



Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 10:05 AM EST

PDB ID : 6MDR
EMDB ID : EMD-9104
Title : Cryo-EM structure of the Ceru+32/GFP-17 protomer
Authors : Simon, A.J.; Zhou, Y.; Ramasubramani, V.; Glaser, J.; Pothukuchy, A.; Goli-
har, J.; Gerberich, J.C.; Leggere, J.C.; Morrow, B.R.; Jung, C.; Glotzer, S.C.;
Taylor, D.W.; Ellington, A.D.
Deposited on : 2018-09-05
Resolution : 3.47 Å(reported)
Based on initial model : 2B3P

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

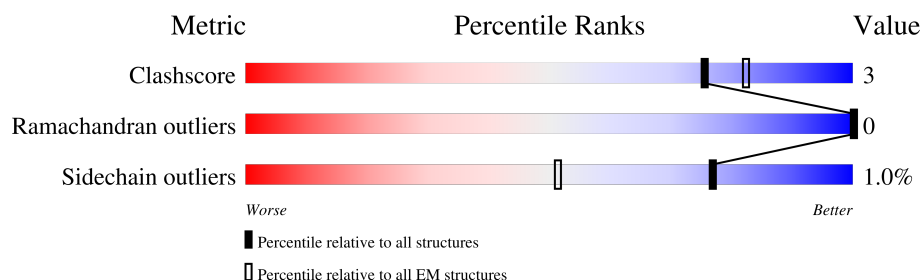
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

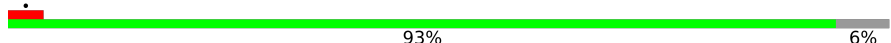
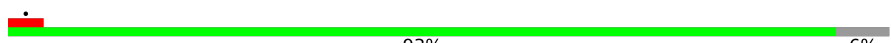
The reported resolution of this entry is 3.47 Å.

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



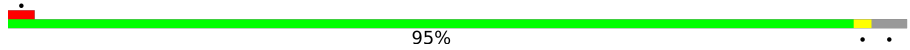
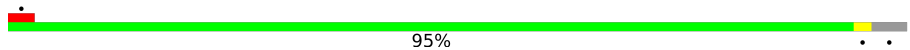
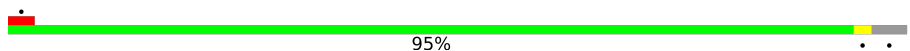
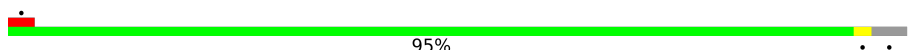
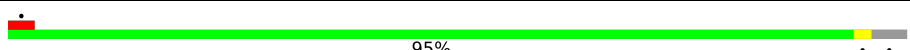
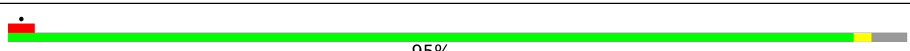
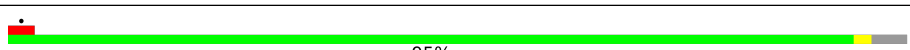
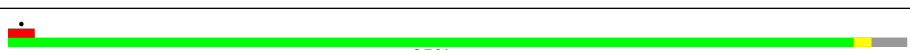
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	a	247	
1	c	247	
1	e	247	
1	g	247	
1	i	247	
1	k	247	
1	m	247	
1	o	247	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	b	240	
2	d	240	
2	f	240	
2	h	240	
2	j	240	
2	l	240	
2	n	240	
2	p	240	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 29456 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 Ceru+32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	231	Total	C	N	O	S	0	0
			1852	1183	349	315	5		
1	c	231	Total	C	N	O	S	0	0
			1852	1183	349	315	5		
1	e	231	Total	C	N	O	S	0	0
			1852	1183	349	315	5		
1	g	231	Total	C	N	O	S	0	0
			1852	1183	349	315	5		
1	i	231	Total	C	N	O	S	0	0
			1852	1183	349	315	5		
1	k	231	Total	C	N	O	S	0	0
			1852	1183	349	315	5		
1	m	231	Total	C	N	O	S	0	0
			1852	1183	349	315	5		
1	o	231	Total	C	N	O	S	0	0
			1852	1183	349	315	5		

