



wwPDB EM Validation Summary Report i

Jan 17, 2024 – 06:51 am GMT

PDB ID : 7ZHS
EMDB ID : EMD-14736
Title : 3D reconstruction of the cylindrical assembly of DnaJA2 delta G/F by imposing D5 symmetry
Authors : Cuellar, J.; Velasco-Carneros, L.; Santiago, C.; Martin-Benito, J.; Valpuesta, J.; Muga, A.
Deposited on : 2022-04-07
Resolution : 6.90 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 i 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](#) ①) were used in the production of this report:

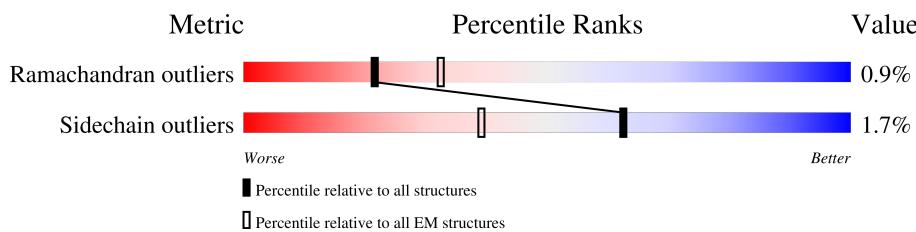
EMDB validation analysis : 0.0.1.dev70
MolProbit : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

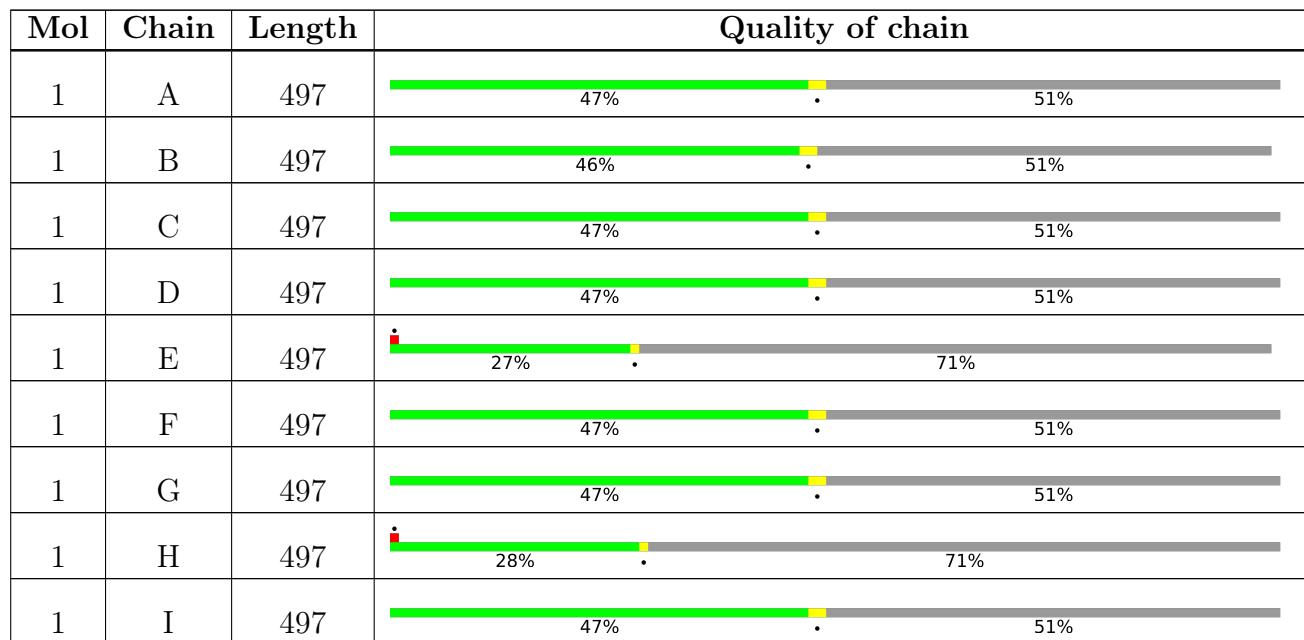
The reported resolution of this entry is 6.90 Å.

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



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

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



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Mol	Chain	Length	Quality of chain		
1	J	497	46%	.	51%
1	K	497	47%	.	51%
1	L	497	47%	.	51%
1	M	497	47%	.	51%
1	N	497	47%	.	51%
1	O	497	47%	.	51%
1	P	497	47%	.	51%
1	Q	497	47%	.	51%
1	R	497	47%	.	51%
1	S	497	47%	.	51%
1	T	497	47%	.	51%
1	U	497	47%	.	51%
1	V	497	47%	.	51%
1	W	497	47%	.	51%
1	X	497	47%	.	51%
1	Y	497	27%	.	71%
1	Z	497	27%	.	71%
1	a	497	27%	.	71%
1	b	497	27%	.	71%
1	c	497	47%	.	51%
1	d	497	47%	.	51%
1	e	497	47%	.	51%
1	f	497	47%	.	51%
1	g	497	47%	.	51%
1	h	497	47%	.	51%

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Mol	Chain	Length	Quality of chain		
1	i	497	47%	.	51%
1	j	497	47%	.	51%
1	k	497	28%	.	71%
1	l	497	28%	.	71%
1	m	497	28%	.	71%
1	n	497	28%	.	71%

2 Entry composition [\(i\)](#)

There are 2 unique types of molecules in this entry. The entry contains 67465 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 Ubiquitin-like protein SMT3,DnaJ homolog subfamily A member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	C	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	B	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	D	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	E	143	Total	C	N	O	S		
			1073	656	197	206	14	0	0
1	G	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	F	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	H	144	Total	C	N	O	S		
			1082	661	198	209	14	0	0
1	I	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	Q	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	M	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	U	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	Y	143	Total	C	N	O	S		
			1073	656	197	206	14	0	0
1	g	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	c	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	k	144	Total	C	N	O	S		
			1082	661	198	209	14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	R	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	N	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	V	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	Z	143	Total	C	N	O	S		
			1073	656	197	206	14	0	0
1	h	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	d	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	l	144	Total	C	N	O	S		
			1082	661	198	209	14	0	0
1	K	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	S	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	O	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	W	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	a	143	Total	C	N	O	S		
			1073	656	197	206	14	0	0
1	i	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	e	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	m	144	Total	C	N	O	S		
			1082	661	198	209	14	0	0
1	L	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	T	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	P	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	X	242	Total	C	N	O	S		
			1887	1180	335	354	18	0	0
1	b	143	Total	C	N	O	S		
			1073	656	197	206	14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	j	242	Total	C	N	O	S	0	0
			1887	1180	335	354	18		
1	f	242	Total	C	N	O	S	0	0
			1887	1180	335	354	18		
1	n	144	Total	C	N	O	S	0	0
			1082	661	198	209	14		

