



Full wwPDB EM Validation Report ⓘ

Sep 16, 2026 – 12:26 am BST

PDB ID : 9SM4 / pdb_00009sm4
EMDB ID : EMD-55026
Title : Zuzalysin active dodecahedral complex
Authors : Rodriguez-Banqueri, A.; Madej, M.; Eckhard, U.; Koziej, L.; Glatt, S.;
Potempa, J.; Gomis Ruth, F.X.
Deposited on : 2025-09-05
Resolution : 1.83 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>.

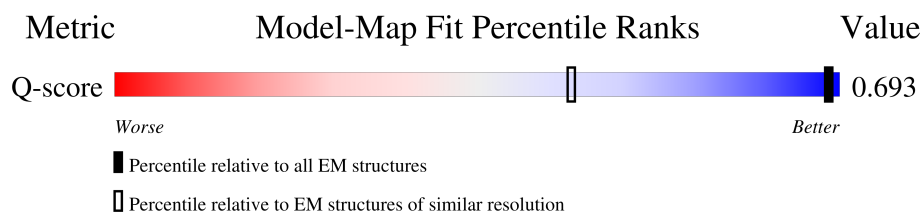
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.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

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ELECTRON MICROSCOPY

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	903 (1.33 - 2.33)

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 419328 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	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	A2	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	A3	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	A4	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	A5	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	B1	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	B2	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	B3	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	B4	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	B5	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	C1	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	C2	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	C3	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	C4	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	C5	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	D1	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		
1	D2	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	D3	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	D4	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	D5	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	E1	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	E2	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	E3	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	E4	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	E5	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	F1	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	F2	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	F3	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	F4	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	F5	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	G1	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	G2	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	G3	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	G4	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	G5	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	H1	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	H2	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	H3	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	H4	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	H5	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	I1	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	I2	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	I3	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	I4	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	I5	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	J1	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	J2	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	J3	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	J4	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	J5	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	K1	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	K2	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	K3	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	K4	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	K5	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	L1	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	L2	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	L3	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0
1	L4	775	Total 6335	C 4047	N 1089	O 1170	S 29	14	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	L5	775	Total	C	N	O	S	14	0
			6335	4047	1089	1170	29		