There are 448 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1	MET	-	expression tag	UNP P42212
a	2	ALA	-	expression tag	UNP P42212
a	3	SER	-	expression tag	UNP P42212
a	7	ARG	GLU	engineered mutation	UNP P42212
a	10	ARG	THR	engineered mutation	UNP P42212
a	12	LYS	VAL	engineered mutation	UNP P42212
a	20	LYS	ASP	engineered mutation	UNP P42212
a	31	ARG	SER	engineered mutation	UNP P42212
a	33	LYS	GLU	engineered mutation	UNP P42212
a	35	LYS	GLU	engineered mutation	UNP P42212
a	40	ASN	TYR	engineered mutation	UNP P42212
a	65	LEU	PHE	engineered mutation	UNP P42212
a	66	THR	SER	engineered mutation	UNP P42212
a	67	TRP	TYR	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
a	73	ALA	SER	engineered mutation	UNP P42212
a	77	LYS	ASP	engineered mutation	UNP P42212
a	81	ARG	GLN	engineered mutation	UNP P42212
a	91	LYS	GLU	engineered mutation	UNP P42212
a	100	SER	PHE	engineered mutation	UNP P42212
a	103	LYS	ASP	engineered mutation	UNP P42212
a	106	THR	ASN	engineered mutation	UNP P42212
a	118	ARG	ASP	engineered mutation	UNP P42212
a	125	LYS	GLU	engineered mutation	UNP P42212
a	129	ARG	ILE	engineered mutation	UNP P42212
a	134	LYS	ASP	engineered mutation	UNP P42212
a	143	ARG	GLU	engineered mutation	UNP P42212
a	146	GLY	TYR	engineered mutation	UNP P42212
a	147	ILE	ASN	engineered mutation	UNP P42212
a	149	ASP	HIS	engineered mutation	UNP P42212
a	150	LYS	ASN	engineered mutation	UNP P42212
a	154	THR	MET	engineered mutation	UNP P42212
a	158	ARG	GLN	engineered mutation	UNP P42212
a	164	ALA	VAL	engineered mutation	UNP P42212
a	165	LYS	ASN	engineered mutation	UNP P42212
a	172	VAL	ILE	engineered mutation	UNP P42212
a	173	LYS	GLU	engineered mutation	UNP P42212
a	191	ARG	ASP	engineered mutation	UNP P42212
a	198	ARG	ASP	engineered mutation	UNP P42212
a	205	ARG	GLN	engineered mutation	UNP P42212
a	207	VAL	ALA	engineered mutation	UNP P42212
a	213	LYS	ASN	engineered mutation	UNP P42212
a	231	LYS	THR	engineered mutation	UNP P42212
a	234	ARG	-	expression tag	UNP P42212
a	235	ASP	-	expression tag	UNP P42212
a	236	GLU	-	expression tag	UNP P42212
a	237	ARG	-	expression tag	UNP P42212
a	238	TYR	-	expression tag	UNP P42212
a	239	LYS	-	expression tag	UNP P42212
a	240	LEU	-	expression tag	UNP P42212
a	241	GLU	-	expression tag	UNP P42212
a	242	HIS	-	expression tag	UNP P42212
a	243	HIS	-	expression tag	UNP P42212
a	244	HIS	-	expression tag	UNP P42212
a	245	HIS	-	expression tag	UNP P42212
a	246	HIS	-	expression tag	UNP P42212
a	247	HIS	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
c	1	MET	-	expression tag	UNP P42212
c	2	ALA	-	expression tag	UNP P42212
c	3	SER	-	expression tag	UNP P42212
c	7	ARG	GLU	engineered mutation	UNP P42212
c	10	ARG	THR	engineered mutation	UNP P42212
c	12	LYS	VAL	engineered mutation	UNP P42212
c	20	LYS	ASP	engineered mutation	UNP P42212
c	31	ARG	SER	engineered mutation	UNP P42212
c	33	LYS	GLU	engineered mutation	UNP P42212
c	35	LYS	GLU	engineered mutation	UNP P42212
c	40	ASN	TYR	engineered mutation	UNP P42212
c	65	LEU	PHE	engineered mutation	UNP P42212
c	66	THR	SER	engineered mutation	UNP P42212
c	67	TRP	TYR	engineered mutation	UNP P42212
c	73	ALA	SER	engineered mutation	UNP P42212
c	77	LYS	ASP	engineered mutation	UNP P42212
c	81	ARG	GLN	engineered mutation	UNP P42212
c	91	LYS	GLU	engineered mutation	UNP P42212
c	100	SER	PHE	engineered mutation	UNP P42212
c	103	LYS	ASP	engineered mutation	UNP P42212
c	106	THR	ASN	engineered mutation	UNP P42212
c	118	ARG	ASP	engineered mutation	UNP P42212
c	125	LYS	GLU	engineered mutation	UNP P42212
c	129	ARG	ILE	engineered mutation	UNP P42212
c	134	LYS	ASP	engineered mutation	UNP P42212
c	143	ARG	GLU	engineered mutation	UNP P42212
c	146	GLY	TYR	engineered mutation	UNP P42212
c	147	ILE	ASN	engineered mutation	UNP P42212
c	149	ASP	HIS	engineered mutation	UNP P42212
c	150	LYS	ASN	engineered mutation	UNP P42212
c	154	THR	MET	engineered mutation	UNP P42212
c	158	ARG	GLN	engineered mutation	UNP P42212
c	164	ALA	VAL	engineered mutation	UNP P42212
c	165	LYS	ASN	engineered mutation	UNP P42212
c	172	VAL	ILE	engineered mutation	UNP P42212
c	173	LYS	GLU	engineered mutation	UNP P42212
c	191	ARG	ASP	engineered mutation	UNP P42212
c	198	ARG	ASP	engineered mutation	UNP P42212
c	205	ARG	GLN	engineered mutation	UNP P42212
c	207	VAL	ALA	engineered mutation	UNP P42212
c	213	LYS	ASN	engineered mutation	UNP P42212
c	231	LYS	THR	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
c	234	ARG	-	expression tag	UNP P42212
c	235	ASP	-	expression tag	UNP P42212
c	236	GLU	-	expression tag	UNP P42212
c	237	ARG	-	expression tag	UNP P42212
c	238	TYR	-	expression tag	UNP P42212
c	239	LYS	-	expression tag	UNP P42212
c	240	LEU	-	expression tag	UNP P42212
c	241	GLU	-	expression tag	UNP P42212
c	242	HIS	-	expression tag	UNP P42212
c	243	HIS	-	expression tag	UNP P42212
c	244	HIS	-	expression tag	UNP P42212
c	245	HIS	-	expression tag	UNP P42212
c	246	HIS	-	expression tag	UNP P42212
c	247	HIS	-	expression tag	UNP P42212
e	1	MET	-	expression tag	UNP P42212
e	2	ALA	-	expression tag	UNP P42212
e	3	SER	-	expression tag	UNP P42212
e	7	ARG	GLU	engineered mutation	UNP P42212
e	10	ARG	THR	engineered mutation	UNP P42212
e	12	LYS	VAL	engineered mutation	UNP P42212
e	20	LYS	ASP	engineered mutation	UNP P42212
e	31	ARG	SER	engineered mutation	UNP P42212
e	33	LYS	GLU	engineered mutation	UNP P42212
e	35	LYS	GLU	engineered mutation	UNP P42212
e	40	ASN	TYR	engineered mutation	UNP P42212
e	65	LEU	PHE	engineered mutation	UNP P42212
e	66	THR	SER	engineered mutation	UNP P42212
e	67	TRP	TYR	engineered mutation	UNP P42212
e	73	ALA	SER	engineered mutation	UNP P42212
e	77	LYS	ASP	engineered mutation	UNP P42212
e	81	ARG	GLN	engineered mutation	UNP P42212
e	91	LYS	GLU	engineered mutation	UNP P42212
e	100	SER	PHE	engineered mutation	UNP P42212
e	103	LYS	ASP	engineered mutation	UNP P42212
e	106	THR	ASN	engineered mutation	UNP P42212
e	118	ARG	ASP	engineered mutation	UNP P42212
e	125	LYS	GLU	engineered mutation	UNP P42212
e	129	ARG	ILE	engineered mutation	UNP P42212
e	134	LYS	ASP	engineered mutation	UNP P42212
e	143	ARG	GLU	engineered mutation	UNP P42212
e	146	GLY	TYR	engineered mutation	UNP P42212
e	147	ILE	ASN	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
e	149	ASP	HIS	engineered mutation	UNP P42212
e	150	LYS	ASN	engineered mutation	UNP P42212
e	154	THR	MET	engineered mutation	UNP P42212
e	158	ARG	GLN	engineered mutation	UNP P42212
e	164	ALA	VAL	engineered mutation	UNP P42212
e	165	LYS	ASN	engineered mutation	UNP P42212
e	172	VAL	ILE	engineered mutation	UNP P42212
e	173	LYS	GLU	engineered mutation	UNP P42212
e	191	ARG	ASP	engineered mutation	UNP P42212
e	198	ARG	ASP	engineered mutation	UNP P42212
e	205	ARG	GLN	engineered mutation	UNP P42212
e	207	VAL	ALA	engineered mutation	UNP P42212
e	213	LYS	ASN	engineered mutation	UNP P42212
e	231	LYS	THR	engineered mutation	UNP P42212
e	234	ARG	-	expression tag	UNP P42212
e	235	ASP	-	expression tag	UNP P42212
e	236	GLU	-	expression tag	UNP P42212
e	237	ARG	-	expression tag	UNP P42212
e	238	TYR	-	expression tag	UNP P42212
e	239	LYS	-	expression tag	UNP P42212
e	240	LEU	-	expression tag	UNP P42212
e	241	GLU	-	expression tag	UNP P42212
e	242	HIS	-	expression tag	UNP P42212
e	243	HIS	-	expression tag	UNP P42212
e	244	HIS	-	expression tag	UNP P42212
e	245	HIS	-	expression tag	UNP P42212
e	246	HIS	-	expression tag	UNP P42212
e	247	HIS	-	expression tag	UNP P42212
g	1	MET	-	expression tag	UNP P42212
g	2	ALA	-	expression tag	UNP P42212
g	3	SER	-	expression tag	UNP P42212
g	7	ARG	GLU	engineered mutation	UNP P42212
g	10	ARG	THR	engineered mutation	UNP P42212
g	12	LYS	VAL	engineered mutation	UNP P42212
g	20	LYS	ASP	engineered mutation	UNP P42212
g	31	ARG	SER	engineered mutation	UNP P42212
g	33	LYS	GLU	engineered mutation	UNP P42212
g	35	LYS	GLU	engineered mutation	UNP P42212
g	40	ASN	TYR	engineered mutation	UNP P42212
g	65	LEU	PHE	engineered mutation	UNP P42212
g	66	THR	SER	engineered mutation	UNP P42212
g	67	TRP	TYR	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
g	73	ALA	SER	engineered mutation	UNP P42212
g	77	LYS	ASP	engineered mutation	UNP P42212
g	81	ARG	GLN	engineered mutation	UNP P42212
g	91	LYS	GLU	engineered mutation	UNP P42212
g	100	SER	PHE	engineered mutation	UNP P42212
g	103	LYS	ASP	engineered mutation	UNP P42212
g	106	THR	ASN	engineered mutation	UNP P42212
g	118	ARG	ASP	engineered mutation	UNP P42212
g	125	LYS	GLU	engineered mutation	UNP P42212
g	129	ARG	ILE	engineered mutation	UNP P42212
g	134	LYS	ASP	engineered mutation	UNP P42212
g	143	ARG	GLU	engineered mutation	UNP P42212
g	146	GLY	TYR	engineered mutation	UNP P42212
g	147	ILE	ASN	engineered mutation	UNP P42212
g	149	ASP	HIS	engineered mutation	UNP P42212
g	150	LYS	ASN	engineered mutation	UNP P42212
g	154	THR	MET	engineered mutation	UNP P42212
g	158	ARG	GLN	engineered mutation	UNP P42212
g	164	ALA	VAL	engineered mutation	UNP P42212
g	165	LYS	ASN	engineered mutation	UNP P42212
g	172	VAL	ILE	engineered mutation	UNP P42212
g	173	LYS	GLU	engineered mutation	UNP P42212
g	191	ARG	ASP	engineered mutation	UNP P42212
g	198	ARG	ASP	engineered mutation	UNP P42212
g	205	ARG	GLN	engineered mutation	UNP P42212
g	207	VAL	ALA	engineered mutation	UNP P42212
g	213	LYS	ASN	engineered mutation	UNP P42212
g	231	LYS	THR	engineered mutation	UNP P42212
g	234	ARG	-	expression tag	UNP P42212
g	235	ASP	-	expression tag	UNP P42212
g	236	GLU	-	expression tag	UNP P42212
g	237	ARG	-	expression tag	UNP P42212
g	238	TYR	-	expression tag	UNP P42212
g	239	LYS	-	expression tag	UNP P42212
g	240	LEU	-	expression tag	UNP P42212
g	241	GLU	-	expression tag	UNP P42212
g	242	HIS	-	expression tag	UNP P42212
g	243	HIS	-	expression tag	UNP P42212
g	244	HIS	-	expression tag	UNP P42212
g	245	HIS	-	expression tag	UNP P42212
g	246	HIS	-	expression tag	UNP P42212