There are 1440 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-154	MET	-	initiating methionine	UNP Q12306
A	-153	GLY	-	expression tag	UNP Q12306
A	-152	HIS	-	expression tag	UNP Q12306
A	-151	HIS	-	expression tag	UNP Q12306
A	-150	HIS	-	expression tag	UNP Q12306
A	-149	HIS	-	expression tag	UNP Q12306
A	-148	HIS	-	expression tag	UNP Q12306
A	-147	HIS	-	expression tag	UNP Q12306
A	-146	GLY	-	expression tag	UNP Q12306
A	-145	SER	-	expression tag	UNP Q12306
A	-144	LEU	-	expression tag	UNP Q12306
A	-143	GLN	-	expression tag	UNP Q12306
A	-68	ALA	THR	conflict	UNP Q12306
A	?	-	SER	deletion	UNP O60884
A	?	-	GLY	deletion	UNP O60884
A	?	-	GLY	deletion	UNP O60884
A	?	-	GLY	deletion	UNP O60884
A	?	-	GLY	deletion	UNP O60884
A	?	-	GLY	deletion	UNP O60884
A	?	-	MET	deletion	UNP O60884
A	?	-	ASP	deletion	UNP O60884
A	?	-	ASP	deletion	UNP O60884
A	?	-	ILE	deletion	UNP O60884
A	?	-	PHE	deletion	UNP O60884
A	?	-	SER	deletion	UNP O60884
A	?	-	HIS	deletion	UNP O60884
A	?	-	ILE	deletion	UNP O60884
A	?	-	PHE	deletion	UNP O60884
A	?	-	GLY	deletion	UNP O60884
A	?	-	GLY	deletion	UNP O60884
A	?	-	GLY	deletion	UNP O60884
A	?	-	LEU	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP O60884
A	?	-	GLY	deletion	UNP O60884
A	?	-	PHE	deletion	UNP O60884
A	?	-	MET	deletion	UNP O60884
C	-154	MET	-	initiating methionine	UNP Q12306
C	-153	GLY	-	expression tag	UNP Q12306
C	-152	HIS	-	expression tag	UNP Q12306
C	-151	HIS	-	expression tag	UNP Q12306
C	-150	HIS	-	expression tag	UNP Q12306
C	-149	HIS	-	expression tag	UNP Q12306
C	-148	HIS	-	expression tag	UNP Q12306
C	-147	HIS	-	expression tag	UNP Q12306
C	-146	GLY	-	expression tag	UNP Q12306
C	-145	SER	-	expression tag	UNP Q12306
C	-144	LEU	-	expression tag	UNP Q12306
C	-143	GLN	-	expression tag	UNP Q12306
C	-68	ALA	THR	conflict	UNP Q12306
C	?	-	SER	deletion	UNP O60884
C	?	-	GLY	deletion	UNP O60884
C	?	-	GLY	deletion	UNP O60884
C	?	-	GLY	deletion	UNP O60884
C	?	-	GLY	deletion	UNP O60884
C	?	-	GLY	deletion	UNP O60884
C	?	-	MET	deletion	UNP O60884
C	?	-	ASP	deletion	UNP O60884
C	?	-	ASP	deletion	UNP O60884
C	?	-	ILE	deletion	UNP O60884
C	?	-	PHE	deletion	UNP O60884
C	?	-	SER	deletion	UNP O60884
C	?	-	HIS	deletion	UNP O60884
C	?	-	ILE	deletion	UNP O60884
C	?	-	PHE	deletion	UNP O60884
C	?	-	GLY	deletion	UNP O60884
C	?	-	GLY	deletion	UNP O60884
C	?	-	GLY	deletion	UNP O60884
C	?	-	LEU	deletion	UNP O60884
C	?	-	PHE	deletion	UNP O60884
C	?	-	GLY	deletion	UNP O60884
C	?	-	PHE	deletion	UNP O60884
C	?	-	MET	deletion	UNP O60884
B	-154	MET	-	initiating methionine	UNP Q12306
B	-153	GLY	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-152	HIS	-	expression tag	UNP Q12306
B	-151	HIS	-	expression tag	UNP Q12306
B	-150	HIS	-	expression tag	UNP Q12306
B	-149	HIS	-	expression tag	UNP Q12306
B	-148	HIS	-	expression tag	UNP Q12306
B	-147	HIS	-	expression tag	UNP Q12306
B	-146	GLY	-	expression tag	UNP Q12306
B	-145	SER	-	expression tag	UNP Q12306
B	-144	LEU	-	expression tag	UNP Q12306
B	-143	GLN	-	expression tag	UNP Q12306
B	-68	ALA	THR	conflict	UNP Q12306
B	?	-	SER	deletion	UNP O60884
B	?	-	GLY	deletion	UNP O60884
B	?	-	GLY	deletion	UNP O60884
B	?	-	GLY	deletion	UNP O60884
B	?	-	GLY	deletion	UNP O60884
B	?	-	GLY	deletion	UNP O60884
B	?	-	MET	deletion	UNP O60884
B	?	-	ASP	deletion	UNP O60884
B	?	-	ASP	deletion	UNP O60884
B	?	-	ILE	deletion	UNP O60884
B	?	-	PHE	deletion	UNP O60884
B	?	-	SER	deletion	UNP O60884
B	?	-	HIS	deletion	UNP O60884
B	?	-	ILE	deletion	UNP O60884
B	?	-	PHE	deletion	UNP O60884
B	?	-	GLY	deletion	UNP O60884
B	?	-	GLY	deletion	UNP O60884
B	?	-	GLY	deletion	UNP O60884
B	?	-	LEU	deletion	UNP O60884
B	?	-	PHE	deletion	UNP O60884
B	?	-	GLY	deletion	UNP O60884
B	?	-	PHE	deletion	UNP O60884
B	?	-	MET	deletion	UNP O60884
D	-154	MET	-	initiating methionine	UNP Q12306
D	-153	GLY	-	expression tag	UNP Q12306
D	-152	HIS	-	expression tag	UNP Q12306
D	-151	HIS	-	expression tag	UNP Q12306
D	-150	HIS	-	expression tag	UNP Q12306
D	-149	HIS	-	expression tag	UNP Q12306
D	-148	HIS	-	expression tag	UNP Q12306
D	-147	HIS	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-146	GLY	-	expression tag	UNP Q12306
D	-145	SER	-	expression tag	UNP Q12306
D	-144	LEU	-	expression tag	UNP Q12306
D	-143	GLN	-	expression tag	UNP Q12306
D	-68	ALA	THR	conflict	UNP Q12306
D	?	-	SER	deletion	UNP O60884
D	?	-	GLY	deletion	UNP O60884
D	?	-	GLY	deletion	UNP O60884
D	?	-	GLY	deletion	UNP O60884
D	?	-	GLY	deletion	UNP O60884
D	?	-	GLY	deletion	UNP O60884
D	?	-	MET	deletion	UNP O60884
D	?	-	ASP	deletion	UNP O60884
D	?	-	ASP	deletion	UNP O60884
D	?	-	ILE	deletion	UNP O60884
D	?	-	PHE	deletion	UNP O60884
D	?	-	SER	deletion	UNP O60884
D	?	-	HIS	deletion	UNP O60884
D	?	-	ILE	deletion	UNP O60884
D	?	-	PHE	deletion	UNP O60884
D	?	-	GLY	deletion	UNP O60884
D	?	-	GLY	deletion	UNP O60884
D	?	-	GLY	deletion	UNP O60884
D	?	-	LEU	deletion	UNP O60884
D	?	-	PHE	deletion	UNP O60884
D	?	-	GLY	deletion	UNP O60884
D	?	-	PHE	deletion	UNP O60884
D	?	-	MET	deletion	UNP O60884
E	-154	MET	-	initiating methionine	UNP Q12306
E	-153	GLY	-	expression tag	UNP Q12306
E	-152	HIS	-	expression tag	UNP Q12306
E	-151	HIS	-	expression tag	UNP Q12306
E	-150	HIS	-	expression tag	UNP Q12306
E	-149	HIS	-	expression tag	UNP Q12306
E	-148	HIS	-	expression tag	UNP Q12306
E	-147	HIS	-	expression tag	UNP Q12306
E	-146	GLY	-	expression tag	UNP Q12306
E	-145	SER	-	expression tag	UNP Q12306
E	-144	LEU	-	expression tag	UNP Q12306
E	-143	GLN	-	expression tag	UNP Q12306
E	-68	ALA	THR	conflict	UNP Q12306
E	?	-	SER	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	GLY	deletion	UNP O60884
E	?	-	GLY	deletion	UNP O60884
E	?	-	GLY	deletion	UNP O60884
E	?	-	GLY	deletion	UNP O60884
E	?	-	GLY	deletion	UNP O60884
E	?	-	MET	deletion	UNP O60884
E	?	-	ASP	deletion	UNP O60884
E	?	-	ASP	deletion	UNP O60884
E	?	-	ILE	deletion	UNP O60884
E	?	-	PHE	deletion	UNP O60884
E	?	-	SER	deletion	UNP O60884
E	?	-	HIS	deletion	UNP O60884
E	?	-	ILE	deletion	UNP O60884
E	?	-	PHE	deletion	UNP O60884
E	?	-	GLY	deletion	UNP O60884
E	?	-	GLY	deletion	UNP O60884
E	?	-	GLY	deletion	UNP O60884
E	?	-	LEU	deletion	UNP O60884
E	?	-	PHE	deletion	UNP O60884
E	?	-	GLY	deletion	UNP O60884
E	?	-	PHE	deletion	UNP O60884
E	?	-	MET	deletion	UNP O60884
G	-154	MET	-	initiating methionine	UNP Q12306
G	-153	GLY	-	expression tag	UNP Q12306
G	-152	HIS	-	expression tag	UNP Q12306
G	-151	HIS	-	expression tag	UNP Q12306
G	-150	HIS	-	expression tag	UNP Q12306
G	-149	HIS	-	expression tag	UNP Q12306
G	-148	HIS	-	expression tag	UNP Q12306
G	-147	HIS	-	expression tag	UNP Q12306
G	-146	GLY	-	expression tag	UNP Q12306
G	-145	SER	-	expression tag	UNP Q12306
G	-144	LEU	-	expression tag	UNP Q12306
G	-143	GLN	-	expression tag	UNP Q12306
G	-68	ALA	THR	conflict	UNP Q12306
G	?	-	SER	deletion	UNP O60884
G	?	-	GLY	deletion	UNP O60884
G	?	-	GLY	deletion	UNP O60884
G	?	-	GLY	deletion	UNP O60884
G	?	-	GLY	deletion	UNP O60884
G	?	-	MET	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	ASP	deletion	UNP O60884
G	?	-	ASP	deletion	UNP O60884
G	?	-	ILE	deletion	UNP O60884
G	?	-	PHE	deletion	UNP O60884
G	?	-	SER	deletion	UNP O60884
G	?	-	HIS	deletion	UNP O60884
G	?	-	ILE	deletion	UNP O60884
G	?	-	PHE	deletion	UNP O60884
G	?	-	GLY	deletion	UNP O60884
G	?	-	GLY	deletion	UNP O60884
G	?	-	GLY	deletion	UNP O60884
G	?	-	LEU	deletion	UNP O60884
G	?	-	PHE	deletion	UNP O60884
G	?	-	GLY	deletion	UNP O60884
G	?	-	PHE	deletion	UNP O60884
G	?	-	MET	deletion	UNP O60884
F	-154	MET	-	initiating methionine	UNP Q12306
F	-153	GLY	-	expression tag	UNP Q12306
F	-152	HIS	-	expression tag	UNP Q12306
F	-151	HIS	-	expression tag	UNP Q12306
F	-150	HIS	-	expression tag	UNP Q12306
F	-149	HIS	-	expression tag	UNP Q12306
F	-148	HIS	-	expression tag	UNP Q12306
F	-147	HIS	-	expression tag	UNP Q12306
F	-146	GLY	-	expression tag	UNP Q12306
F	-145	SER	-	expression tag	UNP Q12306
F	-144	LEU	-	expression tag	UNP Q12306
F	-143	GLN	-	expression tag	UNP Q12306
F	-68	ALA	THR	conflict	UNP Q12306
F	?	-	SER	deletion	UNP O60884
F	?	-	GLY	deletion	UNP O60884
F	?	-	GLY	deletion	UNP O60884
F	?	-	GLY	deletion	UNP O60884
F	?	-	GLY	deletion	UNP O60884
F	?	-	MET	deletion	UNP O60884
F	?	-	ASP	deletion	UNP O60884
F	?	-	ASP	deletion	UNP O60884
F	?	-	ILE	deletion	UNP O60884
F	?	-	PHE	deletion	UNP O60884
F	?	-	SER	deletion	UNP O60884
F	?	-	HIS	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ILE	deletion	UNP O60884
F	?	-	PHE	deletion	UNP O60884
F	?	-	GLY	deletion	UNP O60884
F	?	-	GLY	deletion	UNP O60884
F	?	-	GLY	deletion	UNP O60884
F	?	-	LEU	deletion	UNP O60884
F	?	-	PHE	deletion	UNP O60884
F	?	-	GLY	deletion	UNP O60884
F	?	-	PHE	deletion	UNP O60884
F	?	-	MET	deletion	UNP O60884
H	-154	MET	-	initiating methionine	UNP Q12306
H	-153	GLY	-	expression tag	UNP Q12306
H	-152	HIS	-	expression tag	UNP Q12306
H	-151	HIS	-	expression tag	UNP Q12306
H	-150	HIS	-	expression tag	UNP Q12306
H	-149	HIS	-	expression tag	UNP Q12306
H	-148	HIS	-	expression tag	UNP Q12306
H	-147	HIS	-	expression tag	UNP Q12306
H	-146	GLY	-	expression tag	UNP Q12306
H	-145	SER	-	expression tag	UNP Q12306
H	-144	LEU	-	expression tag	UNP Q12306
H	-143	GLN	-	expression tag	UNP Q12306
H	-68	ALA	THR	conflict	UNP Q12306
H	?	-	SER	deletion	UNP O60884
H	?	-	GLY	deletion	UNP O60884
H	?	-	GLY	deletion	UNP O60884
H	?	-	GLY	deletion	UNP O60884
H	?	-	GLY	deletion	UNP O60884
H	?	-	GLY	deletion	UNP O60884
H	?	-	MET	deletion	UNP O60884
H	?	-	ASP	deletion	UNP O60884
H	?	-	ASP	deletion	UNP O60884
H	?	-	ILE	deletion	UNP O60884
H	?	-	PHE	deletion	UNP O60884
H	?	-	SER	deletion	UNP O60884
H	?	-	HIS	deletion	UNP O60884
H	?	-	ILE	deletion	UNP O60884
H	?	-	PHE	deletion	UNP O60884
H	?	-	GLY	deletion	UNP O60884
H	?	-	GLY	deletion	UNP O60884
H	?	-	GLY	deletion	UNP O60884
H	?	-	LEU	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	PHE	deletion	UNP O60884
H	?	-	GLY	deletion	UNP O60884
H	?	-	PHE	deletion	UNP O60884
H	?	-	MET	deletion	UNP O60884
I	-154	MET	-	initiating methionine	UNP Q12306
I	-153	GLY	-	expression tag	UNP Q12306
I	-152	HIS	-	expression tag	UNP Q12306
I	-151	HIS	-	expression tag	UNP Q12306
I	-150	HIS	-	expression tag	UNP Q12306
I	-149	HIS	-	expression tag	UNP Q12306
I	-148	HIS	-	expression tag	UNP Q12306
I	-147	HIS	-	expression tag	UNP Q12306
I	-146	GLY	-	expression tag	UNP Q12306
I	-145	SER	-	expression tag	UNP Q12306
I	-144	LEU	-	expression tag	UNP Q12306
I	-143	GLN	-	expression tag	UNP Q12306
I	-68	ALA	THR	conflict	UNP Q12306
I	?	-	SER	deletion	UNP O60884
I	?	-	GLY	deletion	UNP O60884
I	?	-	GLY	deletion	UNP O60884
I	?	-	GLY	deletion	UNP O60884
I	?	-	GLY	deletion	UNP O60884
I	?	-	GLY	deletion	UNP O60884
I	?	-	MET	deletion	UNP O60884
I	?	-	ASP	deletion	UNP O60884
I	?	-	ASP	deletion	UNP O60884
I	?	-	ILE	deletion	UNP O60884
I	?	-	PHE	deletion	UNP O60884
I	?	-	SER	deletion	UNP O60884
I	?	-	HIS	deletion	UNP O60884
I	?	-	ILE	deletion	UNP O60884
I	?	-	PHE	deletion	UNP O60884
I	?	-	GLY	deletion	UNP O60884
I	?	-	GLY	deletion	UNP O60884
I	?	-	GLY	deletion	UNP O60884
I	?	-	LEU	deletion	UNP O60884
I	?	-	PHE	deletion	UNP O60884
I	?	-	GLY	deletion	UNP O60884
I	?	-	PHE	deletion	UNP O60884
I	?	-	MET	deletion	UNP O60884
Q	-154	MET	-	initiating methionine	UNP Q12306
Q	-153	GLY	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-152	HIS	-	expression tag	UNP Q12306
Q	-151	HIS	-	expression tag	UNP Q12306
Q	-150	HIS	-	expression tag	UNP Q12306
Q	-149	HIS	-	expression tag	UNP Q12306
Q	-148	HIS	-	expression tag	UNP Q12306
Q	-147	HIS	-	expression tag	UNP Q12306
Q	-146	GLY	-	expression tag	UNP Q12306
Q	-145	SER	-	expression tag	UNP Q12306
Q	-144	LEU	-	expression tag	UNP Q12306
Q	-143	GLN	-	expression tag	UNP Q12306
Q	-68	ALA	THR	conflict	UNP Q12306
Q	?	-	SER	deletion	UNP O60884
Q	?	-	GLY	deletion	UNP O60884
Q	?	-	GLY	deletion	UNP O60884
Q	?	-	GLY	deletion	UNP O60884
Q	?	-	GLY	deletion	UNP O60884
Q	?	-	GLY	deletion	UNP O60884
Q	?	-	MET	deletion	UNP O60884
Q	?	-	ASP	deletion	UNP O60884
Q	?	-	ASP	deletion	UNP O60884
Q	?	-	ILE	deletion	UNP O60884
Q	?	-	PHE	deletion	UNP O60884
Q	?	-	SER	deletion	UNP O60884
Q	?	-	HIS	deletion	UNP O60884
Q	?	-	ILE	deletion	UNP O60884
Q	?	-	PHE	deletion	UNP O60884
Q	?	-	GLY	deletion	UNP O60884
Q	?	-	GLY	deletion	UNP O60884
Q	?	-	GLY	deletion	UNP O60884
Q	?	-	LEU	deletion	UNP O60884
Q	?	-	PHE	deletion	UNP O60884
Q	?	-	GLY	deletion	UNP O60884
Q	?	-	PHE	deletion	UNP O60884
Q	?	-	MET	deletion	UNP O60884
M	-154	MET	-	initiating methionine	UNP Q12306
M	-153	GLY	-	expression tag	UNP Q12306
M	-152	HIS	-	expression tag	UNP Q12306
M	-151	HIS	-	expression tag	UNP Q12306
M	-150	HIS	-	expression tag	UNP Q12306
M	-149	HIS	-	expression tag	UNP Q12306
M	-148	HIS	-	expression tag	UNP Q12306
M	-147	HIS	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-146	GLY	-	expression tag	UNP Q12306
M	-145	SER	-	expression tag	UNP Q12306
M	-144	LEU	-	expression tag	UNP Q12306
M	-143	GLN	-	expression tag	UNP Q12306
M	-68	ALA	THR	conflict	UNP Q12306
M	?	-	SER	deletion	UNP O60884
M	?	-	GLY	deletion	UNP O60884
M	?	-	GLY	deletion	UNP O60884
M	?	-	GLY	deletion	UNP O60884
M	?	-	GLY	deletion	UNP O60884
M	?	-	GLY	deletion	UNP O60884
M	?	-	MET	deletion	UNP O60884
M	?	-	ASP	deletion	UNP O60884
M	?	-	ASP	deletion	UNP O60884
M	?	-	ILE	deletion	UNP O60884
M	?	-	PHE	deletion	UNP O60884
M	?	-	SER	deletion	UNP O60884
M	?	-	HIS	deletion	UNP O60884
M	?	-	ILE	deletion	UNP O60884
M	?	-	PHE	deletion	UNP O60884
M	?	-	GLY	deletion	UNP O60884
M	?	-	GLY	deletion	UNP O60884
M	?	-	GLY	deletion	UNP O60884
M	?	-	LEU	deletion	UNP O60884
M	?	-	PHE	deletion	UNP O60884
M	?	-	GLY	deletion	UNP O60884
M	?	-	PHE	deletion	UNP O60884
M	?	-	MET	deletion	UNP O60884
U	-154	MET	-	initiating methionine	UNP Q12306
U	-153	GLY	-	expression tag	UNP Q12306
U	-152	HIS	-	expression tag	UNP Q12306
U	-151	HIS	-	expression tag	UNP Q12306
U	-150	HIS	-	expression tag	UNP Q12306
U	-149	HIS	-	expression tag	UNP Q12306
U	-148	HIS	-	expression tag	UNP Q12306
U	-147	HIS	-	expression tag	UNP Q12306
U	-146	GLY	-	expression tag	UNP Q12306
U	-145	SER	-	expression tag	UNP Q12306
U	-144	LEU	-	expression tag	UNP Q12306
U	-143	GLN	-	expression tag	UNP Q12306
U	-68	ALA	THR	conflict	UNP Q12306
U	?	-	SER	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
U	?	-	GLY	deletion	UNP O60884
U	?	-	GLY	deletion	UNP O60884
U	?	-	GLY	deletion	UNP O60884
U	?	-	GLY	deletion	UNP O60884
U	?	-	GLY	deletion	UNP O60884
U	?	-	MET	deletion	UNP O60884
U	?	-	ASP	deletion	UNP O60884
U	?	-	ASP	deletion	UNP O60884
U	?	-	ILE	deletion	UNP O60884
U	?	-	PHE	deletion	UNP O60884
U	?	-	SER	deletion	UNP O60884
U	?	-	HIS	deletion	UNP O60884
U	?	-	ILE	deletion	UNP O60884
U	?	-	PHE	deletion	UNP O60884
U	?	-	GLY	deletion	UNP O60884
U	?	-	GLY	deletion	UNP O60884
U	?	-	GLY	deletion	UNP O60884
U	?	-	LEU	deletion	UNP O60884
U	?	-	PHE	deletion	UNP O60884
U	?	-	GLY	deletion	UNP O60884
U	?	-	PHE	deletion	UNP O60884
U	?	-	MET	deletion	UNP O60884
Y	-154	MET	-	initiating methionine	UNP Q12306
Y	-153	GLY	-	expression tag	UNP Q12306
Y	-152	HIS	-	expression tag	UNP Q12306
Y	-151	HIS	-	expression tag	UNP Q12306
Y	-150	HIS	-	expression tag	UNP Q12306
Y	-149	HIS	-	expression tag	UNP Q12306
Y	-148	HIS	-	expression tag	UNP Q12306
Y	-147	HIS	-	expression tag	UNP Q12306
Y	-146	GLY	-	expression tag	UNP Q12306
Y	-145	SER	-	expression tag	UNP Q12306
Y	-144	LEU	-	expression tag	UNP Q12306
Y	-143	GLN	-	expression tag	UNP Q12306
Y	-68	ALA	THR	conflict	UNP Q12306
Y	?	-	SER	deletion	UNP O60884
Y	?	-	GLY	deletion	UNP O60884
Y	?	-	GLY	deletion	UNP O60884
Y	?	-	GLY	deletion	UNP O60884
Y	?	-	GLY	deletion	UNP O60884
Y	?	-	MET	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	?	-	ASP	deletion	UNP O60884
Y	?	-	ASP	deletion	UNP O60884
Y	?	-	ILE	deletion	UNP O60884
Y	?	-	PHE	deletion	UNP O60884
Y	?	-	SER	deletion	UNP O60884
Y	?	-	HIS	deletion	UNP O60884
Y	?	-	ILE	deletion	UNP O60884
Y	?	-	PHE	deletion	UNP O60884
Y	?	-	GLY	deletion	UNP O60884
Y	?	-	GLY	deletion	UNP O60884
Y	?	-	GLY	deletion	UNP O60884
Y	?	-	LEU	deletion	UNP O60884
Y	?	-	PHE	deletion	UNP O60884
Y	?	-	GLY	deletion	UNP O60884
Y	?	-	PHE	deletion	UNP O60884
Y	?	-	MET	deletion	UNP O60884
g	-154	MET	-	initiating methionine	UNP Q12306
g	-153	GLY	-	expression tag	UNP Q12306
g	-152	HIS	-	expression tag	UNP Q12306
g	-151	HIS	-	expression tag	UNP Q12306
g	-150	HIS	-	expression tag	UNP Q12306
g	-149	HIS	-	expression tag	UNP Q12306
g	-148	HIS	-	expression tag	UNP Q12306
g	-147	HIS	-	expression tag	UNP Q12306
g	-146	GLY	-	expression tag	UNP Q12306
g	-145	SER	-	expression tag	UNP Q12306
g	-144	LEU	-	expression tag	UNP Q12306
g	-143	GLN	-	expression tag	UNP Q12306
g	-68	ALA	THR	conflict	UNP Q12306
g	?	-	SER	deletion	UNP O60884
g	?	-	GLY	deletion	UNP O60884
g	?	-	GLY	deletion	UNP O60884
g	?	-	GLY	deletion	UNP O60884
g	?	-	GLY	deletion	UNP O60884
g	?	-	MET	deletion	UNP O60884
g	?	-	ASP	deletion	UNP O60884
g	?	-	ASP	deletion	UNP O60884
g	?	-	ILE	deletion	UNP O60884
g	?	-	PHE	deletion	UNP O60884
g	?	-	SER	deletion	UNP O60884
g	?	-	HIS	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
g	?	-	ILE	deletion	UNP O60884
g	?	-	PHE	deletion	UNP O60884
g	?	-	GLY	deletion	UNP O60884
g	?	-	GLY	deletion	UNP O60884
g	?	-	GLY	deletion	UNP O60884
g	?	-	LEU	deletion	UNP O60884
g	?	-	PHE	deletion	UNP O60884
g	?	-	GLY	deletion	UNP O60884
g	?	-	PHE	deletion	UNP O60884
g	?	-	MET	deletion	UNP O60884
c	-154	MET	-	initiating methionine	UNP Q12306
c	-153	GLY	-	expression tag	UNP Q12306
c	-152	HIS	-	expression tag	UNP Q12306
c	-151	HIS	-	expression tag	UNP Q12306
c	-150	HIS	-	expression tag	UNP Q12306
c	-149	HIS	-	expression tag	UNP Q12306
c	-148	HIS	-	expression tag	UNP Q12306
c	-147	HIS	-	expression tag	UNP Q12306
c	-146	GLY	-	expression tag	UNP Q12306
c	-145	SER	-	expression tag	UNP Q12306
c	-144	LEU	-	expression tag	UNP Q12306
c	-143	GLN	-	expression tag	UNP Q12306
c	-68	ALA	THR	conflict	UNP Q12306
c	?	-	SER	deletion	UNP O60884
c	?	-	GLY	deletion	UNP O60884
c	?	-	GLY	deletion	UNP O60884
c	?	-	GLY	deletion	UNP O60884
c	?	-	GLY	deletion	UNP O60884
c	?	-	MET	deletion	UNP O60884
c	?	-	ASP	deletion	UNP O60884
c	?	-	ASP	deletion	UNP O60884
c	?	-	ILE	deletion	UNP O60884
c	?	-	PHE	deletion	UNP O60884
c	?	-	SER	deletion	UNP O60884
c	?	-	HIS	deletion	UNP O60884
c	?	-	ILE	deletion	UNP O60884
c	?	-	PHE	deletion	UNP O60884
c	?	-	GLY	deletion	UNP O60884
c	?	-	GLY	deletion	UNP O60884
c	?	-	GLY	deletion	UNP O60884
c	?	-	LEU	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
c	?	-	PHE	deletion	UNP O60884
c	?	-	GLY	deletion	UNP O60884
c	?	-	PHE	deletion	UNP O60884
c	?	-	MET	deletion	UNP O60884
k	-154	MET	-	initiating methionine	UNP Q12306
k	-153	GLY	-	expression tag	UNP Q12306
k	-152	HIS	-	expression tag	UNP Q12306
k	-151	HIS	-	expression tag	UNP Q12306
k	-150	HIS	-	expression tag	UNP Q12306
k	-149	HIS	-	expression tag	UNP Q12306
k	-148	HIS	-	expression tag	UNP Q12306
k	-147	HIS	-	expression tag	UNP Q12306
k	-146	GLY	-	expression tag	UNP Q12306
k	-145	SER	-	expression tag	UNP Q12306
k	-144	LEU	-	expression tag	UNP Q12306
k	-143	GLN	-	expression tag	UNP Q12306
k	-68	ALA	THR	conflict	UNP Q12306
k	?	-	SER	deletion	UNP O60884
k	?	-	GLY	deletion	UNP O60884
k	?	-	GLY	deletion	UNP O60884
k	?	-	GLY	deletion	UNP O60884
k	?	-	GLY	deletion	UNP O60884
k	?	-	GLY	deletion	UNP O60884
k	?	-	MET	deletion	UNP O60884
k	?	-	ASP	deletion	UNP O60884
k	?	-	ASP	deletion	UNP O60884
k	?	-	ILE	deletion	UNP O60884
k	?	-	PHE	deletion	UNP O60884
k	?	-	SER	deletion	UNP O60884
k	?	-	HIS	deletion	UNP O60884
k	?	-	ILE	deletion	UNP O60884
k	?	-	PHE	deletion	UNP O60884
k	?	-	GLY	deletion	UNP O60884
k	?	-	GLY	deletion	UNP O60884
k	?	-	GLY	deletion	UNP O60884
k	?	-	LEU	deletion	UNP O60884
k	?	-	PHE	deletion	UNP O60884
k	?	-	GLY	deletion	UNP O60884
k	?	-	PHE	deletion	UNP O60884
k	?	-	MET	deletion	UNP O60884
J	-154	MET	-	initiating methionine	UNP Q12306
J	-153	GLY	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-152	HIS	-	expression tag	UNP Q12306
J	-151	HIS	-	expression tag	UNP Q12306
J	-150	HIS	-	expression tag	UNP Q12306
J	-149	HIS	-	expression tag	UNP Q12306
J	-148	HIS	-	expression tag	UNP Q12306
J	-147	HIS	-	expression tag	UNP Q12306
J	-146	GLY	-	expression tag	UNP Q12306
J	-145	SER	-	expression tag	UNP Q12306
J	-144	LEU	-	expression tag	UNP Q12306
J	-143	GLN	-	expression tag	UNP Q12306
J	-68	ALA	THR	conflict	UNP Q12306
J	?	-	SER	deletion	UNP O60884
J	?	-	GLY	deletion	UNP O60884
J	?	-	GLY	deletion	UNP O60884
J	?	-	GLY	deletion	UNP O60884
J	?	-	GLY	deletion	UNP O60884
J	?	-	MET	deletion	UNP O60884
J	?	-	ASP	deletion	UNP O60884
J	?	-	ASP	deletion	UNP O60884
J	?	-	ILE	deletion	UNP O60884
J	?	-	PHE	deletion	UNP O60884
J	?	-	SER	deletion	UNP O60884
J	?	-	HIS	deletion	UNP O60884
J	?	-	ILE	deletion	UNP O60884
J	?	-	PHE	deletion	UNP O60884
J	?	-	GLY	deletion	UNP O60884
J	?	-	GLY	deletion	UNP O60884
J	?	-	GLY	deletion	UNP O60884
J	?	-	LEU	deletion	UNP O60884
J	?	-	PHE	deletion	UNP O60884
J	?	-	GLY	deletion	UNP O60884
J	?	-	PHE	deletion	UNP O60884
J	?	-	MET	deletion	UNP O60884
R	-154	MET	-	initiating methionine	UNP Q12306
R	-153	GLY	-	expression tag	UNP Q12306
R	-152	HIS	-	expression tag	UNP Q12306
R	-151	HIS	-	expression tag	UNP Q12306
R	-150	HIS	-	expression tag	UNP Q12306
R	-149	HIS	-	expression tag	UNP Q12306
R	-148	HIS	-	expression tag	UNP Q12306
R	-147	HIS	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-146	GLY	-	expression tag	UNP Q12306
R	-145	SER	-	expression tag	UNP Q12306
R	-144	LEU	-	expression tag	UNP Q12306
R	-143	GLN	-	expression tag	UNP Q12306
R	-68	ALA	THR	conflict	UNP Q12306
R	?	-	SER	deletion	UNP O60884
R	?	-	GLY	deletion	UNP O60884
R	?	-	GLY	deletion	UNP O60884
R	?	-	GLY	deletion	UNP O60884
R	?	-	GLY	deletion	UNP O60884
R	?	-	GLY	deletion	UNP O60884
R	?	-	MET	deletion	UNP O60884
R	?	-	ASP	deletion	UNP O60884
R	?	-	ASP	deletion	UNP O60884
R	?	-	ILE	deletion	UNP O60884
R	?	-	PHE	deletion	UNP O60884
R	?	-	SER	deletion	UNP O60884
R	?	-	HIS	deletion	UNP O60884
R	?	-	ILE	deletion	UNP O60884
R	?	-	PHE	deletion	UNP O60884
R	?	-	GLY	deletion	UNP O60884
R	?	-	GLY	deletion	UNP O60884
R	?	-	GLY	deletion	UNP O60884
R	?	-	LEU	deletion	UNP O60884
R	?	-	PHE	deletion	UNP O60884
R	?	-	GLY	deletion	UNP O60884
R	?	-	PHE	deletion	UNP O60884
R	?	-	MET	deletion	UNP O60884
N	-154	MET	-	initiating methionine	UNP Q12306
N	-153	GLY	-	expression tag	UNP Q12306
N	-152	HIS	-	expression tag	UNP Q12306
N	-151	HIS	-	expression tag	UNP Q12306
N	-150	HIS	-	expression tag	UNP Q12306
N	-149	HIS	-	expression tag	UNP Q12306
N	-148	HIS	-	expression tag	UNP Q12306
N	-147	HIS	-	expression tag	UNP Q12306
N	-146	GLY	-	expression tag	UNP Q12306
N	-145	SER	-	expression tag	UNP Q12306
N	-144	LEU	-	expression tag	UNP Q12306
N	-143	GLN	-	expression tag	UNP Q12306
N	-68	ALA	THR	conflict	UNP Q12306
N	?	-	SER	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	GLY	deletion	UNP O60884
N	?	-	GLY	deletion	UNP O60884
N	?	-	GLY	deletion	UNP O60884
N	?	-	GLY	deletion	UNP O60884
N	?	-	GLY	deletion	UNP O60884
N	?	-	MET	deletion	UNP O60884
N	?	-	ASP	deletion	UNP O60884
N	?	-	ASP	deletion	UNP O60884
N	?	-	ILE	deletion	UNP O60884
N	?	-	PHE	deletion	UNP O60884
N	?	-	SER	deletion	UNP O60884
N	?	-	HIS	deletion	UNP O60884
N	?	-	ILE	deletion	UNP O60884
N	?	-	PHE	deletion	UNP O60884
N	?	-	GLY	deletion	UNP O60884
N	?	-	GLY	deletion	UNP O60884
N	?	-	GLY	deletion	UNP O60884
N	?	-	LEU	deletion	UNP O60884
N	?	-	PHE	deletion	UNP O60884
N	?	-	GLY	deletion	UNP O60884
N	?	-	PHE	deletion	UNP O60884
N	?	-	MET	deletion	UNP O60884
V	-154	MET	-	initiating methionine	UNP Q12306
V	-153	GLY	-	expression tag	UNP Q12306
V	-152	HIS	-	expression tag	UNP Q12306
V	-151	HIS	-	expression tag	UNP Q12306
V	-150	HIS	-	expression tag	UNP Q12306
V	-149	HIS	-	expression tag	UNP Q12306
V	-148	HIS	-	expression tag	UNP Q12306
V	-147	HIS	-	expression tag	UNP Q12306
V	-146	GLY	-	expression tag	UNP Q12306
V	-145	SER	-	expression tag	UNP Q12306
V	-144	LEU	-	expression tag	UNP Q12306
V	-143	GLN	-	expression tag	UNP Q12306
V	-68	ALA	THR	conflict	UNP Q12306
V	?	-	SER	deletion	UNP O60884
V	?	-	GLY	deletion	UNP O60884
V	?	-	GLY	deletion	UNP O60884
V	?	-	GLY	deletion	UNP O60884
V	?	-	GLY	deletion	UNP O60884
V	?	-	MET	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
V	?	-	ASP	deletion	UNP O60884
V	?	-	ASP	deletion	UNP O60884
V	?	-	ILE	deletion	UNP O60884
V	?	-	PHE	deletion	UNP O60884
V	?	-	SER	deletion	UNP O60884
