



## Full wwPDB EM Validation Report ⓘ

Jun 27, 2024 – 01:02 AM JST

PDB ID : 8JX3  
EMDB ID : EMD-36689  
Title : alpha-Hemolysin(G122S/K147R/K237C)-SpyTag/SpyCatcher head to head  
14-mer  
Authors : Ishii, Y.; Naito, K.; Yokoyama, T.; Tanaka, Y.; Matsuura, T.  
Deposited on : 2023-06-30  
Resolution : 2.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

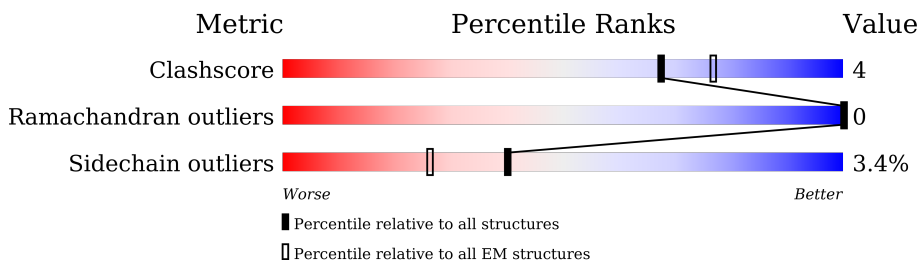
EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 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  $\geq 3$ , 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	421	60% 9% 30%
1	B	421	60% 10% 30%
1	C	421	59% 10% 30%
1	D	421	59% 10% 30%
1	E	421	61% 9% 30%
1	F	421	60% 10% 30%
1	G	421	63% 6% 30%
2	H	324	80% 10% 10%

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Mol	Chain	Length	Quality of chain
2	I	324	 79% 11% 10%
2	J	324	 81% 10% 10%
2	K	324	 80% 10% 10%
2	L	324	 78% 12% 10%
2	M	324	 80% 10% 10%
2	N	324	 78% 12% 10%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 32826 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 alpha hemolysin fused with spy-catcher.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	293	2345	1470	402	465	8	0	0
1	B	293	2345	1470	402	465	8	0	0
1	C	293	2345	1470	402	465	8	0	0
1	D	293	2345	1470	402	465	8	0	0
1	E	293	2345	1470	402	465	8	0	0
1	F	293	2345	1470	402	465	8	0	0
1	G	293	2345	1470	402	465	8	0	0

There are 917 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P09616
A	122	SER	GLY	engineered mutation	UNP P09616
A	147	ARG	LYS	engineered mutation	UNP P09616
A	237	CYS	LYS	engineered mutation	UNP P09616
A	294	GLY	-	expression tag	UNP P09616
A	295	SER	-	expression tag	UNP P09616
A	296	SER	-	expression tag	UNP P09616
A	297	GLY	-	expression tag	UNP P09616
A	298	SER	-	expression tag	UNP P09616
A	299	VAL	-	expression tag	UNP P09616
A	300	THR	-	expression tag	UNP P09616
A	301	THR	-	expression tag	UNP P09616
A	302	LEU	-	expression tag	UNP P09616
A	303	SER	-	expression tag	UNP P09616
A	304	GLY	-	expression tag	UNP P09616
A	305	LEU	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
A	306	SER	-	expression tag	UNP P09616
A	307	GLY	-	expression tag	UNP P09616
A	308	GLU	-	expression tag	UNP P09616
A	309	GLN	-	expression tag	UNP P09616
A	310	GLY	-	expression tag	UNP P09616
A	311	PRO	-	expression tag	UNP P09616
A	312	SER	-	expression tag	UNP P09616
A	313	GLY	-	expression tag	UNP P09616
A	314	ASP	-	expression tag	UNP P09616
A	315	MET	-	expression tag	UNP P09616
A	316	THR	-	expression tag	UNP P09616
A	317	THR	-	expression tag	UNP P09616
A	318	GLU	-	expression tag	UNP P09616
A	319	GLU	-	expression tag	UNP P09616
A	320	ASP	-	expression tag	UNP P09616
A	321	SER	-	expression tag	UNP P09616
A	322	ALA	-	expression tag	UNP P09616
A	323	THR	-	expression tag	UNP P09616
A	324	HIS	-	expression tag	UNP P09616
A	325	ILE	-	expression tag	UNP P09616