g	247	HIS	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
i	1	MET	-	expression tag	UNP P42212
i	2	ALA	-	expression tag	UNP P42212
i	3	SER	-	expression tag	UNP P42212
i	7	ARG	GLU	engineered mutation	UNP P42212
i	10	ARG	THR	engineered mutation	UNP P42212
i	12	LYS	VAL	engineered mutation	UNP P42212
i	20	LYS	ASP	engineered mutation	UNP P42212
i	31	ARG	SER	engineered mutation	UNP P42212
i	33	LYS	GLU	engineered mutation	UNP P42212
i	35	LYS	GLU	engineered mutation	UNP P42212
i	40	ASN	TYR	engineered mutation	UNP P42212
i	65	LEU	PHE	engineered mutation	UNP P42212
i	66	THR	SER	engineered mutation	UNP P42212
i	67	TRP	TYR	engineered mutation	UNP P42212
i	73	ALA	SER	engineered mutation	UNP P42212
i	77	LYS	ASP	engineered mutation	UNP P42212
i	81	ARG	GLN	engineered mutation	UNP P42212
i	91	LYS	GLU	engineered mutation	UNP P42212
i	100	SER	PHE	engineered mutation	UNP P42212
i	103	LYS	ASP	engineered mutation	UNP P42212
i	106	THR	ASN	engineered mutation	UNP P42212
i	118	ARG	ASP	engineered mutation	UNP P42212
i	125	LYS	GLU	engineered mutation	UNP P42212
i	129	ARG	ILE	engineered mutation	UNP P42212
i	134	LYS	ASP	engineered mutation	UNP P42212
i	143	ARG	GLU	engineered mutation	UNP P42212
i	146	GLY	TYR	engineered mutation	UNP P42212
i	147	ILE	ASN	engineered mutation	UNP P42212
i	149	ASP	HIS	engineered mutation	UNP P42212
i	150	LYS	ASN	engineered mutation	UNP P42212
i	154	THR	MET	engineered mutation	UNP P42212
i	158	ARG	GLN	engineered mutation	UNP P42212
i	164	ALA	VAL	engineered mutation	UNP P42212
i	165	LYS	ASN	engineered mutation	UNP P42212
i	172	VAL	ILE	engineered mutation	UNP P42212
i	173	LYS	GLU	engineered mutation	UNP P42212
i	191	ARG	ASP	engineered mutation	UNP P42212
i	198	ARG	ASP	engineered mutation	UNP P42212
i	205	ARG	GLN	engineered mutation	UNP P42212
i	207	VAL	ALA	engineered mutation	UNP P42212
i	213	LYS	ASN	engineered mutation	UNP P42212
i	231	LYS	THR	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
i	234	ARG	-	expression tag	UNP P42212
i	235	ASP	-	expression tag	UNP P42212
i	236	GLU	-	expression tag	UNP P42212
i	237	ARG	-	expression tag	UNP P42212
i	238	TYR	-	expression tag	UNP P42212
i	239	LYS	-	expression tag	UNP P42212
i	240	LEU	-	expression tag	UNP P42212
i	241	GLU	-	expression tag	UNP P42212
i	242	HIS	-	expression tag	UNP P42212
i	243	HIS	-	expression tag	UNP P42212
i	244	HIS	-	expression tag	UNP P42212
i	245	HIS	-	expression tag	UNP P42212
i	246	HIS	-	expression tag	UNP P42212
i	247	HIS	-	expression tag	UNP P42212
k	1	MET	-	expression tag	UNP P42212
k	2	ALA	-	expression tag	UNP P42212
k	3	SER	-	expression tag	UNP P42212
k	7	ARG	GLU	engineered mutation	UNP P42212
k	10	ARG	THR	engineered mutation	UNP P42212
k	12	LYS	VAL	engineered mutation	UNP P42212
k	20	LYS	ASP	engineered mutation	UNP P42212
k	31	ARG	SER	engineered mutation	UNP P42212
k	33	LYS	GLU	engineered mutation	UNP P42212
k	35	LYS	GLU	engineered mutation	UNP P42212
k	40	ASN	TYR	engineered mutation	UNP P42212
k	65	LEU	PHE	engineered mutation	UNP P42212
k	66	THR	SER	engineered mutation	UNP P42212
k	67	TRP	TYR	engineered mutation	UNP P42212
k	73	ALA	SER	engineered mutation	UNP P42212
k	77	LYS	ASP	engineered mutation	UNP P42212
k	81	ARG	GLN	engineered mutation	UNP P42212
k	91	LYS	GLU	engineered mutation	UNP P42212
k	100	SER	PHE	engineered mutation	UNP P42212
k	103	LYS	ASP	engineered mutation	UNP P42212
k	106	THR	ASN	engineered mutation	UNP P42212
k	118	ARG	ASP	engineered mutation	UNP P42212
k	125	LYS	GLU	engineered mutation	UNP P42212
k	129	ARG	ILE	engineered mutation	UNP P42212
k	134	LYS	ASP	engineered mutation	UNP P42212
k	143	ARG	GLU	engineered mutation	UNP P42212
k	146	GLY	TYR	engineered mutation	UNP P42212
k	147	ILE	ASN	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
k	149	ASP	HIS	engineered mutation	UNP P42212
k	150	LYS	ASN	engineered mutation	UNP P42212
k	154	THR	MET	engineered mutation	UNP P42212
k	158	ARG	GLN	engineered mutation	UNP P42212
k	164	ALA	VAL	engineered mutation	UNP P42212
k	165	LYS	ASN	engineered mutation	UNP P42212
k	172	VAL	ILE	engineered mutation	UNP P42212
k	173	LYS	GLU	engineered mutation	UNP P42212
k	191	ARG	ASP	engineered mutation	UNP P42212
k	198	ARG	ASP	engineered mutation	UNP P42212
k	205	ARG	GLN	engineered mutation	UNP P42212
k	207	VAL	ALA	engineered mutation	UNP P42212
k	213	LYS	ASN	engineered mutation	UNP P42212
k	231	LYS	THR	engineered mutation	UNP P42212
k	234	ARG	-	expression tag	UNP P42212
k	235	ASP	-	expression tag	UNP P42212
k	236	GLU	-	expression tag	UNP P42212
k	237	ARG	-	expression tag	UNP P42212
k	238	TYR	-	expression tag	UNP P42212
k	239	LYS	-	expression tag	UNP P42212
k	240	LEU	-	expression tag	UNP P42212
k	241	GLU	-	expression tag	UNP P42212
k	242	HIS	-	expression tag	UNP P42212
k	243	HIS	-	expression tag	UNP P42212
k	244	HIS	-	expression tag	UNP P42212
k	245	HIS	-	expression tag	UNP P42212
k	246	HIS	-	expression tag	UNP P42212
k	247	HIS	-	expression tag	UNP P42212
m	1	MET	-	expression tag	UNP P42212
m	2	ALA	-	expression tag	UNP P42212
m	3	SER	-	expression tag	UNP P42212
m	7	ARG	GLU	engineered mutation	UNP P42212
m	10	ARG	THR	engineered mutation	UNP P42212
m	12	LYS	VAL	engineered mutation	UNP P42212
m	20	LYS	ASP	engineered mutation	UNP P42212
m	31	ARG	SER	engineered mutation	UNP P42212
m	33	LYS	GLU	engineered mutation	UNP P42212
m	35	LYS	GLU	engineered mutation	UNP P42212
m	40	ASN	TYR	engineered mutation	UNP P42212
m	65	LEU	PHE	engineered mutation	UNP P42212
m	66	THR	SER	engineered mutation	UNP P42212
m	67	TRP	TYR	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
m	73	ALA	SER	engineered mutation	UNP P42212
m	77	LYS	ASP	engineered mutation	UNP P42212
m	81	ARG	GLN	engineered mutation	UNP P42212
m	91	LYS	GLU	engineered mutation	UNP P42212
m	100	SER	PHE	engineered mutation	UNP P42212
m	103	LYS	ASP	engineered mutation	UNP P42212
m	106	THR	ASN	engineered mutation	UNP P42212
m	118	ARG	ASP	engineered mutation	UNP P42212
m	125	LYS	GLU	engineered mutation	UNP P42212
m	129	ARG	ILE	engineered mutation	UNP P42212
m	134	LYS	ASP	engineered mutation	UNP P42212
m	143	ARG	GLU	engineered mutation	UNP P42212
m	146	GLY	TYR	engineered mutation	UNP P42212
m	147	ILE	ASN	engineered mutation	UNP P42212
m	149	ASP	HIS	engineered mutation	UNP P42212
m	150	LYS	ASN	engineered mutation	UNP P42212
m	154	THR	MET	engineered mutation	UNP P42212
m	158	ARG	GLN	engineered mutation	UNP P42212
m	164	ALA	VAL	engineered mutation	UNP P42212
m	165	LYS	ASN	engineered mutation	UNP P42212
m	172	VAL	ILE	engineered mutation	UNP P42212
m	173	LYS	GLU	engineered mutation	UNP P42212
m	191	ARG	ASP	engineered mutation	UNP P42212
m	198	ARG	ASP	engineered mutation	UNP P42212
m	205	ARG	GLN	engineered mutation	UNP P42212
m	207	VAL	ALA	engineered mutation	UNP P42212
m	213	LYS	ASN	engineered mutation	UNP P42212
m	231	LYS	THR	engineered mutation	UNP P42212
m	234	ARG	-	expression tag	UNP P42212
m	235	ASP	-	expression tag	UNP P42212
m	236	GLU	-	expression tag	UNP P42212
m	237	ARG	-	expression tag	UNP P42212
m	238	TYR	-	expression tag	UNP P42212
m	239	LYS	-	expression tag	UNP P42212
m	240	LEU	-	expression tag	UNP P42212
m	241	GLU	-	expression tag	UNP P42212
m	242	HIS	-	expression tag	UNP P42212
m	243	HIS	-	expression tag	UNP P42212
m	244	HIS	-	expression tag	UNP P42212
m	245	HIS	-	expression tag	UNP P42212
m	246	HIS	-	expression tag	UNP P42212
m	247	HIS	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
o	1	MET	-	expression tag	UNP P42212
o	2	ALA	-	expression tag	UNP P42212
o	3	SER	-	expression tag	UNP P42212
o	7	ARG	GLU	engineered mutation	UNP P42212
o	10	ARG	THR	engineered mutation	UNP P42212
o	12	LYS	VAL	engineered mutation	UNP P42212
o	20	LYS	ASP	engineered mutation	UNP P42212
o	31	ARG	SER	engineered mutation	UNP P42212
o	33	LYS	GLU	engineered mutation	UNP P42212
o	35	LYS	GLU	engineered mutation	UNP P42212
o	40	ASN	TYR	engineered mutation	UNP P42212
o	65	LEU	PHE	engineered mutation	UNP P42212
o	66	THR	SER	engineered mutation	UNP P42212
o	67	TRP	TYR	engineered mutation	UNP P42212
o	73	ALA	SER	engineered mutation	UNP P42212
o	77	LYS	ASP	engineered mutation	UNP P42212
o	81	ARG	GLN	engineered mutation	UNP P42212
o	91	LYS	GLU	engineered mutation	UNP P42212
o	100	SER	PHE	engineered mutation	UNP P42212
o	103	LYS	ASP	engineered mutation	UNP P42212
o	106	THR	ASN	engineered mutation	UNP P42212
o	118	ARG	ASP	engineered mutation	UNP P42212
o	125	LYS	GLU	engineered mutation	UNP P42212
o	129	ARG	ILE	engineered mutation	UNP P42212
o	134	LYS	ASP	engineered mutation	UNP P42212
o	143	ARG	GLU	engineered mutation	UNP P42212
o	146	GLY	TYR	engineered mutation	UNP P42212
o	147	ILE	ASN	engineered mutation	UNP P42212
o	149	ASP	HIS	engineered mutation	UNP P42212
o	150	LYS	ASN	engineered mutation	UNP P42212
o	154	THR	MET	engineered mutation	UNP P42212
o	158	ARG	GLN	engineered mutation	UNP P42212
o	164	ALA	VAL	engineered mutation	UNP P42212
o	165	LYS	ASN	engineered mutation	UNP P42212
o	172	VAL	ILE	engineered mutation	UNP P42212
o	173	LYS	GLU	engineered mutation	UNP P42212
o	191	ARG	ASP	engineered mutation	UNP P42212
o	198	ARG	ASP	engineered mutation	UNP P42212
o	205	ARG	GLN	engineered mutation	UNP P42212
o	207	VAL	ALA	engineered mutation	UNP P42212
o	213	LYS	ASN	engineered mutation	UNP P42212
o	231	LYS	THR	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
o	234	ARG	-	expression tag	UNP P42212
o	235	ASP	-	expression tag	UNP P42212
o	236	GLU	-	expression tag	UNP P42212
o	237	ARG	-	expression tag	UNP P42212
o	238	TYR	-	expression tag	UNP P42212
o	239	LYS	-	expression tag	UNP P42212
o	240	LEU	-	expression tag	UNP P42212
o	241	GLU	-	expression tag	UNP P42212
o	242	HIS	-	expression tag	UNP P42212
o	243	HIS	-	expression tag	UNP P42212
o	244	HIS	-	expression tag	UNP P42212
o	245	HIS	-	expression tag	UNP P42212
o	246	HIS	-	expression tag	UNP P42212
o	247	HIS	-	expression tag	UNP P42212

