
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

8.2 Q-score mapped to coordinate model [i](#)



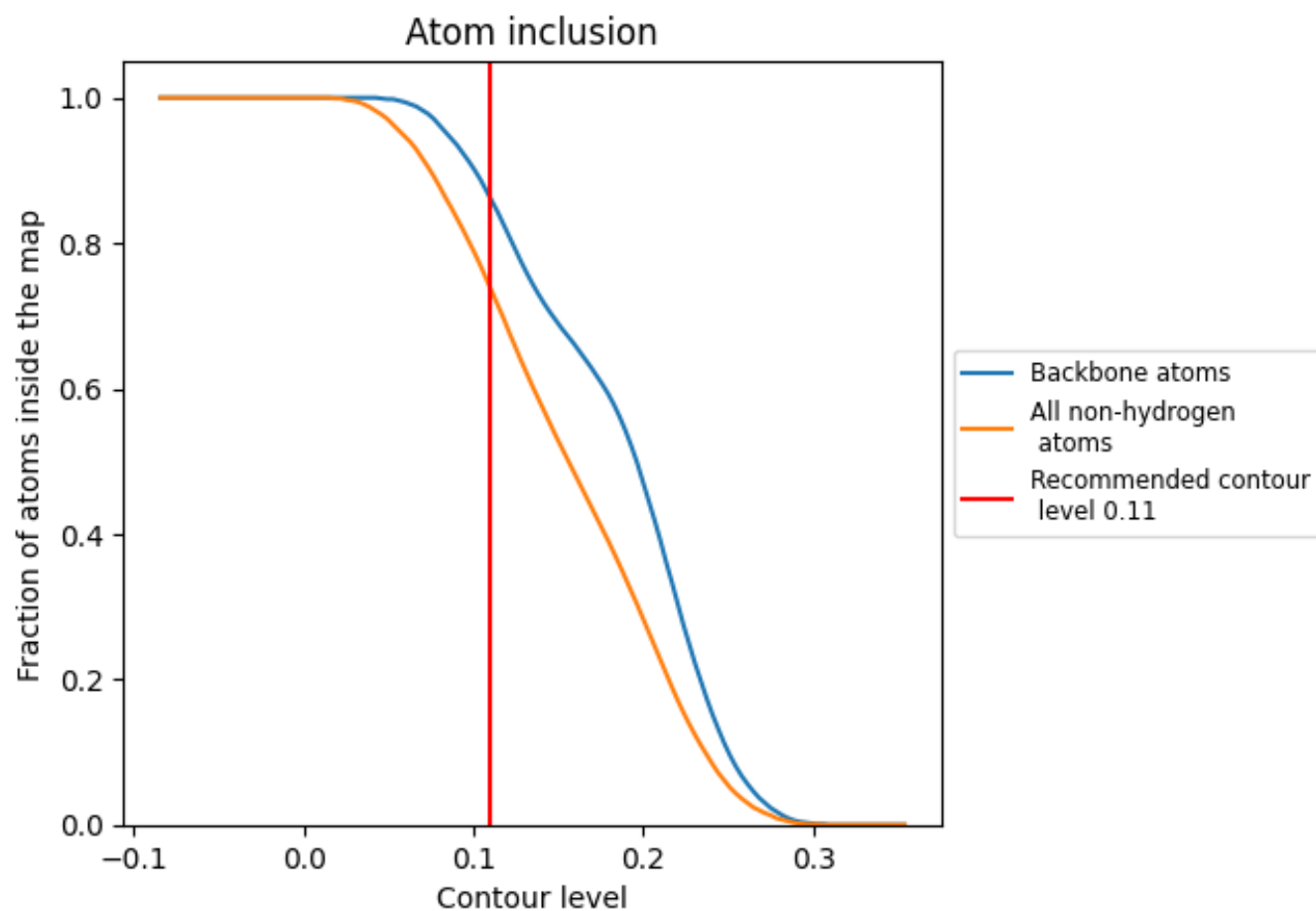
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.11).

8.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7380	 0.5270
A1	 0.7320	 0.5260
A2	 0.7480	 0.5310
A3	 0.7440	 0.5190
A4	 0.7390	 0.5320
A5	 0.7310	 0.5290
B1	 0.7490	 0.5310
B2	 0.7500	 0.5280
B3	 0.7360	 0.5260
B4	 0.7290	 0.5260
B5	 0.7350	 0.5260
C1	 0.7360	 0.5310
C2	 0.7410	 0.5260
C3	 0.7410	 0.5200
C4	 0.7300	 0.5220
C5	 0.7290	 0.5270
D1	 0.7310	 0.5200
D2	 0.7260	 0.5250
D3	 0.7320	 0.5260
D4	 0.7490	 0.5300
D5	 0.7490	 0.5290
E1	 0.7520	 0.5320
E2	 0.7360	 0.5320
E3	 0.7270	 0.5270
E4	 0.7390	 0.5290
E5	 0.7440	 0.5300
F1	 0.7300	 0.5280
F2	 0.7380	 0.5300
F3	 0.7460	 0.5270
F4	 0.7460	 0.5280
F5	 0.7370	 0.5300
G1	 0.7360	 0.5330
G2	 0.7450	 0.5280
G3	 0.7490	 0.5260
G4	 0.7360	 0.5300



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Chain	Atom inclusion	Q-score
G5	 0.7260	 0.5260
H1	 0.7360	 0.5320
H2	 0.7290	 0.5300
H3	 0.7280	 0.5200
H4	 0.7490	 0.5300
H5	 0.7510	 0.5300
I1	 0.7380	 0.5320
I2	 0.7490	 0.5310
I3	 0.7430	 0.5240
I4	 0.7390	 0.5310
I5	 0.7300	 0.5300
J1	 0.7470	 0.5290
J2	 0.7390	 0.5310
J3	 0.7210	 0.5210
J4	 0.7370	 0.5260
J5	 0.7280	 0.5010
K1	 0.7500	 0.5300
K2	 0.7460	 0.5270
K3	 0.7310	 0.5180
K4	 0.7300	 0.5300
K5	 0.7360	 0.5260
L1	 0.7450	 0.5220
L2	 0.7450	 0.5200
L3	 0.7390	 0.5250
L4	 0.7280	 0.5310
L5	 0.7380	 0.5310