A	326	LYS	-	expression tag	UNP P09616
A	327	PHE	-	expression tag	UNP P09616
A	328	SER	-	expression tag	UNP P09616
A	329	LYS	-	expression tag	UNP P09616
A	330	ARG	-	expression tag	UNP P09616
A	331	ASP	-	expression tag	UNP P09616
A	332	GLU	-	expression tag	UNP P09616
A	333	ASP	-	expression tag	UNP P09616
A	334	GLY	-	expression tag	UNP P09616
A	335	ARG	-	expression tag	UNP P09616
A	336	GLU	-	expression tag	UNP P09616
A	337	LEU	-	expression tag	UNP P09616
A	338	ALA	-	expression tag	UNP P09616
A	339	GLY	-	expression tag	UNP P09616
A	340	ALA	-	expression tag	UNP P09616
A	341	THR	-	expression tag	UNP P09616
A	342	MET	-	expression tag	UNP P09616
A	343	GLU	-	expression tag	UNP P09616
A	344	LEU	-	expression tag	UNP P09616
A	345	ARG	-	expression tag	UNP P09616
A	346	ASP	-	expression tag	UNP P09616
A	347	SER	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
A	348	SER	-	expression tag	UNP P09616
A	349	GLY	-	expression tag	UNP P09616
A	350	LYS	-	expression tag	UNP P09616
A	351	THR	-	expression tag	UNP P09616
A	352	ILE	-	expression tag	UNP P09616
A	353	SER	-	expression tag	UNP P09616
A	354	THR	-	expression tag	UNP P09616
A	355	TRP	-	expression tag	UNP P09616
A	356	ILE	-	expression tag	UNP P09616
A	357	SER	-	expression tag	UNP P09616
A	358	ASP	-	expression tag	UNP P09616
A	359	GLY	-	expression tag	UNP P09616
A	360	HIS	-	expression tag	UNP P09616
A	361	VAL	-	expression tag	UNP P09616
A	362	LYS	-	expression tag	UNP P09616
A	363	ASP	-	expression tag	UNP P09616
A	364	PHE	-	expression tag	UNP P09616
A	365	TYR	-	expression tag	UNP P09616
A	366	LEU	-	expression tag	UNP P09616
A	367	TYR	-	expression tag	UNP P09616
A	368	PRO	-	expression tag	UNP P09616
A	369	GLY	-	expression tag	UNP P09616
A	370	LYS	-	expression tag	UNP P09616
A	371	TYR	-	expression tag	UNP P09616
A	372	THR	-	expression tag	UNP P09616
A	373	PHE	-	expression tag	UNP P09616
A	374	VAL	-	expression tag	UNP P09616
A	375	GLU	-	expression tag	UNP P09616
A	376	THR	-	expression tag	UNP P09616
A	377	ALA	-	expression tag	UNP P09616
A	378	ALA	-	expression tag	UNP P09616
A	379	PRO	-	expression tag	UNP P09616
A	380	ASP	-	expression tag	UNP P09616
A	381	GLY	-	expression tag	UNP P09616
A	382	TYR	-	expression tag	UNP P09616
A	383	GLU	-	expression tag	UNP P09616
A	384	VAL	-	expression tag	UNP P09616
A	385	ALA	-	expression tag	UNP P09616
A	386	THR	-	expression tag	UNP P09616
A	387	PRO	-	expression tag	UNP P09616
A	388	ILE	-	expression tag	UNP P09616
A	389	GLU	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
A	390	PHE	-	expression tag	UNP P09616
A	391	THR	-	expression tag	UNP P09616
A	392	VAL	-	expression tag	UNP P09616
A	393	ASN	-	expression tag	UNP P09616
A	394	GLU	-	expression tag	UNP P09616
A	395	ASP	-	expression tag	UNP P09616
A	396	GLY	-	expression tag	UNP P09616
A	397	GLN	-	expression tag	UNP P09616
A	398	VAL	-	expression tag	UNP P09616