There are 1140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	-13	MET	-	initiating methionine	UNP A0AAF0BD41
A1	-12	HIS	-	expression tag	UNP A0AAF0BD41
A1	-11	HIS	-	expression tag	UNP A0AAF0BD41
A1	-10	HIS	-	expression tag	UNP A0AAF0BD41
A1	-9	HIS	-	expression tag	UNP A0AAF0BD41
A1	-8	HIS	-	expression tag	UNP A0AAF0BD41
A1	-7	HIS	-	expression tag	UNP A0AAF0BD41
A1	-6	GLU	-	expression tag	UNP A0AAF0BD41
A1	-5	ASN	-	expression tag	UNP A0AAF0BD41
A1	-4	LEU	-	expression tag	UNP A0AAF0BD41
A1	-3	TYR	-	expression tag	UNP A0AAF0BD41
A1	-2	PHE	-	expression tag	UNP A0AAF0BD41
A1	-1	GLN	-	expression tag	UNP A0AAF0BD41
A1	197	MET	VAL	conflict	UNP A0AAF0BD41
A1	298	PRO	LEU	conflict	UNP A0AAF0BD41
A1	306	VAL	ILE	conflict	UNP A0AAF0BD41
A1	751	HIS	TYR	conflict	UNP A0AAF0BD41
A1	774	HIS	TYR	conflict	UNP A0AAF0BD41
A1	805	ALA	SER	conflict	UNP A0AAF0BD41
A2	-13	MET	-	initiating methionine	UNP A0AAF0BD41
A2	-12	HIS	-	expression tag	UNP A0AAF0BD41
A2	-11	HIS	-	expression tag	UNP A0AAF0BD41
A2	-10	HIS	-	expression tag	UNP A0AAF0BD41
A2	-9	HIS	-	expression tag	UNP A0AAF0BD41
A2	-8	HIS	-	expression tag	UNP A0AAF0BD41
A2	-7	HIS	-	expression tag	UNP A0AAF0BD41
A2	-6	GLU	-	expression tag	UNP A0AAF0BD41
A2	-5	ASN	-	expression tag	UNP A0AAF0BD41
A2	-4	LEU	-	expression tag	UNP A0AAF0BD41
A2	-3	TYR	-	expression tag	UNP A0AAF0BD41
A2	-2	PHE	-	expression tag	UNP A0AAF0BD41
A2	-1	GLN	-	expression tag	UNP A0AAF0BD41
A2	197	MET	VAL	conflict	UNP A0AAF0BD41
A2	298	PRO	LEU	conflict	UNP A0AAF0BD41
A2	306	VAL	ILE	conflict	UNP A0AAF0BD41
A2	751	HIS	TYR	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
A2	774	HIS	TYR	conflict	UNP A0AAF0BD41
A2	805	ALA	SER	conflict	UNP A0AAF0BD41
A3	-13	MET	-	initiating methionine	UNP A0AAF0BD41
A3	-12	HIS	-	expression tag	UNP A0AAF0BD41
A3	-11	HIS	-	expression tag	UNP A0AAF0BD41
A3	-10	HIS	-	expression tag	UNP A0AAF0BD41
A3	-9	HIS	-	expression tag	UNP A0AAF0BD41
A3	-8	HIS	-	expression tag	UNP A0AAF0BD41
A3	-7	HIS	-	expression tag	UNP A0AAF0BD41
A3	-6	GLU	-	expression tag	UNP A0AAF0BD41
A3	-5	ASN	-	expression tag	UNP A0AAF0BD41
A3	-4	LEU	-	expression tag	UNP A0AAF0BD41
A3	-3	TYR	-	expression tag	UNP A0AAF0BD41
A3	-2	PHE	-	expression tag	UNP A0AAF0BD41
A3	-1	GLN	-	expression tag	UNP A0AAF0BD41
A3	197	MET	VAL	conflict	UNP A0AAF0BD41
A3	298	PRO	LEU	conflict	UNP A0AAF0BD41
A3	306	VAL	ILE	conflict	UNP A0AAF0BD41
A3	751	HIS	TYR	conflict	UNP A0AAF0BD41
A3	774	HIS	TYR	conflict	UNP A0AAF0BD41
A3	805	ALA	SER	conflict	UNP A0AAF0BD41
A4	-13	MET	-	initiating methionine	UNP A0AAF0BD41
A4	-12	HIS	-	expression tag	UNP A0AAF0BD41
A4	-11	HIS	-	expression tag	UNP A0AAF0BD41
A4	-10	HIS	-	expression tag	UNP A0AAF0BD41
A4	-9	HIS	-	expression tag	UNP A0AAF0BD41
A4	-8	HIS	-	expression tag	UNP A0AAF0BD41
A4	-7	HIS	-	expression tag	UNP A0AAF0BD41
A4	-6	GLU	-	expression tag	UNP A0AAF0BD41
A4	-5	ASN	-	expression tag	UNP A0AAF0BD41
A4	-4	LEU	-	expression tag	UNP A0AAF0BD41
A4	-3	TYR	-	expression tag	UNP A0AAF0BD41
A4	-2	PHE	-	expression tag	UNP A0AAF0BD41
A4	-1	GLN	-	expression tag	UNP A0AAF0BD41
A4	197	MET	VAL	conflict	UNP A0AAF0BD41
A4	298	PRO	LEU	conflict	UNP A0AAF0BD41
A4	306	VAL	ILE	conflict	UNP A0AAF0BD41
A4	751	HIS	TYR	conflict	UNP A0AAF0BD41
A4	774	HIS	TYR	conflict	UNP A0AAF0BD41
A4	805	ALA	SER	conflict	UNP A0AAF0BD41
A5	-13	MET	-	initiating methionine	UNP A0AAF0BD41
A5	-12	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
A5	-11	HIS	-	expression tag	UNP A0AAF0BD41
A5	-10	HIS	-	expression tag	UNP A0AAF0BD41
A5	-9	HIS	-	expression tag	UNP A0AAF0BD41
A5	-8	HIS	-	expression tag	UNP A0AAF0BD41
A5	-7	HIS	-	expression tag	UNP A0AAF0BD41
A5	-6	GLU	-	expression tag	UNP A0AAF0BD41
A5	-5	ASN	-	expression tag	UNP A0AAF0BD41
A5	-4	LEU	-	expression tag	UNP A0AAF0BD41
A5	-3	TYR	-	expression tag	UNP A0AAF0BD41
A5	-2	PHE	-	expression tag	UNP A0AAF0BD41
A5	-1	GLN	-	expression tag	UNP A0AAF0BD41
A5	197	MET	VAL	conflict	UNP A0AAF0BD41
A5	298	PRO	LEU	conflict	UNP A0AAF0BD41
A5	306	VAL	ILE	conflict	UNP A0AAF0BD41
A5	751	HIS	TYR	conflict	UNP A0AAF0BD41
A5	774	HIS	TYR	conflict	UNP A0AAF0BD41
A5	805	ALA	SER	conflict	UNP A0AAF0BD41
B1	-13	MET	-	initiating methionine	UNP A0AAF0BD41
B1	-12	HIS	-	expression tag	UNP A0AAF0BD41
B1	-11	HIS	-	expression tag	UNP A0AAF0BD41
B1	-10	HIS	-	expression tag	UNP A0AAF0BD41
B1	-9	HIS	-	expression tag	UNP A0AAF0BD41
B1	-8	HIS	-	expression tag	UNP A0AAF0BD41
B1	-7	HIS	-	expression tag	UNP A0AAF0BD41
B1	-6	GLU	-	expression tag	UNP A0AAF0BD41
B1	-5	ASN	-	expression tag	UNP A0AAF0BD41
B1	-4	LEU	-	expression tag	UNP A0AAF0BD41
B1	-3	TYR	-	expression tag	UNP A0AAF0BD41
B1	-2	PHE	-	expression tag	UNP A0AAF0BD41
B1	-1	GLN	-	expression tag	UNP A0AAF0BD41
B1	197	MET	VAL	conflict	UNP A0AAF0BD41
B1	298	PRO	LEU	conflict	UNP A0AAF0BD41
B1	306	VAL	ILE	conflict	UNP A0AAF0BD41
B1	751	HIS	TYR	conflict	UNP A0AAF0BD41
B1	774	HIS	TYR	conflict	UNP A0AAF0BD41
B1	805	ALA	SER	conflict	UNP A0AAF0BD41
B2	-13	MET	-	initiating methionine	UNP A0AAF0BD41
B2	-12	HIS	-	expression tag	UNP A0AAF0BD41
B2	-11	HIS	-	expression tag	UNP A0AAF0BD41
B2	-10	HIS	-	expression tag	UNP A0AAF0BD41
B2	-9	HIS	-	expression tag	UNP A0AAF0BD41
B2	-8	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
B2	-7	HIS	-	expression tag	UNP A0AAF0BD41
B2	-6	GLU	-	expression tag	UNP A0AAF0BD41
B2	-5	ASN	-	expression tag	UNP A0AAF0BD41
B2	-4	LEU	-	expression tag	UNP A0AAF0BD41
B2	-3	TYR	-	expression tag	UNP A0AAF0BD41
B2	-2	PHE	-	expression tag	UNP A0AAF0BD41
B2	-1	GLN	-	expression tag	UNP A0AAF0BD41
B2	197	MET	VAL	conflict	UNP A0AAF0BD41
B2	298	PRO	LEU	conflict	UNP A0AAF0BD41
B2	306	VAL	ILE	conflict	UNP A0AAF0BD41
B2	751	HIS	TYR	conflict	UNP A0AAF0BD41
B2	774	HIS	TYR	conflict	UNP A0AAF0BD41
B2	805	ALA	SER	conflict	UNP A0AAF0BD41
B3	-13	MET	-	initiating methionine	UNP A0AAF0BD41
B3	-12	HIS	-	expression tag	UNP A0AAF0BD41
B3	-11	HIS	-	expression tag	UNP A0AAF0BD41
B3	-10	HIS	-	expression tag	UNP A0AAF0BD41
B3	-9	HIS	-	expression tag	UNP A0AAF0BD41
B3	-8	HIS	-	expression tag	UNP A0AAF0BD41
B3	-7	HIS	-	expression tag	UNP A0AAF0BD41
B3	-6	GLU	-	expression tag	UNP A0AAF0BD41
B3	-5	ASN	-	expression tag	UNP A0AAF0BD41
B3	-4	LEU	-	expression tag	UNP A0AAF0BD41
B3	-3	TYR	-	expression tag	UNP A0AAF0BD41
B3	-2	PHE	-	expression tag	UNP A0AAF0BD41
B3	-1	GLN	-	expression tag	UNP A0AAF0BD41
B3	197	MET	VAL	conflict	UNP A0AAF0BD41
B3	298	PRO	LEU	conflict	UNP A0AAF0BD41
B3	306	VAL	ILE	conflict	UNP A0AAF0BD41
B3	751	HIS	TYR	conflict	UNP A0AAF0BD41
B3	774	HIS	TYR	conflict	UNP A0AAF0BD41
B3	805	ALA	SER	conflict	UNP A0AAF0BD41
B4	-13	MET	-	initiating methionine	UNP A0AAF0BD41
B4	-12	HIS	-	expression tag	UNP A0AAF0BD41
B4	-11	HIS	-	expression tag	UNP A0AAF0BD41
B4	-10	HIS	-	expression tag	UNP A0AAF0BD41
B4	-9	HIS	-	expression tag	UNP A0AAF0BD41
B4	-8	HIS	-	expression tag	UNP A0AAF0BD41
B4	-7	HIS	-	expression tag	UNP A0AAF0BD41
B4	-6	GLU	-	expression tag	UNP A0AAF0BD41
B4	-5	ASN	-	expression tag	UNP A0AAF0BD41
B4	-4	LEU	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
B4	-3	TYR	-	expression tag	UNP A0AAF0BD41
B4	-2	PHE	-	expression tag	UNP A0AAF0BD41
B4	-1	GLN	-	expression tag	UNP A0AAF0BD41
B4	197	MET	VAL	conflict	UNP A0AAF0BD41
B4	298	PRO	LEU	conflict	UNP A0AAF0BD41
B4	306	VAL	ILE	conflict	UNP A0AAF0BD41
B4	751	HIS	TYR	conflict	UNP A0AAF0BD41
B4	774	HIS	TYR	conflict	UNP A0AAF0BD41
B4	805	ALA	SER	conflict	UNP A0AAF0BD41
B5	-13	MET	-	initiating methionine	UNP A0AAF0BD41
B5	-12	HIS	-	expression tag	UNP A0AAF0BD41
B5	-11	HIS	-	expression tag	UNP A0AAF0BD41
B5	-10	HIS	-	expression tag	UNP A0AAF0BD41
B5	-9	HIS	-	expression tag	UNP A0AAF0BD41
B5	-8	HIS	-	expression tag	UNP A0AAF0BD41
B5	-7	HIS	-	expression tag	UNP A0AAF0BD41
B5	-6	GLU	-	expression tag	UNP A0AAF0BD41
B5	-5	ASN	-	expression tag	UNP A0AAF0BD41
B5	-4	LEU	-	expression tag	UNP A0AAF0BD41
B5	-3	TYR	-	expression tag	UNP A0AAF0BD41
B5	-2	PHE	-	expression tag	UNP A0AAF0BD41
B5	-1	GLN	-	expression tag	UNP A0AAF0BD41
B5	197	MET	VAL	conflict	UNP A0AAF0BD41
B5	298	PRO	LEU	conflict	UNP A0AAF0BD41
B5	306	VAL	ILE	conflict	UNP A0AAF0BD41
B5	751	HIS	TYR	conflict	UNP A0AAF0BD41
B5	774	HIS	TYR	conflict	UNP A0AAF0BD41
B5	805	ALA	SER	conflict	UNP A0AAF0BD41
C1	-13	MET	-	initiating methionine	UNP A0AAF0BD41
C1	-12	HIS	-	expression tag	UNP A0AAF0BD41
C1	-11	HIS	-	expression tag	UNP A0AAF0BD41
C1	-10	HIS	-	expression tag	UNP A0AAF0BD41
C1	-9	HIS	-	expression tag	UNP A0AAF0BD41
C1	-8	HIS	-	expression tag	UNP A0AAF0BD41
C1	-7	HIS	-	expression tag	UNP A0AAF0BD41
C1	-6	GLU	-	expression tag	UNP A0AAF0BD41
C1	-5	ASN	-	expression tag	UNP A0AAF0BD41
C1	-4	LEU	-	expression tag	UNP A0AAF0BD41
C1	-3	TYR	-	expression tag	UNP A0AAF0BD41
C1	-2	PHE	-	expression tag	UNP A0AAF0BD41
C1	-1	GLN	-	expression tag	UNP A0AAF0BD41
C1	197	MET	VAL	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
C1	298	PRO	LEU	conflict	UNP A0AAF0BD41
C1	306	VAL	ILE	conflict	UNP A0AAF0BD41
C1	751	HIS	TYR	conflict	UNP A0AAF0BD41
C1	774	HIS	TYR	conflict	UNP A0AAF0BD41
C1	805	ALA	SER	conflict	UNP A0AAF0BD41
C2	-13	MET	-	initiating methionine	UNP A0AAF0BD41
C2	-12	HIS	-	expression tag	UNP A0AAF0BD41
C2	-11	HIS	-	expression tag	UNP A0AAF0BD41
C2	-10	HIS	-	expression tag	UNP A0AAF0BD41
C2	-9	HIS	-	expression tag	UNP A0AAF0BD41
C2	-8	HIS	-	expression tag	UNP A0AAF0BD41
C2	-7	HIS	-	expression tag	UNP A0AAF0BD41
C2	-6	GLU	-	expression tag	UNP A0AAF0BD41
C2	-5	ASN	-	expression tag	UNP A0AAF0BD41
C2	-4	LEU	-	expression tag	UNP A0AAF0BD41
C2	-3	TYR	-	expression tag	UNP A0AAF0BD41
C2	-2	PHE	-	expression tag	UNP A0AAF0BD41
C2	-1	GLN	-	expression tag	UNP A0AAF0BD41
C2	197	MET	VAL	conflict	UNP A0AAF0BD41
C2	298	PRO	LEU	conflict	UNP A0AAF0BD41
C2	306	VAL	ILE	conflict	UNP A0AAF0BD41
C2	751	HIS	TYR	conflict	UNP A0AAF0BD41
C2	774	HIS	TYR	conflict	UNP A0AAF0BD41
C2	805	ALA	SER	conflict	UNP A0AAF0BD41
C3	-13	MET	-	initiating methionine	UNP A0AAF0BD41
C3	-12	HIS	-	expression tag	UNP A0AAF0BD41
C3	-11	HIS	-	expression tag	UNP A0AAF0BD41
C3	-10	HIS	-	expression tag	UNP A0AAF0BD41
C3	-9	HIS	-	expression tag	UNP A0AAF0BD41
C3	-8	HIS	-	expression tag	UNP A0AAF0BD41
C3	-7	HIS	-	expression tag	UNP A0AAF0BD41
C3	-6	GLU	-	expression tag	UNP A0AAF0BD41
C3	-5	ASN	-	expression tag	UNP A0AAF0BD41
C3	-4	LEU	-	expression tag	UNP A0AAF0BD41
C3	-3	TYR	-	expression tag	UNP A0AAF0BD41
C3	-2	PHE	-	expression tag	UNP A0AAF0BD41
C3	-1	GLN	-	expression tag	UNP A0AAF0BD41
C3	197	MET	VAL	conflict	UNP A0AAF0BD41
C3	298	PRO	LEU	conflict	UNP A0AAF0BD41
C3	306	VAL	ILE	conflict	UNP A0AAF0BD41
C3	751	HIS	TYR	conflict	UNP A0AAF0BD41
C3	774	HIS	TYR	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
C3	805	ALA	SER	conflict	UNP A0AAF0BD41
C4	-13	MET	-	initiating methionine	UNP A0AAF0BD41
C4	-12	HIS	-	expression tag	UNP A0AAF0BD41
C4	-11	HIS	-	expression tag	UNP A0AAF0BD41
C4	-10	HIS	-	expression tag	UNP A0AAF0BD41
C4	-9	HIS	-	expression tag	UNP A0AAF0BD41
C4	-8	HIS	-	expression tag	UNP A0AAF0BD41
C4	-7	HIS	-	expression tag	UNP A0AAF0BD41
C4	-6	GLU	-	expression tag	UNP A0AAF0BD41
C4	-5	ASN	-	expression tag	UNP A0AAF0BD41
C4	-4	LEU	-	expression tag	UNP A0AAF0BD41
C4	-3	TYR	-	expression tag	UNP A0AAF0BD41
C4	-2	PHE	-	expression tag	UNP A0AAF0BD41
C4	-1	GLN	-	expression tag	UNP A0AAF0BD41
C4	197	MET	VAL	conflict	UNP A0AAF0BD41
C4	298	PRO	LEU	conflict	UNP A0AAF0BD41
C4	306	VAL	ILE	conflict	UNP A0AAF0BD41
C4	751	HIS	TYR	conflict	UNP A0AAF0BD41
C4	774	HIS	TYR	conflict	UNP A0AAF0BD41
C4	805	ALA	SER	conflict	UNP A0AAF0BD41
C5	-13	MET	-	initiating methionine	UNP A0AAF0BD41
C5	-12	HIS	-	expression tag	UNP A0AAF0BD41
C5	-11	HIS	-	expression tag	UNP A0AAF0BD41
C5	-10	HIS	-	expression tag	UNP A0AAF0BD41
C5	-9	HIS	-	expression tag	UNP A0AAF0BD41
C5	-8	HIS	-	expression tag	UNP A0AAF0BD41
C5	-7	HIS	-	expression tag	UNP A0AAF0BD41
C5	-6	GLU	-	expression tag	UNP A0AAF0BD41
C5	-5	ASN	-	expression tag	UNP A0AAF0BD41
C5	-4	LEU	-	expression tag	UNP A0AAF0BD41
C5	-3	TYR	-	expression tag	UNP A0AAF0BD41
C5	-2	PHE	-	expression tag	UNP A0AAF0BD41
C5	-1	GLN	-	expression tag	UNP A0AAF0BD41
C5	197	MET	VAL	conflict	UNP A0AAF0BD41
C5	298	PRO	LEU	conflict	UNP A0AAF0BD41
C5	306	VAL	ILE	conflict	UNP A0AAF0BD41
C5	751	HIS	TYR	conflict	UNP A0AAF0BD41
C5	774	HIS	TYR	conflict	UNP A0AAF0BD41
C5	805	ALA	SER	conflict	UNP A0AAF0BD41
D1	-13	MET	-	initiating methionine	UNP A0AAF0BD41
D1	-12	HIS	-	expression tag	UNP A0AAF0BD41
D1	-11	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
D1	-10	HIS	-	expression tag	UNP A0AAF0BD41
D1	-9	HIS	-	expression tag	UNP A0AAF0BD41
D1	-8	HIS	-	expression tag	UNP A0AAF0BD41
D1	-7	HIS	-	expression tag	UNP A0AAF0BD41
D1	-6	GLU	-	expression tag	UNP A0AAF0BD41
D1	-5	ASN	-	expression tag	UNP A0AAF0BD41
D1	-4	LEU	-	expression tag	UNP A0AAF0BD41
D1	-3	TYR	-	expression tag	UNP A0AAF0BD41
D1	-2	PHE	-	expression tag	UNP A0AAF0BD41
D1	-1	GLN	-	expression tag	UNP A0AAF0BD41
D1	197	MET	VAL	conflict	UNP A0AAF0BD41
D1	298	PRO	LEU	conflict	UNP A0AAF0BD41
D1	306	VAL	ILE	conflict	UNP A0AAF0BD41
D1	751	HIS	TYR	conflict	UNP A0AAF0BD41
D1	774	HIS	TYR	conflict	UNP A0AAF0BD41
D1	805	ALA	SER	conflict	UNP A0AAF0BD41
D2	-13	MET	-	initiating methionine	UNP A0AAF0BD41
D2	-12	HIS	-	expression tag	UNP A0AAF0BD41
D2	-11	HIS	-	expression tag	UNP A0AAF0BD41
D2	-10	HIS	-	expression tag	UNP A0AAF0BD41
D2	-9	HIS	-	expression tag	UNP A0AAF0BD41
D2	-8	HIS	-	expression tag	UNP A0AAF0BD41
D2	-7	HIS	-	expression tag	UNP A0AAF0BD41
D2	-6	GLU	-	expression tag	UNP A0AAF0BD41
D2	-5	ASN	-	expression tag	UNP A0AAF0BD41
D2	-4	LEU	-	expression tag	UNP A0AAF0BD41
D2	-3	TYR	-	expression tag	UNP A0AAF0BD41
D2	-2	PHE	-	expression tag	UNP A0AAF0BD41
D2	-1	GLN	-	expression tag	UNP A0AAF0BD41
D2	197	MET	VAL	conflict	UNP A0AAF0BD41
D2	298	PRO	LEU	conflict	UNP A0AAF0BD41
D2	306	VAL	ILE	conflict	UNP A0AAF0BD41
D2	751	HIS	TYR	conflict	UNP A0AAF0BD41
D2	774	HIS	TYR	conflict	UNP A0AAF0BD41
D2	805	ALA	SER	conflict	UNP A0AAF0BD41
D3	-13	MET	-	initiating methionine	UNP A0AAF0BD41
D3	-12	HIS	-	expression tag	UNP A0AAF0BD41
D3	-11	HIS	-	expression tag	UNP A0AAF0BD41
D3	-10	HIS	-	expression tag	UNP A0AAF0BD41
D3	-9	HIS	-	expression tag	UNP A0AAF0BD41
D3	-8	HIS	-	expression tag	UNP A0AAF0BD41
D3	-7	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
D3	-6	GLU	-	expression tag	UNP A0AAF0BD41
D3	-5	ASN	-	expression tag	UNP A0AAF0BD41
D3	-4	LEU	-	expression tag	UNP A0AAF0BD41
D3	-3	TYR	-	expression tag	UNP A0AAF0BD41
D3	-2	PHE	-	expression tag	UNP A0AAF0BD41
D3	-1	GLN	-	expression tag	UNP A0AAF0BD41
D3	197	MET	VAL	conflict	UNP A0AAF0BD41
D3	298	PRO	LEU	conflict	UNP A0AAF0BD41
D3	306	VAL	ILE	conflict	UNP A0AAF0BD41
D3	751	HIS	TYR	conflict	UNP A0AAF0BD41
D3	774	HIS	TYR	conflict	UNP A0AAF0BD41
D3	805	ALA	SER	conflict	UNP A0AAF0BD41
D4	-13	MET	-	initiating methionine	UNP A0AAF0BD41
D4	-12	HIS	-	expression tag	UNP A0AAF0BD41
D4	-11	HIS	-	expression tag	UNP A0AAF0BD41
D4	-10	HIS	-	expression tag	UNP A0AAF0BD41
D4	-9	HIS	-	expression tag	UNP A0AAF0BD41
D4	-8	HIS	-	expression tag	UNP A0AAF0BD41
D4	-7	HIS	-	expression tag	UNP A0AAF0BD41
D4	-6	GLU	-	expression tag	UNP A0AAF0BD41
D4	-5	ASN	-	expression tag	UNP A0AAF0BD41
D4	-4	LEU	-	expression tag	UNP A0AAF0BD41
D4	-3	TYR	-	expression tag	UNP A0AAF0BD41
D4	-2	PHE	-	expression tag	UNP A0AAF0BD41
D4	-1	GLN	-	expression tag	UNP A0AAF0BD41
D4	197	MET	VAL	conflict	UNP A0AAF0BD41
D4	298	PRO	LEU	conflict	UNP A0AAF0BD41
D4	306	VAL	ILE	conflict	UNP A0AAF0BD41
D4	751	HIS	TYR	conflict	UNP A0AAF0BD41
D4	774	HIS	TYR	conflict	UNP A0AAF0BD41
D4	805	ALA	SER	conflict	UNP A0AAF0BD41
D5	-13	MET	-	initiating methionine	UNP A0AAF0BD41
D5	-12	HIS	-	expression tag	UNP A0AAF0BD41
D5	-11	HIS	-	expression tag	UNP A0AAF0BD41
D5	-10	HIS	-	expression tag	UNP A0AAF0BD41
D5	-9	HIS	-	expression tag	UNP A0AAF0BD41
D5	-8	HIS	-	expression tag	UNP A0AAF0BD41
D5	-7	HIS	-	expression tag	UNP A0AAF0BD41
D5	-6	GLU	-	expression tag	UNP A0AAF0BD41
D5	-5	ASN	-	expression tag	UNP A0AAF0BD41
D5	-4	LEU	-	expression tag	UNP A0AAF0BD41
D5	-3	TYR	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
D5	-2	PHE	-	expression tag	UNP A0AAF0BD41
D5	-1	GLN	-	expression tag	UNP A0AAF0BD41