V	?	-	HIS	deletion	UNP O60884
V	?	-	ILE	deletion	UNP O60884
V	?	-	PHE	deletion	UNP O60884
V	?	-	GLY	deletion	UNP O60884
V	?	-	GLY	deletion	UNP O60884
V	?	-	GLY	deletion	UNP O60884
V	?	-	LEU	deletion	UNP O60884
V	?	-	PHE	deletion	UNP O60884
V	?	-	GLY	deletion	UNP O60884
V	?	-	PHE	deletion	UNP O60884
V	?	-	MET	deletion	UNP O60884
Z	-154	MET	-	initiating methionine	UNP Q12306
Z	-153	GLY	-	expression tag	UNP Q12306
Z	-152	HIS	-	expression tag	UNP Q12306
Z	-151	HIS	-	expression tag	UNP Q12306
Z	-150	HIS	-	expression tag	UNP Q12306
Z	-149	HIS	-	expression tag	UNP Q12306
Z	-148	HIS	-	expression tag	UNP Q12306
Z	-147	HIS	-	expression tag	UNP Q12306
Z	-146	GLY	-	expression tag	UNP Q12306
Z	-145	SER	-	expression tag	UNP Q12306
Z	-144	LEU	-	expression tag	UNP Q12306
Z	-143	GLN	-	expression tag	UNP Q12306
Z	-68	ALA	THR	conflict	UNP Q12306
Z	?	-	SER	deletion	UNP O60884
Z	?	-	GLY	deletion	UNP O60884
Z	?	-	GLY	deletion	UNP O60884
Z	?	-	GLY	deletion	UNP O60884
Z	?	-	GLY	deletion	UNP O60884
Z	?	-	MET	deletion	UNP O60884
Z	?	-	ASP	deletion	UNP O60884
Z	?	-	ASP	deletion	UNP O60884
Z	?	-	ILE	deletion	UNP O60884
Z	?	-	PHE	deletion	UNP O60884
Z	?	-	SER	deletion	UNP O60884
Z	?	-	HIS	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	?	-	ILE	deletion	UNP O60884
Z	?	-	PHE	deletion	UNP O60884
Z	?	-	GLY	deletion	UNP O60884
Z	?	-	GLY	deletion	UNP O60884
Z	?	-	GLY	deletion	UNP O60884
Z	?	-	LEU	deletion	UNP O60884
Z	?	-	PHE	deletion	UNP O60884
Z	?	-	GLY	deletion	UNP O60884
Z	?	-	PHE	deletion	UNP O60884
Z	?	-	MET	deletion	UNP O60884
h	-154	MET	-	initiating methionine	UNP Q12306
h	-153	GLY	-	expression tag	UNP Q12306
h	-152	HIS	-	expression tag	UNP Q12306
h	-151	HIS	-	expression tag	UNP Q12306
h	-150	HIS	-	expression tag	UNP Q12306
h	-149	HIS	-	expression tag	UNP Q12306
h	-148	HIS	-	expression tag	UNP Q12306
h	-147	HIS	-	expression tag	UNP Q12306
h	-146	GLY	-	expression tag	UNP Q12306
h	-145	SER	-	expression tag	UNP Q12306
h	-144	LEU	-	expression tag	UNP Q12306
h	-143	GLN	-	expression tag	UNP Q12306
h	-68	ALA	THR	conflict	UNP Q12306
h	?	-	SER	deletion	UNP O60884
h	?	-	GLY	deletion	UNP O60884
h	?	-	GLY	deletion	UNP O60884
h	?	-	GLY	deletion	UNP O60884
h	?	-	GLY	deletion	UNP O60884
h	?	-	GLY	deletion	UNP O60884
h	?	-	MET	deletion	UNP O60884
h	?	-	ASP	deletion	UNP O60884
h	?	-	ASP	deletion	UNP O60884
h	?	-	ILE	deletion	UNP O60884
h	?	-	PHE	deletion	UNP O60884
h	?	-	SER	deletion	UNP O60884
h	?	-	HIS	deletion	UNP O60884
h	?	-	ILE	deletion	UNP O60884
h	?	-	PHE	deletion	UNP O60884
h	?	-	GLY	deletion	UNP O60884
h	?	-	GLY	deletion	UNP O60884
h	?	-	GLY	deletion	UNP O60884
h	?	-	LEU	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
h	?	-	PHE	deletion	UNP O60884
h	?	-	GLY	deletion	UNP O60884
h	?	-	PHE	deletion	UNP O60884
h	?	-	MET	deletion	UNP O60884
d	-154	MET	-	initiating methionine	UNP Q12306
d	-153	GLY	-	expression tag	UNP Q12306
d	-152	HIS	-	expression tag	UNP Q12306
d	-151	HIS	-	expression tag	UNP Q12306
d	-150	HIS	-	expression tag	UNP Q12306
d	-149	HIS	-	expression tag	UNP Q12306
d	-148	HIS	-	expression tag	UNP Q12306
d	-147	HIS	-	expression tag	UNP Q12306
d	-146	GLY	-	expression tag	UNP Q12306
d	-145	SER	-	expression tag	UNP Q12306
d	-144	LEU	-	expression tag	UNP Q12306
d	-143	GLN	-	expression tag	UNP Q12306
d	-68	ALA	THR	conflict	UNP Q12306
d	?	-	SER	deletion	UNP O60884
d	?	-	GLY	deletion	UNP O60884
d	?	-	GLY	deletion	UNP O60884
d	?	-	GLY	deletion	UNP O60884
d	?	-	GLY	deletion	UNP O60884
d	?	-	GLY	deletion	UNP O60884
d	?	-	MET	deletion	UNP O60884
d	?	-	ASP	deletion	UNP O60884
d	?	-	ASP	deletion	UNP O60884
d	?	-	ILE	deletion	UNP O60884
d	?	-	PHE	deletion	UNP O60884
d	?	-	SER	deletion	UNP O60884
d	?	-	HIS	deletion	UNP O60884
d	?	-	ILE	deletion	UNP O60884
d	?	-	PHE	deletion	UNP O60884
d	?	-	GLY	deletion	UNP O60884
d	?	-	GLY	deletion	UNP O60884
d	?	-	GLY	deletion	UNP O60884
d	?	-	LEU	deletion	UNP O60884
d	?	-	PHE	deletion	UNP O60884
d	?	-	GLY	deletion	UNP O60884
d	?	-	PHE	deletion	UNP O60884
d	?	-	MET	deletion	UNP O60884
l	-154	MET	-	initiating methionine	UNP Q12306
l	-153	GLY	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
1	-152	HIS	-	expression tag	UNP Q12306
1	-151	HIS	-	expression tag	UNP Q12306
1	-150	HIS	-	expression tag	UNP Q12306
1	-149	HIS	-	expression tag	UNP Q12306
1	-148	HIS	-	expression tag	UNP Q12306
1	-147	HIS	-	expression tag	UNP Q12306
1	-146	GLY	-	expression tag	UNP Q12306
1	-145	SER	-	expression tag	UNP Q12306
1	-144	LEU	-	expression tag	UNP Q12306
1	-143	GLN	-	expression tag	UNP Q12306
1	-68	ALA	THR	conflict	UNP Q12306
1	?	-	SER	deletion	UNP O60884
1	?	-	GLY	deletion	UNP O60884
1	?	-	GLY	deletion	UNP O60884
1	?	-	GLY	deletion	UNP O60884
1	?	-	GLY	deletion	UNP O60884
1	?	-	GLY	deletion	UNP O60884
1	?	-	MET	deletion	UNP O60884
1	?	-	ASP	deletion	UNP O60884
1	?	-	ASP	deletion	UNP O60884
1	?	-	ILE	deletion	UNP O60884
1	?	-	PHE	deletion	UNP O60884
1	?	-	SER	deletion	UNP O60884
1	?	-	HIS	deletion	UNP O60884
1	?	-	ILE	deletion	UNP O60884
1	?	-	PHE	deletion	UNP O60884
1	?	-	GLY	deletion	UNP O60884
1	?	-	GLY	deletion	UNP O60884
1	?	-	GLY	deletion	UNP O60884
1	?	-	LEU	deletion	UNP O60884
1	?	-	PHE	deletion	UNP O60884
1	?	-	GLY	deletion	UNP O60884
1	?	-	PHE	deletion	UNP O60884
1	?	-	MET	deletion	UNP O60884
K	-154	MET	-	initiating methionine	UNP Q12306
K	-153	GLY	-	expression tag	UNP Q12306
K	-152	HIS	-	expression tag	UNP Q12306
K	-151	HIS	-	expression tag	UNP Q12306
K	-150	HIS	-	expression tag	UNP Q12306
K	-149	HIS	-	expression tag	UNP Q12306
K	-148	HIS	-	expression tag	UNP Q12306
K	-147	HIS	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-146	GLY	-	expression tag	UNP Q12306
K	-145	SER	-	expression tag	UNP Q12306
K	-144	LEU	-	expression tag	UNP Q12306
K	-143	GLN	-	expression tag	UNP Q12306
K	-68	ALA	THR	conflict	UNP Q12306
K	?	-	SER	deletion	UNP O60884
K	?	-	GLY	deletion	UNP O60884
K	?	-	GLY	deletion	UNP O60884
K	?	-	GLY	deletion	UNP O60884
K	?	-	GLY	deletion	UNP O60884
K	?	-	GLY	deletion	UNP O60884
K	?	-	MET	deletion	UNP O60884
K	?	-	ASP	deletion	UNP O60884
K	?	-	ASP	deletion	UNP O60884
K	?	-	ILE	deletion	UNP O60884
K	?	-	PHE	deletion	UNP O60884
K	?	-	SER	deletion	UNP O60884
K	?	-	HIS	deletion	UNP O60884
K	?	-	ILE	deletion	UNP O60884
K	?	-	PHE	deletion	UNP O60884
K	?	-	GLY	deletion	UNP O60884
K	?	-	GLY	deletion	UNP O60884
K	?	-	GLY	deletion	UNP O60884
K	?	-	LEU	deletion	UNP O60884
K	?	-	PHE	deletion	UNP O60884
K	?	-	GLY	deletion	UNP O60884
K	?	-	PHE	deletion	UNP O60884
K	?	-	MET	deletion	UNP O60884
S	-154	MET	-	initiating methionine	UNP Q12306
S	-153	GLY	-	expression tag	UNP Q12306
S	-152	HIS	-	expression tag	UNP Q12306
S	-151	HIS	-	expression tag	UNP Q12306
S	-150	HIS	-	expression tag	UNP Q12306
S	-149	HIS	-	expression tag	UNP Q12306
S	-148	HIS	-	expression tag	UNP Q12306
S	-147	HIS	-	expression tag	UNP Q12306
S	-146	GLY	-	expression tag	UNP Q12306
S	-145	SER	-	expression tag	UNP Q12306
S	-144	LEU	-	expression tag	UNP Q12306
S	-143	GLN	-	expression tag	UNP Q12306
S	-68	ALA	THR	conflict	UNP Q12306
S	?	-	SER	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
S	?	-	GLY	deletion	UNP O60884
S	?	-	GLY	deletion	UNP O60884
S	?	-	GLY	deletion	UNP O60884
S	?	-	GLY	deletion	UNP O60884
S	?	-	GLY	deletion	UNP O60884
S	?	-	MET	deletion	UNP O60884
S	?	-	ASP	deletion	UNP O60884
S	?	-	ASP	deletion	UNP O60884
S	?	-	ILE	deletion	UNP O60884
S	?	-	PHE	deletion	UNP O60884
S	?	-	SER	deletion	UNP O60884
S	?	-	HIS	deletion	UNP O60884
S	?	-	ILE	deletion	UNP O60884
S	?	-	PHE	deletion	UNP O60884
S	?	-	GLY	deletion	UNP O60884
S	?	-	GLY	deletion	UNP O60884
S	?	-	GLY	deletion	UNP O60884
S	?	-	LEU	deletion	UNP O60884
S	?	-	PHE	deletion	UNP O60884
S	?	-	GLY	deletion	UNP O60884
S	?	-	PHE	deletion	UNP O60884
S	?	-	MET	deletion	UNP O60884
O	-154	MET	-	initiating methionine	UNP Q12306
O	-153	GLY	-	expression tag	UNP Q12306
O	-152	HIS	-	expression tag	UNP Q12306
O	-151	HIS	-	expression tag	UNP Q12306
O	-150	HIS	-	expression tag	UNP Q12306
O	-149	HIS	-	expression tag	UNP Q12306
O	-148	HIS	-	expression tag	UNP Q12306
O	-147	HIS	-	expression tag	UNP Q12306
O	-146	GLY	-	expression tag	UNP Q12306
O	-145	SER	-	expression tag	UNP Q12306
O	-144	LEU	-	expression tag	UNP Q12306
O	-143	GLN	-	expression tag	UNP Q12306
O	-68	ALA	THR	conflict	UNP Q12306
O	?	-	SER	deletion	UNP O60884
O	?	-	GLY	deletion	UNP O60884
O	?	-	GLY	deletion	UNP O60884
O	?	-	GLY	deletion	UNP O60884
O	?	-	GLY	deletion	UNP O60884
O	?	-	MET	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
O	?	-	ASP	deletion	UNP O60884
O	?	-	ASP	deletion	UNP O60884
O	?	-	ILE	deletion	UNP O60884
O	?	-	PHE	deletion	UNP O60884
O	?	-	SER	deletion	UNP O60884
O	?	-	HIS	deletion	UNP O60884
O	?	-	ILE	deletion	UNP O60884
O	?	-	PHE	deletion	UNP O60884
O	?	-	GLY	deletion	UNP O60884
O	?	-	GLY	deletion	UNP O60884
O	?	-	GLY	deletion	UNP O60884
O	?	-	LEU	deletion	UNP O60884
O	?	-	PHE	deletion	UNP O60884
O	?	-	GLY	deletion	UNP O60884
O	?	-	PHE	deletion	UNP O60884
O	?	-	MET	deletion	UNP O60884
W	-154	MET	-	initiating methionine	UNP Q12306
W	-153	GLY	-	expression tag	UNP Q12306
W	-152	HIS	-	expression tag	UNP Q12306
W	-151	HIS	-	expression tag	UNP Q12306
W	-150	HIS	-	expression tag	UNP Q12306
W	-149	HIS	-	expression tag	UNP Q12306
W	-148	HIS	-	expression tag	UNP Q12306
W	-147	HIS	-	expression tag	UNP Q12306
W	-146	GLY	-	expression tag	UNP Q12306
W	-145	SER	-	expression tag	UNP Q12306
W	-144	LEU	-	expression tag	UNP Q12306
W	-143	GLN	-	expression tag	UNP Q12306
W	-68	ALA	THR	conflict	UNP Q12306
W	?	-	SER	deletion	UNP O60884
W	?	-	GLY	deletion	UNP O60884
W	?	-	GLY	deletion	UNP O60884
W	?	-	GLY	deletion	UNP O60884
W	?	-	GLY	deletion	UNP O60884
W	?	-	MET	deletion	UNP O60884
W	?	-	ASP	deletion	UNP O60884
W	?	-	ASP	deletion	UNP O60884
W	?	-	ILE	deletion	UNP O60884
W	?	-	PHE	deletion	UNP O60884
W	?	-	SER	deletion	UNP O60884
W	?	-	HIS	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
W	?	-	ILE	deletion	UNP O60884
W	?	-	PHE	deletion	UNP O60884
W	?	-	GLY	deletion	UNP O60884
W	?	-	GLY	deletion	UNP O60884
W	?	-	GLY	deletion	UNP O60884
W	?	-	LEU	deletion	UNP O60884
W	?	-	PHE	deletion	UNP O60884
W	?	-	GLY	deletion	UNP O60884
W	?	-	PHE	deletion	UNP O60884
W	?	-	MET	deletion	UNP O60884
a	-154	MET	-	initiating methionine	UNP Q12306
a	-153	GLY	-	expression tag	UNP Q12306
a	-152	HIS	-	expression tag	UNP Q12306
a	-151	HIS	-	expression tag	UNP Q12306
a	-150	HIS	-	expression tag	UNP Q12306
a	-149	HIS	-	expression tag	UNP Q12306
a	-148	HIS	-	expression tag	UNP Q12306
a	-147	HIS	-	expression tag	UNP Q12306
a	-146	GLY	-	expression tag	UNP Q12306
a	-145	SER	-	expression tag	UNP Q12306
a	-144	LEU	-	expression tag	UNP Q12306
a	-143	GLN	-	expression tag	UNP Q12306
a	-68	ALA	THR	conflict	UNP Q12306
a	?	-	SER	deletion	UNP O60884
a	?	-	GLY	deletion	UNP O60884
a	?	-	GLY	deletion	UNP O60884
a	?	-	GLY	deletion	UNP O60884
a	?	-	GLY	deletion	UNP O60884
a	?	-	GLY	deletion	UNP O60884
a	?	-	MET	deletion	UNP O60884
a	?	-	ASP	deletion	UNP O60884
a	?	-	ASP	deletion	UNP O60884
a	?	-	ILE	deletion	UNP O60884
a	?	-	PHE	deletion	UNP O60884
a	?	-	SER	deletion	UNP O60884
a	?	-	HIS	deletion	UNP O60884
a	?	-	ILE	deletion	UNP O60884
a	?	-	PHE	deletion	UNP O60884
a	?	-	GLY	deletion	UNP O60884
a	?	-	GLY	deletion	UNP O60884
a	?	-	GLY	deletion	UNP O60884
a	?	-	LEU	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
a	?	-	PHE	deletion	UNP O60884
a	?	-	GLY	deletion	UNP O60884
a	?	-	PHE	deletion	UNP O60884
a	?	-	MET	deletion	UNP O60884
i	-154	MET	-	initiating methionine	UNP Q12306
i	-153	GLY	-	expression tag	UNP Q12306
i	-152	HIS	-	expression tag	UNP Q12306
i	-151	HIS	-	expression tag	UNP Q12306
i	-150	HIS	-	expression tag	UNP Q12306
i	-149	HIS	-	expression tag	UNP Q12306
i	-148	HIS	-	expression tag	UNP Q12306
i	-147	HIS	-	expression tag	UNP Q12306
i	-146	GLY	-	expression tag	UNP Q12306
i	-145	SER	-	expression tag	UNP Q12306
i	-144	LEU	-	expression tag	UNP Q12306
i	-143	GLN	-	expression tag	UNP Q12306
i	-68	ALA	THR	conflict	UNP Q12306
i	?	-	SER	deletion	UNP O60884
i	?	-	GLY	deletion	UNP O60884
i	?	-	GLY	deletion	UNP O60884
i	?	-	GLY	deletion	UNP O60884
i	?	-	GLY	deletion	UNP O60884
i	?	-	GLY	deletion	UNP O60884
i	?	-	MET	deletion	UNP O60884
i	?	-	ASP	deletion	UNP O60884
i	?	-	ASP	deletion	UNP O60884
i	?	-	ILE	deletion	UNP O60884
i	?	-	PHE	deletion	UNP O60884
i	?	-	SER	deletion	UNP O60884
i	?	-	HIS	deletion	UNP O60884
i	?	-	ILE	deletion	UNP O60884
i	?	-	PHE	deletion	UNP O60884
i	?	-	GLY	deletion	UNP O60884
i	?	-	GLY	deletion	UNP O60884
i	?	-	GLY	deletion	UNP O60884
i	?	-	LEU	deletion	UNP O60884
i	?	-	PHE	deletion	UNP O60884
i	?	-	GLY	deletion	UNP O60884
i	?	-	PHE	deletion	UNP O60884
i	?	-	MET	deletion	UNP O60884
e	-154	MET	-	initiating methionine	UNP Q12306
e	-153	GLY	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
e	-152	HIS	-	expression tag	UNP Q12306
e	-151	HIS	-	expression tag	UNP Q12306
e	-150	HIS	-	expression tag	UNP Q12306
e	-149	HIS	-	expression tag	UNP Q12306
e	-148	HIS	-	expression tag	UNP Q12306
e	-147	HIS	-	expression tag	UNP Q12306
e	-146	GLY	-	expression tag	UNP Q12306
e	-145	SER	-	expression tag	UNP Q12306
e	-144	LEU	-	expression tag	UNP Q12306
e	-143	GLN	-	expression tag	UNP Q12306
e	-68	ALA	THR	conflict	UNP Q12306
e	?	-	SER	deletion	UNP O60884
e	?	-	GLY	deletion	UNP O60884
e	?	-	GLY	deletion	UNP O60884
e	?	-	GLY	deletion	UNP O60884
e	?	-	GLY	deletion	UNP O60884
e	?	-	GLY	deletion	UNP O60884
e	?	-	MET	deletion	UNP O60884
e	?	-	ASP	deletion	UNP O60884
e	?	-	ASP	deletion	UNP O60884
e	?	-	ILE	deletion	UNP O60884
e	?	-	PHE	deletion	UNP O60884
e	?	-	SER	deletion	UNP O60884
e	?	-	HIS	deletion	UNP O60884
e	?	-	ILE	deletion	UNP O60884
e	?	-	PHE	deletion	UNP O60884
e	?	-	GLY	deletion	UNP O60884
e	?	-	GLY	deletion	UNP O60884
e	?	-	GLY	deletion	UNP O60884
e	?	-	LEU	deletion	UNP O60884
e	?	-	PHE	deletion	UNP O60884
e	?	-	GLY	deletion	UNP O60884
e	?	-	PHE	deletion	UNP O60884
e	?	-	MET	deletion	UNP O60884
m	-154	MET	-	initiating methionine	UNP Q12306
m	-153	GLY	-	expression tag	UNP Q12306
m	-152	HIS	-	expression tag	UNP Q12306
m	-151	HIS	-	expression tag	UNP Q12306
m	-150	HIS	-	expression tag	UNP Q12306
m	-149	HIS	-	expression tag	UNP Q12306
m	-148	HIS	-	expression tag	UNP Q12306
m	-147	HIS	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
m	-146	GLY	-	expression tag	UNP Q12306
m	-145	SER	-	expression tag	UNP Q12306
m	-144	LEU	-	expression tag	UNP Q12306
m	-143	GLN	-	expression tag	UNP Q12306
m	-68	ALA	THR	conflict	UNP Q12306
m	?	-	SER	deletion	UNP O60884
m	?	-	GLY	deletion	UNP O60884
m	?	-	GLY	deletion	UNP O60884
m	?	-	GLY	deletion	UNP O60884
m	?	-	GLY	deletion	UNP O60884
m	?	-	GLY	deletion	UNP O60884
m	?	-	MET	deletion	UNP O60884
m	?	-	ASP	deletion	UNP O60884
m	?	-	ASP	deletion	UNP O60884
m	?	-	ILE	deletion	UNP O60884
m	?	-	PHE	deletion	UNP O60884
m	?	-	SER	deletion	UNP O60884
m	?	-	HIS	deletion	UNP O60884
m	?	-	ILE	deletion	UNP O60884
m	?	-	PHE	deletion	UNP O60884
m	?	-	GLY	deletion	UNP O60884
m	?	-	GLY	deletion	UNP O60884
m	?	-	GLY	deletion	UNP O60884
m	?	-	LEU	deletion	UNP O60884
m	?	-	PHE	deletion	UNP O60884
m	?	-	GLY	deletion	UNP O60884
m	?	-	PHE	deletion	UNP O60884
m	?	-	MET	deletion	UNP O60884
L	-154	MET	-	initiating methionine	UNP Q12306
L	-153	GLY	-	expression tag	UNP Q12306
L	-152	HIS	-	expression tag	UNP Q12306
L	-151	HIS	-	expression tag	UNP Q12306
L	-150	HIS	-	expression tag	UNP Q12306
L	-149	HIS	-	expression tag	UNP Q12306
L	-148	HIS	-	expression tag	UNP Q12306
L	-147	HIS	-	expression tag	UNP Q12306
L	-146	GLY	-	expression tag	UNP Q12306
L	-145	SER	-	expression tag	UNP Q12306
L	-144	LEU	-	expression tag	UNP Q12306
L	-143	GLN	-	expression tag	UNP Q12306
L	-68	ALA	THR	conflict	UNP Q12306
L	?	-	SER	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	GLY	deletion	UNP O60884
L	?	-	GLY	deletion	UNP O60884
L	?	-	GLY	deletion	UNP O60884
L	?	-	GLY	deletion	UNP O60884
L	?	-	GLY	deletion	UNP O60884
L	?	-	MET	deletion	UNP O60884
L	?	-	ASP	deletion	UNP O60884
L	?	-	ASP	deletion	UNP O60884
L	?	-	ILE	deletion	UNP O60884
L	?	-	PHE	deletion	UNP O60884
L	?	-	SER	deletion	UNP O60884
L	?	-	HIS	deletion	UNP O60884
L	?	-	ILE	deletion	UNP O60884
L	?	-	PHE	deletion	UNP O60884
L	?	-	GLY	deletion	UNP O60884
L	?	-	GLY	deletion	UNP O60884
L	?	-	GLY	deletion	UNP O60884
L	?	-	LEU	deletion	UNP O60884
L	?	-	PHE	deletion	UNP O60884
L	?	-	GLY	deletion	UNP O60884
L	?	-	PHE	deletion	UNP O60884
L	?	-	MET	deletion	UNP O60884
T	-154	MET	-	initiating methionine	UNP Q12306
T	-153	GLY	-	expression tag	UNP Q12306
T	-152	HIS	-	expression tag	UNP Q12306
T	-151	HIS	-	expression tag	UNP Q12306
T	-150	HIS	-	expression tag	UNP Q12306
T	-149	HIS	-	expression tag	UNP Q12306
T	-148	HIS	-	expression tag	UNP Q12306
T	-147	HIS	-	expression tag	UNP Q12306
T	-146	GLY	-	expression tag	UNP Q12306
T	-145	SER	-	expression tag	UNP Q12306
T	-144	LEU	-	expression tag	UNP Q12306
T	-143	GLN	-	expression tag	UNP Q12306
T	-68	ALA	THR	conflict	UNP Q12306
T	?	-	SER	deletion	UNP O60884
T	?	-	GLY	deletion	UNP O60884
T	?	-	GLY	deletion	UNP O60884
T	?	-	GLY	deletion	UNP O60884
T	?	-	GLY	deletion	UNP O60884
T	?	-	MET	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
T	?	-	ASP	deletion	UNP O60884
T	?	-	ASP	deletion	UNP O60884
T	?	-	ILE	deletion	UNP O60884
T	?	-	PHE	deletion	UNP O60884
T	?	-	SER	deletion	UNP O60884
T	?	-	HIS	deletion	UNP O60884
T	?	-	ILE	deletion	UNP O60884
T	?	-	PHE	deletion	UNP O60884
T	?	-	GLY	deletion	UNP O60884
T	?	-	GLY	deletion	UNP O60884
T	?	-	GLY	deletion	UNP O60884
T	?	-	LEU	deletion	UNP O60884
T	?	-	PHE	deletion	UNP O60884
T	?	-	GLY	deletion	UNP O60884
T	?	-	PHE	deletion	UNP O60884
T	?	-	MET	deletion	UNP O60884
P	-154	MET	-	initiating methionine	UNP Q12306
P	-153	GLY	-	expression tag	UNP Q12306
P	-152	HIS	-	expression tag	UNP Q12306
P	-151	HIS	-	expression tag	UNP Q12306
P	-150	HIS	-	expression tag	UNP Q12306
P	-149	HIS	-	expression tag	UNP Q12306
P	-148	HIS	-	expression tag	UNP Q12306
P	-147	HIS	-	expression tag	UNP Q12306
P	-146	GLY	-	expression tag	UNP Q12306
P	-145	SER	-	expression tag	UNP Q12306
P	-144	LEU	-	expression tag	UNP Q12306
P	-143	GLN	-	expression tag	UNP Q12306
P	-68	ALA	THR	conflict	UNP Q12306
P	?	-	SER	deletion	UNP O60884
P	?	-	GLY	deletion	UNP O60884
P	?	-	GLY	deletion	UNP O60884
P	?	-	GLY	deletion	UNP O60884
P	?	-	GLY	deletion	UNP O60884
P	?	-	MET	deletion	UNP O60884
P	?	-	ASP	deletion	UNP O60884
P	?	-	ASP	deletion	UNP O60884
P	?	-	ILE	deletion	UNP O60884
P	?	-	PHE	deletion	UNP O60884
P	?	-	SER	deletion	UNP O60884
P	?	-	HIS	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
P	?	-	ILE	deletion	UNP O60884
P	?	-	PHE	deletion	UNP O60884
P	?	-	GLY	deletion	UNP O60884
P	?	-	GLY	deletion	UNP O60884
P	?	-	GLY	deletion	UNP O60884
P	?	-	LEU	deletion	UNP O60884
P	?	-	PHE	deletion	UNP O60884
P	?	-	GLY	deletion	UNP O60884
P	?	-	PHE	deletion	UNP O60884
P	?	-	MET	deletion	UNP O60884
X	-154	MET	-	initiating methionine	UNP Q12306
X	-153	GLY	-	expression tag	UNP Q12306
X	-152	HIS	-	expression tag	UNP Q12306
X	-151	HIS	-	expression tag	UNP Q12306
X	-150	HIS	-	expression tag	UNP Q12306
X	-149	HIS	-	expression tag	UNP Q12306
X	-148	HIS	-	expression tag	UNP Q12306
X	-147	HIS	-	expression tag	UNP Q12306
X	-146	GLY	-	expression tag	UNP Q12306
X	-145	SER	-	expression tag	UNP Q12306
X	-144	LEU	-	expression tag	UNP Q12306
X	-143	GLN	-	expression tag	UNP Q12306
X	-68	ALA	THR	conflict	UNP Q12306
X	?	-	SER	deletion	UNP O60884
X	?	-	GLY	deletion	UNP O60884
X	?	-	GLY	deletion	UNP O60884
X	?	-	GLY	deletion	UNP O60884
X	?	-	GLY	deletion	UNP O60884
X	?	-	GLY	deletion	UNP O60884
X	?	-	MET	deletion	UNP O60884
X	?	-	ASP	deletion	UNP O60884
X	?	-	ASP	deletion	UNP O60884
X	?	-	ILE	deletion	UNP O60884
X	?	-	PHE	deletion	UNP O60884
X	?	-	SER	deletion	UNP O60884
X	?	-	HIS	deletion	UNP O60884
X	?	-	ILE	deletion	UNP O60884
X	?	-	PHE	deletion	UNP O60884
X	?	-	GLY	deletion	UNP O60884
X	?	-	GLY	deletion	UNP O60884
X	?	-	GLY	deletion	UNP O60884
X	?	-	LEU	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
X	?	-	PHE	deletion	UNP O60884
X	?	-	GLY	deletion	UNP O60884
X	?	-	PHE	deletion	UNP O60884
X	?	-	MET	deletion	UNP O60884
b	-154	MET	-	initiating methionine	UNP Q12306
b	-153	GLY	-	expression tag	UNP Q12306
b	-152	HIS	-	expression tag	UNP Q12306
b	-151	HIS	-	expression tag	UNP Q12306
b	-150	HIS	-	expression tag	UNP Q12306
b	-149	HIS	-	expression tag	UNP Q12306
b	-148	HIS	-	expression tag	UNP Q12306
b	-147	HIS	-	expression tag	UNP Q12306
b	-146	GLY	-	expression tag	UNP Q12306
b	-145	SER	-	expression tag	UNP Q12306
b	-144	LEU	-	expression tag	UNP Q12306
b	-143	GLN	-	expression tag	UNP Q12306
b	-68	ALA	THR	conflict	UNP Q12306
b	?	-	SER	deletion	UNP O60884
b	?	-	GLY	deletion	UNP O60884
b	?	-	GLY	deletion	UNP O60884
b	?	-	GLY	deletion	UNP O60884
b	?	-	GLY	deletion	UNP O60884
b	?	-	GLY	deletion	UNP O60884
b	?	-	MET	deletion	UNP O60884
b	?	-	ASP	deletion	UNP O60884
b	?	-	ASP	deletion	UNP O60884
b	?	-	ILE	deletion	UNP O60884
b	?	-	PHE	deletion	UNP O60884
b	?	-	SER	deletion	UNP O60884
b	?	-	HIS	deletion	UNP O60884
b	?	-	ILE	deletion	UNP O60884
b	?	-	PHE	deletion	UNP O60884
b	?	-	GLY	deletion	UNP O60884
b	?	-	GLY	deletion	UNP O60884
b	?	-	GLY	deletion	UNP O60884
b	?	-	LEU	deletion	UNP O60884
b	?	-	PHE	deletion	UNP O60884
b	?	-	GLY	deletion	UNP O60884
b	?	-	PHE	deletion	UNP O60884
b	?	-	MET	deletion	UNP O60884
j	-154	MET	-	initiating methionine	UNP Q12306
j	-153	GLY	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
j	-152	HIS	-	expression tag	UNP Q12306
j	-151	HIS	-	expression tag	UNP Q12306
j	-150	HIS	-	expression tag	UNP Q12306
j	-149	HIS	-	expression tag	UNP Q12306
j	-148	HIS	-	expression tag	UNP Q12306
j	-147	HIS	-	expression tag	UNP Q12306
j	-146	GLY	-	expression tag	UNP Q12306
j	-145	SER	-	expression tag	UNP Q12306
j	-144	LEU	-	expression tag	UNP Q12306
j	-143	GLN	-	expression tag	UNP Q12306
j	-68	ALA	THR	conflict	UNP Q12306
j	?	-	SER	deletion	UNP O60884
j	?	-	GLY	deletion	UNP O60884
j	?	-	GLY	deletion	UNP O60884
j	?	-	GLY	deletion	UNP O60884
j	?	-	GLY	deletion	UNP O60884
j	?	-	GLY	deletion	UNP O60884
j	?	-	MET	deletion	UNP O60884
j	?	-	ASP	deletion	UNP O60884
j	?	-	ASP	deletion	UNP O60884
j	?	-	ILE	deletion	UNP O60884
j	?	-	PHE	deletion	UNP O60884
j	?	-	SER	deletion	UNP O60884
j	?	-	HIS	deletion	UNP O60884
j	?	-	ILE	deletion	UNP O60884
j	?	-	PHE	deletion	UNP O60884
j	?	-	GLY	deletion	UNP O60884
j	?	-	GLY	deletion	UNP O60884
j	?	-	GLY	deletion	UNP O60884
j	?	-	LEU	deletion	UNP O60884
j	?	-	PHE	deletion	UNP O60884
j	?	-	GLY	deletion	UNP O60884
j	?	-	PHE	deletion	UNP O60884
j	?	-	MET	deletion	UNP O60884
f	-154	MET	-	initiating methionine	UNP Q12306
f	-153	GLY	-	expression tag	UNP Q12306
f	-152	HIS	-	expression tag	UNP Q12306
f	-151	HIS	-	expression tag	UNP Q12306
f	-150	HIS	-	expression tag	UNP Q12306
f	-149	HIS	-	expression tag	UNP Q12306
f	-148	HIS	-	expression tag	UNP Q12306
f	-147	HIS	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
f	-146	GLY	-	expression tag	UNP Q12306
f	-145	SER	-	expression tag	UNP Q12306
f	-144	LEU	-	expression tag	UNP Q12306
f	-143	GLN	-	expression tag	UNP Q12306
f	-68	ALA	THR	conflict	UNP Q12306
f	?	-	SER	deletion	UNP O60884
f	?	-	GLY	deletion	UNP O60884
f	?	-	GLY	deletion	UNP O60884
f	?	-	GLY	deletion	UNP O60884
f	?	-	GLY	deletion	UNP O60884
f	?	-	GLY	deletion	UNP O60884
f	?	-	MET	deletion	UNP O60884
f	?	-	ASP	deletion	UNP O60884
f	?	-	ASP	deletion	UNP O60884
f	?	-	ILE	deletion	UNP O60884
f	?	-	PHE	deletion	UNP O60884
f	?	-	SER	deletion	UNP O60884
f	?	-	HIS	deletion	UNP O60884
f	?	-	ILE	deletion	UNP O60884
f	?	-	PHE	deletion	UNP O60884
f	?	-	GLY	deletion	UNP O60884
f	?	-	GLY	deletion	UNP O60884
f	?	-	GLY	deletion	UNP O60884
f	?	-	LEU	deletion	UNP O60884
f	?	-	PHE	deletion	UNP O60884
f	?	-	GLY	deletion	UNP O60884
f	?	-	PHE	deletion	UNP O60884
f	?	-	MET	deletion	UNP O60884
n	-154	MET	-	initiating methionine	UNP Q12306
n	-153	GLY	-	expression tag	UNP Q12306
n	-152	HIS	-	expression tag	UNP Q12306
n	-151	HIS	-	expression tag	UNP Q12306
n	-150	HIS	-	expression tag	UNP Q12306
n	-149	HIS	-	expression tag	UNP Q12306
n	-148	HIS	-	expression tag	UNP Q12306
n	-147	HIS	-	expression tag	UNP Q12306
n	-146	GLY	-	expression tag	UNP Q12306
n	-145	SER	-	expression tag	UNP Q12306
n	-144	LEU	-	expression tag	UNP Q12306
n	-143	GLN	-	expression tag	UNP Q12306
n	-68	ALA	THR	conflict	UNP Q12306
n	?	-	SER	deletion	UNP O60884