A	399	THR	-	expression tag	UNP P09616
A	400	VAL	-	expression tag	UNP P09616
A	401	ASP	-	expression tag	UNP P09616
A	402	GLY	-	expression tag	UNP P09616
A	403	GLU	-	expression tag	UNP P09616
A	404	ALA	-	expression tag	UNP P09616
A	405	THR	-	expression tag	UNP P09616
A	406	GLU	-	expression tag	UNP P09616
A	407	GLY	-	expression tag	UNP P09616
A	408	ASP	-	expression tag	UNP P09616
A	409	ALA	-	expression tag	UNP P09616
A	410	HIS	-	expression tag	UNP P09616
A	411	THR	-	expression tag	UNP P09616
A	412	GLY	-	expression tag	UNP P09616
A	413	GLY	-	expression tag	UNP P09616
A	414	SER	-	expression tag	UNP P09616
A	415	HIS	-	expression tag	UNP P09616
A	416	HIS	-	expression tag	UNP P09616
A	417	HIS	-	expression tag	UNP P09616
A	418	HIS	-	expression tag	UNP P09616
A	419	HIS	-	expression tag	UNP P09616
A	420	HIS	-	expression tag	UNP P09616
B	0	MET	-	initiating methionine	UNP P09616
B	122	SER	GLY	engineered mutation	UNP P09616
B	147	ARG	LYS	engineered mutation	UNP P09616
B	237	CYS	LYS	engineered mutation	UNP P09616
B	294	GLY	-	expression tag	UNP P09616
B	295	SER	-	expression tag	UNP P09616
B	296	SER	-	expression tag	UNP P09616
B	297	GLY	-	expression tag	UNP P09616
B	298	SER	-	expression tag	UNP P09616
B	299	VAL	-	expression tag	UNP P09616
B	300	THR	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
B	301	THR	-	expression tag	UNP P09616
B	302	LEU	-	expression tag	UNP P09616
B	303	SER	-	expression tag	UNP P09616
B	304	GLY	-	expression tag	UNP P09616
B	305	LEU	-	expression tag	UNP P09616
B	306	SER	-	expression tag	UNP P09616
B	307	GLY	-	expression tag	UNP P09616
B	308	GLU	-	expression tag	UNP P09616
B	309	GLN	-	expression tag	UNP P09616
B	310	GLY	-	expression tag	UNP P09616
B	311	PRO	-	expression tag	UNP P09616
B	312	SER	-	expression tag	UNP P09616
B	313	GLY	-	expression tag	UNP P09616
B	314	ASP	-	expression tag	UNP P09616
B	315	MET	-	expression tag	UNP P09616
B	316	THR	-	expression tag	UNP P09616
B	317	THR	-	expression tag	UNP P09616
B	318	GLU	-	expression tag	UNP P09616
B	319	GLU	-	expression tag	UNP P09616
B	320	ASP	-	expression tag	UNP P09616
B	321	SER	-	expression tag	UNP P09616
B	322	ALA	-	expression tag	UNP P09616
B	323	THR	-	expression tag	UNP P09616
B	324	HIS	-	expression tag	UNP P09616
B	325	ILE	-	expression tag	UNP P09616
B	326	LYS	-	expression tag	UNP P09616
B	327	PHE	-	expression tag	UNP P09616
B	328	SER	-	expression tag	UNP P09616
B	329	LYS	-	expression tag	UNP P09616
B	330	ARG	-	expression tag	UNP P09616
B	331	ASP	-	expression tag	UNP P09616
B	332	GLU	-	expression tag	UNP P09616
B	333	ASP	-	expression tag	UNP P09616
B	334	GLY	-	expression tag	UNP P09616
B	335	ARG	-	expression tag	UNP P09616
B	336	GLU	-	expression tag	UNP P09616
B	337	LEU	-	expression tag	UNP P09616
B	338	ALA	-	expression tag	UNP P09616
B	339	GLY	-	expression tag	UNP P09616