D5	197	MET	VAL	conflict	UNP A0AAF0BD41
D5	298	PRO	LEU	conflict	UNP A0AAF0BD41
D5	306	VAL	ILE	conflict	UNP A0AAF0BD41
D5	751	HIS	TYR	conflict	UNP A0AAF0BD41
D5	774	HIS	TYR	conflict	UNP A0AAF0BD41
D5	805	ALA	SER	conflict	UNP A0AAF0BD41
E1	-13	MET	-	initiating methionine	UNP A0AAF0BD41
E1	-12	HIS	-	expression tag	UNP A0AAF0BD41
E1	-11	HIS	-	expression tag	UNP A0AAF0BD41
E1	-10	HIS	-	expression tag	UNP A0AAF0BD41
E1	-9	HIS	-	expression tag	UNP A0AAF0BD41
E1	-8	HIS	-	expression tag	UNP A0AAF0BD41
E1	-7	HIS	-	expression tag	UNP A0AAF0BD41
E1	-6	GLU	-	expression tag	UNP A0AAF0BD41
E1	-5	ASN	-	expression tag	UNP A0AAF0BD41
E1	-4	LEU	-	expression tag	UNP A0AAF0BD41
E1	-3	TYR	-	expression tag	UNP A0AAF0BD41
E1	-2	PHE	-	expression tag	UNP A0AAF0BD41
E1	-1	GLN	-	expression tag	UNP A0AAF0BD41
E1	197	MET	VAL	conflict	UNP A0AAF0BD41
E1	298	PRO	LEU	conflict	UNP A0AAF0BD41
E1	306	VAL	ILE	conflict	UNP A0AAF0BD41
E1	751	HIS	TYR	conflict	UNP A0AAF0BD41
E1	774	HIS	TYR	conflict	UNP A0AAF0BD41
E1	805	ALA	SER	conflict	UNP A0AAF0BD41
E2	-13	MET	-	initiating methionine	UNP A0AAF0BD41
E2	-12	HIS	-	expression tag	UNP A0AAF0BD41
E2	-11	HIS	-	expression tag	UNP A0AAF0BD41
E2	-10	HIS	-	expression tag	UNP A0AAF0BD41
E2	-9	HIS	-	expression tag	UNP A0AAF0BD41
E2	-8	HIS	-	expression tag	UNP A0AAF0BD41
E2	-7	HIS	-	expression tag	UNP A0AAF0BD41
E2	-6	GLU	-	expression tag	UNP A0AAF0BD41
E2	-5	ASN	-	expression tag	UNP A0AAF0BD41
E2	-4	LEU	-	expression tag	UNP A0AAF0BD41
E2	-3	TYR	-	expression tag	UNP A0AAF0BD41
E2	-2	PHE	-	expression tag	UNP A0AAF0BD41
E2	-1	GLN	-	expression tag	UNP A0AAF0BD41
E2	197	MET	VAL	conflict	UNP A0AAF0BD41
E2	298	PRO	LEU	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
E2	306	VAL	ILE	conflict	UNP A0AAF0BD41
E2	751	HIS	TYR	conflict	UNP A0AAF0BD41
E2	774	HIS	TYR	conflict	UNP A0AAF0BD41
E2	805	ALA	SER	conflict	UNP A0AAF0BD41
E3	-13	MET	-	initiating methionine	UNP A0AAF0BD41
E3	-12	HIS	-	expression tag	UNP A0AAF0BD41
E3	-11	HIS	-	expression tag	UNP A0AAF0BD41
E3	-10	HIS	-	expression tag	UNP A0AAF0BD41
E3	-9	HIS	-	expression tag	UNP A0AAF0BD41
E3	-8	HIS	-	expression tag	UNP A0AAF0BD41
E3	-7	HIS	-	expression tag	UNP A0AAF0BD41
E3	-6	GLU	-	expression tag	UNP A0AAF0BD41
E3	-5	ASN	-	expression tag	UNP A0AAF0BD41
E3	-4	LEU	-	expression tag	UNP A0AAF0BD41
E3	-3	TYR	-	expression tag	UNP A0AAF0BD41
E3	-2	PHE	-	expression tag	UNP A0AAF0BD41
E3	-1	GLN	-	expression tag	UNP A0AAF0BD41
E3	197	MET	VAL	conflict	UNP A0AAF0BD41
E3	298	PRO	LEU	conflict	UNP A0AAF0BD41
E3	306	VAL	ILE	conflict	UNP A0AAF0BD41
E3	751	HIS	TYR	conflict	UNP A0AAF0BD41
E3	774	HIS	TYR	conflict	UNP A0AAF0BD41
E3	805	ALA	SER	conflict	UNP A0AAF0BD41
E4	-13	MET	-	initiating methionine	UNP A0AAF0BD41
E4	-12	HIS	-	expression tag	UNP A0AAF0BD41
E4	-11	HIS	-	expression tag	UNP A0AAF0BD41
E4	-10	HIS	-	expression tag	UNP A0AAF0BD41
E4	-9	HIS	-	expression tag	UNP A0AAF0BD41
E4	-8	HIS	-	expression tag	UNP A0AAF0BD41
E4	-7	HIS	-	expression tag	UNP A0AAF0BD41
E4	-6	GLU	-	expression tag	UNP A0AAF0BD41
E4	-5	ASN	-	expression tag	UNP A0AAF0BD41
E4	-4	LEU	-	expression tag	UNP A0AAF0BD41
E4	-3	TYR	-	expression tag	UNP A0AAF0BD41
E4	-2	PHE	-	expression tag	UNP A0AAF0BD41
E4	-1	GLN	-	expression tag	UNP A0AAF0BD41
E4	197	MET	VAL	conflict	UNP A0AAF0BD41
E4	298	PRO	LEU	conflict	UNP A0AAF0BD41
E4	306	VAL	ILE	conflict	UNP A0AAF0BD41
E4	751	HIS	TYR	conflict	UNP A0AAF0BD41
E4	774	HIS	TYR	conflict	UNP A0AAF0BD41
E4	805	ALA	SER	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
E5	-13	MET	-	initiating methionine	UNP A0AAF0BD41
E5	-12	HIS	-	expression tag	UNP A0AAF0BD41
E5	-11	HIS	-	expression tag	UNP A0AAF0BD41
E5	-10	HIS	-	expression tag	UNP A0AAF0BD41
E5	-9	HIS	-	expression tag	UNP A0AAF0BD41
E5	-8	HIS	-	expression tag	UNP A0AAF0BD41
E5	-7	HIS	-	expression tag	UNP A0AAF0BD41
E5	-6	GLU	-	expression tag	UNP A0AAF0BD41
E5	-5	ASN	-	expression tag	UNP A0AAF0BD41
E5	-4	LEU	-	expression tag	UNP A0AAF0BD41
E5	-3	TYR	-	expression tag	UNP A0AAF0BD41
E5	-2	PHE	-	expression tag	UNP A0AAF0BD41
E5	-1	GLN	-	expression tag	UNP A0AAF0BD41
E5	197	MET	VAL	conflict	UNP A0AAF0BD41
E5	298	PRO	LEU	conflict	UNP A0AAF0BD41
E5	306	VAL	ILE	conflict	UNP A0AAF0BD41
E5	751	HIS	TYR	conflict	UNP A0AAF0BD41
E5	774	HIS	TYR	conflict	UNP A0AAF0BD41
E5	805	ALA	SER	conflict	UNP A0AAF0BD41
F1	-13	MET	-	initiating methionine	UNP A0AAF0BD41
F1	-12	HIS	-	expression tag	UNP A0AAF0BD41
F1	-11	HIS	-	expression tag	UNP A0AAF0BD41
F1	-10	HIS	-	expression tag	UNP A0AAF0BD41
F1	-9	HIS	-	expression tag	UNP A0AAF0BD41
F1	-8	HIS	-	expression tag	UNP A0AAF0BD41
F1	-7	HIS	-	expression tag	UNP A0AAF0BD41
F1	-6	GLU	-	expression tag	UNP A0AAF0BD41
F1	-5	ASN	-	expression tag	UNP A0AAF0BD41
F1	-4	LEU	-	expression tag	UNP A0AAF0BD41
F1	-3	TYR	-	expression tag	UNP A0AAF0BD41
F1	-2	PHE	-	expression tag	UNP A0AAF0BD41
F1	-1	GLN	-	expression tag	UNP A0AAF0BD41
F1	197	MET	VAL	conflict	UNP A0AAF0BD41
F1	298	PRO	LEU	conflict	UNP A0AAF0BD41
F1	306	VAL	ILE	conflict	UNP A0AAF0BD41
F1	751	HIS	TYR	conflict	UNP A0AAF0BD41
F1	774	HIS	TYR	conflict	UNP A0AAF0BD41
F1	805	ALA	SER	conflict	UNP A0AAF0BD41
F2	-13	MET	-	initiating methionine	UNP A0AAF0BD41
F2	-12	HIS	-	expression tag	UNP A0AAF0BD41
F2	-11	HIS	-	expression tag	UNP A0AAF0BD41
F2	-10	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
F2	-9	HIS	-	expression tag	UNP A0AAF0BD41
F2	-8	HIS	-	expression tag	UNP A0AAF0BD41
F2	-7	HIS	-	expression tag	UNP A0AAF0BD41
F2	-6	GLU	-	expression tag	UNP A0AAF0BD41
F2	-5	ASN	-	expression tag	UNP A0AAF0BD41
F2	-4	LEU	-	expression tag	UNP A0AAF0BD41
F2	-3	TYR	-	expression tag	UNP A0AAF0BD41
F2	-2	PHE	-	expression tag	UNP A0AAF0BD41
F2	-1	GLN	-	expression tag	UNP A0AAF0BD41
F2	197	MET	VAL	conflict	UNP A0AAF0BD41
F2	298	PRO	LEU	conflict	UNP A0AAF0BD41
F2	306	VAL	ILE	conflict	UNP A0AAF0BD41
F2	751	HIS	TYR	conflict	UNP A0AAF0BD41
F2	774	HIS	TYR	conflict	UNP A0AAF0BD41
F2	805	ALA	SER	conflict	UNP A0AAF0BD41
F3	-13	MET	-	initiating methionine	UNP A0AAF0BD41
F3	-12	HIS	-	expression tag	UNP A0AAF0BD41
F3	-11	HIS	-	expression tag	UNP A0AAF0BD41
F3	-10	HIS	-	expression tag	UNP A0AAF0BD41
F3	-9	HIS	-	expression tag	UNP A0AAF0BD41
F3	-8	HIS	-	expression tag	UNP A0AAF0BD41
F3	-7	HIS	-	expression tag	UNP A0AAF0BD41
F3	-6	GLU	-	expression tag	UNP A0AAF0BD41
F3	-5	ASN	-	expression tag	UNP A0AAF0BD41
F3	-4	LEU	-	expression tag	UNP A0AAF0BD41
F3	-3	TYR	-	expression tag	UNP A0AAF0BD41
F3	-2	PHE	-	expression tag	UNP A0AAF0BD41
F3	-1	GLN	-	expression tag	UNP A0AAF0BD41
F3	197	MET	VAL	conflict	UNP A0AAF0BD41
F3	298	PRO	LEU	conflict	UNP A0AAF0BD41
F3	306	VAL	ILE	conflict	UNP A0AAF0BD41
F3	751	HIS	TYR	conflict	UNP A0AAF0BD41
F3	774	HIS	TYR	conflict	UNP A0AAF0BD41
F3	805	ALA	SER	conflict	UNP A0AAF0BD41
F4	-13	MET	-	initiating methionine	UNP A0AAF0BD41
F4	-12	HIS	-	expression tag	UNP A0AAF0BD41
F4	-11	HIS	-	expression tag	UNP A0AAF0BD41
F4	-10	HIS	-	expression tag	UNP A0AAF0BD41
F4	-9	HIS	-	expression tag	UNP A0AAF0BD41
F4	-8	HIS	-	expression tag	UNP A0AAF0BD41
F4	-7	HIS	-	expression tag	UNP A0AAF0BD41
F4	-6	GLU	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
F4	-5	ASN	-	expression tag	UNP A0AAF0BD41
F4	-4	LEU	-	expression tag	UNP A0AAF0BD41
F4	-3	TYR	-	expression tag	UNP A0AAF0BD41
F4	-2	PHE	-	expression tag	UNP A0AAF0BD41
F4	-1	GLN	-	expression tag	UNP A0AAF0BD41
F4	197	MET	VAL	conflict	UNP A0AAF0BD41
F4	298	PRO	LEU	conflict	UNP A0AAF0BD41
F4	306	VAL	ILE	conflict	UNP A0AAF0BD41
F4	751	HIS	TYR	conflict	UNP A0AAF0BD41
F4	774	HIS	TYR	conflict	UNP A0AAF0BD41
F4	805	ALA	SER	conflict	UNP A0AAF0BD41
F5	-13	MET	-	initiating methionine	UNP A0AAF0BD41
F5	-12	HIS	-	expression tag	UNP A0AAF0BD41
F5	-11	HIS	-	expression tag	UNP A0AAF0BD41
F5	-10	HIS	-	expression tag	UNP A0AAF0BD41
F5	-9	HIS	-	expression tag	UNP A0AAF0BD41
F5	-8	HIS	-	expression tag	UNP A0AAF0BD41
F5	-7	HIS	-	expression tag	UNP A0AAF0BD41
F5	-6	GLU	-	expression tag	UNP A0AAF0BD41
F5	-5	ASN	-	expression tag	UNP A0AAF0BD41
F5	-4	LEU	-	expression tag	UNP A0AAF0BD41
F5	-3	TYR	-	expression tag	UNP A0AAF0BD41
F5	-2	PHE	-	expression tag	UNP A0AAF0BD41
F5	-1	GLN	-	expression tag	UNP A0AAF0BD41
F5	197	MET	VAL	conflict	UNP A0AAF0BD41
F5	298	PRO	LEU	conflict	UNP A0AAF0BD41
F5	306	VAL	ILE	conflict	UNP A0AAF0BD41
F5	751	HIS	TYR	conflict	UNP A0AAF0BD41
F5	774	HIS	TYR	conflict	UNP A0AAF0BD41
F5	805	ALA	SER	conflict	UNP A0AAF0BD41
G1	-13	MET	-	initiating methionine	UNP A0AAF0BD41
G1	-12	HIS	-	expression tag	UNP A0AAF0BD41
G1	-11	HIS	-	expression tag	UNP A0AAF0BD41
G1	-10	HIS	-	expression tag	UNP A0AAF0BD41
G1	-9	HIS	-	expression tag	UNP A0AAF0BD41
G1	-8	HIS	-	expression tag	UNP A0AAF0BD41
G1	-7	HIS	-	expression tag	UNP A0AAF0BD41
G1	-6	GLU	-	expression tag	UNP A0AAF0BD41
G1	-5	ASN	-	expression tag	UNP A0AAF0BD41
G1	-4	LEU	-	expression tag	UNP A0AAF0BD41
G1	-3	TYR	-	expression tag	UNP A0AAF0BD41
G1	-2	PHE	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
G1	-1	GLN	-	expression tag	UNP A0AAF0BD41
G1	197	MET	VAL	conflict	UNP A0AAF0BD41
G1	298	PRO	LEU	conflict	UNP A0AAF0BD41
G1	306	VAL	ILE	conflict	UNP A0AAF0BD41
G1	751	HIS	TYR	conflict	UNP A0AAF0BD41
G1	774	HIS	TYR	conflict	UNP A0AAF0BD41
G1	805	ALA	SER	conflict	UNP A0AAF0BD41
G2	-13	MET	-	initiating methionine	UNP A0AAF0BD41
G2	-12	HIS	-	expression tag	UNP A0AAF0BD41
G2	-11	HIS	-	expression tag	UNP A0AAF0BD41
G2	-10	HIS	-	expression tag	UNP A0AAF0BD41
G2	-9	HIS	-	expression tag	UNP A0AAF0BD41
G2	-8	HIS	-	expression tag	UNP A0AAF0BD41
G2	-7	HIS	-	expression tag	UNP A0AAF0BD41
G2	-6	GLU	-	expression tag	UNP A0AAF0BD41
G2	-5	ASN	-	expression tag	UNP A0AAF0BD41
G2	-4	LEU	-	expression tag	UNP A0AAF0BD41
G2	-3	TYR	-	expression tag	UNP A0AAF0BD41
G2	-2	PHE	-	expression tag	UNP A0AAF0BD41
G2	-1	GLN	-	expression tag	UNP A0AAF0BD41
G2	197	MET	VAL	conflict	UNP A0AAF0BD41
G2	298	PRO	LEU	conflict	UNP A0AAF0BD41
G2	306	VAL	ILE	conflict	UNP A0AAF0BD41
G2	751	HIS	TYR	conflict	UNP A0AAF0BD41
G2	774	HIS	TYR	conflict	UNP A0AAF0BD41
G2	805	ALA	SER	conflict	UNP A0AAF0BD41
G3	-13	MET	-	initiating methionine	UNP A0AAF0BD41
G3	-12	HIS	-	expression tag	UNP A0AAF0BD41
G3	-11	HIS	-	expression tag	UNP A0AAF0BD41
G3	-10	HIS	-	expression tag	UNP A0AAF0BD41
G3	-9	HIS	-	expression tag	UNP A0AAF0BD41
G3	-8	HIS	-	expression tag	UNP A0AAF0BD41
G3	-7	HIS	-	expression tag	UNP A0AAF0BD41
G3	-6	GLU	-	expression tag	UNP A0AAF0BD41
G3	-5	ASN	-	expression tag	UNP A0AAF0BD41
G3	-4	LEU	-	expression tag	UNP A0AAF0BD41
G3	-3	TYR	-	expression tag	UNP A0AAF0BD41
G3	-2	PHE	-	expression tag	UNP A0AAF0BD41
G3	-1	GLN	-	expression tag	UNP A0AAF0BD41
G3	197	MET	VAL	conflict	UNP A0AAF0BD41
G3	298	PRO	LEU	conflict	UNP A0AAF0BD41
G3	306	VAL	ILE	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
G4	-13	MET	-	initiating methionine	UNP A0AAF0BD41
G4	-12	HIS	-	expression tag	UNP A0AAF0BD41
G4	-11	HIS	-	expression tag	UNP A0AAF0BD41
G4	-10	HIS	-	expression tag	UNP A0AAF0BD41
G4	-9	HIS	-	expression tag	UNP A0AAF0BD41
G4	-8	HIS	-	expression tag	UNP A0AAF0BD41
G4	-7	HIS	-	expression tag	UNP A0AAF0BD41
G4	-6	GLU	-	expression tag	UNP A0AAF0BD41
G4	-5	ASN	-	expression tag	UNP A0AAF0BD41
G4	-4	LEU	-	expression tag	UNP A0AAF0BD41
G4	-3	TYR	-	expression tag	UNP A0AAF0BD41
G4	-2	PHE	-	expression tag	UNP A0AAF0BD41
G4	-1	GLN	-	expression tag	UNP A0AAF0BD41
G4	197	MET	VAL	conflict	UNP A0AAF0BD41
G4	298	PRO	LEU	conflict	UNP A0AAF0BD41
G4	306	VAL	ILE	conflict	UNP A0AAF0BD41
G4	751	HIS	TYR	conflict	UNP A0AAF0BD41
G4	774	HIS	TYR	conflict	UNP A0AAF0BD41
G4	805	ALA	SER	conflict	UNP A0AAF0BD41
G5	-13	MET	-	initiating methionine	UNP A0AAF0BD41
G5	-12	HIS	-	expression tag	UNP A0AAF0BD41
G5	-11	HIS	-	expression tag	UNP A0AAF0BD41
G5	-10	HIS	-	expression tag	UNP A0AAF0BD41
G5	-9	HIS	-	expression tag	UNP A0AAF0BD41
G5	-8	HIS	-	expression tag	UNP A0AAF0BD41
G5	-7	HIS	-	expression tag	UNP A0AAF0BD41
G5	-6	GLU	-	expression tag	UNP A0AAF0BD41
G5	-5	ASN	-	expression tag	UNP A0AAF0BD41
G5	-4	LEU	-	expression tag	UNP A0AAF0BD41
G5	-3	TYR	-	expression tag	UNP A0AAF0BD41
G5	-2	PHE	-	expression tag	UNP A0AAF0BD41
G5	-1	GLN	-	expression tag	UNP A0AAF0BD41
G5	197	MET	VAL	conflict	UNP A0AAF0BD41
G5	298	PRO	LEU	conflict	UNP A0AAF0BD41
G5	306	VAL	ILE	conflict	UNP A0AAF0BD41
G5	751	HIS	TYR	conflict	UNP A0AAF0BD41
G5	774	HIS	TYR	conflict	UNP A0AAF0BD41
G5	805	ALA	SER	conflict	UNP A0AAF0BD41
H1	-13	MET	-	initiating methionine	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
H1	-12	HIS	-	expression tag	UNP A0AAF0BD41
H1	-11	HIS	-	expression tag	UNP A0AAF0BD41
H1	-10	HIS	-	expression tag	UNP A0AAF0BD41
H1	-9	HIS	-	expression tag	UNP A0AAF0BD41
H1	-8	HIS	-	expression tag	UNP A0AAF0BD41
H1	-7	HIS	-	expression tag	UNP A0AAF0BD41
H1	-6	GLU	-	expression tag	UNP A0AAF0BD41
H1	-5	ASN	-	expression tag	UNP A0AAF0BD41
H1	-4	LEU	-	expression tag	UNP A0AAF0BD41
H1	-3	TYR	-	expression tag	UNP A0AAF0BD41
H1	-2	PHE	-	expression tag	UNP A0AAF0BD41
H1	-1	GLN	-	expression tag	UNP A0AAF0BD41
H1	197	MET	VAL	conflict	UNP A0AAF0BD41
H1	298	PRO	LEU	conflict	UNP A0AAF0BD41
H1	306	VAL	ILE	conflict	UNP A0AAF0BD41
H1	751	HIS	TYR	conflict	UNP A0AAF0BD41
H1	774	HIS	TYR	conflict	UNP A0AAF0BD41
H1	805	ALA	SER	conflict	UNP A0AAF0BD41
H2	-13	MET	-	initiating methionine	UNP A0AAF0BD41
H2	-12	HIS	-	expression tag	UNP A0AAF0BD41
H2	-11	HIS	-	expression tag	UNP A0AAF0BD41
H2	-10	HIS	-	expression tag	UNP A0AAF0BD41
H2	-9	HIS	-	expression tag	UNP A0AAF0BD41
H2	-8	HIS	-	expression tag	UNP A0AAF0BD41
H2	-7	HIS	-	expression tag	UNP A0AAF0BD41
H2	-6	GLU	-	expression tag	UNP A0AAF0BD41
H2	-5	ASN	-	expression tag	UNP A0AAF0BD41
H2	-4	LEU	-	expression tag	UNP A0AAF0BD41
H2	-3	TYR	-	expression tag	UNP A0AAF0BD41
H2	-2	PHE	-	expression tag	UNP A0AAF0BD41
H2	-1	GLN	-	expression tag	UNP A0AAF0BD41
H2	197	MET	VAL	conflict	UNP A0AAF0BD41
H2	298	PRO	LEU	conflict	UNP A0AAF0BD41
H2	306	VAL	ILE	conflict	UNP A0AAF0BD41
H2	751	HIS	TYR	conflict	UNP A0AAF0BD41
H2	774	HIS	TYR	conflict	UNP A0AAF0BD41
H2	805	ALA	SER	conflict	UNP A0AAF0BD41
H3	-13	MET	-	initiating methionine	UNP A0AAF0BD41
H3	-12	HIS	-	expression tag	UNP A0AAF0BD41
H3	-11	HIS	-	expression tag	UNP A0AAF0BD41
H3	-10	HIS	-	expression tag	UNP A0AAF0BD41
H3	-9	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
H3	-8	HIS	-	expression tag	UNP A0AAF0BD41
H3	-7	HIS	-	expression tag	UNP A0AAF0BD41
H3	-6	GLU	-	expression tag	UNP A0AAF0BD41
H3	-5	ASN	-	expression tag	UNP A0AAF0BD41
H3	-4	LEU	-	expression tag	UNP A0AAF0BD41
H3	-3	TYR	-	expression tag	UNP A0AAF0BD41
H3	-2	PHE	-	expression tag	UNP A0AAF0BD41
H3	-1	GLN	-	expression tag	UNP A0AAF0BD41
H3	197	MET	VAL	conflict	UNP A0AAF0BD41
H3	298	PRO	LEU	conflict	UNP A0AAF0BD41
H3	306	VAL	ILE	conflict	UNP A0AAF0BD41
H3	751	HIS	TYR	conflict	UNP A0AAF0BD41
H3	774	HIS	TYR	conflict	UNP A0AAF0BD41
H3	805	ALA	SER	conflict	UNP A0AAF0BD41
H4	-13	MET	-	initiating methionine	UNP A0AAF0BD41
H4	-12	HIS	-	expression tag	UNP A0AAF0BD41
H4	-11	HIS	-	expression tag	UNP A0AAF0BD41
H4	-10	HIS	-	expression tag	UNP A0AAF0BD41
H4	-9	HIS	-	expression tag	UNP A0AAF0BD41
H4	-8	HIS	-	expression tag	UNP A0AAF0BD41
H4	-7	HIS	-	expression tag	UNP A0AAF0BD41
H4	-6	GLU	-	expression tag	UNP A0AAF0BD41
H4	-5	ASN	-	expression tag	UNP A0AAF0BD41
H4	-4	LEU	-	expression tag	UNP A0AAF0BD41
H4	-3	TYR	-	expression tag	UNP A0AAF0BD41
H4	-2	PHE	-	expression tag	UNP A0AAF0BD41
H4	-1	GLN	-	expression tag	UNP A0AAF0BD41
H4	197	MET	VAL	conflict	UNP A0AAF0BD41
H4	298	PRO	LEU	conflict	UNP A0AAF0BD41
H4	306	VAL	ILE	conflict	UNP A0AAF0BD41
H4	751	HIS	TYR	conflict	UNP A0AAF0BD41
H4	774	HIS	TYR	conflict	UNP A0AAF0BD41
H4	805	ALA	SER	conflict	UNP A0AAF0BD41
H5	-13	MET	-	initiating methionine	UNP A0AAF0BD41
H5	-12	HIS	-	expression tag	UNP A0AAF0BD41
H5	-11	HIS	-	expression tag	UNP A0AAF0BD41
H5	-10	HIS	-	expression tag	UNP A0AAF0BD41
H5	-9	HIS	-	expression tag	UNP A0AAF0BD41
H5	-8	HIS	-	expression tag	UNP A0AAF0BD41
H5	-7	HIS	-	expression tag	UNP A0AAF0BD41
H5	-6	GLU	-	expression tag	UNP A0AAF0BD41
H5	-5	ASN	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
H5	-4	LEU	-	expression tag	UNP A0AAF0BD41
H5	-3	TYR	-	expression tag	UNP A0AAF0BD41