- Molecule 2 is a protein called GFP-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	231	Total	C	N	O	S	0	0
			1830	1153	305	367	5		
2	d	231	Total	C	N	O	S	0	0
			1830	1153	305	367	5		
2	f	231	Total	C	N	O	S	0	0
			1830	1153	305	367	5		
2	h	231	Total	C	N	O	S	0	0
			1830	1153	305	367	5		
2	j	231	Total	C	N	O	S	0	0
			1830	1153	305	367	5		
2	l	231	Total	C	N	O	S	0	0
			1830	1153	305	367	5		
2	n	231	Total	C	N	O	S	0	0
			1830	1153	305	367	5		
2	p	231	Total	C	N	O	S	0	0
			1830	1153	305	367	5		

There are 248 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	3	MET	-	initiating methionine	UNP P42212
b	32	ARG	SER	engineered mutation	UNP P42212
b	40	ASP	THR	engineered mutation	UNP P42212
b	41	ASN	TYR	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
b	45	ASP	THR	engineered mutation	UNP P42212
b	66	LEU	PHE	engineered mutation	UNP P42212
b	67	THR	SER	engineered mutation	UNP P42212
b	82	GLU	GLN	engineered mutation	UNP P42212
b	101	SER	PHE	engineered mutation	UNP P42212
b	107	THR	ASN	engineered mutation	UNP P42212
b	147	PHE	TYR	engineered mutation	UNP P42212
b	151	GLU	ASN	engineered mutation	UNP P42212
b	155	THR	MET	engineered mutation	UNP P42212
b	158	ASP	LYS	engineered mutation	UNP P42212
b	159	GLU	GLN	engineered mutation	UNP P42212
b	165	ALA	VAL	engineered mutation	UNP P42212
b	166	GLU	ASN	engineered mutation	UNP P42212
b	173	VAL	ILE	engineered mutation	UNP P42212
b	195	ASP	VAL	engineered mutation	UNP P42212
b	200	GLU	ASN	engineered mutation	UNP P42212
b	208	VAL	ALA	engineered mutation	UNP P42212
b	229	ASP	ALA	engineered mutation	UNP P42212
b	233	GLU	HIS	engineered mutation	UNP P42212
b	235	HIS	-	expression tag	UNP P42212
b	236	HIS	-	expression tag	UNP P42212
b	237	HIS	-	expression tag	UNP P42212
b	238	HIS	-	expression tag	UNP P42212
b	239	HIS	-	expression tag	UNP P42212
b	240	HIS	-	expression tag	UNP P42212
b	241	HIS	-	expression tag	UNP P42212
b	242	HIS	-	expression tag	UNP P42212
d	3	MET	-	initiating methionine	UNP P42212
d	32	ARG	SER	engineered mutation	UNP P42212
d	40	ASP	THR	engineered mutation	UNP P42212
d	41	ASN	TYR	engineered mutation	UNP P42212
d	45	ASP	THR	engineered mutation	UNP P42212
d	66	LEU	PHE	engineered mutation	UNP P42212
d	67	THR	SER	engineered mutation	UNP P42212
d	82	GLU	GLN	engineered mutation	UNP P42212
d	101	SER	PHE	engineered mutation	UNP P42212
d	107	THR	ASN	engineered mutation	UNP P42212
d	147	PHE	TYR	engineered mutation	UNP P42212
d	151	GLU	ASN	engineered mutation	UNP P42212
d	155	THR	MET	engineered mutation	UNP P42212
d	158	ASP	LYS	engineered mutation	UNP P42212
d	159	GLU	GLN	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
d	165	ALA	VAL	engineered mutation	UNP P42212
d	166	GLU	ASN	engineered mutation	UNP P42212
d	173	VAL	ILE	engineered mutation	UNP P42212
d	195	ASP	VAL	engineered mutation	UNP P42212
d	200	GLU	ASN	engineered mutation	UNP P42212
d	208	VAL	ALA	engineered mutation	UNP P42212
d	229	ASP	ALA	engineered mutation	UNP P42212
d	233	GLU	HIS	engineered mutation	UNP P42212
d	235	HIS	-	expression tag	UNP P42212
d	236	HIS	-	expression tag	UNP P42212
d	237	HIS	-	expression tag	UNP P42212
d	238	HIS	-	expression tag	UNP P42212
d	239	HIS	-	expression tag	UNP P42212
d	240	HIS	-	expression tag	UNP P42212
d	241	HIS	-	expression tag	UNP P42212
d	242	HIS	-	expression tag	UNP P42212
f	3	MET	-	initiating methionine	UNP P42212
f	32	ARG	SER	engineered mutation	UNP P42212
f	40	ASP	THR	engineered mutation	UNP P42212
f	41	ASN	TYR	engineered mutation	UNP P42212
f	45	ASP	THR	engineered mutation	UNP P42212
f	66	LEU	PHE	engineered mutation	UNP P42212
f	67	THR	SER	engineered mutation	UNP P42212
f	82	GLU	GLN	engineered mutation	UNP P42212
f	101	SER	PHE	engineered mutation	UNP P42212
f	107	THR	ASN	engineered mutation	UNP P42212
f	147	PHE	TYR	engineered mutation	UNP P42212
f	151	GLU	ASN	engineered mutation	UNP P42212
f	155	THR	MET	engineered mutation	UNP P42212
f	158	ASP	LYS	engineered mutation	UNP P42212
f	159	GLU	GLN	engineered mutation	UNP P42212
f	165	ALA	VAL	engineered mutation	UNP P42212
f	166	GLU	ASN	engineered mutation	UNP P42212
f	173	VAL	ILE	engineered mutation	UNP P42212
f	195	ASP	VAL	engineered mutation	UNP P42212
f	200	GLU	ASN	engineered mutation	UNP P42212
f	208	VAL	ALA	engineered mutation	UNP P42212
f	229	ASP	ALA	engineered mutation	UNP P42212
f	233	GLU	HIS	engineered mutation	UNP P42212
f	235	HIS	-	expression tag	UNP P42212
f	236	HIS	-	expression tag	UNP P42212
f	237	HIS	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
f	238	HIS	-	expression tag	UNP P42212
f	239	HIS	-	expression tag	UNP P42212
f	240	HIS	-	expression tag	UNP P42212
f	241	HIS	-	expression tag	UNP P42212
f	242	HIS	-	expression tag	UNP P42212
h	3	MET	-	initiating methionine	UNP P42212
h	32	ARG	SER	engineered mutation	UNP P42212
h	40	ASP	THR	engineered mutation	UNP P42212
h	41	ASN	TYR	engineered mutation	UNP P42212
h	45	ASP	THR	engineered mutation	UNP P42212
h	66	LEU	PHE	engineered mutation	UNP P42212
h	67	THR	SER	engineered mutation	UNP P42212
h	82	GLU	GLN	engineered mutation	UNP P42212
h	101	SER	PHE	engineered mutation	UNP P42212
h	107	THR	ASN	engineered mutation	UNP P42212
h	147	PHE	TYR	engineered mutation	UNP P42212
h	151	GLU	ASN	engineered mutation	UNP P42212
h	155	THR	MET	engineered mutation	UNP P42212
h	158	ASP	LYS	engineered mutation	UNP P42212
h	159	GLU	GLN	engineered mutation	UNP P42212
h	165	ALA	VAL	engineered mutation	UNP P42212
h	166	GLU	ASN	engineered mutation	UNP P42212
h	173	VAL	ILE	engineered mutation	UNP P42212
h	195	ASP	VAL	engineered mutation	UNP P42212
h	200	GLU	ASN	engineered mutation	UNP P42212
h	208	VAL	ALA	engineered mutation	UNP P42212
h	229	ASP	ALA	engineered mutation	UNP P42212
h	233	GLU	HIS	engineered mutation	UNP P42212
h	235	HIS	-	expression tag	UNP P42212
h	236	HIS	-	expression tag	UNP P42212
h	237	HIS	-	expression tag	UNP P42212
h	238	HIS	-	expression tag	UNP P42212
h	239	HIS	-	expression tag	UNP P42212
h	240	HIS	-	expression tag	UNP P42212
h	241	HIS	-	expression tag	UNP P42212
h	242	HIS	-	expression tag	UNP P42212
j	3	MET	-	initiating methionine	UNP P42212
j	32	ARG	SER	engineered mutation	UNP P42212
j	40	ASP	THR	engineered mutation	UNP P42212
j	41	ASN	TYR	engineered mutation	UNP P42212
j	45	ASP	THR	engineered mutation	UNP P42212
j	66	LEU	PHE	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
j	67	THR	SER	engineered mutation	UNP P42212
j	82	GLU	GLN	engineered mutation	UNP P42212
j	101	SER	PHE	engineered mutation	UNP P42212
j	107	THR	ASN	engineered mutation	UNP P42212
j	147	PHE	TYR	engineered mutation	UNP P42212
j	151	GLU	ASN	engineered mutation	UNP P42212
j	155	THR	MET	engineered mutation	UNP P42212
j	158	ASP	LYS	engineered mutation	UNP P42212
j	159	GLU	GLN	engineered mutation	UNP P42212
j	165	ALA	VAL	engineered mutation	UNP P42212
j	166	GLU	ASN	engineered mutation	UNP P42212
j	173	VAL	ILE	engineered mutation	UNP P42212
j	195	ASP	VAL	engineered mutation	UNP P42212
j	200	GLU	ASN	engineered mutation	UNP P42212
j	208	VAL	ALA	engineered mutation	UNP P42212
j	229	ASP	ALA	engineered mutation	UNP P42212
j	233	GLU	HIS	engineered mutation	UNP P42212
j	235	HIS	-	expression tag	UNP P42212
j	236	HIS	-	expression tag	UNP P42212
j	237	HIS	-	expression tag	UNP P42212
j	238	HIS	-	expression tag	UNP P42212
j	239	HIS	-	expression tag	UNP P42212
j	240	HIS	-	expression tag	UNP P42212
j	241	HIS	-	expression tag	UNP P42212
j	242	HIS	-	expression tag	UNP P42212
l	3	MET	-	initiating methionine	UNP P42212
l	32	ARG	SER	engineered mutation	UNP P42212
l	40	ASP	THR	engineered mutation	UNP P42212
l	41	ASN	TYR	engineered mutation	UNP P42212
l	45	ASP	THR	engineered mutation	UNP P42212
l	66	LEU	PHE	engineered mutation	UNP P42212
l	67	THR	SER	engineered mutation	UNP P42212
l	82	GLU	GLN	engineered mutation	UNP P42212
l	101	SER	PHE	engineered mutation	UNP P42212
l	107	THR	ASN	engineered mutation	UNP P42212
l	147	PHE	TYR	engineered mutation	UNP P42212
l	151	GLU	ASN	engineered mutation	UNP P42212
l	155	THR	MET	engineered mutation	UNP P42212
l	158	ASP	LYS	engineered mutation	UNP P42212
l	159	GLU	GLN	engineered mutation	UNP P42212
l	165	ALA	VAL	engineered mutation	UNP P42212
l	166	GLU	ASN	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
l	173	VAL	ILE	engineered mutation	UNP P42212
l	195	ASP	VAL	engineered mutation	UNP P42212
l	200	GLU	ASN	engineered mutation	UNP P42212
l	208	VAL	ALA	engineered mutation	UNP P42212
l	229	ASP	ALA	engineered mutation	UNP P42212
l	233	GLU	HIS	engineered mutation	UNP P42212
l	235	HIS	-	expression tag	UNP P42212
l	236	HIS	-	expression tag	UNP P42212
l	237	HIS	-	expression tag	UNP P42212
l	238	HIS	-	expression tag	UNP P42212
l	239	HIS	-	expression tag	UNP P42212
l	240	HIS	-	expression tag	UNP P42212
l	241	HIS	-	expression tag	UNP P42212
l	242	HIS	-	expression tag	UNP P42212
n	3	MET	-	initiating methionine	UNP P42212
n	32	ARG	SER	engineered mutation	UNP P42212
n	40	ASP	THR	engineered mutation	UNP P42212
n	41	ASN	TYR	engineered mutation	UNP P42212
n	45	ASP	THR	engineered mutation	UNP P42212
n	66	LEU	PHE	engineered mutation	UNP P42212
n	67	THR	SER	engineered mutation	UNP P42212
n	82	GLU	GLN	engineered mutation	UNP P42212
n	101	SER	PHE	engineered mutation	UNP P42212
n	107	THR	ASN	engineered mutation	UNP P42212
n	147	PHE	TYR	engineered mutation	UNP P42212
n	151	GLU	ASN	engineered mutation	UNP P42212
n	155	THR	MET	engineered mutation	UNP P42212
n	158	ASP	LYS	engineered mutation	UNP P42212
n	159	GLU	GLN	engineered mutation	UNP P42212
n	165	ALA	VAL	engineered mutation	UNP P42212
n	166	GLU	ASN	engineered mutation	UNP P42212
n	173	VAL	ILE	engineered mutation	UNP P42212
n	195	ASP	VAL	engineered mutation	UNP P42212
n	200	GLU	ASN	engineered mutation	UNP P42212
n	208	VAL	ALA	engineered mutation	UNP P42212
n	229	ASP	ALA	engineered mutation	UNP P42212
n	233	GLU	HIS	engineered mutation	UNP P42212
n	235	HIS	-	expression tag	UNP P42212
n	236	HIS	-	expression tag	UNP P42212
n	237	HIS	-	expression tag	UNP P42212
n	238	HIS	-	expression tag	UNP P42212
n	239	HIS	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