B	340	ALA	-	expression tag	UNP P09616
B	341	THR	-	expression tag	UNP P09616
B	342	MET	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
B	343	GLU	-	expression tag	UNP P09616
B	344	LEU	-	expression tag	UNP P09616
B	345	ARG	-	expression tag	UNP P09616
B	346	ASP	-	expression tag	UNP P09616
B	347	SER	-	expression tag	UNP P09616
B	348	SER	-	expression tag	UNP P09616
B	349	GLY	-	expression tag	UNP P09616
B	350	LYS	-	expression tag	UNP P09616
B	351	THR	-	expression tag	UNP P09616
B	352	ILE	-	expression tag	UNP P09616
B	353	SER	-	expression tag	UNP P09616
B	354	THR	-	expression tag	UNP P09616
B	355	TRP	-	expression tag	UNP P09616
B	356	ILE	-	expression tag	UNP P09616
B	357	SER	-	expression tag	UNP P09616
B	358	ASP	-	expression tag	UNP P09616
B	359	GLY	-	expression tag	UNP P09616
B	360	HIS	-	expression tag	UNP P09616
B	361	VAL	-	expression tag	UNP P09616
B	362	LYS	-	expression tag	UNP P09616
B	363	ASP	-	expression tag	UNP P09616
B	364	PHE	-	expression tag	UNP P09616
B	365	TYR	-	expression tag	UNP P09616
B	366	LEU	-	expression tag	UNP P09616
B	367	TYR	-	expression tag	UNP P09616
B	368	PRO	-	expression tag	UNP P09616
B	369	GLY	-	expression tag	UNP P09616
B	370	LYS	-	expression tag	UNP P09616
B	371	TYR	-	expression tag	UNP P09616
B	372	THR	-	expression tag	UNP P09616
B	373	PHE	-	expression tag	UNP P09616
B	374	VAL	-	expression tag	UNP P09616
B	375	GLU	-	expression tag	UNP P09616
B	376	THR	-	expression tag	UNP P09616
B	377	ALA	-	expression tag	UNP P09616
B	378	ALA	-	expression tag	UNP P09616
B	379	PRO	-	expression tag	UNP P09616
B	380	ASP	-	expression tag	UNP P09616
B	381	GLY	-	expression tag	UNP P09616
B	382	TYR	-	expression tag	UNP P09616
B	383	GLU	-	expression tag	UNP P09616
B	384	VAL	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
B	385	ALA	-	expression tag	UNP P09616
B	386	THR	-	expression tag	UNP P09616
B	387	PRO	-	expression tag	UNP P09616
B	388	ILE	-	expression tag	UNP P09616
B	389	GLU	-	expression tag	UNP P09616
B	390	PHE	-	expression tag	UNP P09616
B	391	THR	-	expression tag	UNP P09616
B	392	VAL	-	expression tag	UNP P09616
B	393	ASN	-	expression tag	UNP P09616
B	394	GLU	-	expression tag	UNP P09616
B	395	ASP	-	expression tag	UNP P09616
B	396	GLY	-	expression tag	UNP P09616
B	397	GLN	-	expression tag	UNP P09616
B	398	VAL	-	expression tag	UNP P09616
B	399	THR	-	expression tag	UNP P09616
B	400	VAL	-	expression tag	UNP P09616
B	401	ASP	-	expression tag	UNP P09616
B	402	GLY	-	expression tag	UNP P09616
B	403	GLU	-	expression tag	UNP P09616
B	404	ALA	-	expression tag	UNP P09616
B	405	THR	-	expression tag	UNP P09616
B	406	GLU	-	expression tag	UNP P09616
B	407	GLY	-	expression tag	UNP P09616
B	408	ASP	-	expression tag	UNP P09616
B	409	ALA	-	expression tag	UNP P09616
B	410	HIS	-	expression tag	UNP P09616
B	411	THR	-	expression tag	UNP P09616
B	412	GLY	-	expression tag	UNP P09616