H5	-2	PHE	-	expression tag	UNP A0AAF0BD41
H5	-1	GLN	-	expression tag	UNP A0AAF0BD41
H5	197	MET	VAL	conflict	UNP A0AAF0BD41
H5	298	PRO	LEU	conflict	UNP A0AAF0BD41
H5	306	VAL	ILE	conflict	UNP A0AAF0BD41
H5	751	HIS	TYR	conflict	UNP A0AAF0BD41
H5	774	HIS	TYR	conflict	UNP A0AAF0BD41
H5	805	ALA	SER	conflict	UNP A0AAF0BD41
I1	-13	MET	-	initiating methionine	UNP A0AAF0BD41
I1	-12	HIS	-	expression tag	UNP A0AAF0BD41
I1	-11	HIS	-	expression tag	UNP A0AAF0BD41
I1	-10	HIS	-	expression tag	UNP A0AAF0BD41
I1	-9	HIS	-	expression tag	UNP A0AAF0BD41
I1	-8	HIS	-	expression tag	UNP A0AAF0BD41
I1	-7	HIS	-	expression tag	UNP A0AAF0BD41
I1	-6	GLU	-	expression tag	UNP A0AAF0BD41
I1	-5	ASN	-	expression tag	UNP A0AAF0BD41
I1	-4	LEU	-	expression tag	UNP A0AAF0BD41
I1	-3	TYR	-	expression tag	UNP A0AAF0BD41
I1	-2	PHE	-	expression tag	UNP A0AAF0BD41
I1	-1	GLN	-	expression tag	UNP A0AAF0BD41
I1	197	MET	VAL	conflict	UNP A0AAF0BD41
I1	298	PRO	LEU	conflict	UNP A0AAF0BD41
I1	306	VAL	ILE	conflict	UNP A0AAF0BD41
I1	751	HIS	TYR	conflict	UNP A0AAF0BD41
I1	774	HIS	TYR	conflict	UNP A0AAF0BD41
I1	805	ALA	SER	conflict	UNP A0AAF0BD41
I2	-13	MET	-	initiating methionine	UNP A0AAF0BD41
I2	-12	HIS	-	expression tag	UNP A0AAF0BD41
I2	-11	HIS	-	expression tag	UNP A0AAF0BD41
I2	-10	HIS	-	expression tag	UNP A0AAF0BD41
I2	-9	HIS	-	expression tag	UNP A0AAF0BD41
I2	-8	HIS	-	expression tag	UNP A0AAF0BD41
I2	-7	HIS	-	expression tag	UNP A0AAF0BD41
I2	-6	GLU	-	expression tag	UNP A0AAF0BD41
I2	-5	ASN	-	expression tag	UNP A0AAF0BD41
I2	-4	LEU	-	expression tag	UNP A0AAF0BD41
I2	-3	TYR	-	expression tag	UNP A0AAF0BD41
I2	-2	PHE	-	expression tag	UNP A0AAF0BD41
I2	-1	GLN	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
I2	197	MET	VAL	conflict	UNP A0AAF0BD41
I2	298	PRO	LEU	conflict	UNP A0AAF0BD41
I2	306	VAL	ILE	conflict	UNP A0AAF0BD41
I2	751	HIS	TYR	conflict	UNP A0AAF0BD41
I2	774	HIS	TYR	conflict	UNP A0AAF0BD41
I2	805	ALA	SER	conflict	UNP A0AAF0BD41
I3	-13	MET	-	initiating methionine	UNP A0AAF0BD41
I3	-12	HIS	-	expression tag	UNP A0AAF0BD41
I3	-11	HIS	-	expression tag	UNP A0AAF0BD41
I3	-10	HIS	-	expression tag	UNP A0AAF0BD41
I3	-9	HIS	-	expression tag	UNP A0AAF0BD41
I3	-8	HIS	-	expression tag	UNP A0AAF0BD41
I3	-7	HIS	-	expression tag	UNP A0AAF0BD41
I3	-6	GLU	-	expression tag	UNP A0AAF0BD41
I3	-5	ASN	-	expression tag	UNP A0AAF0BD41
I3	-4	LEU	-	expression tag	UNP A0AAF0BD41
I3	-3	TYR	-	expression tag	UNP A0AAF0BD41
I3	-2	PHE	-	expression tag	UNP A0AAF0BD41
I3	-1	GLN	-	expression tag	UNP A0AAF0BD41
I3	197	MET	VAL	conflict	UNP A0AAF0BD41
I3	298	PRO	LEU	conflict	UNP A0AAF0BD41
I3	306	VAL	ILE	conflict	UNP A0AAF0BD41
I3	751	HIS	TYR	conflict	UNP A0AAF0BD41
I3	774	HIS	TYR	conflict	UNP A0AAF0BD41
I3	805	ALA	SER	conflict	UNP A0AAF0BD41
I4	-13	MET	-	initiating methionine	UNP A0AAF0BD41
I4	-12	HIS	-	expression tag	UNP A0AAF0BD41
I4	-11	HIS	-	expression tag	UNP A0AAF0BD41
I4	-10	HIS	-	expression tag	UNP A0AAF0BD41
I4	-9	HIS	-	expression tag	UNP A0AAF0BD41
I4	-8	HIS	-	expression tag	UNP A0AAF0BD41
I4	-7	HIS	-	expression tag	UNP A0AAF0BD41
I4	-6	GLU	-	expression tag	UNP A0AAF0BD41
I4	-5	ASN	-	expression tag	UNP A0AAF0BD41
I4	-4	LEU	-	expression tag	UNP A0AAF0BD41
I4	-3	TYR	-	expression tag	UNP A0AAF0BD41
I4	-2	PHE	-	expression tag	UNP A0AAF0BD41
I4	-1	GLN	-	expression tag	UNP A0AAF0BD41
I4	197	MET	VAL	conflict	UNP A0AAF0BD41
I4	298	PRO	LEU	conflict	UNP A0AAF0BD41
I4	306	VAL	ILE	conflict	UNP A0AAF0BD41
I4	751	HIS	TYR	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
I4	774	HIS	TYR	conflict	UNP A0AAF0BD41
I4	805	ALA	SER	conflict	UNP A0AAF0BD41
I5	-13	MET	-	initiating methionine	UNP A0AAF0BD41
I5	-12	HIS	-	expression tag	UNP A0AAF0BD41
I5	-11	HIS	-	expression tag	UNP A0AAF0BD41
I5	-10	HIS	-	expression tag	UNP A0AAF0BD41
I5	-9	HIS	-	expression tag	UNP A0AAF0BD41
I5	-8	HIS	-	expression tag	UNP A0AAF0BD41
I5	-7	HIS	-	expression tag	UNP A0AAF0BD41
I5	-6	GLU	-	expression tag	UNP A0AAF0BD41
I5	-5	ASN	-	expression tag	UNP A0AAF0BD41
I5	-4	LEU	-	expression tag	UNP A0AAF0BD41
I5	-3	TYR	-	expression tag	UNP A0AAF0BD41
I5	-2	PHE	-	expression tag	UNP A0AAF0BD41
I5	-1	GLN	-	expression tag	UNP A0AAF0BD41
I5	197	MET	VAL	conflict	UNP A0AAF0BD41
I5	298	PRO	LEU	conflict	UNP A0AAF0BD41
I5	306	VAL	ILE	conflict	UNP A0AAF0BD41
I5	751	HIS	TYR	conflict	UNP A0AAF0BD41
I5	774	HIS	TYR	conflict	UNP A0AAF0BD41
I5	805	ALA	SER	conflict	UNP A0AAF0BD41
J1	-13	MET	-	initiating methionine	UNP A0AAF0BD41
J1	-12	HIS	-	expression tag	UNP A0AAF0BD41
J1	-11	HIS	-	expression tag	UNP A0AAF0BD41
J1	-10	HIS	-	expression tag	UNP A0AAF0BD41
J1	-9	HIS	-	expression tag	UNP A0AAF0BD41
J1	-8	HIS	-	expression tag	UNP A0AAF0BD41
J1	-7	HIS	-	expression tag	UNP A0AAF0BD41
J1	-6	GLU	-	expression tag	UNP A0AAF0BD41
J1	-5	ASN	-	expression tag	UNP A0AAF0BD41
J1	-4	LEU	-	expression tag	UNP A0AAF0BD41
J1	-3	TYR	-	expression tag	UNP A0AAF0BD41
J1	-2	PHE	-	expression tag	UNP A0AAF0BD41
J1	-1	GLN	-	expression tag	UNP A0AAF0BD41
J1	197	MET	VAL	conflict	UNP A0AAF0BD41
J1	298	PRO	LEU	conflict	UNP A0AAF0BD41
J1	306	VAL	ILE	conflict	UNP A0AAF0BD41
J1	751	HIS	TYR	conflict	UNP A0AAF0BD41
J1	774	HIS	TYR	conflict	UNP A0AAF0BD41
J1	805	ALA	SER	conflict	UNP A0AAF0BD41
J2	-13	MET	-	initiating methionine	UNP A0AAF0BD41
J2	-12	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
J2	-11	HIS	-	expression tag	UNP A0AAF0BD41
J2	-10	HIS	-	expression tag	UNP A0AAF0BD41
J2	-9	HIS	-	expression tag	UNP A0AAF0BD41
J2	-8	HIS	-	expression tag	UNP A0AAF0BD41
J2	-7	HIS	-	expression tag	UNP A0AAF0BD41
J2	-6	GLU	-	expression tag	UNP A0AAF0BD41
J2	-5	ASN	-	expression tag	UNP A0AAF0BD41
J2	-4	LEU	-	expression tag	UNP A0AAF0BD41
J2	-3	TYR	-	expression tag	UNP A0AAF0BD41
J2	-2	PHE	-	expression tag	UNP A0AAF0BD41
J2	-1	GLN	-	expression tag	UNP A0AAF0BD41
J2	197	MET	VAL	conflict	UNP A0AAF0BD41
J2	298	PRO	LEU	conflict	UNP A0AAF0BD41
J2	306	VAL	ILE	conflict	UNP A0AAF0BD41
J2	751	HIS	TYR	conflict	UNP A0AAF0BD41
J2	774	HIS	TYR	conflict	UNP A0AAF0BD41
J2	805	ALA	SER	conflict	UNP A0AAF0BD41
J3	-13	MET	-	initiating methionine	UNP A0AAF0BD41
J3	-12	HIS	-	expression tag	UNP A0AAF0BD41
J3	-11	HIS	-	expression tag	UNP A0AAF0BD41
J3	-10	HIS	-	expression tag	UNP A0AAF0BD41
J3	-9	HIS	-	expression tag	UNP A0AAF0BD41
J3	-8	HIS	-	expression tag	UNP A0AAF0BD41
J3	-7	HIS	-	expression tag	UNP A0AAF0BD41
J3	-6	GLU	-	expression tag	UNP A0AAF0BD41
J3	-5	ASN	-	expression tag	UNP A0AAF0BD41
J3	-4	LEU	-	expression tag	UNP A0AAF0BD41
J3	-3	TYR	-	expression tag	UNP A0AAF0BD41
J3	-2	PHE	-	expression tag	UNP A0AAF0BD41
J3	-1	GLN	-	expression tag	UNP A0AAF0BD41
J3	197	MET	VAL	conflict	UNP A0AAF0BD41
J3	298	PRO	LEU	conflict	UNP A0AAF0BD41
J3	306	VAL	ILE	conflict	UNP A0AAF0BD41
J3	751	HIS	TYR	conflict	UNP A0AAF0BD41
J3	774	HIS	TYR	conflict	UNP A0AAF0BD41
J3	805	ALA	SER	conflict	UNP A0AAF0BD41
J4	-13	MET	-	initiating methionine	UNP A0AAF0BD41
J4	-12	HIS	-	expression tag	UNP A0AAF0BD41
J4	-11	HIS	-	expression tag	UNP A0AAF0BD41
J4	-10	HIS	-	expression tag	UNP A0AAF0BD41
J4	-9	HIS	-	expression tag	UNP A0AAF0BD41
J4	-8	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
J4	-7	HIS	-	expression tag	UNP A0AAF0BD41
J4	-6	GLU	-	expression tag	UNP A0AAF0BD41
J4	-5	ASN	-	expression tag	UNP A0AAF0BD41
J4	-4	LEU	-	expression tag	UNP A0AAF0BD41
J4	-3	TYR	-	expression tag	UNP A0AAF0BD41
J4	-2	PHE	-	expression tag	UNP A0AAF0BD41
J4	-1	GLN	-	expression tag	UNP A0AAF0BD41
J4	197	MET	VAL	conflict	UNP A0AAF0BD41
J4	298	PRO	LEU	conflict	UNP A0AAF0BD41
J4	306	VAL	ILE	conflict	UNP A0AAF0BD41
J4	751	HIS	TYR	conflict	UNP A0AAF0BD41
J4	774	HIS	TYR	conflict	UNP A0AAF0BD41
J4	805	ALA	SER	conflict	UNP A0AAF0BD41
J5	-13	MET	-	initiating methionine	UNP A0AAF0BD41
J5	-12	HIS	-	expression tag	UNP A0AAF0BD41
J5	-11	HIS	-	expression tag	UNP A0AAF0BD41
J5	-10	HIS	-	expression tag	UNP A0AAF0BD41
J5	-9	HIS	-	expression tag	UNP A0AAF0BD41
J5	-8	HIS	-	expression tag	UNP A0AAF0BD41
J5	-7	HIS	-	expression tag	UNP A0AAF0BD41
J5	-6	GLU	-	expression tag	UNP A0AAF0BD41
J5	-5	ASN	-	expression tag	UNP A0AAF0BD41
J5	-4	LEU	-	expression tag	UNP A0AAF0BD41
J5	-3	TYR	-	expression tag	UNP A0AAF0BD41
J5	-2	PHE	-	expression tag	UNP A0AAF0BD41
J5	-1	GLN	-	expression tag	UNP A0AAF0BD41
J5	197	MET	VAL	conflict	UNP A0AAF0BD41
J5	298	PRO	LEU	conflict	UNP A0AAF0BD41
J5	306	VAL	ILE	conflict	UNP A0AAF0BD41
J5	751	HIS	TYR	conflict	UNP A0AAF0BD41
J5	774	HIS	TYR	conflict	UNP A0AAF0BD41
J5	805	ALA	SER	conflict	UNP A0AAF0BD41
K1	-13	MET	-	initiating methionine	UNP A0AAF0BD41
K1	-12	HIS	-	expression tag	UNP A0AAF0BD41
K1	-11	HIS	-	expression tag	UNP A0AAF0BD41
K1	-10	HIS	-	expression tag	UNP A0AAF0BD41
K1	-9	HIS	-	expression tag	UNP A0AAF0BD41
K1	-8	HIS	-	expression tag	UNP A0AAF0BD41
K1	-7	HIS	-	expression tag	UNP A0AAF0BD41
K1	-6	GLU	-	expression tag	UNP A0AAF0BD41
K1	-5	ASN	-	expression tag	UNP A0AAF0BD41
K1	-4	LEU	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
K1	-3	TYR	-	expression tag	UNP A0AAF0BD41
K1	-2	PHE	-	expression tag	UNP A0AAF0BD41
K1	-1	GLN	-	expression tag	UNP A0AAF0BD41
K1	197	MET	VAL	conflict	UNP A0AAF0BD41
K1	298	PRO	LEU	conflict	UNP A0AAF0BD41
K1	306	VAL	ILE	conflict	UNP A0AAF0BD41
K1	751	HIS	TYR	conflict	UNP A0AAF0BD41
K1	774	HIS	TYR	conflict	UNP A0AAF0BD41
K1	805	ALA	SER	conflict	UNP A0AAF0BD41
K2	-13	MET	-	initiating methionine	UNP A0AAF0BD41
K2	-12	HIS	-	expression tag	UNP A0AAF0BD41
K2	-11	HIS	-	expression tag	UNP A0AAF0BD41
K2	-10	HIS	-	expression tag	UNP A0AAF0BD41
K2	-9	HIS	-	expression tag	UNP A0AAF0BD41
K2	-8	HIS	-	expression tag	UNP A0AAF0BD41
K2	-7	HIS	-	expression tag	UNP A0AAF0BD41
K2	-6	GLU	-	expression tag	UNP A0AAF0BD41
K2	-5	ASN	-	expression tag	UNP A0AAF0BD41
K2	-4	LEU	-	expression tag	UNP A0AAF0BD41
K2	-3	TYR	-	expression tag	UNP A0AAF0BD41
K2	-2	PHE	-	expression tag	UNP A0AAF0BD41
K2	-1	GLN	-	expression tag	UNP A0AAF0BD41
K2	197	MET	VAL	conflict	UNP A0AAF0BD41
K2	298	PRO	LEU	conflict	UNP A0AAF0BD41
K2	306	VAL	ILE	conflict	UNP A0AAF0BD41
K2	751	HIS	TYR	conflict	UNP A0AAF0BD41
K2	774	HIS	TYR	conflict	UNP A0AAF0BD41
K2	805	ALA	SER	conflict	UNP A0AAF0BD41
K3	-13	MET	-	initiating methionine	UNP A0AAF0BD41
K3	-12	HIS	-	expression tag	UNP A0AAF0BD41
K3	-11	HIS	-	expression tag	UNP A0AAF0BD41
K3	-10	HIS	-	expression tag	UNP A0AAF0BD41
K3	-9	HIS	-	expression tag	UNP A0AAF0BD41
K3	-8	HIS	-	expression tag	UNP A0AAF0BD41
K3	-7	HIS	-	expression tag	UNP A0AAF0BD41
K3	-6	GLU	-	expression tag	UNP A0AAF0BD41
K3	-5	ASN	-	expression tag	UNP A0AAF0BD41
K3	-4	LEU	-	expression tag	UNP A0AAF0BD41
K3	-3	TYR	-	expression tag	UNP A0AAF0BD41
K3	-2	PHE	-	expression tag	UNP A0AAF0BD41
K3	-1	GLN	-	expression tag	UNP A0AAF0BD41
K3	197	MET	VAL	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
K3	298	PRO	LEU	conflict	UNP A0AAF0BD41
K3	306	VAL	ILE	conflict	UNP A0AAF0BD41
K3	751	HIS	TYR	conflict	UNP A0AAF0BD41
K3	774	HIS	TYR	conflict	UNP A0AAF0BD41
K3	805	ALA	SER	conflict	UNP A0AAF0BD41
K4	-13	MET	-	initiating methionine	UNP A0AAF0BD41
K4	-12	HIS	-	expression tag	UNP A0AAF0BD41
K4	-11	HIS	-	expression tag	UNP A0AAF0BD41
K4	-10	HIS	-	expression tag	UNP A0AAF0BD41
K4	-9	HIS	-	expression tag	UNP A0AAF0BD41
K4	-8	HIS	-	expression tag	UNP A0AAF0BD41
K4	-7	HIS	-	expression tag	UNP A0AAF0BD41
K4	-6	GLU	-	expression tag	UNP A0AAF0BD41
K4	-5	ASN	-	expression tag	UNP A0AAF0BD41
K4	-4	LEU	-	expression tag	UNP A0AAF0BD41
K4	-3	TYR	-	expression tag	UNP A0AAF0BD41
K4	-2	PHE	-	expression tag	UNP A0AAF0BD41
K4	-1	GLN	-	expression tag	UNP A0AAF0BD41
K4	197	MET	VAL	conflict	UNP A0AAF0BD41
K4	298	PRO	LEU	conflict	UNP A0AAF0BD41
K4	306	VAL	ILE	conflict	UNP A0AAF0BD41
K4	751	HIS	TYR	conflict	UNP A0AAF0BD41
K4	774	HIS	TYR	conflict	UNP A0AAF0BD41
K4	805	ALA	SER	conflict	UNP A0AAF0BD41
K5	-13	MET	-	initiating methionine	UNP A0AAF0BD41
K5	-12	HIS	-	expression tag	UNP A0AAF0BD41
K5	-11	HIS	-	expression tag	UNP A0AAF0BD41
K5	-10	HIS	-	expression tag	UNP A0AAF0BD41
K5	-9	HIS	-	expression tag	UNP A0AAF0BD41
K5	-8	HIS	-	expression tag	UNP A0AAF0BD41
K5	-7	HIS	-	expression tag	UNP A0AAF0BD41
K5	-6	GLU	-	expression tag	UNP A0AAF0BD41
K5	-5	ASN	-	expression tag	UNP A0AAF0BD41
K5	-4	LEU	-	expression tag	UNP A0AAF0BD41
K5	-3	TYR	-	expression tag	UNP A0AAF0BD41
K5	-2	PHE	-	expression tag	UNP A0AAF0BD41
K5	-1	GLN	-	expression tag	UNP A0AAF0BD41
K5	197	MET	VAL	conflict	UNP A0AAF0BD41
K5	298	PRO	LEU	conflict	UNP A0AAF0BD41
K5	306	VAL	ILE	conflict	UNP A0AAF0BD41
K5	751	HIS	TYR	conflict	UNP A0AAF0BD41
K5	774	HIS	TYR	conflict	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
K5	805	ALA	SER	conflict	UNP A0AAF0BD41
L1	-13	MET	-	initiating methionine	UNP A0AAF0BD41
L1	-12	HIS	-	expression tag	UNP A0AAF0BD41
L1	-11	HIS	-	expression tag	UNP A0AAF0BD41
L1	-10	HIS	-	expression tag	UNP A0AAF0BD41
L1	-9	HIS	-	expression tag	UNP A0AAF0BD41
L1	-8	HIS	-	expression tag	UNP A0AAF0BD41
L1	-7	HIS	-	expression tag	UNP A0AAF0BD41
L1	-6	GLU	-	expression tag	UNP A0AAF0BD41
L1	-5	ASN	-	expression tag	UNP A0AAF0BD41
L1	-4	LEU	-	expression tag	UNP A0AAF0BD41
L1	-3	TYR	-	expression tag	UNP A0AAF0BD41
L1	-2	PHE	-	expression tag	UNP A0AAF0BD41
L1	-1	GLN	-	expression tag	UNP A0AAF0BD41
L1	197	MET	VAL	conflict	UNP A0AAF0BD41
L1	298	PRO	LEU	conflict	UNP A0AAF0BD41
L1	306	VAL	ILE	conflict	UNP A0AAF0BD41
L1	751	HIS	TYR	conflict	UNP A0AAF0BD41
L1	774	HIS	TYR	conflict	UNP A0AAF0BD41
L1	805	ALA	SER	conflict	UNP A0AAF0BD41
L2	-13	MET	-	initiating methionine	UNP A0AAF0BD41
L2	-12	HIS	-	expression tag	UNP A0AAF0BD41
L2	-11	HIS	-	expression tag	UNP A0AAF0BD41
L2	-10	HIS	-	expression tag	UNP A0AAF0BD41
L2	-9	HIS	-	expression tag	UNP A0AAF0BD41
L2	-8	HIS	-	expression tag	UNP A0AAF0BD41
L2	-7	HIS	-	expression tag	UNP A0AAF0BD41
L2	-6	GLU	-	expression tag	UNP A0AAF0BD41
L2	-5	ASN	-	expression tag	UNP A0AAF0BD41
L2	-4	LEU	-	expression tag	UNP A0AAF0BD41
L2	-3	TYR	-	expression tag	UNP A0AAF0BD41
L2	-2	PHE	-	expression tag	UNP A0AAF0BD41
L2	-1	GLN	-	expression tag	UNP A0AAF0BD41
L2	197	MET	VAL	conflict	UNP A0AAF0BD41
L2	298	PRO	LEU	conflict	UNP A0AAF0BD41
L2	306	VAL	ILE	conflict	UNP A0AAF0BD41
L2	751	HIS	TYR	conflict	UNP A0AAF0BD41
L2	774	HIS	TYR	conflict	UNP A0AAF0BD41
L2	805	ALA	SER	conflict	UNP A0AAF0BD41
L3	-13	MET	-	initiating methionine	UNP A0AAF0BD41
L3	-12	HIS	-	expression tag	UNP A0AAF0BD41
L3	-11	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
L3	-10	HIS	-	expression tag	UNP A0AAF0BD41
L3	-9	HIS	-	expression tag	UNP A0AAF0BD41
L3	-8	HIS	-	expression tag	UNP A0AAF0BD41
L3	-7	HIS	-	expression tag	UNP A0AAF0BD41
L3	-6	GLU	-	expression tag	UNP A0AAF0BD41
L3	-5	ASN	-	expression tag	UNP A0AAF0BD41
L3	-4	LEU	-	expression tag	UNP A0AAF0BD41
L3	-3	TYR	-	expression tag	UNP A0AAF0BD41
L3	-2	PHE	-	expression tag	UNP A0AAF0BD41
L3	-1	GLN	-	expression tag	UNP A0AAF0BD41
L3	197	MET	VAL	conflict	UNP A0AAF0BD41
L3	298	PRO	LEU	conflict	UNP A0AAF0BD41
L3	306	VAL	ILE	conflict	UNP A0AAF0BD41
L3	751	HIS	TYR	conflict	UNP A0AAF0BD41
L3	774	HIS	TYR	conflict	UNP A0AAF0BD41
L3	805	ALA	SER	conflict	UNP A0AAF0BD41
L4	-13	MET	-	initiating methionine	UNP A0AAF0BD41
L4	-12	HIS	-	expression tag	UNP A0AAF0BD41
L4	-11	HIS	-	expression tag	UNP A0AAF0BD41
L4	-10	HIS	-	expression tag	UNP A0AAF0BD41
L4	-9	HIS	-	expression tag	UNP A0AAF0BD41
L4	-8	HIS	-	expression tag	UNP A0AAF0BD41
L4	-7	HIS	-	expression tag	UNP A0AAF0BD41
L4	-6	GLU	-	expression tag	UNP A0AAF0BD41
L4	-5	ASN	-	expression tag	UNP A0AAF0BD41
L4	-4	LEU	-	expression tag	UNP A0AAF0BD41
L4	-3	TYR	-	expression tag	UNP A0AAF0BD41
L4	-2	PHE	-	expression tag	UNP A0AAF0BD41
L4	-1	GLN	-	expression tag	UNP A0AAF0BD41
L4	197	MET	VAL	conflict	UNP A0AAF0BD41
L4	298	PRO	LEU	conflict	UNP A0AAF0BD41
L4	306	VAL	ILE	conflict	UNP A0AAF0BD41
L4	751	HIS	TYR	conflict	UNP A0AAF0BD41
L4	774	HIS	TYR	conflict	UNP A0AAF0BD41
L4	805	ALA	SER	conflict	UNP A0AAF0BD41
L5	-13	MET	-	initiating methionine	UNP A0AAF0BD41
L5	-12	HIS	-	expression tag	UNP A0AAF0BD41
L5	-11	HIS	-	expression tag	UNP A0AAF0BD41
L5	-10	HIS	-	expression tag	UNP A0AAF0BD41
L5	-9	HIS	-	expression tag	UNP A0AAF0BD41
L5	-8	HIS	-	expression tag	UNP A0AAF0BD41
L5	-7	HIS	-	expression tag	UNP A0AAF0BD41