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Chain	Residue	Modelled	Actual	Comment	Reference
n	?	-	GLY	deletion	UNP O60884
n	?	-	GLY	deletion	UNP O60884
n	?	-	GLY	deletion	UNP O60884
n	?	-	GLY	deletion	UNP O60884
n	?	-	GLY	deletion	UNP O60884
n	?	-	MET	deletion	UNP O60884
n	?	-	ASP	deletion	UNP O60884
n	?	-	ASP	deletion	UNP O60884
n	?	-	ILE	deletion	UNP O60884
n	?	-	PHE	deletion	UNP O60884
n	?	-	SER	deletion	UNP O60884
n	?	-	HIS	deletion	UNP O60884
n	?	-	ILE	deletion	UNP O60884
n	?	-	PHE	deletion	UNP O60884
n	?	-	GLY	deletion	UNP O60884
n	?	-	GLY	deletion	UNP O60884
n	?	-	GLY	deletion	UNP O60884
n	?	-	LEU	deletion	UNP O60884
n	?	-	PHE	deletion	UNP O60884
n	?	-	GLY	deletion	UNP O60884
n	?	-	PHE	deletion	UNP O60884
n	?	-	MET	deletion	UNP O60884

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	A	2	Total Zn 2 2	0
2	C	2	Total Zn 2 2	0
2	B	2	Total Zn 2 2	0
2	D	2	Total Zn 2 2	0
2	E	2	Total Zn 2 2	0
2	G	2	Total Zn 2 2	0
2	F	2	Total Zn 2 2	0
2	H	2	Total Zn 2 2	0