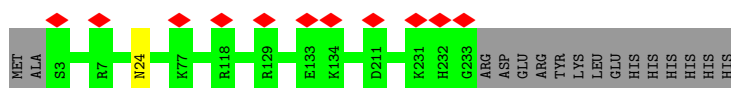
Chain	Residue	Modelled	Actual	Comment	Reference
n	240	HIS	-	expression tag	UNP P42212
n	241	HIS	-	expression tag	UNP P42212
n	242	HIS	-	expression tag	UNP P42212
p	3	MET	-	initiating methionine	UNP P42212
p	32	ARG	SER	engineered mutation	UNP P42212
p	40	ASP	THR	engineered mutation	UNP P42212
p	41	ASN	TYR	engineered mutation	UNP P42212
p	45	ASP	THR	engineered mutation	UNP P42212
p	66	LEU	PHE	engineered mutation	UNP P42212
p	67	THR	SER	engineered mutation	UNP P42212
p	82	GLU	GLN	engineered mutation	UNP P42212
p	101	SER	PHE	engineered mutation	UNP P42212
p	107	THR	ASN	engineered mutation	UNP P42212
p	147	PHE	TYR	engineered mutation	UNP P42212
p	151	GLU	ASN	engineered mutation	UNP P42212
p	155	THR	MET	engineered mutation	UNP P42212
p	158	ASP	LYS	engineered mutation	UNP P42212
p	159	GLU	GLN	engineered mutation	UNP P42212
p	165	ALA	VAL	engineered mutation	UNP P42212
p	166	GLU	ASN	engineered mutation	UNP P42212
p	173	VAL	ILE	engineered mutation	UNP P42212
p	195	ASP	VAL	engineered mutation	UNP P42212
p	200	GLU	ASN	engineered mutation	UNP P42212
p	208	VAL	ALA	engineered mutation	UNP P42212
p	229	ASP	ALA	engineered mutation	UNP P42212
p	233	GLU	HIS	engineered mutation	UNP P42212
p	235	HIS	-	expression tag	UNP P42212
p	236	HIS	-	expression tag	UNP P42212
p	237	HIS	-	expression tag	UNP P42212
p	238	HIS	-	expression tag	UNP P42212
p	239	HIS	-	expression tag	UNP P42212
p	240	HIS	-	expression tag	UNP P42212
p	241	HIS	-	expression tag	UNP P42212
p	242	HIS	-	expression tag	UNP P42212

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ceru+32

Chain a: 



- Molecule 1: Ceru+32

Chain c: 



- Molecule 1: Ceru+32

Chain e: 

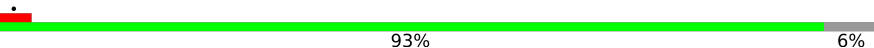


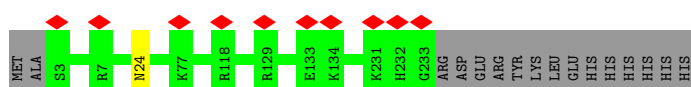
- Molecule 1: Ceru+32

Chain g: 



- Molecule 1: Ceru+32

Chain i: 



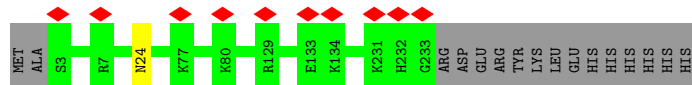
- Molecule 1: Ceru+32

Chain k:  93% 6%



- Molecule 1: Ceru+32

Chain m:  93% 6%



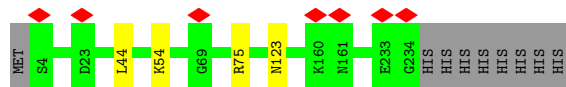
- Molecule 1: Ceru+32

Chain o:  93% 6%



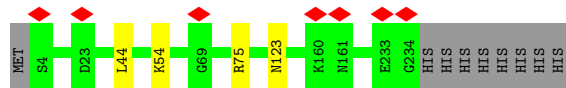
- Molecule 2: GFP-17

Chain b:  95% ..



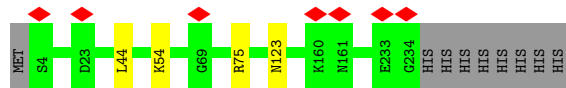
- Molecule 2: GFP-17

Chain d:  95% ..



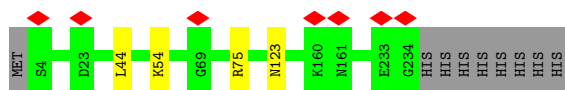
- Molecule 2: GFP-17

Chain f:  95% ..

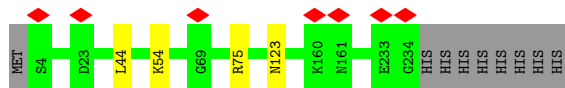


- Molecule 2: GFP-17

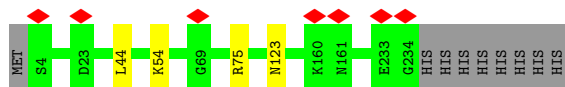
Chain h:  95% ..



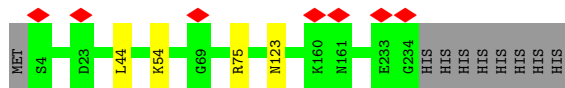
- Molecule 2: GFP-17



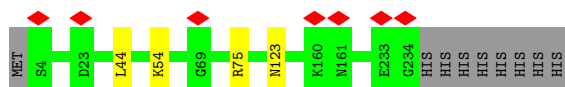
- Molecule 2: GFP-17



- Molecule 2: GFP-17



- Molecule 2: GFP-17



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126822	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.330	Depositor
Minimum map value	-0.250	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	246.40001, 246.40001, 246.40001	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.36	0/1892	0.57	0/2533
1	c	0.36	0/1892	0.57	0/2533
1	e	0.36	0/1892	0.57	0/2533
1	g	0.36	0/1892	0.57	0/2533
1	i	0.36	0/1892	0.57	0/2533
1	k	0.36	0/1892	0.57	0/2533
1	m	0.36	0/1892	0.57	0/2533
1	o	0.36	0/1892	0.57	0/2533
2	b	0.37	0/1870	0.60	1/2528 (0.0%)
2	d	0.37	0/1870	0.60	1/2528 (0.0%)
2	f	0.37	0/1870	0.60	1/2528 (0.0%)
2	h	0.37	0/1870	0.60	1/2528 (0.0%)
2	j	0.37	0/1870	0.60	1/2528 (0.0%)
2	l	0.37	0/1870	0.60	1/2528 (0.0%)
2	n	0.37	0/1870	0.60	1/2528 (0.0%)
2	p	0.37	0/1870	0.60	1/2528 (0.0%)
All	All	0.37	0/30096	0.58	8/40488 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	44	LEU	CA-CB-CG	5.77	128.56	115.30
2	d	44	LEU	CA-CB-CG	5.76	128.54	115.30
2	f	44	LEU	CA-CB-CG	5.76	128.55	115.30
2	j	44	LEU	CA-CB-CG	5.75	128.53	115.30
2	b	44	LEU	CA-CB-CG	5.75	128.52	115.30
2	p	44	LEU	CA-CB-CG	5.75	128.51	115.30
2	n	44	LEU	CA-CB-CG	5.75	128.51	115.30
2	h	44	LEU	CA-CB-CG	5.73	128.49	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	1852	0	1941	0	0
1	c	1852	0	1941	0	0
1	e	1852	0	1941	0	0
1	g	1852	0	1941	0	0
1	i	1852	0	1941	0	0
1	k	1852	0	1941	0	0
1	m	1852	0	1941	0	0
1	o	1852	0	1941	0	0
2	b	1830	0	1752	0	0
2	d	1830	0	1752	0	0
2	f	1830	0	1752	0	0
2	h	1830	0	1752	0	0
2	j	1830	0	1752	0	0
2	l	1830	0	1752	0	0
2	n	1830	0	1752	0	0
2	p	1830	0	1752	0	0
All	All	29456	0	29544	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	229/247 (93%)	214 (93%)	15 (7%)	0	100	100
1	c	229/247 (93%)	214 (93%)	15 (7%)	0	100	100
1	e	229/247 (93%)	214 (93%)	15 (7%)	0	100	100
1	g	229/247 (93%)	214 (93%)	15 (7%)	0	100	100
1	i	229/247 (93%)	214 (93%)	15 (7%)	0	100	100
1	k	229/247 (93%)	214 (93%)	15 (7%)	0	100	100
1	m	229/247 (93%)	214 (93%)	15 (7%)	0	100	100
1	o	229/247 (93%)	214 (93%)	15 (7%)	0	100	100
2	b	229/240 (95%)	214 (93%)	15 (7%)	0	100	100
2	d	229/240 (95%)	214 (93%)	15 (7%)	0	100	100
2	f	229/240 (95%)	214 (93%)	15 (7%)	0	100	100
2	h	229/240 (95%)	214 (93%)	15 (7%)	0	100	100
2	j	229/240 (95%)	214 (93%)	15 (7%)	0	100	100
2	l	229/240 (95%)	214 (93%)	15 (7%)	0	100	100
2	n	229/240 (95%)	214 (93%)	15 (7%)	0	100	100
2	p	229/240 (95%)	214 (93%)	15 (7%)	0	100	100
All	All	3664/3896 (94%)	3424 (93%)	240 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	199/214 (93%)	198 (100%)	1 (0%)	88	95
1	c	199/214 (93%)	198 (100%)	1 (0%)	88	95
1	e	199/214 (93%)	198 (100%)	1 (0%)	88	95
1	g	199/214 (93%)	198 (100%)	1 (0%)	88	95
1	i	199/214 (93%)	198 (100%)	1 (0%)	88	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	k	199/214 (93%)	198 (100%)	1 (0%)	88	95
1	m	199/214 (93%)	198 (100%)	1 (0%)	88	95
1	o	199/214 (93%)	198 (100%)	1 (0%)	88	95
2	b	202/211 (96%)	199 (98%)	3 (2%)	65	84
2	d	202/211 (96%)	199 (98%)	3 (2%)	65	84
2	f	202/211 (96%)	199 (98%)	3 (2%)	65	84
2	h	202/211 (96%)	199 (98%)	3 (2%)	65	84
2	j	202/211 (96%)	199 (98%)	3 (2%)	65	84
2	l	202/211 (96%)	199 (98%)	3 (2%)	65	84
2	n	202/211 (96%)	199 (98%)	3 (2%)	65	84
2	p	202/211 (96%)	199 (98%)	3 (2%)	65	84
All	All	3208/3400 (94%)	3176 (99%)	32 (1%)	77	89