B	413	GLY	-	expression tag	UNP P09616
B	414	SER	-	expression tag	UNP P09616
B	415	HIS	-	expression tag	UNP P09616
B	416	HIS	-	expression tag	UNP P09616
B	417	HIS	-	expression tag	UNP P09616
B	418	HIS	-	expression tag	UNP P09616
B	419	HIS	-	expression tag	UNP P09616
B	420	HIS	-	expression tag	UNP P09616
C	0	MET	-	initiating methionine	UNP P09616
C	122	SER	GLY	engineered mutation	UNP P09616
C	147	ARG	LYS	engineered mutation	UNP P09616
C	237	CYS	LYS	engineered mutation	UNP P09616
C	294	GLY	-	expression tag	UNP P09616
C	295	SER	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
C	296	SER	-	expression tag	UNP P09616
C	297	GLY	-	expression tag	UNP P09616
C	298	SER	-	expression tag	UNP P09616
C	299	VAL	-	expression tag	UNP P09616
C	300	THR	-	expression tag	UNP P09616
C	301	THR	-	expression tag	UNP P09616
C	302	LEU	-	expression tag	UNP P09616
C	303	SER	-	expression tag	UNP P09616
C	304	GLY	-	expression tag	UNP P09616
C	305	LEU	-	expression tag	UNP P09616
C	306	SER	-	expression tag	UNP P09616
C	307	GLY	-	expression tag	UNP P09616
C	308	GLU	-	expression tag	UNP P09616
C	309	GLN	-	expression tag	UNP P09616
C	310	GLY	-	expression tag	UNP P09616
C	311	PRO	-	expression tag	UNP P09616
C	312	SER	-	expression tag	UNP P09616
C	313	GLY	-	expression tag	UNP P09616
C	314	ASP	-	expression tag	UNP P09616
C	315	MET	-	expression tag	UNP P09616
C	316	THR	-	expression tag	UNP P09616
C	317	THR	-	expression tag	UNP P09616
C	318	GLU	-	expression tag	UNP P09616
C	319	GLU	-	expression tag	UNP P09616
C	320	ASP	-	expression tag	UNP P09616
C	321	SER	-	expression tag	UNP P09616
C	322	ALA	-	expression tag	UNP P09616
C	323	THR	-	expression tag	UNP P09616
C	324	HIS	-	expression tag	UNP P09616
C	325	ILE	-	expression tag	UNP P09616
C	326	LYS	-	expression tag	UNP P09616
C	327	PHE	-	expression tag	UNP P09616
C	328	SER	-	expression tag	UNP P09616
C	329	LYS	-	expression tag	UNP P09616
C	330	ARG	-	expression tag	UNP P09616
C	331	ASP	-	expression tag	UNP P09616
C	332	GLU	-	expression tag	UNP P09616
C	333	ASP	-	expression tag	UNP P09616
C	334	GLY	-	expression tag	UNP P09616
C	335	ARG	-	expression tag	UNP P09616
C	336	GLU	-	expression tag	UNP P09616
C	337	LEU	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
C	338	ALA	-	expression tag	UNP P09616
C	339	GLY	-	expression tag	UNP P09616
C	340	ALA	-	expression tag	UNP P09616
C	341	THR	-	expression tag	UNP P09616
C	342	MET	-	expression tag	UNP P09616
C	343	GLU	-	expression tag	UNP P09616
C	344	LEU	-	expression tag	UNP P09616
C	345	ARG	-	expression tag	UNP P09616
C	346	ASP	-	expression tag	UNP P09616
C	347	SER	-	expression tag	UNP P09616
C	348	SER	-	expression tag	UNP P09616
C	349	GLY	-	expression tag	UNP P09616
C	350	LYS	-	expression tag	UNP P09616
C	351	THR	-	expression tag	UNP P09616
C	352	ILE	-	expression tag	UNP P09616
C	353	SER	-	expression tag	UNP P09616