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Mol	Chain	Residues	Atoms	AltConf
2	I	2	Total Zn 2 2	0
2	Q	2	Total Zn 2 2	0
2	M	2	Total Zn 2 2	0
2	U	2	Total Zn 2 2	0
2	Y	2	Total Zn 2 2	0
2	g	2	Total Zn 2 2	0
2	c	2	Total Zn 2 2	0
2	k	2	Total Zn 2 2	0
2	J	2	Total Zn 2 2	0
2	R	2	Total Zn 2 2	0
2	N	2	Total Zn 2 2	0
2	V	2	Total Zn 2 2	0
2	Z	2	Total Zn 2 2	0
2	h	2	Total Zn 2 2	0
2	d	2	Total Zn 2 2	0
2	l	2	Total Zn 2 2	0
2	K	2	Total Zn 2 2	0
2	S	2	Total Zn 2 2	0
2	O	2	Total Zn 2 2	0
2	W	2	Total Zn 2 2	0
2	a	2	Total Zn 2 2	0

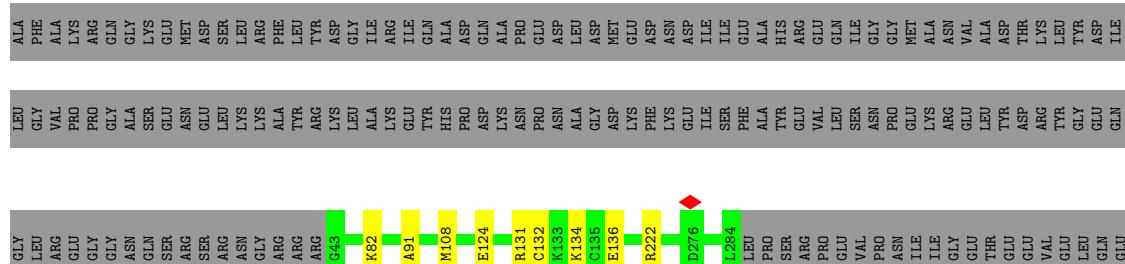
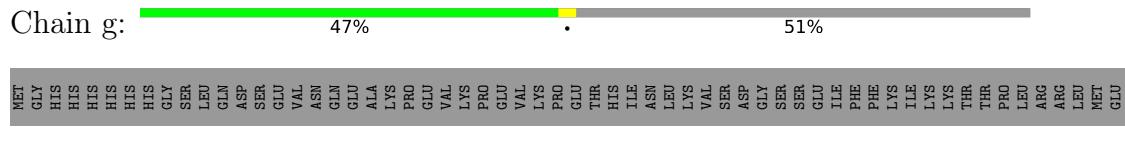
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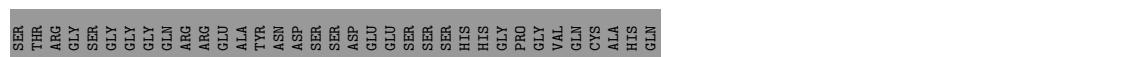
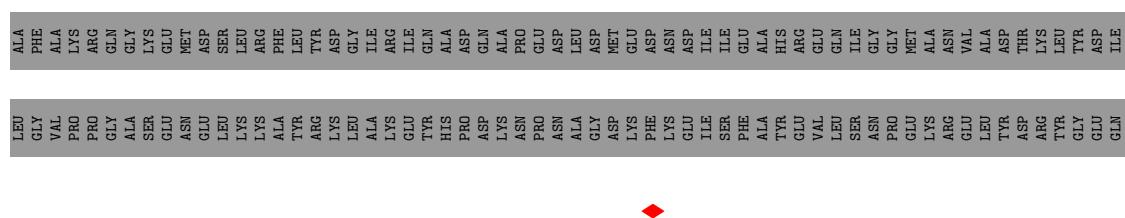
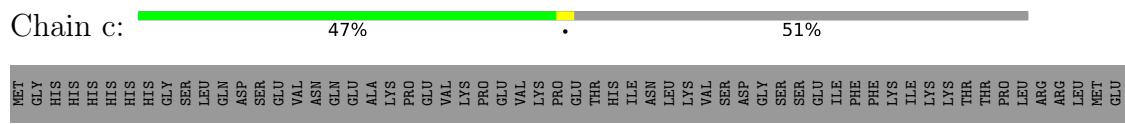
Mol	Chain	Residues	Atoms	AltConf
2	i	2	Total Zn 2 2	0
2	e	2	Total Zn 2 2	0
2	m	2	Total Zn 2 2	0
2	L	2	Total Zn 2 2	0
2	T	2	Total Zn 2 2	0
2	P	2	Total Zn 2 2	0
2	X	2	Total Zn 2 2	0
2	b	2	Total Zn 2 2	0
2	j	2	Total Zn 2 2	0
2	f	2	Total Zn 2 2	0
2	n	2	Total Zn 2 2	0

SER	ALA	MET	ALA	PHE	GLY	GLY	GLY	GLY	GLU
	GLY	GLY	HIS	ALA	VAL	ALA	ALA	SER	
	ALA	HIS	HIS	ARG	GLU	GLY	GLY	ASP	
	ALA	ALA	LYS	PRO	GLU	CLY	VAL	ASP	
						GLY	PRO		

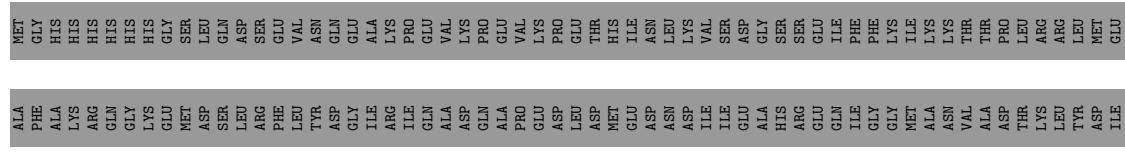
- Molecule 1: Ubiquitin-like protein SMT3,DnaJ homolog subfamily A member 2

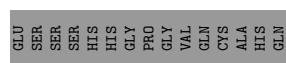
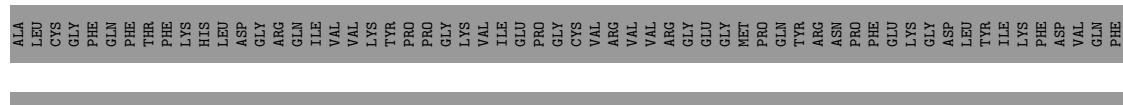
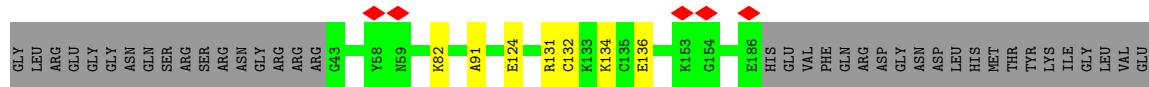


- Molecule 1: Ubiquitin-like protein SMT3,DnaJ homolog subfamily A member 2

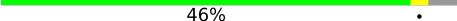
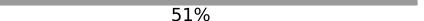