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	24	ASN
2	b	54	LYS
2	b	75	ARG
2	b	123	ASN
1	c	24	ASN
2	d	54	LYS
2	d	75	ARG
2	d	123	ASN
1	e	24	ASN
2	f	54	LYS
2	f	75	ARG
2	f	123	ASN
1	g	24	ASN
2	h	54	LYS
2	h	75	ARG
2	h	123	ASN
1	i	24	ASN
2	j	54	LYS
2	j	75	ARG
2	j	123	ASN
1	k	24	ASN
2	l	54	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	l	75	ARG
2	l	123	ASN
1	m	24	ASN
2	n	54	LYS
2	n	75	ARG
2	n	123	ASN
1	o	24	ASN
2	p	54	LYS
2	p	75	ARG
2	p	123	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	24	ASN
2	b	123	ASN
2	b	137	ASN
2	b	179	GLN
1	c	24	ASN
2	d	123	ASN
2	d	137	ASN
2	d	179	GLN
1	e	24	ASN
2	f	123	ASN
2	f	137	ASN
2	f	179	GLN
1	g	24	ASN
2	h	123	ASN
2	h	137	ASN
2	h	179	GLN
1	i	24	ASN
2	j	123	ASN
2	j	137	ASN
2	j	179	GLN
1	k	24	ASN
2	l	123	ASN
2	l	137	ASN
2	l	179	GLN
1	m	24	ASN
2	n	123	ASN
2	n	137	ASN
2	n	179	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	o	24	ASN
2	p	123	ASN
2	p	137	ASN
2	p	179	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

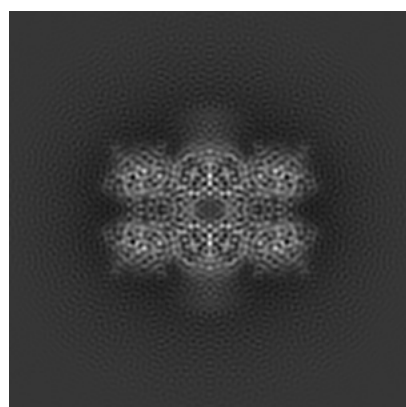
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9104. These allow visual inspection of the internal detail of the map and identification of artifacts.

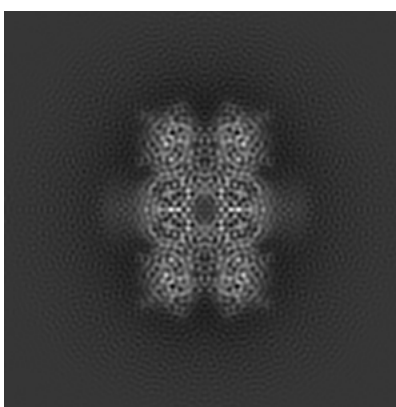
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

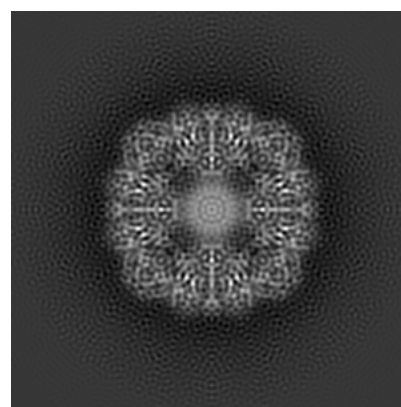
6.1.1 Primary map



X



Y

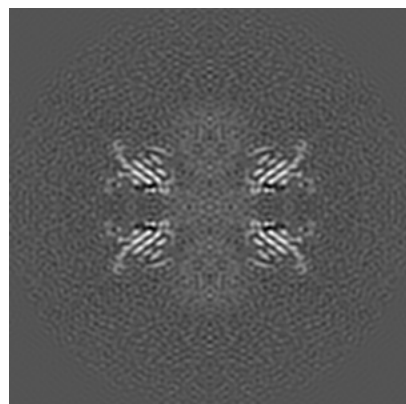


Z

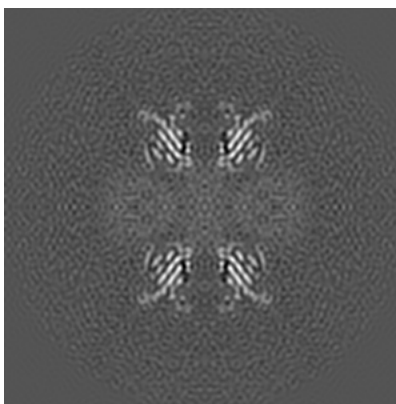
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

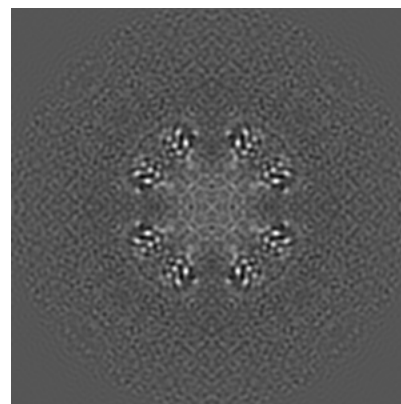
6.2.1 Primary map



X Index: 112



Y Index: 112

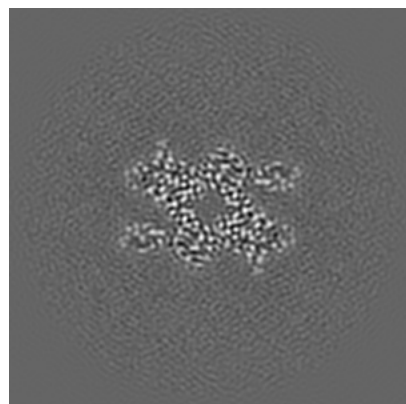


Z Index: 112

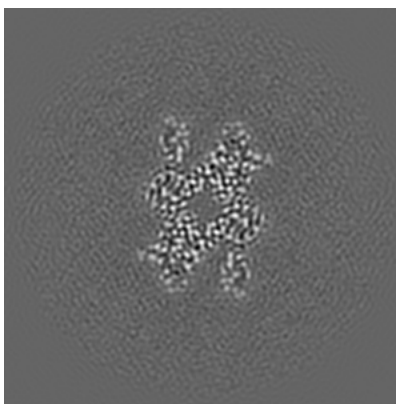
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

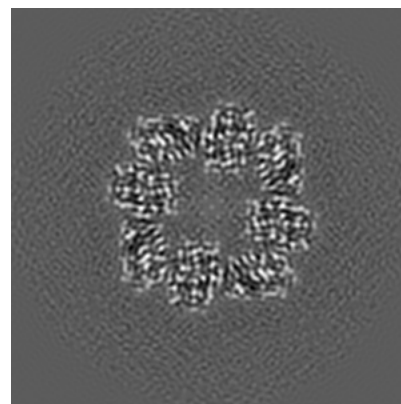
6.3.1 Primary map



X Index: 73



Y Index: 73



Z Index: 130

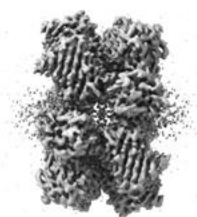
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

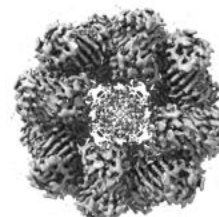
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