C	354	THR	-	expression tag	UNP P09616
C	355	TRP	-	expression tag	UNP P09616
C	356	ILE	-	expression tag	UNP P09616
C	357	SER	-	expression tag	UNP P09616
C	358	ASP	-	expression tag	UNP P09616
C	359	GLY	-	expression tag	UNP P09616
C	360	HIS	-	expression tag	UNP P09616
C	361	VAL	-	expression tag	UNP P09616
C	362	LYS	-	expression tag	UNP P09616
C	363	ASP	-	expression tag	UNP P09616
C	364	PHE	-	expression tag	UNP P09616
C	365	TYR	-	expression tag	UNP P09616
C	366	LEU	-	expression tag	UNP P09616
C	367	TYR	-	expression tag	UNP P09616
C	368	PRO	-	expression tag	UNP P09616
C	369	GLY	-	expression tag	UNP P09616
C	370	LYS	-	expression tag	UNP P09616
C	371	TYR	-	expression tag	UNP P09616
C	372	THR	-	expression tag	UNP P09616
C	373	PHE	-	expression tag	UNP P09616
C	374	VAL	-	expression tag	UNP P09616
C	375	GLU	-	expression tag	UNP P09616
C	376	THR	-	expression tag	UNP P09616
C	377	ALA	-	expression tag	UNP P09616
C	378	ALA	-	expression tag	UNP P09616
C	379	PRO	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
C	380	ASP	-	expression tag	UNP P09616
C	381	GLY	-	expression tag	UNP P09616
C	382	TYR	-	expression tag	UNP P09616
C	383	GLU	-	expression tag	UNP P09616
C	384	VAL	-	expression tag	UNP P09616
C	385	ALA	-	expression tag	UNP P09616
C	386	THR	-	expression tag	UNP P09616
C	387	PRO	-	expression tag	UNP P09616
C	388	ILE	-	expression tag	UNP P09616
C	389	GLU	-	expression tag	UNP P09616
C	390	PHE	-	expression tag	UNP P09616
C	391	THR	-	expression tag	UNP P09616
C	392	VAL	-	expression tag	UNP P09616
C	393	ASN	-	expression tag	UNP P09616
C	394	GLU	-	expression tag	UNP P09616
C	395	ASP	-	expression tag	UNP P09616
C	396	GLY	-	expression tag	UNP P09616
C	397	GLN	-	expression tag	UNP P09616
C	398	VAL	-	expression tag	UNP P09616
C	399	THR	-	expression tag	UNP P09616
C	400	VAL	-	expression tag	UNP P09616
C	401	ASP	-	expression tag	UNP P09616
C	402	GLY	-	expression tag	UNP P09616
C	403	GLU	-	expression tag	UNP P09616
C	404	ALA	-	expression tag	UNP P09616
C	405	THR	-	expression tag	UNP P09616
C	406	GLU	-	expression tag	UNP P09616
C	407	GLY	-	expression tag	UNP P09616
C	408	ASP	-	expression tag	UNP P09616
C	409	ALA	-	expression tag	UNP P09616
C	410	HIS	-	expression tag	UNP P09616
C	411	THR	-	expression tag	UNP P09616
C	412	GLY	-	expression tag	UNP P09616
C	413	GLY	-	expression tag	UNP P09616
C	414	SER	-	expression tag	UNP P09616
C	415	HIS	-	expression tag	UNP P09616
C	416	HIS	-	expression tag	UNP P09616
C	417	HIS	-	expression tag	UNP P09616
C	418	HIS	-	expression tag	UNP P09616
C	419	HIS	-	expression tag	UNP P09616
C	420	HIS	-	expression tag	UNP P09616
D	0	MET	-	initiating methionine	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
D	122	SER	GLY	engineered mutation	UNP P09616
D	147	ARG	LYS	engineered mutation	UNP P09616
D	237	CYS	LYS	engineered mutation	UNP P09616
D	294	GLY	-	expression tag	UNP P09616