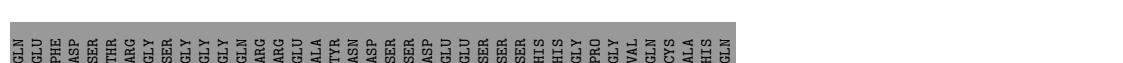
- Molecule 1: Ubiquitin-like protein SMT3,DnaJ homolog subfamily A member 2



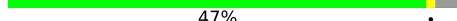
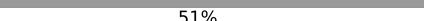


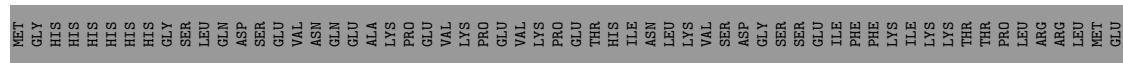
- Molecule 1: Ubiquitin-like protein SMT3,DnaJ homolog subfamily A member 2

Chain J:  • 

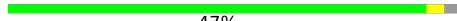
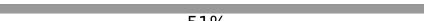


- Molecule 1: Ubiquitin-like protein SMT3,DnaJ homolog subfamily A member 2

Chain R:  • 



- Molecule 1: Ubiquitin-like protein SMT3,DnaJ homolog subfamily A member 2

Chain N:  • 



ASP	
GLU	
GLU	
SER	
SER	
HIS	
HIS	
GLY	
PRO	
GLY	
VAL	
GLN	
CYS	
ALA	
HIS	
GLN	

4 Experimental information i

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D5	Depositor
Number of particles used	47396	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.443	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.088	Depositor
Map size (Å)	316.2, 316.2, 316.2	wwPDB
Map dimensions	150, 150, 150	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.108, 2.108, 2.108	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	2/1918 (0.1%)	0.76	4/2572 (0.2%)
1	B	0.56	3/1918 (0.2%)	0.79	5/2572 (0.2%)
1	C	0.47	0/1918	0.80	4/2572 (0.2%)
1	D	0.48	1/1918 (0.1%)	0.76	3/2572 (0.1%)
1	E	0.45	1/1081 (0.1%)	0.75	1/1440 (0.1%)
1	F	0.42	1/1918 (0.1%)	0.74	3/2572 (0.1%)
1	G	0.43	1/1918 (0.1%)	0.75	4/2572 (0.2%)
1	H	0.47	1/1090 (0.1%)	0.75	1/1452 (0.1%)
1	I	0.54	3/1918 (0.2%)	0.79	5/2572 (0.2%)
1	J	0.55	2/1918 (0.1%)	0.80	5/2572 (0.2%)
1	K	0.47	1/1918 (0.1%)	0.76	3/2572 (0.1%)
1	L	0.51	2/1918 (0.1%)	0.80	6/2572 (0.2%)
1	M	0.56	4/1918 (0.2%)	0.79	5/2572 (0.2%)
1	N	0.53	2/1918 (0.1%)	0.77	4/2572 (0.2%)
1	O	0.51	2/1918 (0.1%)	0.77	4/2572 (0.2%)
1	P	0.48	1/1918 (0.1%)	0.76	3/2572 (0.1%)
1	Q	0.46	0/1918	0.75	3/2572 (0.1%)
1	R	0.47	0/1918	0.76	3/2572 (0.1%)
1	S	0.46	0/1918	0.75	3/2572 (0.1%)
1	T	0.54	2/1918 (0.1%)	0.79	6/2572 (0.2%)
1	U	0.46	1/1918 (0.1%)	0.76	3/2572 (0.1%)
1	V	0.48	2/1918 (0.1%)	0.79	4/2572 (0.2%)
1	W	0.51	3/1918 (0.2%)	0.79	5/2572 (0.2%)
1	X	0.46	1/1918 (0.1%)	0.75	3/2572 (0.1%)
1	Y	0.47	1/1081 (0.1%)	0.79	2/1440 (0.1%)
1	Z	0.45	1/1081 (0.1%)	0.76	1/1440 (0.1%)
1	a	0.45	1/1081 (0.1%)	0.76	1/1440 (0.1%)
1	b	0.46	1/1081 (0.1%)	0.75	1/1440 (0.1%)
1	c	0.43	1/1918 (0.1%)	0.74	3/2572 (0.1%)
1	d	0.43	1/1918 (0.1%)	0.74	3/2572 (0.1%)
1	e	0.42	1/1918 (0.1%)	0.74	3/2572 (0.1%)
1	f	0.43	1/1918 (0.1%)	0.74	3/2572 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	g	0.44	1/1918 (0.1%)	0.76	4/2572 (0.2%)
1	h	0.43	1/1918 (0.1%)	0.75	4/2572 (0.2%)
1	i	0.44	1/1918 (0.1%)	0.75	4/2572 (0.2%)
1	j	0.43	1/1918 (0.1%)	0.75	4/2572 (0.2%)
1	k	0.47	1/1090 (0.1%)	0.76	1/1452 (0.1%)
1	l	0.46	1/1090 (0.1%)	0.75	1/1452 (0.1%)
1	m	0.46	1/1090 (0.1%)	0.75	1/1452 (0.1%)
1	n	0.46	1/1090 (0.1%)	0.76	1/1452 (0.1%)
All	All	0.48	52/68395 (0.1%)	0.76	127/91620 (0.1%)

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	93	ARG	NE-CZ	11.68	1.48	1.33
1	B	243	ARG	CZ-NH1	10.88	1.47	1.33
1	J	243	ARG	CZ-NH1	10.46	1.46	1.33
1	M	93	ARG	NE-CZ	9.37	1.45	1.33
1	I	93	ARG	NE-CZ	9.33	1.45	1.33

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	ARG	NE-CZ-NH2	11.30	125.95	120.30
1	M	93	ARG	NE-CZ-NH2	10.50	125.55	120.30
1	I	93	ARG	NE-CZ-NH2	10.34	125.47	120.30
1	W	93	ARG	NE-CZ-NH2	10.11	125.35	120.30
1	T	93	ARG	NE-CZ-NH2	9.28	124.94	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	B	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	C	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	D	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	E	141/497 (28%)	133 (94%)	6 (4%)	2 (1%)	11 46
1	F	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	G	240/497 (48%)	229 (95%)	9 (4%)	2 (1%)	19 60
1	H	142/497 (29%)	134 (94%)	6 (4%)	2 (1%)	11 46
1	I	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	J	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	K	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	L	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	M	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	N	240/497 (48%)	229 (95%)	9 (4%)	2 (1%)	19 60
1	O	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	P	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	Q	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	R	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	S	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	T	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	U	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	V	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	W	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	X	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	Y	141/497 (28%)	132 (94%)	7 (5%)	2 (1%)	11 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Z	141/497 (28%)	133 (94%)	6 (4%)	2 (1%)	11 46
1	a	141/497 (28%)	133 (94%)	6 (4%)	2 (1%)	11 46
1	b	141/497 (28%)	133 (94%)	6 (4%)	2 (1%)	11 46
1	c	240/497 (48%)	229 (95%)	9 (4%)	2 (1%)	19 60
1	d	240/497 (48%)	229 (95%)	9 (4%)	2 (1%)	19 60
1	e	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	f	240/497 (48%)	230 (96%)	8 (3%)	2 (1%)	19 60
1	g	240/497 (48%)	229 (95%)	9 (4%)	2 (1%)	19 60
1	h	240/497 (48%)	229 (95%)	9 (4%)	2 (1%)	19 60
1	i	240/497 (48%)	229 (95%)	9 (4%)	2 (1%)	19 60
1	j	240/497 (48%)	229 (95%)	9 (4%)	2 (1%)	19 60
1	k	142/497 (29%)	134 (94%)	6 (4%)	2 (1%)	11 46
1	l	142/497 (29%)	134 (94%)	6 (4%)	2 (1%)	11 46
1	m	142/497 (29%)	134 (94%)	6 (4%)	2 (1%)	11 46
1	n	142/497 (29%)	134 (94%)	6 (4%)	2 (1%)	11 46
All	All	8615/19880 (43%)	8226 (96%)	309 (4%)	80 (1%)	21 57

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	CYS
1	A	136	GLU
1	C	132	CYS
1	C	136	GLU
1	B	132	CYS

5.3.2 Protein sidechains [\(i\)](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	209/427 (49%)	205 (98%)	4 (2%)	57 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	209/427 (49%)	205 (98%)	4 (2%)	57 75
1	C	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	D	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	E	120/427 (28%)	117 (98%)	3 (2%)	47 68
1	F	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	G	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	H	121/427 (28%)	118 (98%)	3 (2%)	47 68
1	I	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	J	209/427 (49%)	205 (98%)	4 (2%)	57 75
1	K	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	L	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	M	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	N	209/427 (49%)	205 (98%)	4 (2%)	57 75
1	O	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	P	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	Q	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	R	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	S	209/427 (49%)	205 (98%)	4 (2%)	57 75
1	T	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	U	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	V	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	W	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	X	209/427 (49%)	205 (98%)	4 (2%)	57 75
1	Y	120/427 (28%)	117 (98%)	3 (2%)	47 68
1	Z	120/427 (28%)	117 (98%)	3 (2%)	47 68
1	a	120/427 (28%)	117 (98%)	3 (2%)	47 68
1	b	120/427 (28%)	117 (98%)	3 (2%)	47 68
1	c	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	d	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	e	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	f	209/427 (49%)	206 (99%)	3 (1%)	67 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	g	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	h	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	i	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	j	209/427 (49%)	206 (99%)	3 (1%)	67 80
1	k	121/427 (28%)	118 (98%)	3 (2%)	47 68
1	l	121/427 (28%)	118 (98%)	3 (2%)	47 68
1	m	121/427 (28%)	118 (98%)	3 (2%)	47 68
1	n	121/427 (28%)	118 (98%)	3 (2%)	47 68
All	All	7475/17080 (44%)	7349 (98%)	126 (2%)	62 78

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	82	LYS
1	X	82	LYS
1	d	131	ARG
1	P	134	LYS
1	j	131	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
1	d	103	GLN
1	W	113	GLN
1	n	110	GLN
1	l	79	GLN
1	S	103	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 80 ligands modelled in this entry, 80 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.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

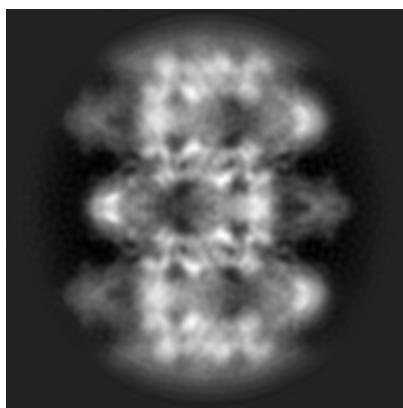
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14736. These allow visual inspection of the internal detail of the map and identification of artifacts.

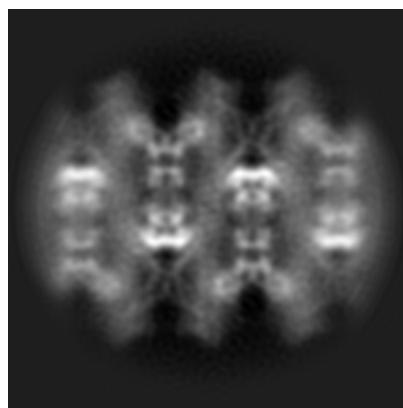
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

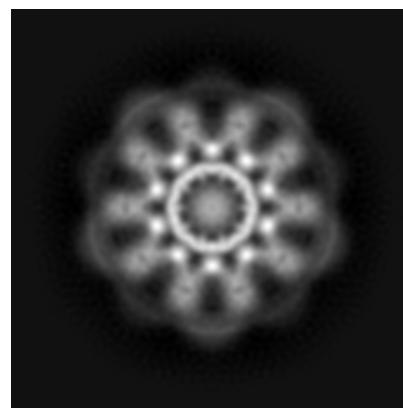
6.1.1 Primary map



X

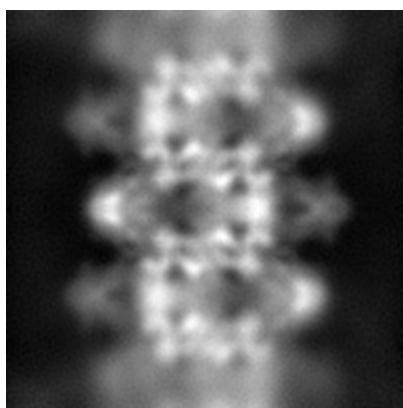


Y

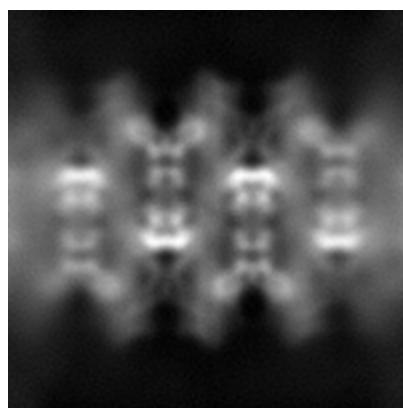


Z

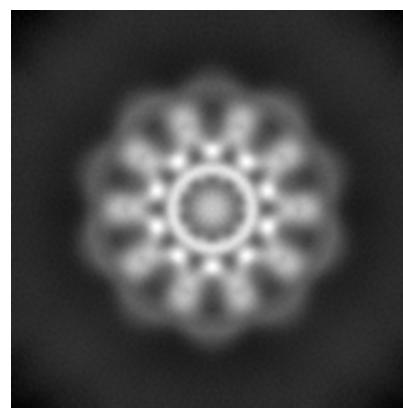
6.1.2 Raw map



X



Y

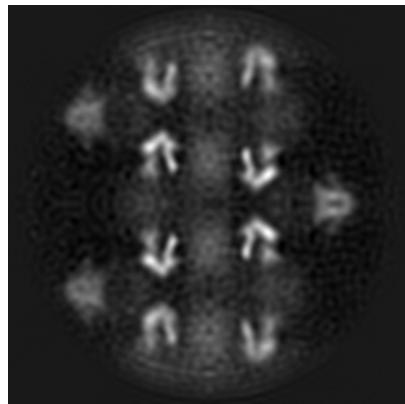


Z

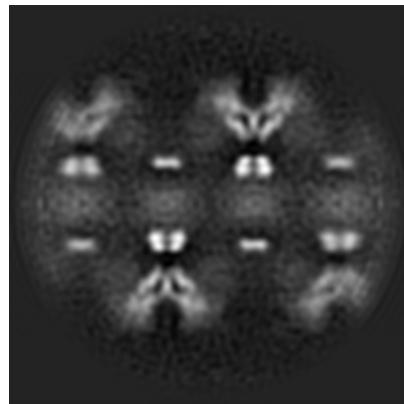
The images above show the map projected in three orthogonal directions.

6.2 Central slices [\(i\)](#)

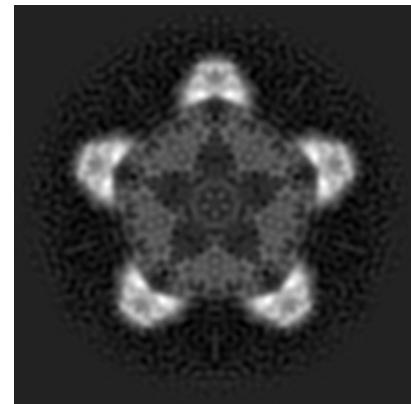
6.2.1 Primary map



X Index: 75

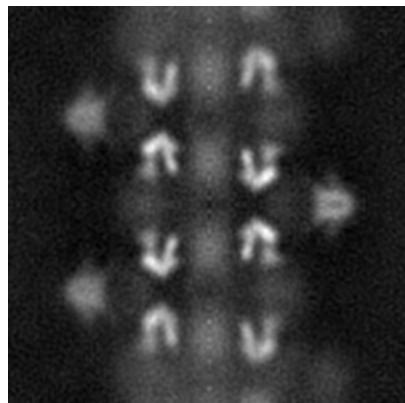


Y Index: 75

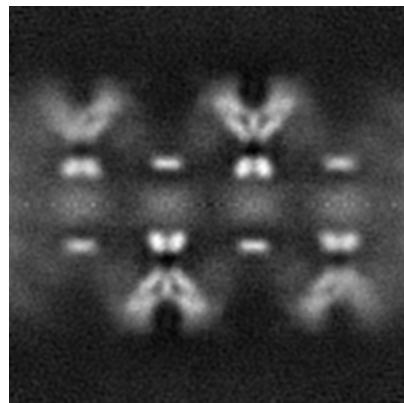


Z Index: 75

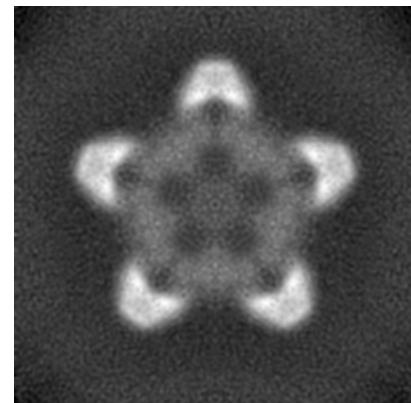
6.2.2 Raw map



X Index: 75



Y Index: 75

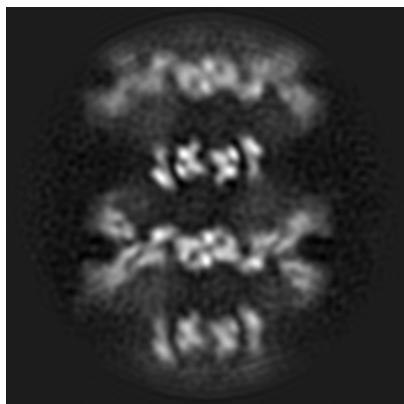


Z Index: 75

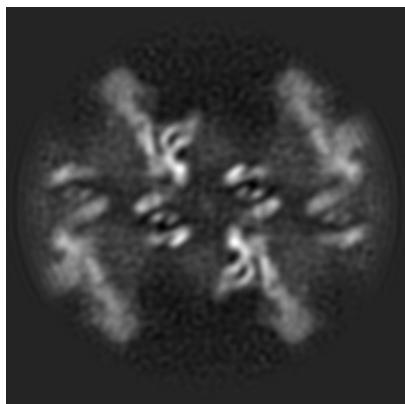
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