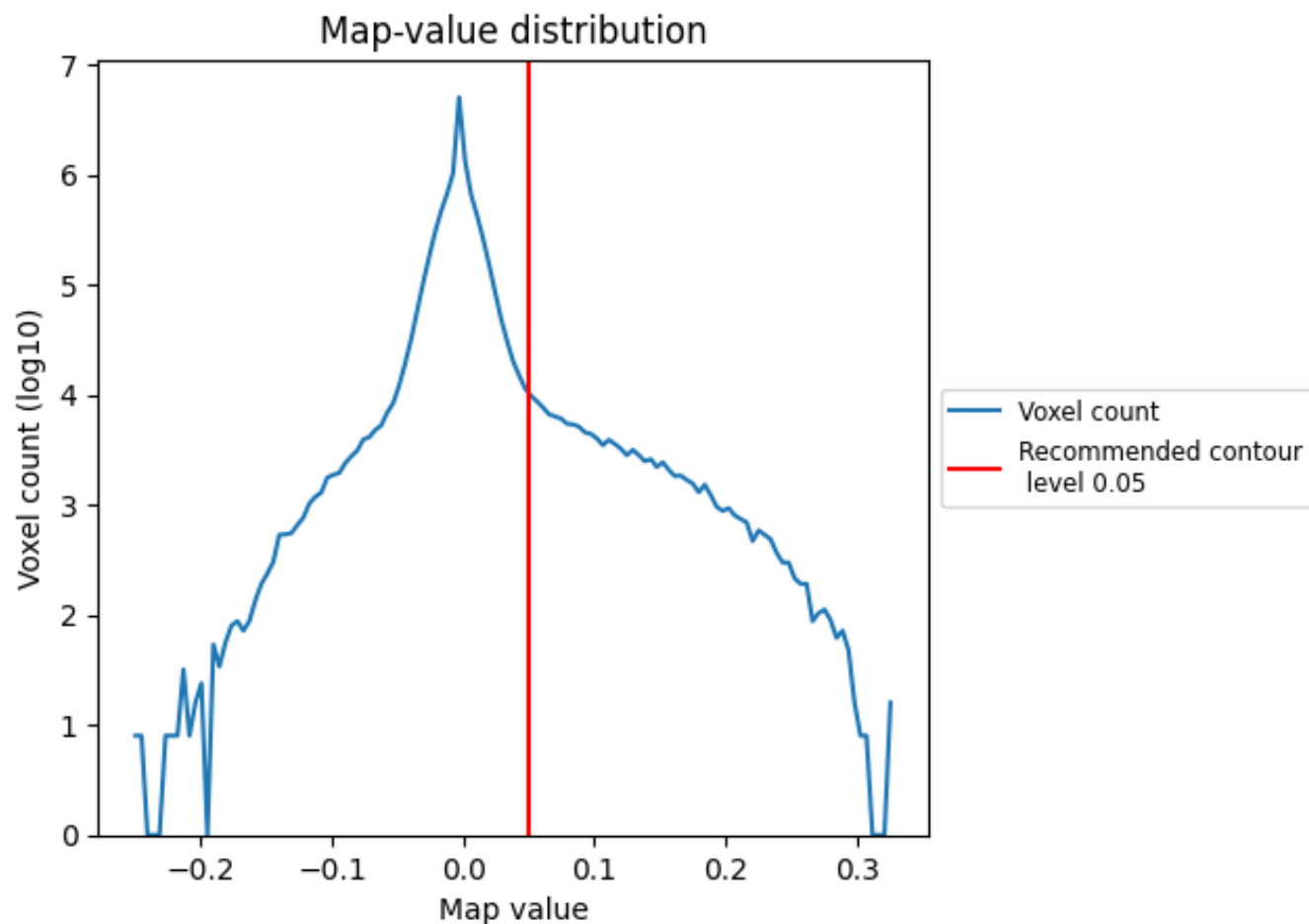
6.5 Mask visualisation

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

7 Map analysis [i](#)

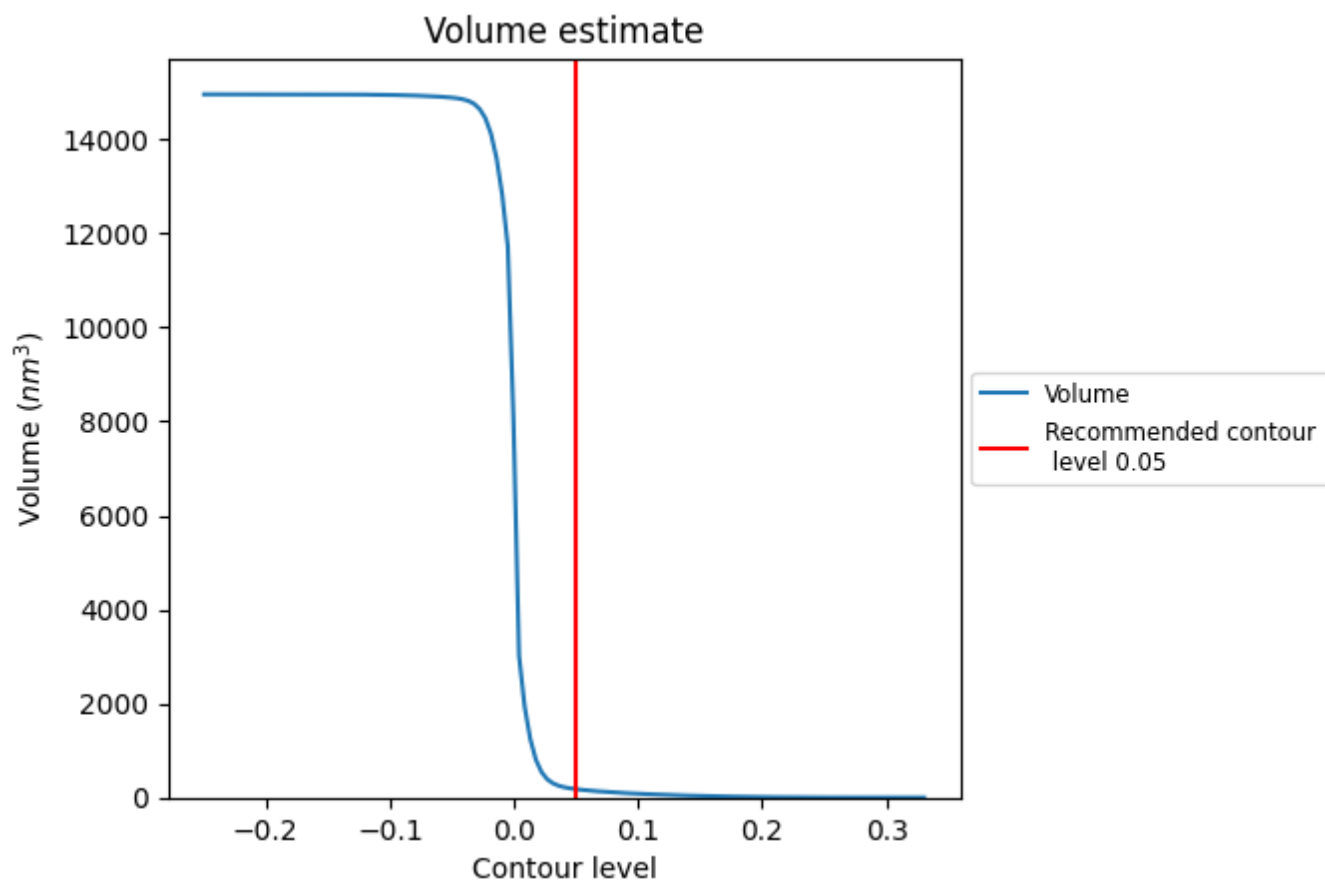
This section contains the results of statistical analysis of the map.

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.

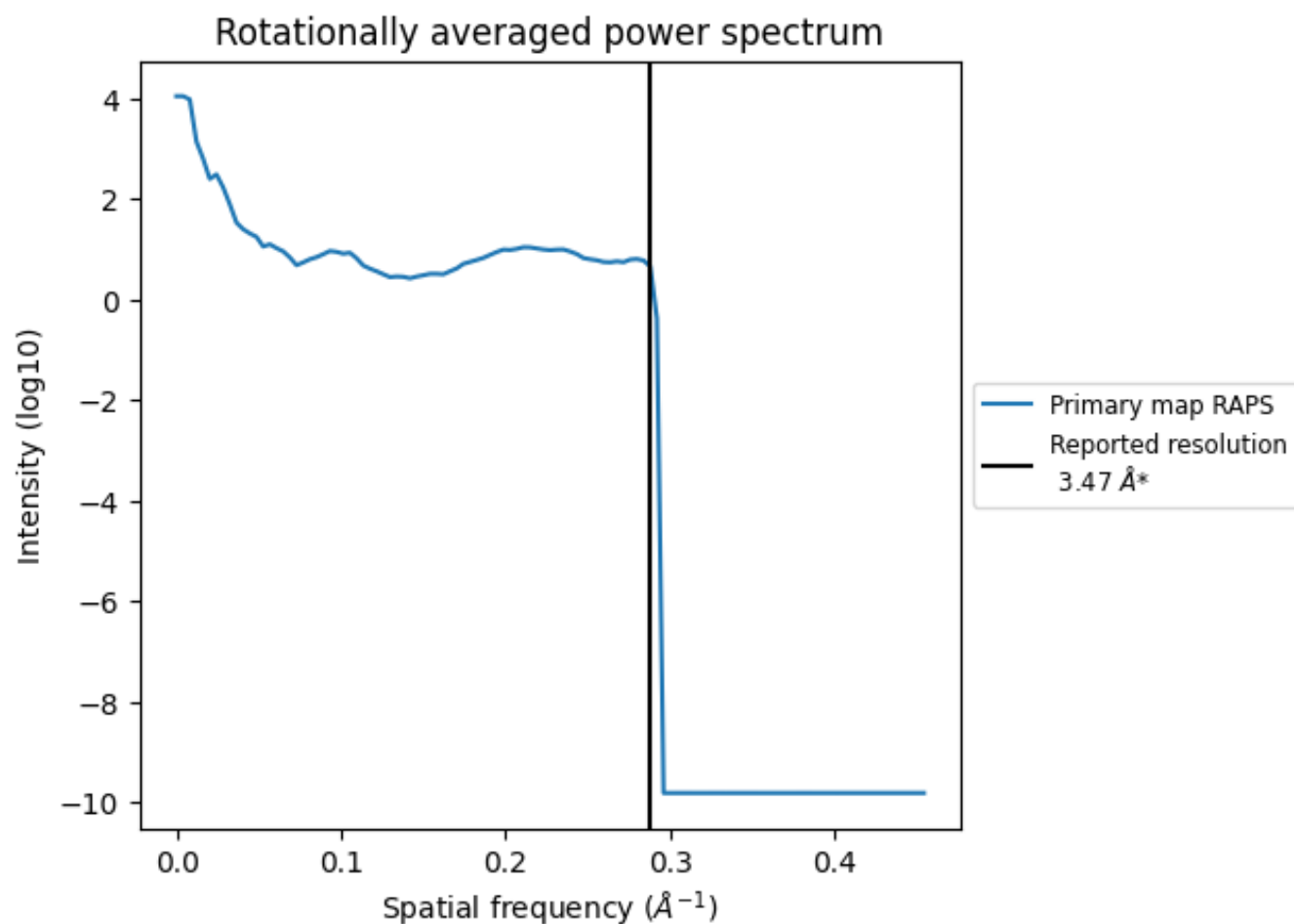
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 178 nm³; this corresponds to an approximate mass of 161 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