D	295	SER	-	expression tag	UNP P09616
D	296	SER	-	expression tag	UNP P09616
D	297	GLY	-	expression tag	UNP P09616
D	298	SER	-	expression tag	UNP P09616
D	299	VAL	-	expression tag	UNP P09616
D	300	THR	-	expression tag	UNP P09616
D	301	THR	-	expression tag	UNP P09616
D	302	LEU	-	expression tag	UNP P09616
D	303	SER	-	expression tag	UNP P09616
D	304	GLY	-	expression tag	UNP P09616
D	305	LEU	-	expression tag	UNP P09616
D	306	SER	-	expression tag	UNP P09616
D	307	GLY	-	expression tag	UNP P09616
D	308	GLU	-	expression tag	UNP P09616
D	309	GLN	-	expression tag	UNP P09616
D	310	GLY	-	expression tag	UNP P09616
D	311	PRO	-	expression tag	UNP P09616
D	312	SER	-	expression tag	UNP P09616
D	313	GLY	-	expression tag	UNP P09616
D	314	ASP	-	expression tag	UNP P09616
D	315	MET	-	expression tag	UNP P09616
D	316	THR	-	expression tag	UNP P09616
D	317	THR	-	expression tag	UNP P09616
D	318	GLU	-	expression tag	UNP P09616
D	319	GLU	-	expression tag	UNP P09616
D	320	ASP	-	expression tag	UNP P09616
D	321	SER	-	expression tag	UNP P09616
D	322	ALA	-	expression tag	UNP P09616
D	323	THR	-	expression tag	UNP P09616
D	324	HIS	-	expression tag	UNP P09616
D	325	ILE	-	expression tag	UNP P09616
D	326	LYS	-	expression tag	UNP P09616
D	327	PHE	-	expression tag	UNP P09616
D	328	SER	-	expression tag	UNP P09616
D	329	LYS	-	expression tag	UNP P09616
D	330	ARG	-	expression tag	UNP P09616
D	331	ASP	-	expression tag	UNP P09616
D	332	GLU	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
D	333	ASP	-	expression tag	UNP P09616
D	334	GLY	-	expression tag	UNP P09616
D	335	ARG	-	expression tag	UNP P09616
D	336	GLU	-	expression tag	UNP P09616
D	337	LEU	-	expression tag	UNP P09616
D	338	ALA	-	expression tag	UNP P09616
D	339	GLY	-	expression tag	UNP P09616
D	340	ALA	-	expression tag	UNP P09616
D	341	THR	-	expression tag	UNP P09616
D	342	MET	-	expression tag	UNP P09616
D	343	GLU	-	expression tag	UNP P09616
D	344	LEU	-	expression tag	UNP P09616
D	345	ARG	-	expression tag	UNP P09616
D	346	ASP	-	expression tag	UNP P09616
D	347	SER	-	expression tag	UNP P09616
D	348	SER	-	expression tag	UNP P09616
D	349	GLY	-	expression tag	UNP P09616
D	350	LYS	-	expression tag	UNP P09616
D	351	THR	-	expression tag	UNP P09616
D	352	ILE	-	expression tag	UNP P09616
D	353	SER	-	expression tag	UNP P09616
D	354	THR	-	expression tag	UNP P09616
D	355	TRP	-	expression tag	UNP P09616
D	356	ILE	-	expression tag	UNP P09616
D	357	SER	-	expression tag	UNP P09616
D	358	ASP	-	expression tag	UNP P09616
D	359	GLY	-	expression tag	UNP P09616
D	360	HIS	-	expression tag	UNP P09616
D	361	VAL	-	expression tag	UNP P09616
D	362	LYS	-	expression tag	UNP P09616
D	363	ASP	-	expression tag	UNP P09616
D	364	PHE	-	expression tag	UNP P09616
D	365	TYR	-	expression tag	UNP P09616
D	366	LEU	-	expression tag	UNP P09616
D	367	TYR	-	expression tag	UNP P09616