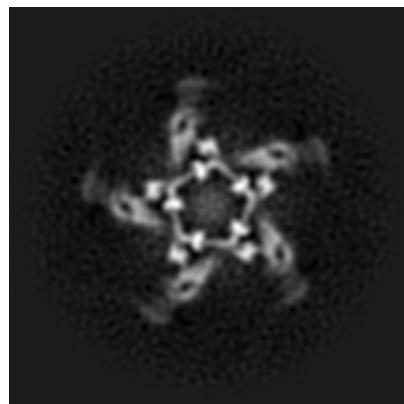
6.3.1 Primary map



X Index: 62

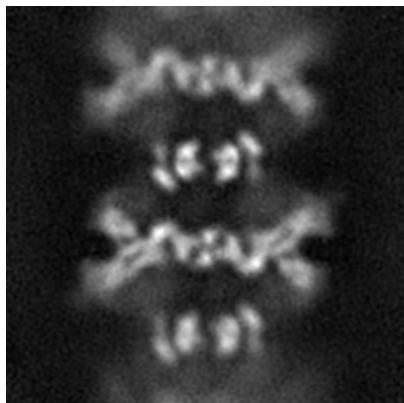


Y Index: 58

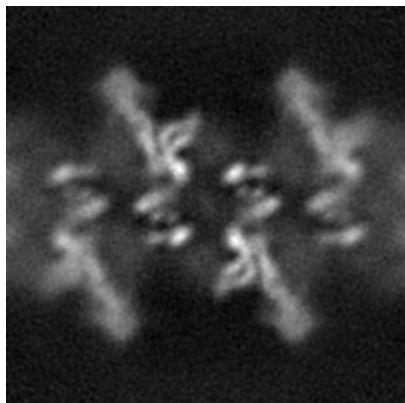


Z Index: 63

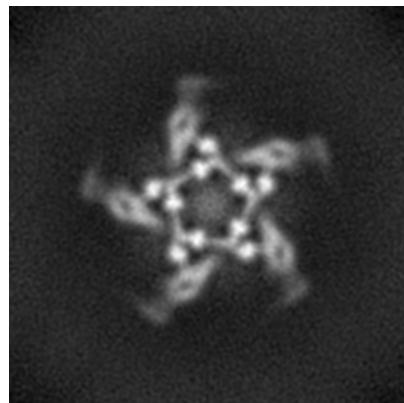
6.3.2 Raw map



X Index: 63



Y Index: 58

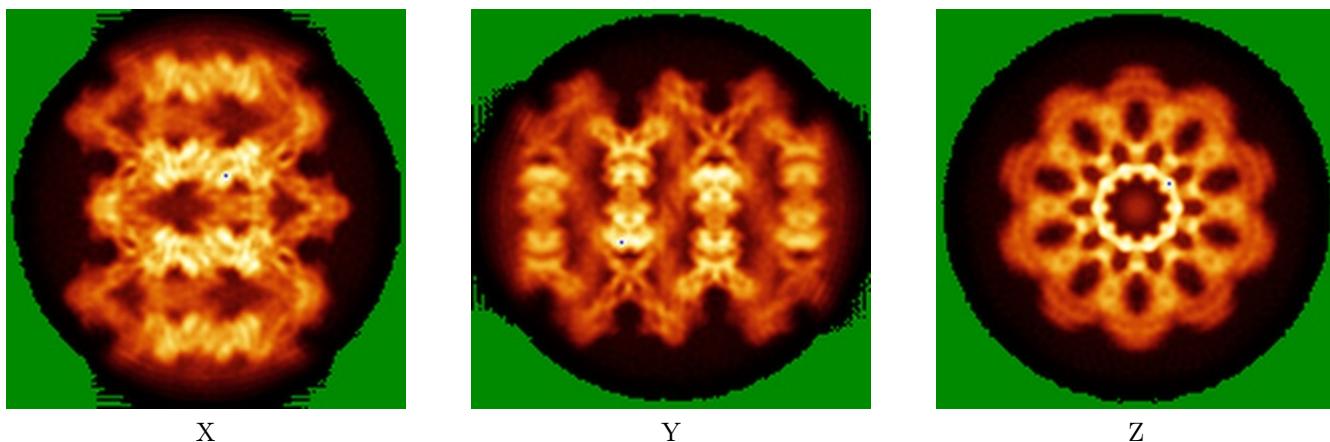


Z Index: 63

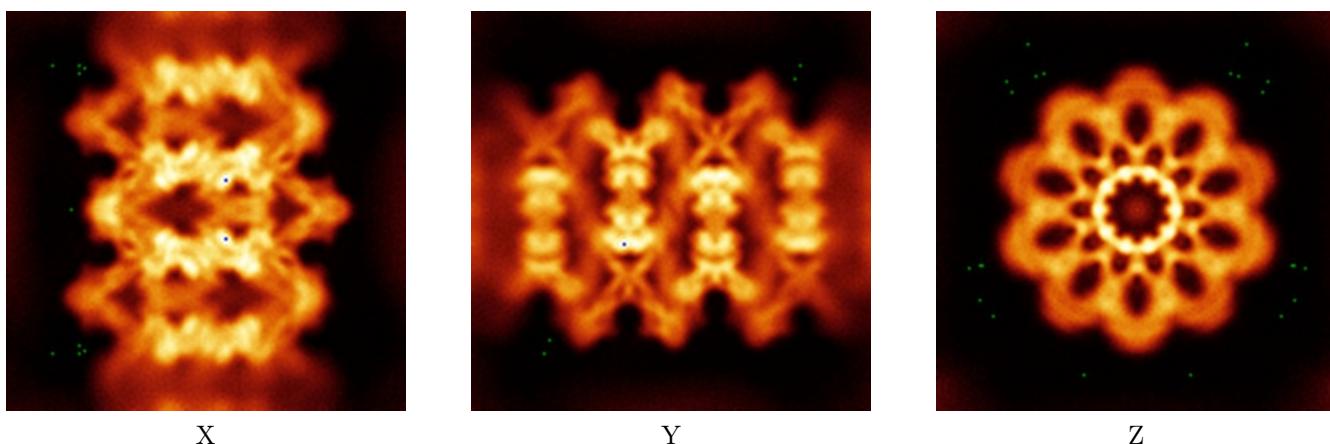
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



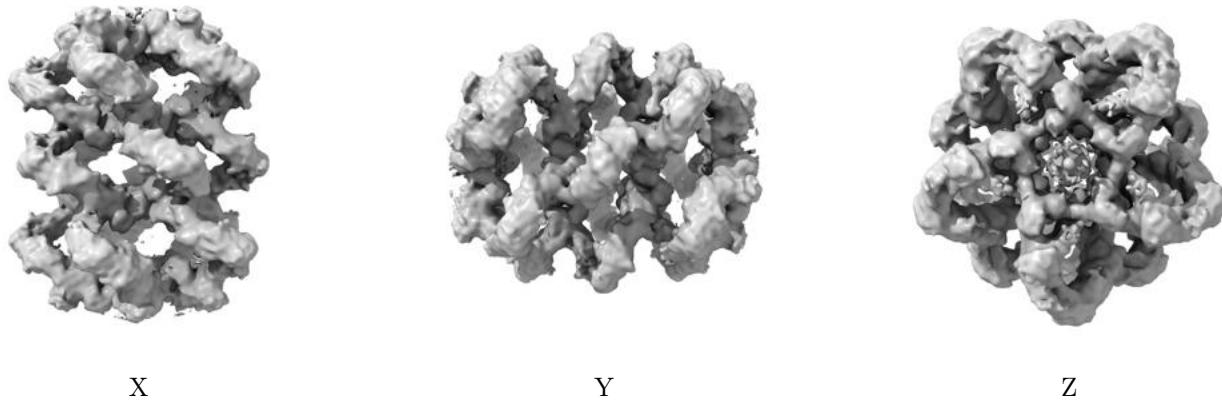
6.4.2 Raw map



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

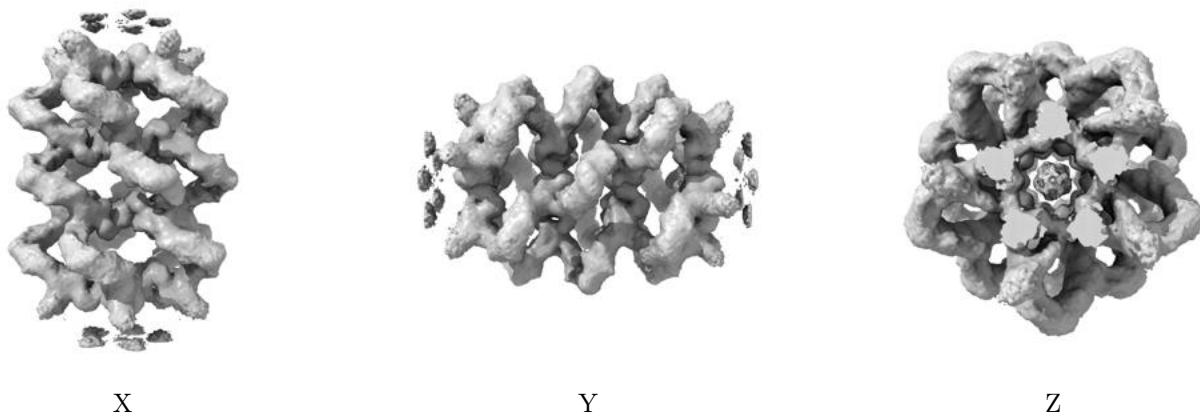
6.5 Orthogonal surface views [\(i\)](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.088. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

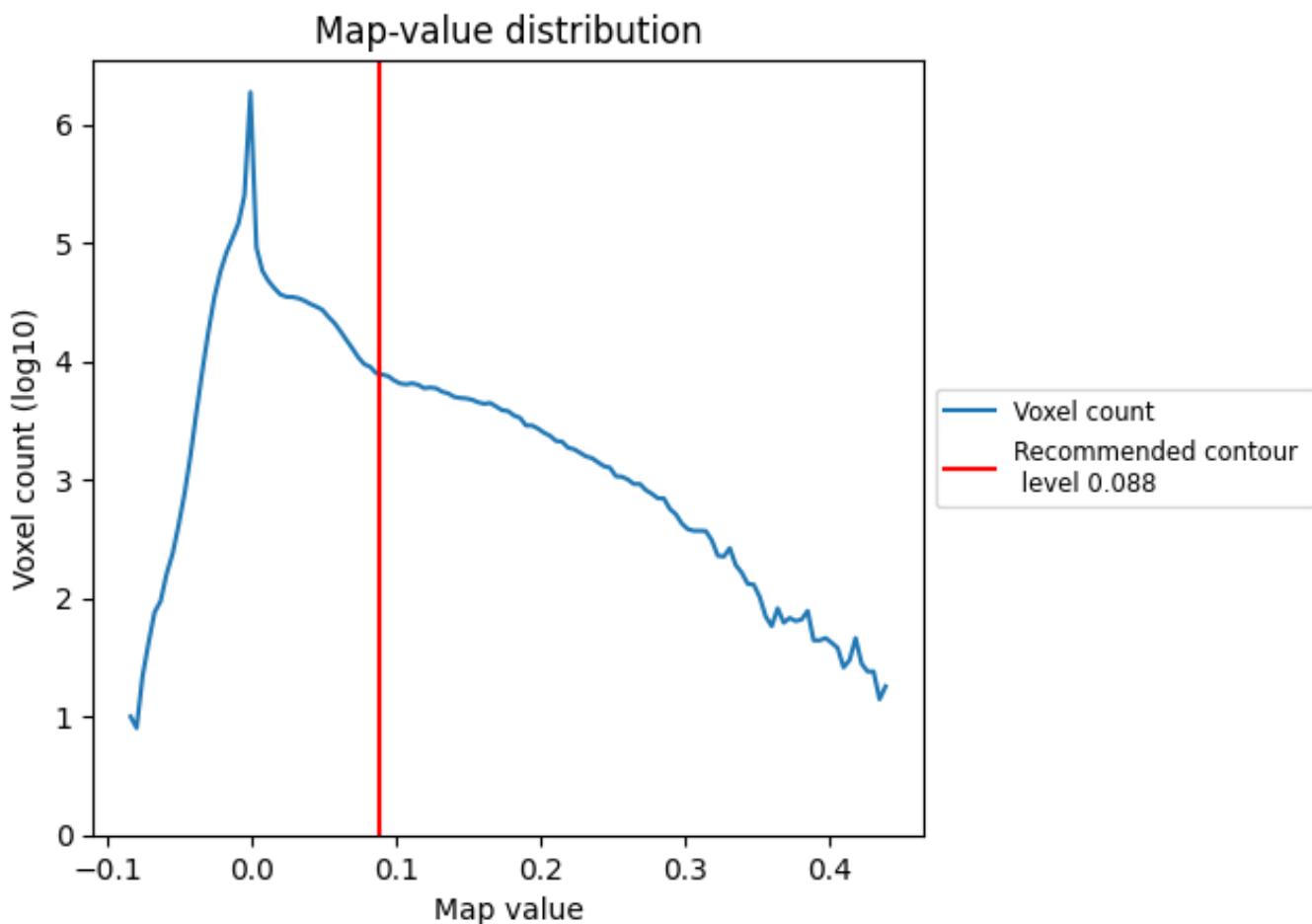
6.6 Mask visualisation [\(i\)](#)

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

7 Map analysis (i)

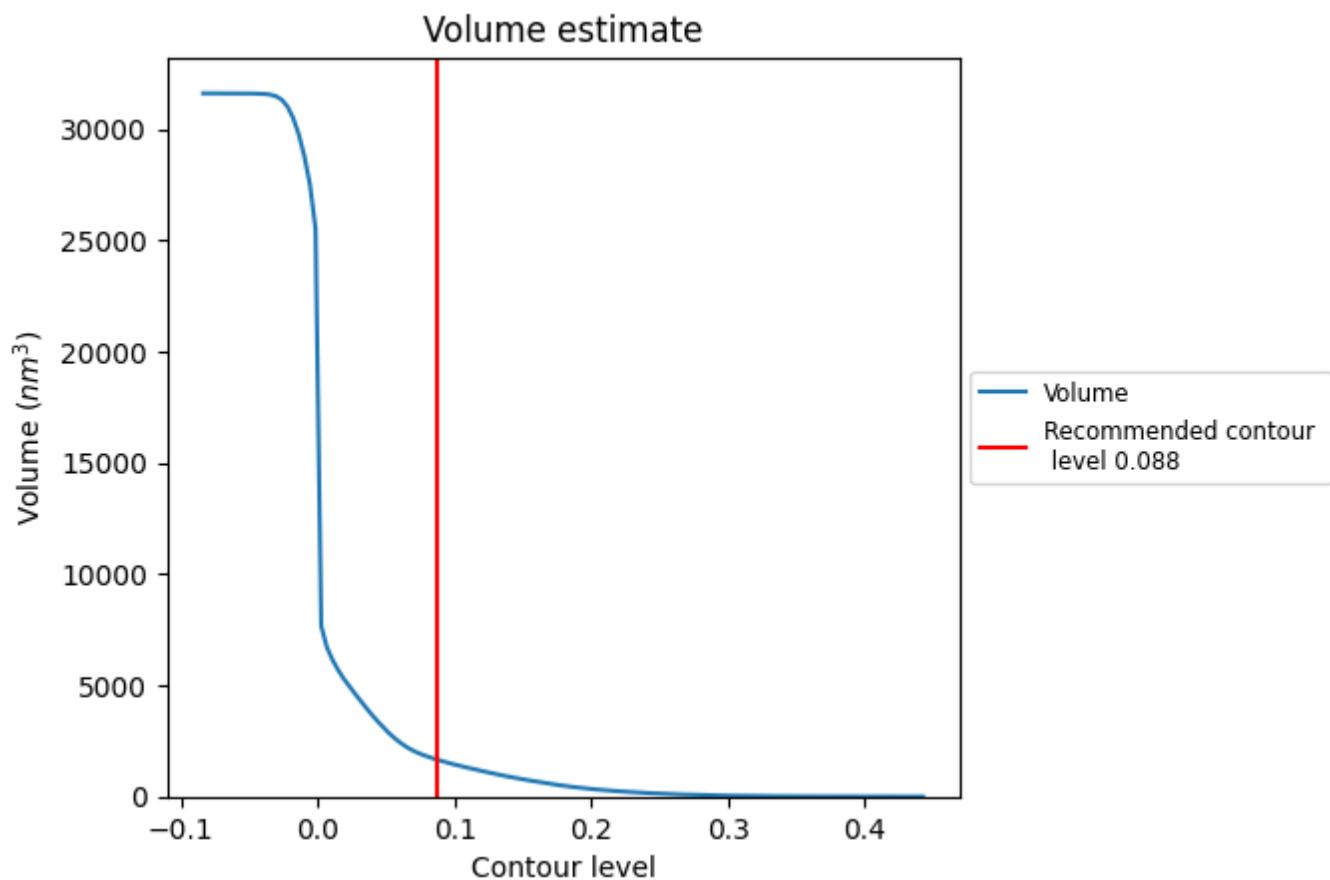
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