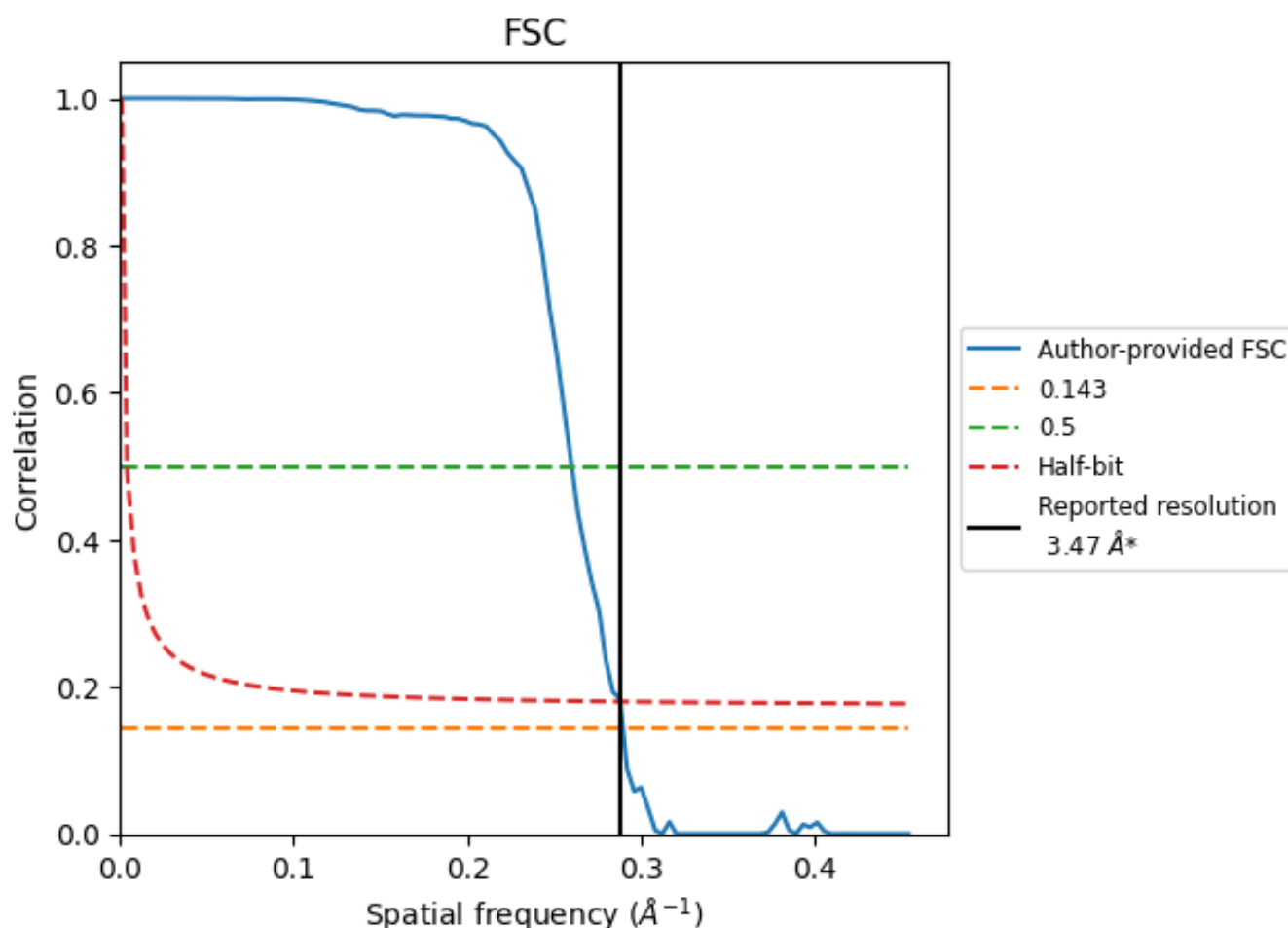


*Reported resolution corresponds to spatial frequency of 0.288 \AA^{-1}

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 0.288 \AA^{-1}

8.2 Resolution estimates [i](#)

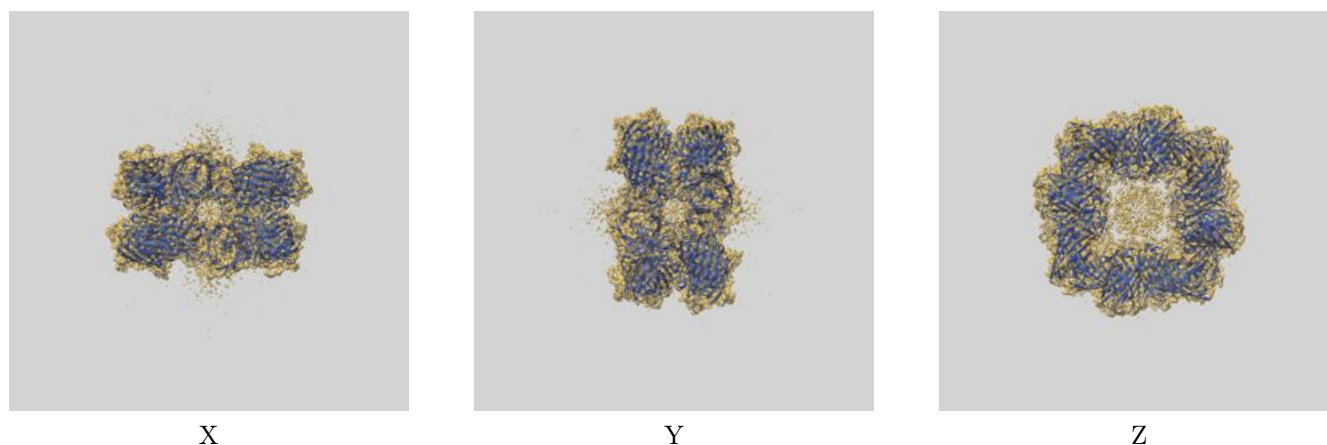
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	3.45	3.84	3.47
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

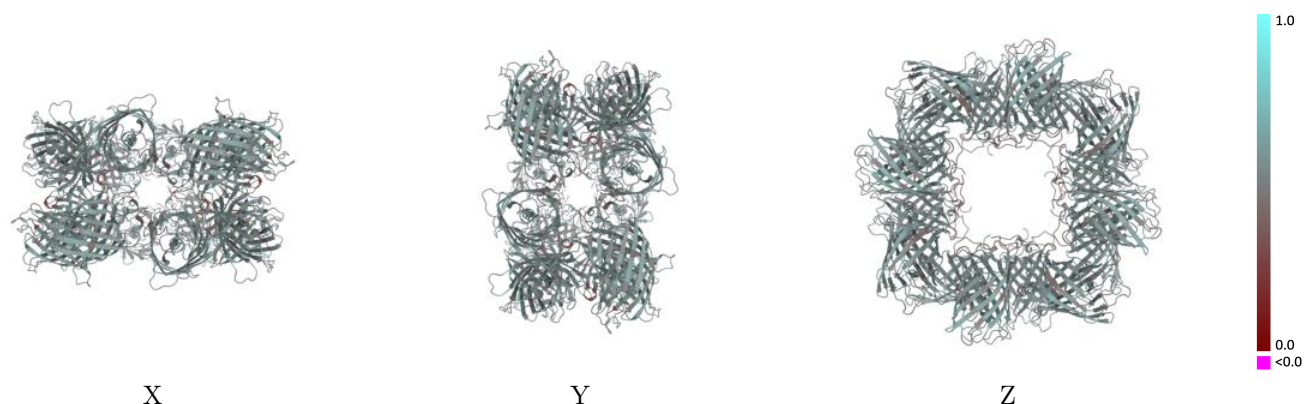
This section contains information regarding the fit between EMDB map EMD-9104 and PDB model 6MDR. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



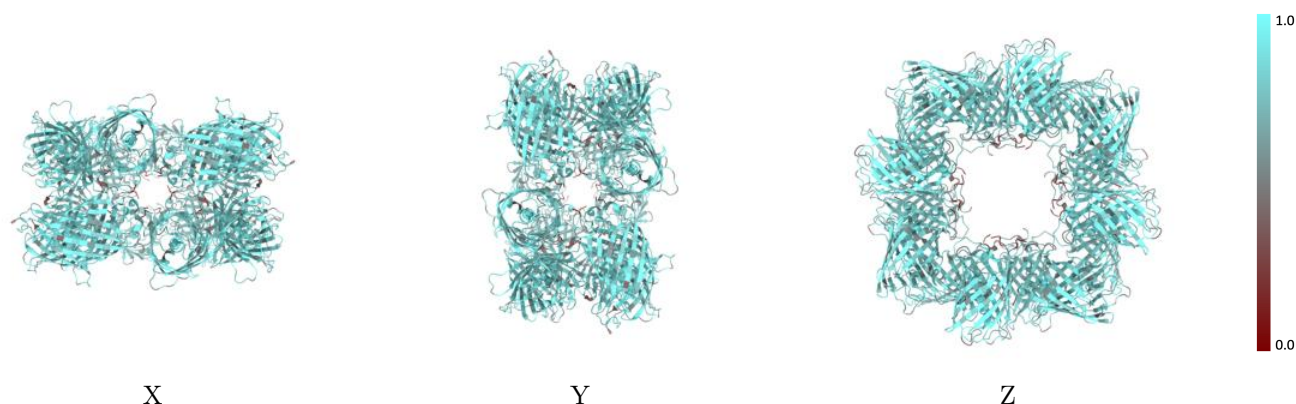
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



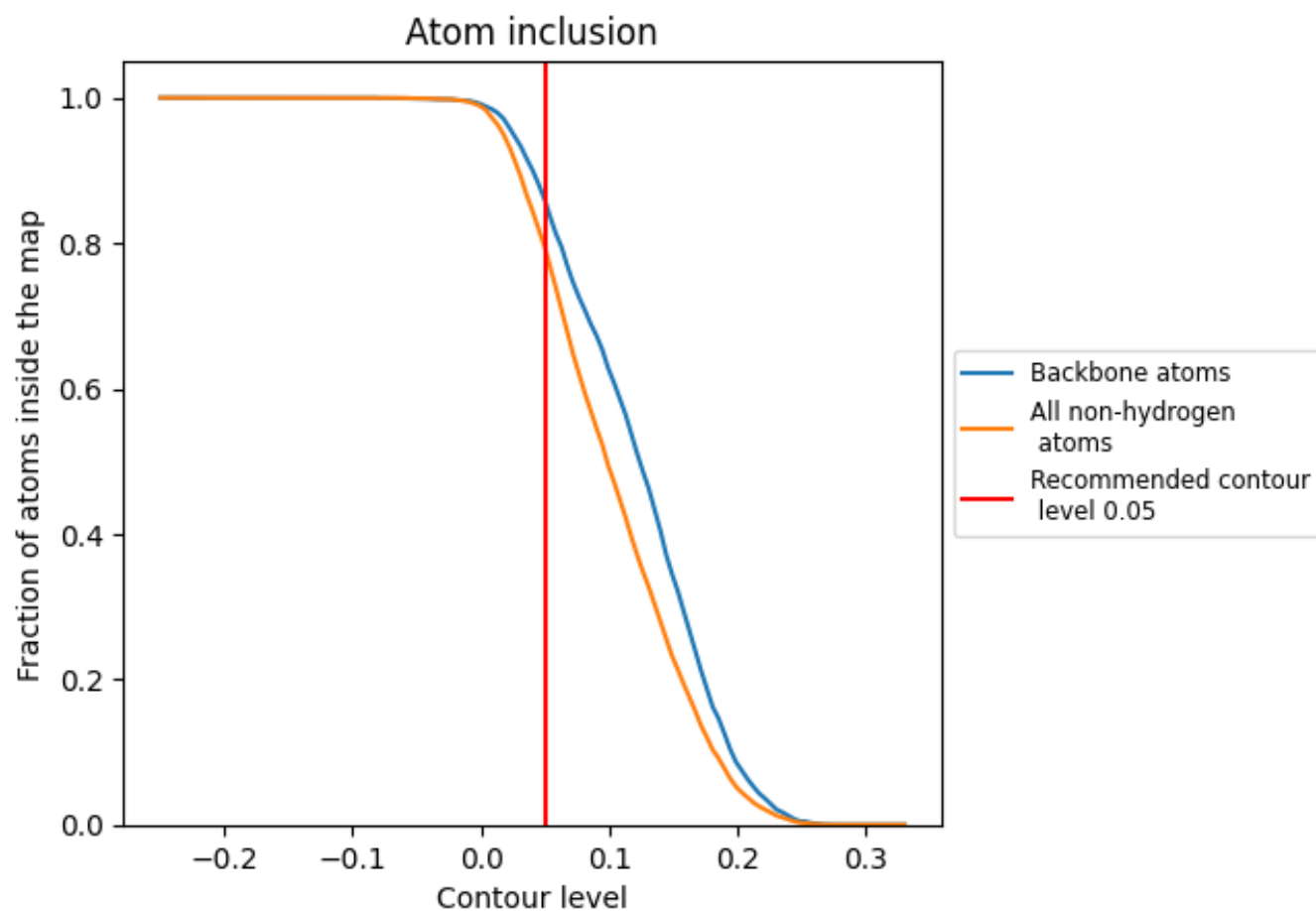
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.05).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 79% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7936	 0.5180
a	 0.7927	 0.5190
b	 0.7958	 0.5160
c	 0.7927	 0.5210
d	 0.7925	 0.5150
e	 0.7922	 0.5210
f	 0.7952	 0.5140
g	 0.7922	 0.5210
h	 0.7963	 0.5170
i	 0.7894	 0.5220
j	 0.7963	 0.5160
k	 0.7922	 0.5210
l	 0.7925	 0.5160
m	 0.7922	 0.5210
n	 0.7947	 0.5160
o	 0.7949	 0.5200
p	 0.7963	 0.5140