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Chain	Residue	Modelled	Actual	Comment	Reference
L5	-6	GLU	-	expression tag	UNP A0AAF0BD41
L5	-5	ASN	-	expression tag	UNP A0AAF0BD41
L5	-4	LEU	-	expression tag	UNP A0AAF0BD41
L5	-3	TYR	-	expression tag	UNP A0AAF0BD41
L5	-2	PHE	-	expression tag	UNP A0AAF0BD41
L5	-1	GLN	-	expression tag	UNP A0AAF0BD41
L5	197	MET	VAL	conflict	UNP A0AAF0BD41
L5	298	PRO	LEU	conflict	UNP A0AAF0BD41
L5	306	VAL	ILE	conflict	UNP A0AAF0BD41
L5	751	HIS	TYR	conflict	UNP A0AAF0BD41
L5	774	HIS	TYR	conflict	UNP A0AAF0BD41
L5	805	ALA	SER	conflict	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

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Mol	Chain	Residues	Atoms		AltConf
2	C4	2	Total 2	Ca 2	0
2	C5	2	Total 2	Ca 2	0
2	D1	2	Total 2	Ca 2	0
2	D2	2	Total 2	Ca 2	0
2	D3	2	Total 2	Ca 2	0
2	D4	2	Total 2	Ca 2	0
2	D5	2	Total 2	Ca 2	0
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