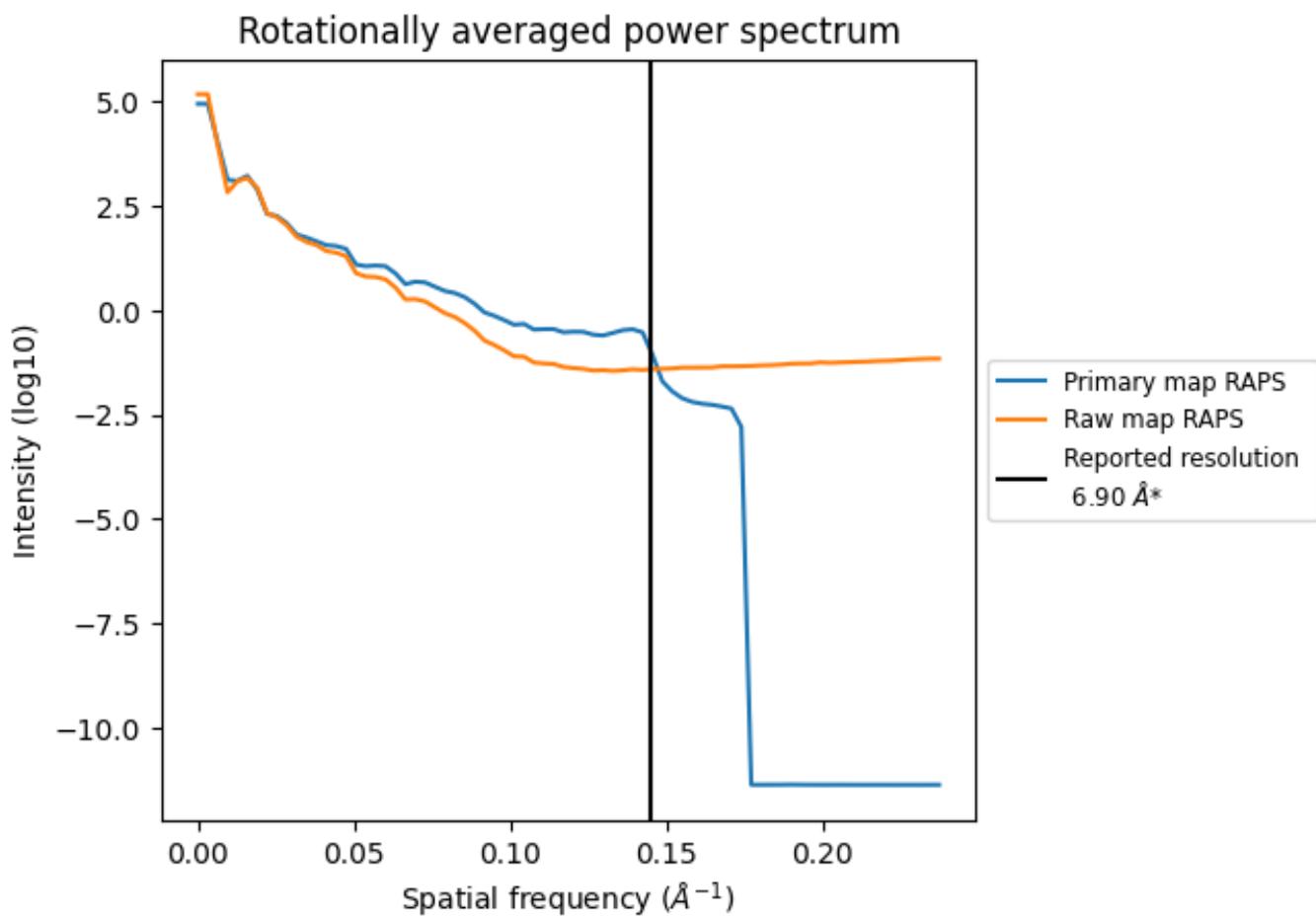
7.2 Volume estimate (i)



The volume at the recommended contour level is 1647 nm³; this corresponds to an approximate mass of 1488 kDa.

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

7.3 Rotationally averaged power spectrum [\(i\)](#)

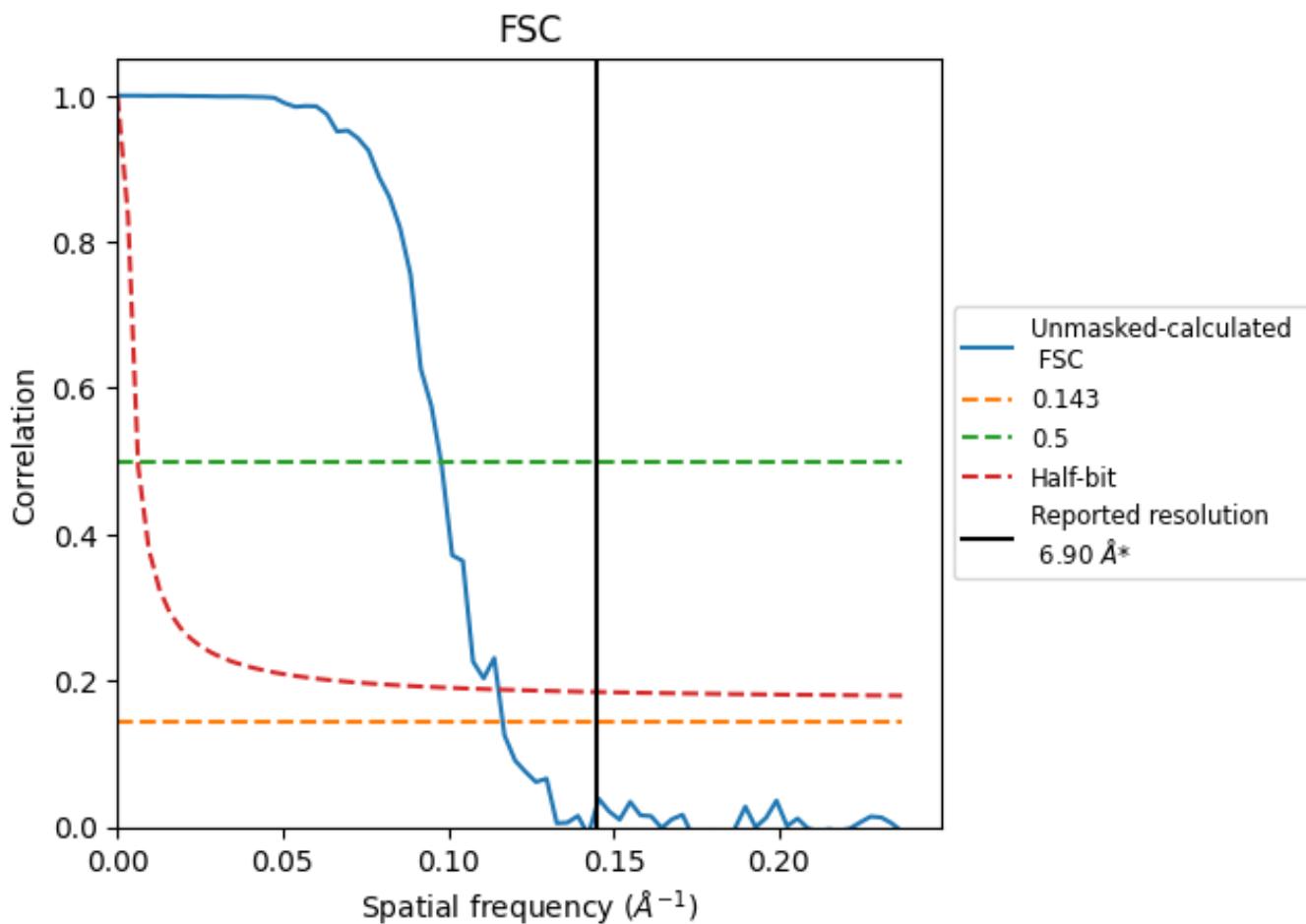


*Reported resolution corresponds to spatial frequency of 0.145\AA^{-1}

8 Fourier-Shell correlation [\(i\)](#)

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

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.145 \AA^{-1}

8.2 Resolution estimates [\(i\)](#)

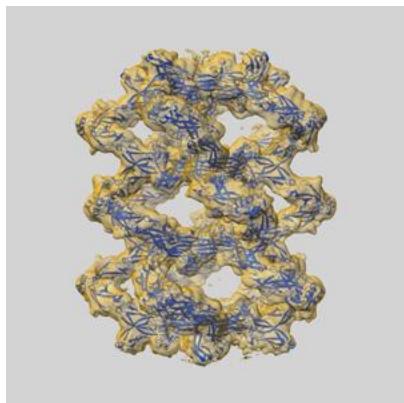
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.58	10.22	8.69

*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 8.58 differs from the reported value 6.9 by more than 10 %

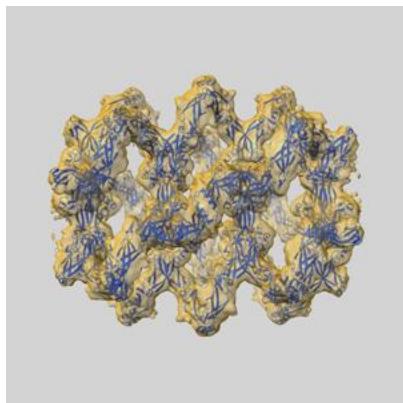
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14736 and PDB model 7ZHS. Per-residue inclusion information can be found in section 3 on page 44.

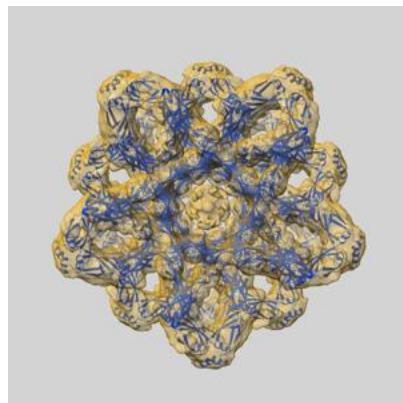
9.1 Map-model overlay (i)



X



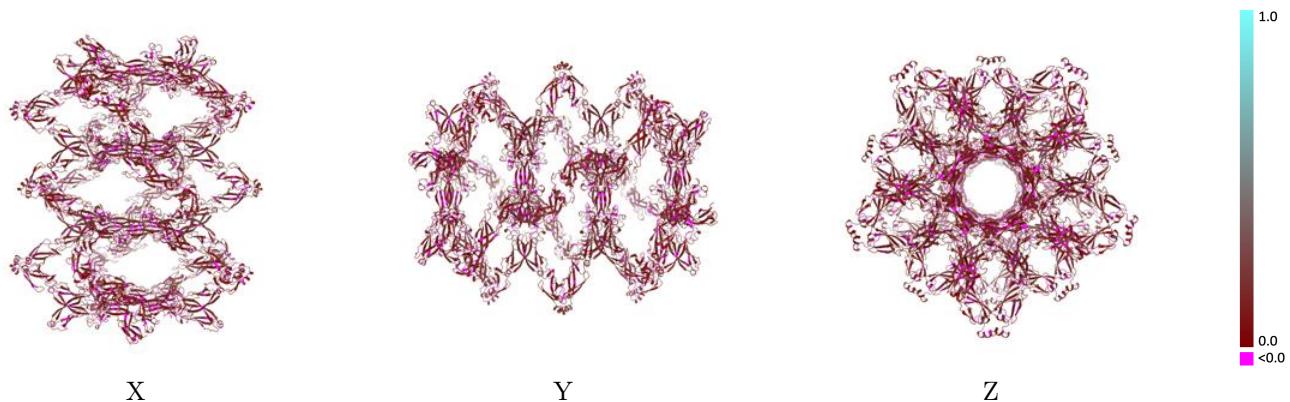
Y



Z

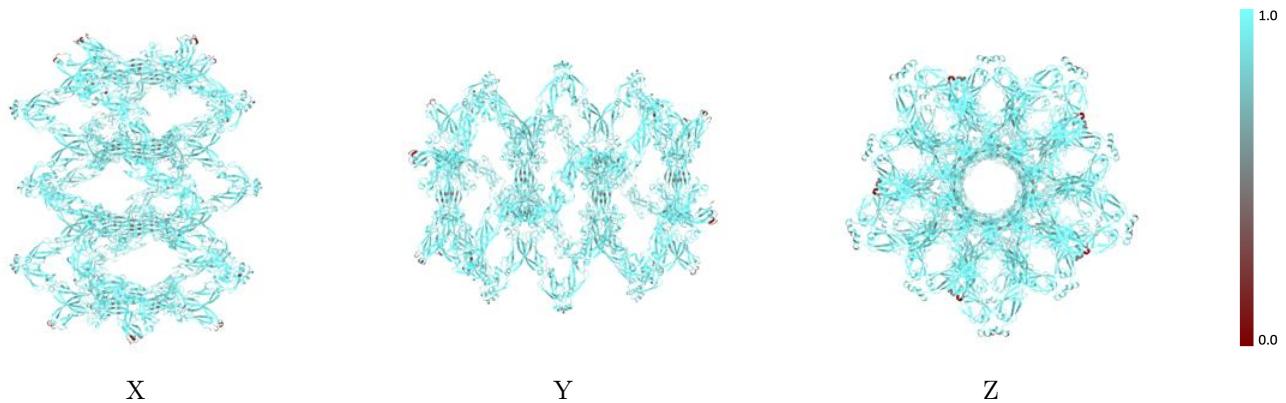
The images above show the 3D surface view of the map at the recommended contour level 0.088 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



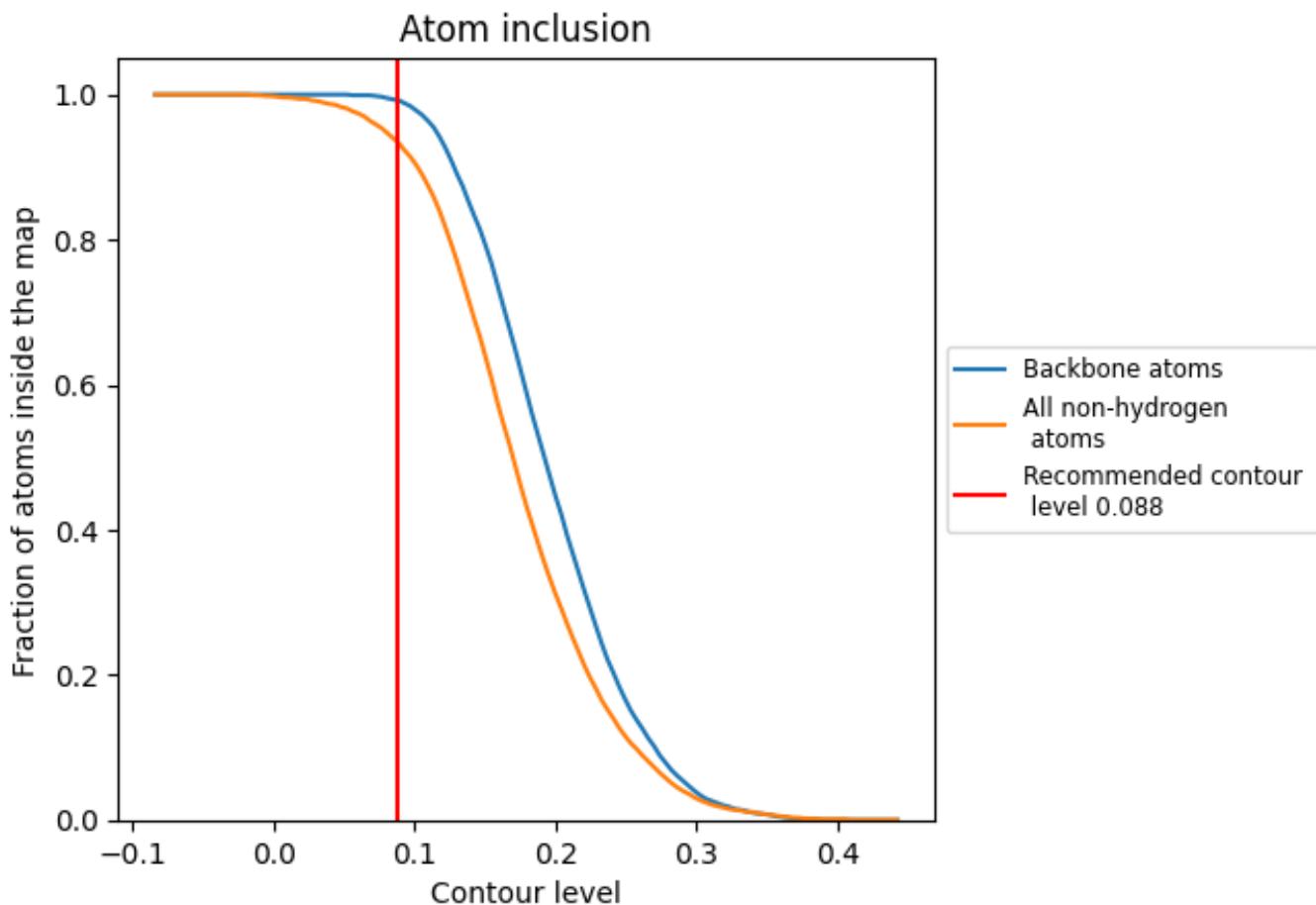
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.088).

9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 99% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.088) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9350	0.1210
A	0.9450	0.1310
B	0.9440	0.1300
C	0.9390	0.1250
D	0.9390	0.1280
E	0.9030	0.1150
F	0.9440	0.1090
G	0.9430	0.1120
H	0.8970	0.1130
I	0.9430	0.1320
J	0.9440	0.1290
K	0.9450	0.1300
L	0.9450	0.1310
M	0.9440	0.1340
N	0.9460	0.1340
O	0.9450	0.1330
P	0.9460	0.1330
Q	0.9380	0.1260
R	0.9390	0.1240
S	0.9380	0.1250
T	0.9350	0.1250
U	0.9380	0.1270
V	0.9400	0.1260
W	0.9370	0.1280
X	0.9380	0.1290
Y	0.9050	0.1110
Z	0.9030	0.1140
a	0.9040	0.1120
b	0.9020	0.1130
c	0.9440	0.1120
d	0.9440	0.1100
e	0.9430	0.1120
f	0.9440	0.1110
g	0.9440	0.1140
h	0.9460	0.1090



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Chain	Atom inclusion	Q-score
i	0.9430	0.1110
j	0.9400	0.1110
k	0.8970	0.1130
l	0.8930	0.1140
m	0.8940	0.1150
n	0.8930	0.1120