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Mol	Chain	Residues	Atoms		AltConf
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
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

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Mol	Chain	Residues	Atoms		AltConf
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

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Mol	Chain	Residues	Atoms		AltConf
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
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

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Mol	Chain	Residues	Atoms		AltConf
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
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

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Mol	Chain	Residues	Atoms		AltConf
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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A1	651	Total 651	O 651	0
4	A2	646	Total 646	O 646	0
4	A3	641	Total 641	O 641	0
4	A4	652	Total 652	O 652	0
4	A5	651	Total 651	O 651	0
4	B1	651	Total 651	O 651	0
4	B2	650	Total 650	O 650	0
4	B3	644	Total 644	O 644	0
4	B4	655	Total 655	O 655	0
4	B5	654	Total 654	O 654	0
4	C1	656	Total 656	O 656	0
4	C2	650	Total 650	O 650	0
4	C3	645	Total 645	O 645	0
4	C4	656	Total 656	O 656	0
4	C5	654	Total 654	O 654	0

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Mol	Chain	Residues	Atoms		AltConf
4	D1	655	Total 655	O 655	0
4	D2	650	Total 650	O 650	0
4	D3	645	Total 645	O 645	0
4	D4	654	Total 654	O 654	0
4	D5	654	Total 654	O 654	0
4	E1	653	Total 653	O 653	0
4	E2	650	Total 650	O 650	0
4	E3	644	Total 644	O 644	0
4	E4	655	Total 655	O 655	0
4	E5	654	Total 654	O 654	0
4	F1	653	Total 653	O 653	0
4	F2	650	Total 650	O 650	0
4	F3	640	Total 640	O 640	0
4	F4	656	Total 656	O 656	0
4	F5	654	Total 654	O 654	0
4	G1	656	Total 656	O 656	0
4	G2	650	Total 650	O 650	0
4	G3	640	Total 640	O 640	0
4	G4	655	Total 655	O 655	0
4	G5	653	Total 653	O 653	0
4	H1	656	Total 656	O 656	0

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Mol	Chain	Residues	Atoms		AltConf
4	H2	652	Total 652	O 652	0
4	H3	645	Total 645	O 645	0
4	H4	651	Total 651	O 651	0
4	H5	655	Total 655	O 655	0
4	I1	654	Total 654	O 654	0
4	I2	651	Total 651	O 651	0
4	I3	643	Total 643	O 643	0
4	I4	651	Total 651	O 651	0
4	I5	653	Total 653	O 653	0
4	J1	654	Total 654	O 654	0
4	J2	651	Total 651	O 651	0
4	J3	644	Total 644	O 644	0
4	J4	651	Total 651	O 651	0
4	J5	653	Total 653	O 653	0
4	K1	654	Total 654	O 654	0
4	K2	652	Total 652	O 652	0
4	K3	643	Total 643	O 643	0
4	K4	654	Total 654	O 654	0
4	K5	650	Total 650	O 650	0
4	L1	654	Total 654	O 654	0
4	L2	650	Total 650	O 650	0

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Mol	Chain	Residues	Atoms		AltConf
4	L3	643	Total 643	O 643	0
4	L4	654	Total 654	O 654	0
4	L5	653	Total 653	O 653	0

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

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64886	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.88	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.841	Depositor
Minimum map value	-0.195	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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.

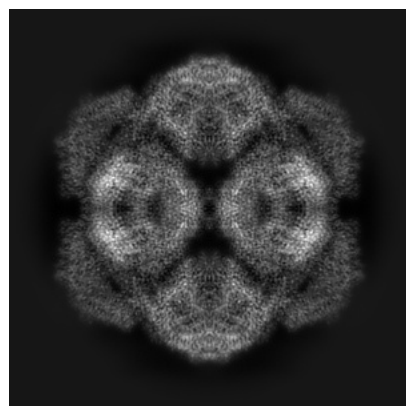
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55026. These allow visual inspection of the internal detail of the map and identification of artifacts.

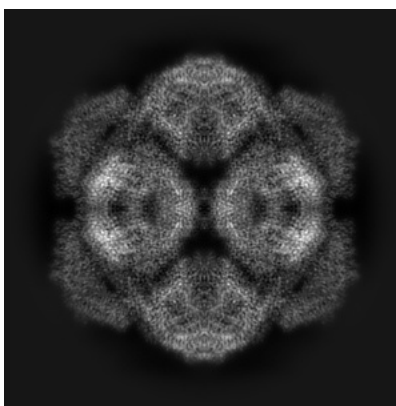
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

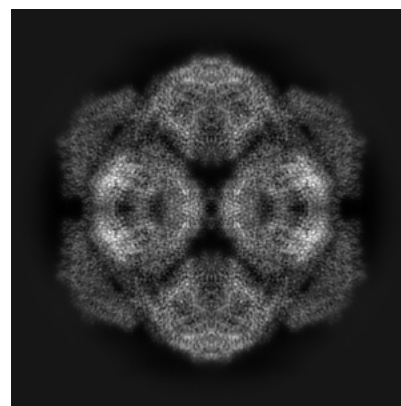
5.1.1 Primary map



X

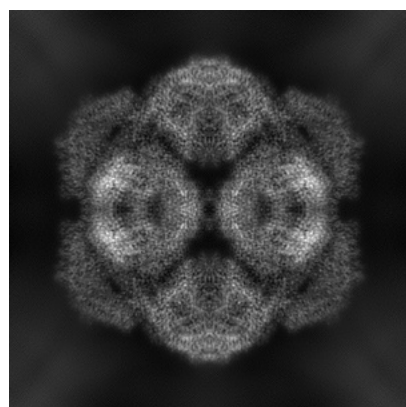


Y

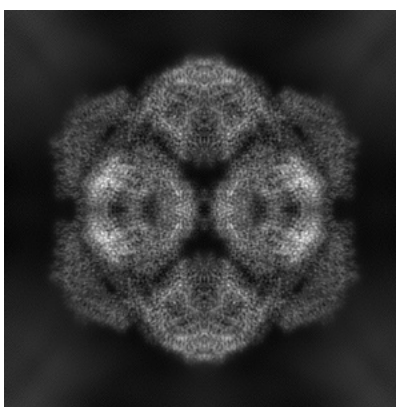


Z

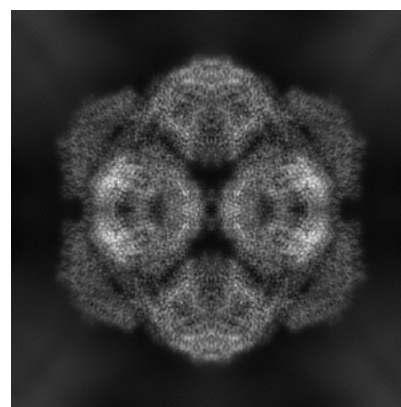
5.1.2 Raw map



X



Y

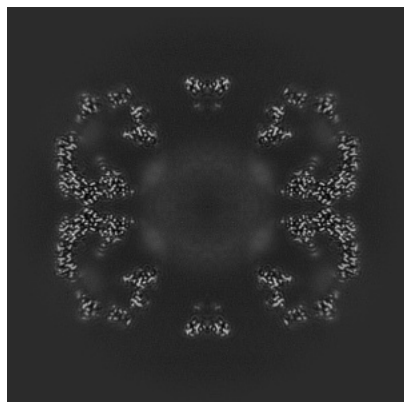


Z

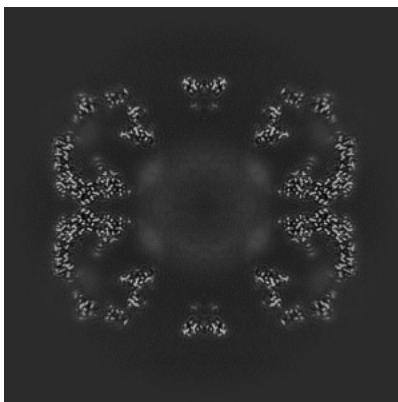
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

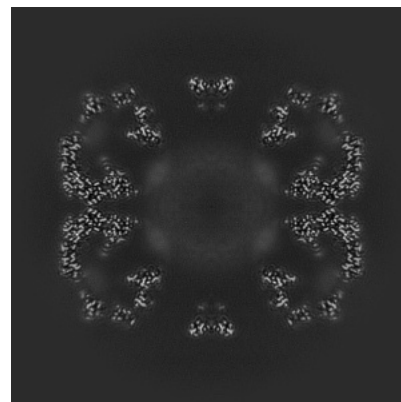
5.2.1 Primary map



X Index: 250

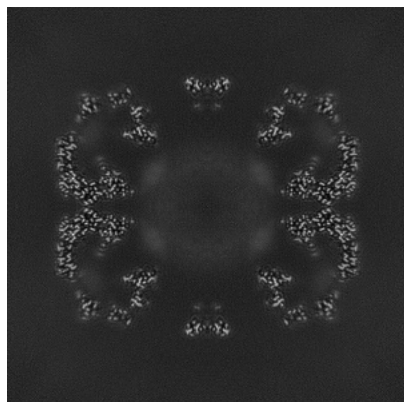


Y Index: 250

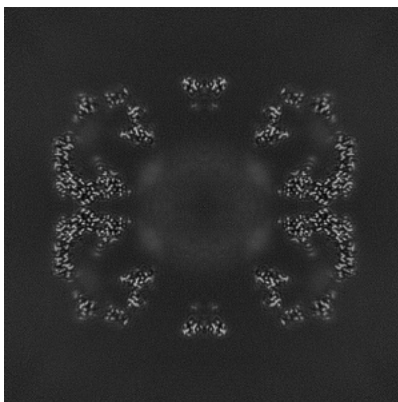


Z Index: 250

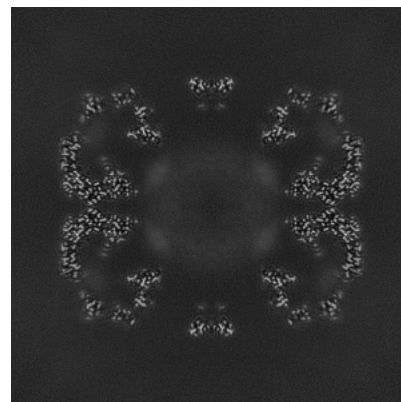
5.2.2 Raw map



X Index: 250



Y Index: 250

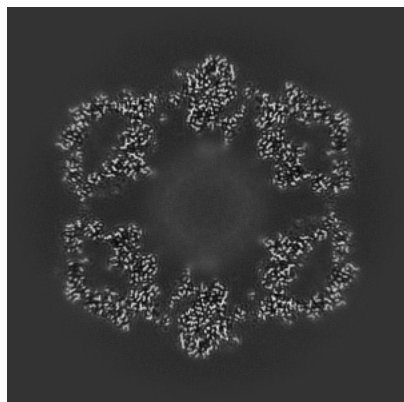


Z Index: 250

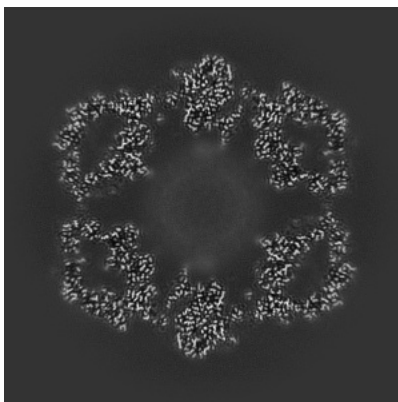
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

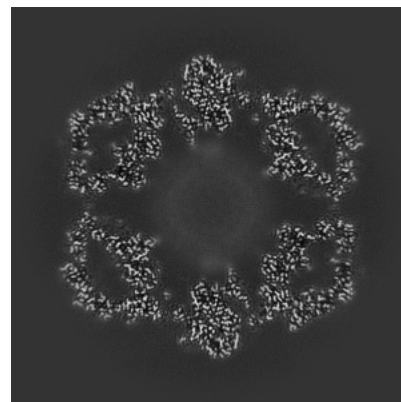
5.3.1 Primary map



X Index: 221

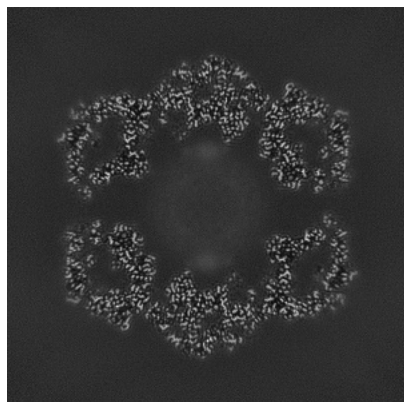


Y Index: 221

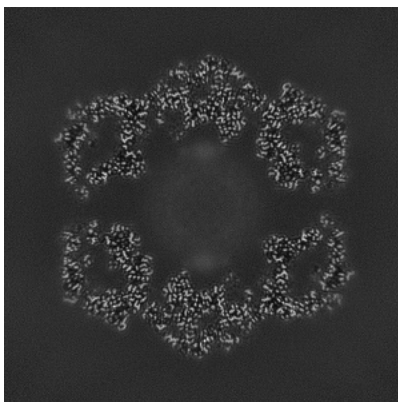


Z Index: 279

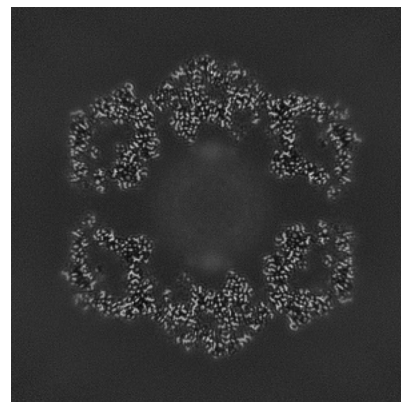
5.3.2 Raw map



X Index: 215



Y Index: 215

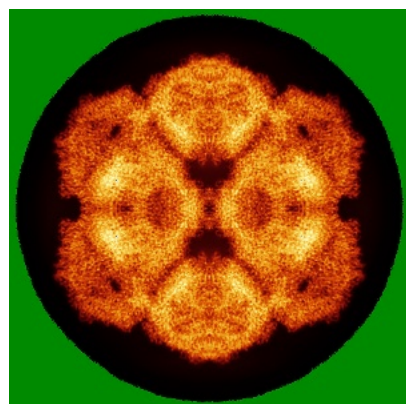


Z Index: 285

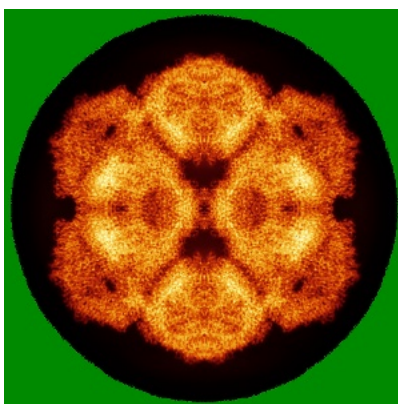
The images above show the largest variance slices of the map in three orthogonal directions.

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

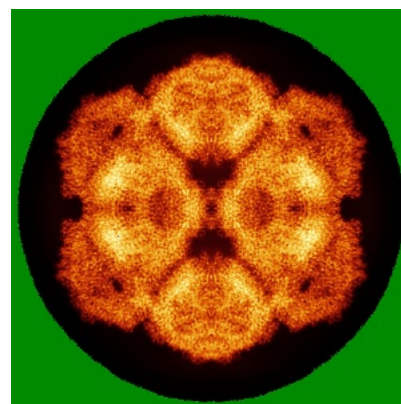
5.4.1 Primary map



X

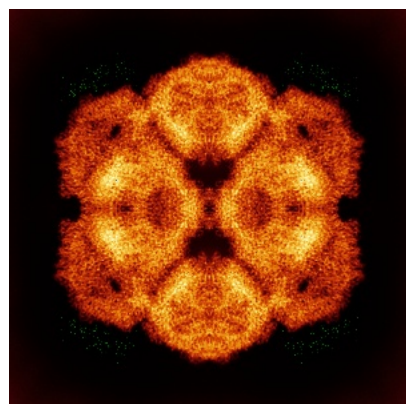


Y

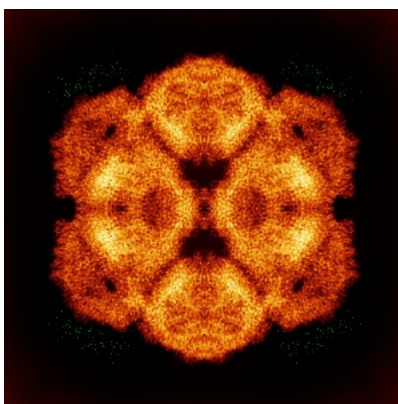


Z

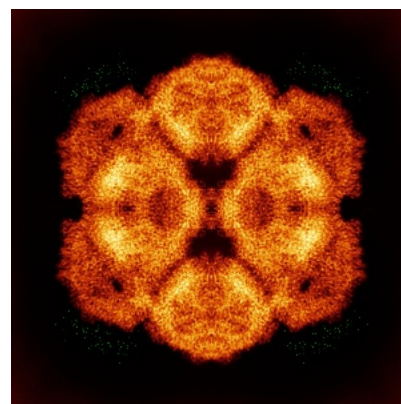
5.4.2 Raw map



X



Y

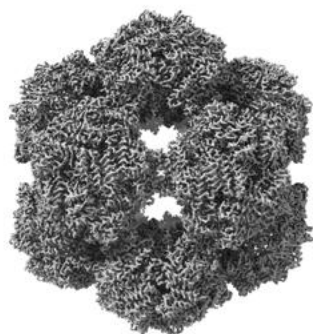


Z

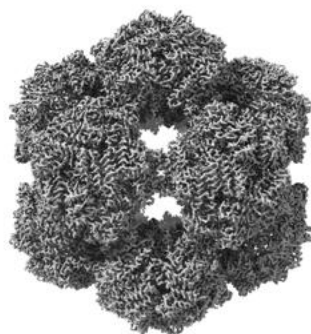
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views [i](#)

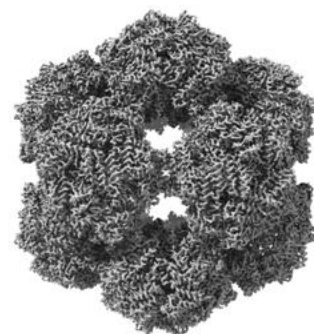
5.5.1 Primary map



X



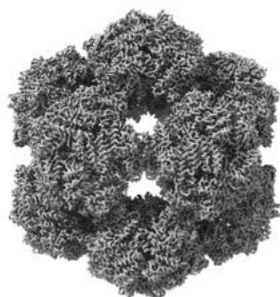
Y



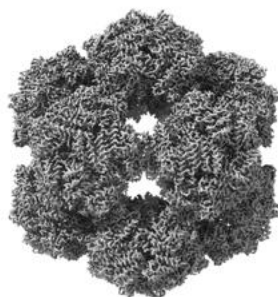
Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

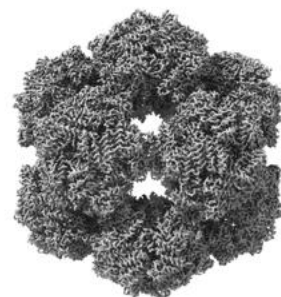
5.5.2 Raw map



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.

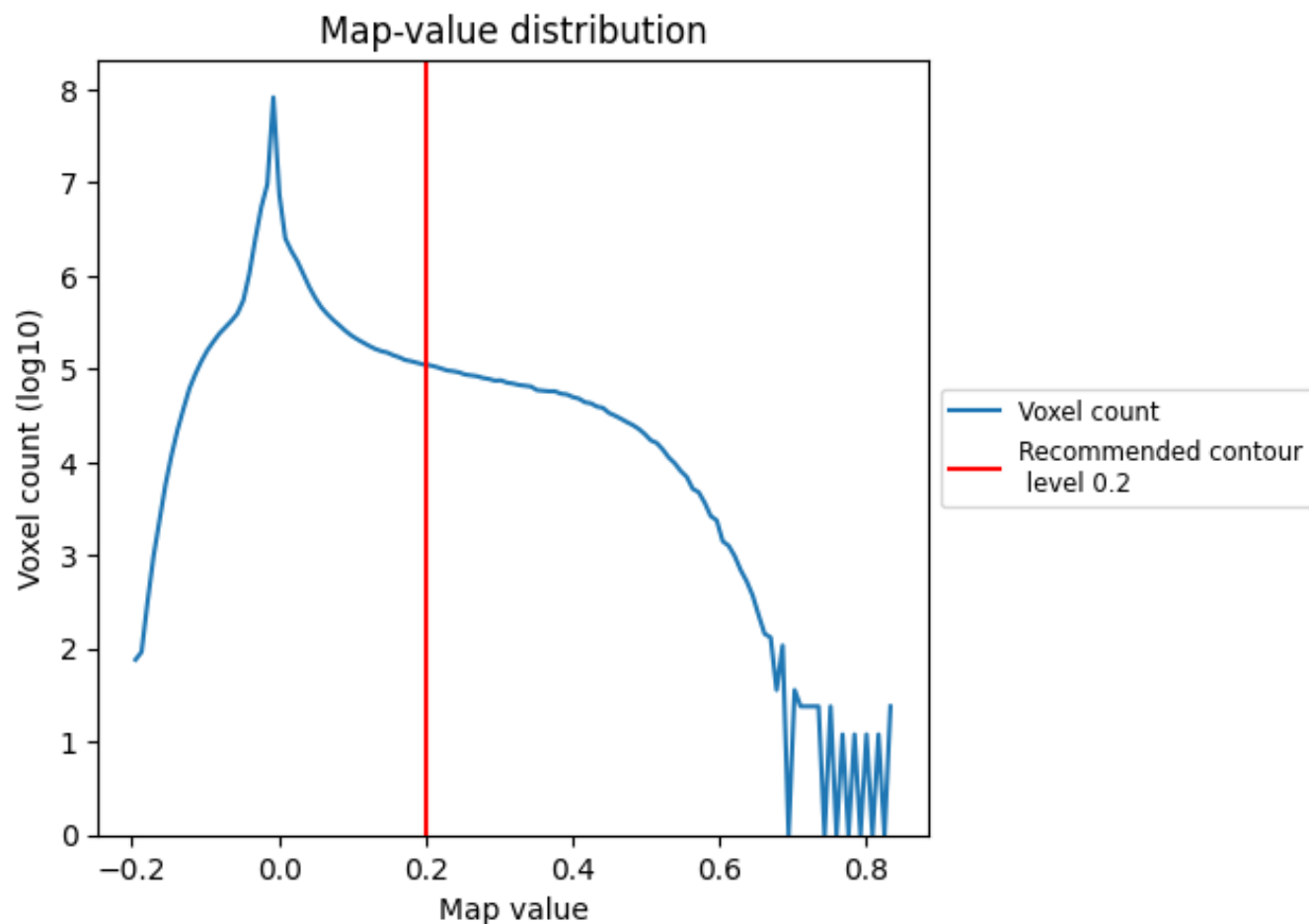
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

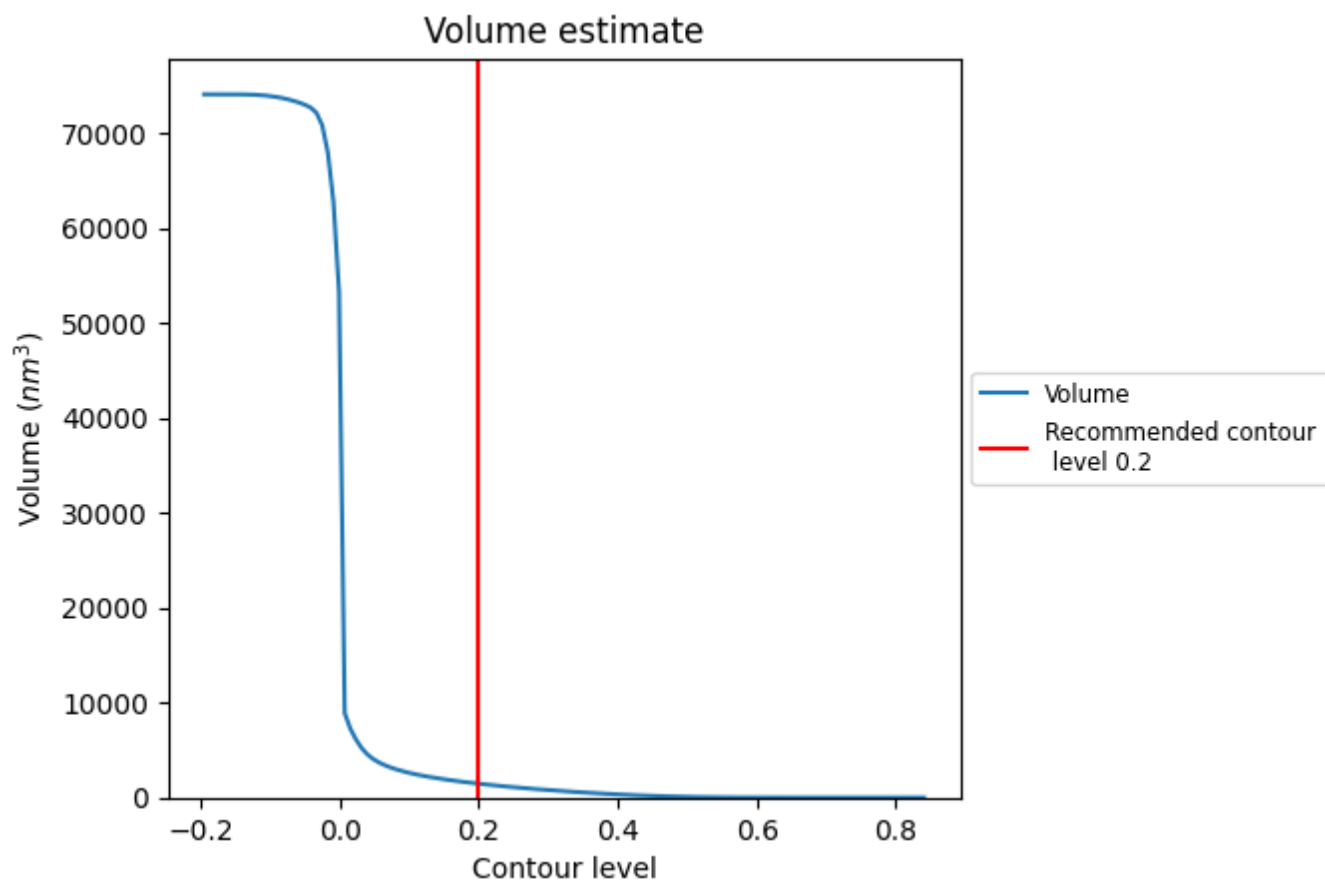
This section contains the results of statistical analysis of the map.

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.

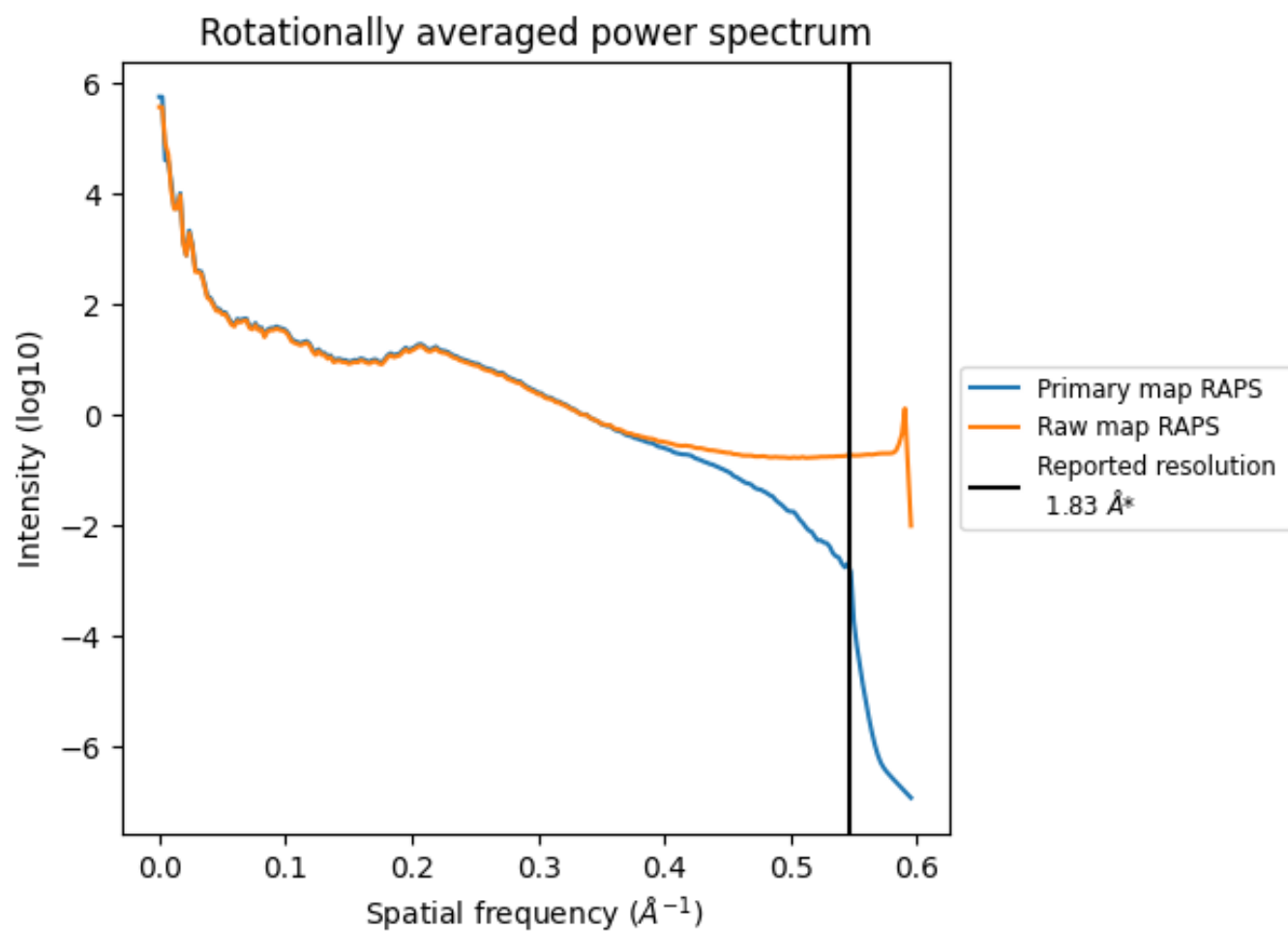
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 1463 nm^3 ; this corresponds to an approximate mass of 1322 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 ⓘ

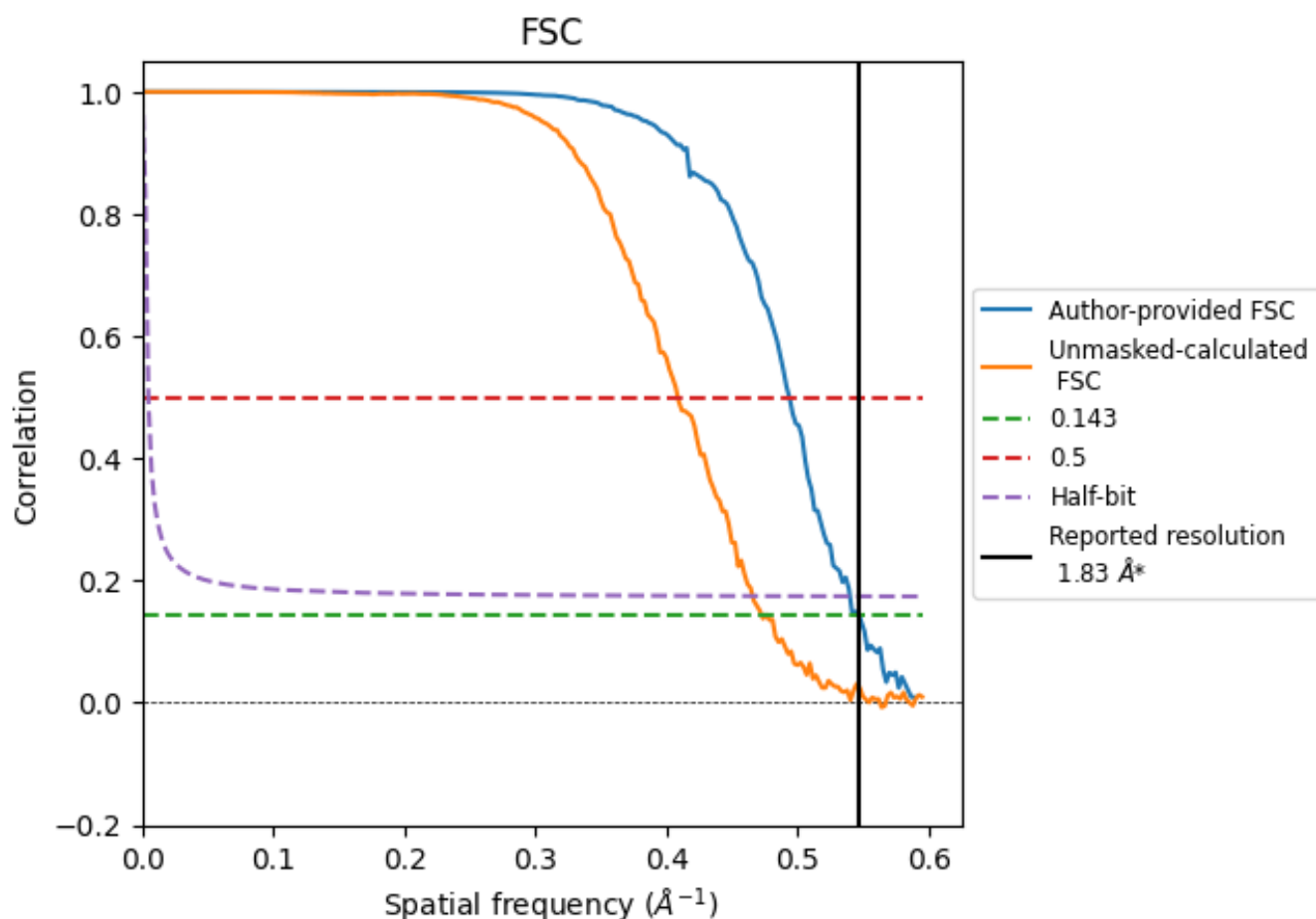


*Reported resolution corresponds to spatial frequency of 0.546 Å⁻¹

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 0.546 Å⁻¹

7.2 Resolution estimates [i](#)

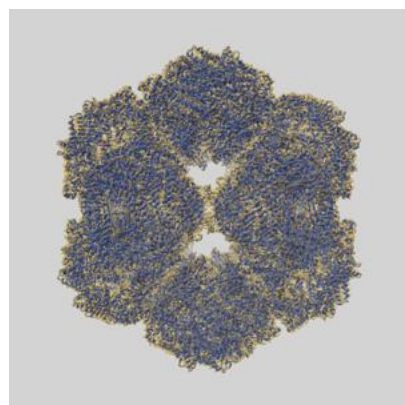
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.83	-	-
Author-provided FSC curve	1.83	2.02	1.85
Unmasked-calculated*	2.12	2.45	2.15

*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 2.12 differs from the reported value 1.83 by more than 10 %

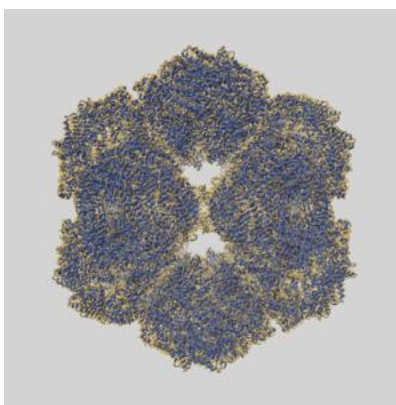
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55026 and PDB model 9SM4. Per-residue inclusion information can be found in section ?? on page ??.

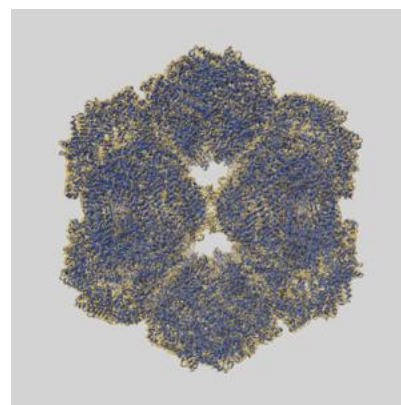
8.1 Map-model overlay [i](#)



X



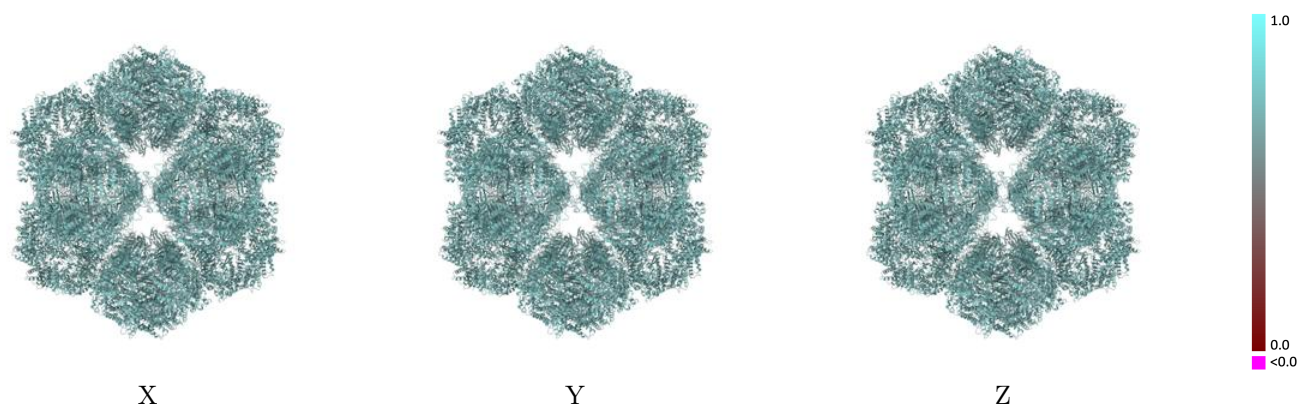
Y



Z

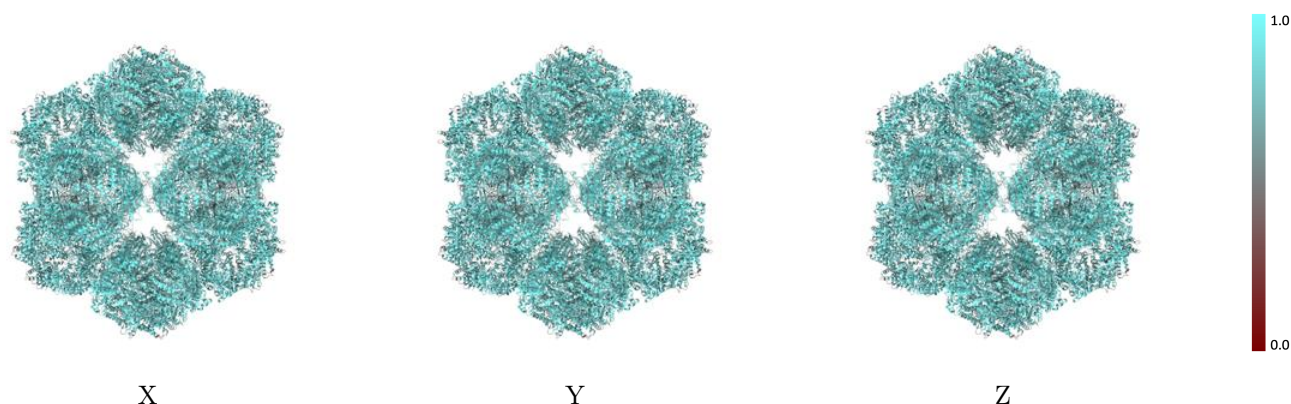
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



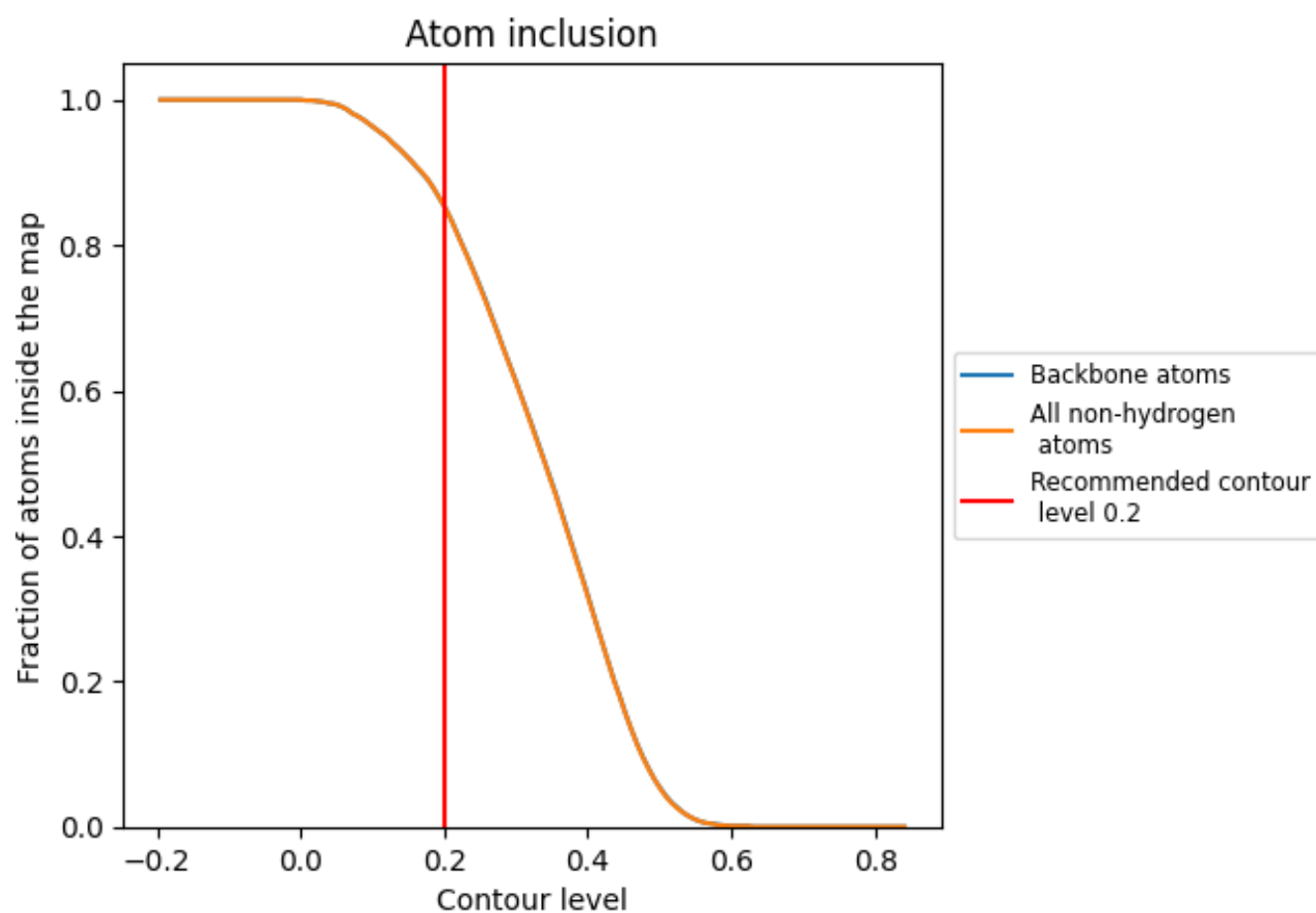
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

8.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8540	 0.6930
A1	 0.8590	 0.6940
A2	 0.8600	 0.6940
A3	 0.8600	 0.6920
A4	 0.8610	 0.6920
A5	 0.8590	 0.6920
B1	 0.8590	 0.6940
B2	 0.8610	 0.6930
B3	 0.8600	 0.6940
B4	 0.8620	 0.6930
B5	 0.8590	 0.6930
C1	 0.8600	 0.6940
C2	 0.8600	 0.6930
C3	 0.8590	 0.6930
C4	 0.8590	 0.6940
C5	 0.8630	 0.6940
D1	 0.8610	 0.6930
D2	 0.8590	 0.6940
D3	 0.8610	 0.6930
D4	 0.8590	 0.6940
D5	 0.8600	 0.6930
E1	 0.8600	 0.6930
E2	 0.8590	 0.6920
E3	 0.8620	 0.6930
E4	 0.8600	 0.6930
E5	 0.8600	 0.6930
F1	 0.8600	 0.6930
F2	 0.8570	 0.6940
F3	 0.8590	 0.6940
F4	 0.8620	 0.6950
F5	 0.8610	 0.6940
G1	 0.8590	 0.6940
G2	 0.8600	 0.6940
G3	 0.8590	 0.6930
G4	 0.8620	 0.6940



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Chain	Atom inclusion	Q-score
G5	 0.8600	 0.6950
H1	 0.8620	 0.6930
H2	 0.8610	 0.6930
H3	 0.8590	 0.6930
H4	 0.8580	 0.6940
H5	 0.8590	 0.6950
I1	 0.8610	 0.6930
I2	 0.8590	 0.6930
I3	 0.8580	 0.6930
I4	 0.8600	 0.6930
I5	 0.8600	 0.6920
J1	 0.8610	 0.6930
J2	 0.8610	 0.6920
J3	 0.8560	 0.6920
J4	 0.8580	 0.6920
J5	 0.8610	 0.6920
K1	 0.8600	 0.6930
K2	 0.8620	 0.6940
K3	 0.8600	 0.6940
K4	 0.8610	 0.6950
K5	 0.8590	 0.6930
L1	 0.8610	 0.6930
L2	 0.8600	 0.6940
L3	 0.8590	 0.6950
L4	 0.8600	 0.6930
L5	 0.8600	 0.6930