D	368	PRO	-	expression tag	UNP P09616
D	369	GLY	-	expression tag	UNP P09616
D	370	LYS	-	expression tag	UNP P09616
D	371	TYR	-	expression tag	UNP P09616
D	372	THR	-	expression tag	UNP P09616
D	373	PHE	-	expression tag	UNP P09616
D	374	VAL	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
D	375	GLU	-	expression tag	UNP P09616
D	376	THR	-	expression tag	UNP P09616
D	377	ALA	-	expression tag	UNP P09616
D	378	ALA	-	expression tag	UNP P09616
D	379	PRO	-	expression tag	UNP P09616
D	380	ASP	-	expression tag	UNP P09616
D	381	GLY	-	expression tag	UNP P09616
D	382	TYR	-	expression tag	UNP P09616
D	383	GLU	-	expression tag	UNP P09616
D	384	VAL	-	expression tag	UNP P09616
D	385	ALA	-	expression tag	UNP P09616
D	386	THR	-	expression tag	UNP P09616
D	387	PRO	-	expression tag	UNP P09616
D	388	ILE	-	expression tag	UNP P09616
D	389	GLU	-	expression tag	UNP P09616
D	390	PHE	-	expression tag	UNP P09616
D	391	THR	-	expression tag	UNP P09616
D	392	VAL	-	expression tag	UNP P09616
D	393	ASN	-	expression tag	UNP P09616
D	394	GLU	-	expression tag	UNP P09616
D	395	ASP	-	expression tag	UNP P09616
D	396	GLY	-	expression tag	UNP P09616
D	397	GLN	-	expression tag	UNP P09616
D	398	VAL	-	expression tag	UNP P09616
D	399	THR	-	expression tag	UNP P09616
D	400	VAL	-	expression tag	UNP P09616
D	401	ASP	-	expression tag	UNP P09616
D	402	GLY	-	expression tag	UNP P09616
D	403	GLU	-	expression tag	UNP P09616
D	404	ALA	-	expression tag	UNP P09616
D	405	THR	-	expression tag	UNP P09616
D	406	GLU	-	expression tag	UNP P09616
D	407	GLY	-	expression tag	UNP P09616
D	408	ASP	-	expression tag	UNP P09616
D	409	ALA	-	expression tag	UNP P09616
D	410	HIS	-	expression tag	UNP P09616
D	411	THR	-	expression tag	UNP P09616
D	412	GLY	-	expression tag	UNP P09616
D	413	GLY	-	expression tag	UNP P09616
D	414	SER	-	expression tag	UNP P09616
D	415	HIS	-	expression tag	UNP P09616
D	416	HIS	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
D	417	HIS	-	expression tag	UNP P09616
D	418	HIS	-	expression tag	UNP P09616
D	419	HIS	-	expression tag	UNP P09616
D	420	HIS	-	expression tag	UNP P09616
E	0	MET	-	initiating methionine	UNP P09616
E	122	SER	GLY	engineered mutation	UNP P09616
E	147	ARG	LYS	engineered mutation	UNP P09616
E	237	CYS	LYS	engineered mutation	UNP P09616
E	294	GLY	-	expression tag	UNP P09616
E	295	SER	-	expression tag	UNP P09616
E	296	SER	-	expression tag	UNP P09616
E	297	GLY	-	expression tag	UNP P09616
E	298	SER	-	expression tag	UNP P09616
E	299	VAL	-	expression tag	UNP P09616
E	300	THR	-	expression tag	UNP P09616
E	301	THR	-	expression tag	UNP P09616
E	302	LEU	-	expression tag	UNP P09616
E	303	SER	-	expression tag	UNP P09616
E	304	GLY	-	expression tag	UNP P09616
E	305	LEU	-	expression tag	UNP P09616
E	306	SER	-	expression tag	UNP P09616
E	307	GLY	-	expression tag	UNP P09616
E	308	GLU	-	expression tag	UNP P09616
E	309	GLN	-	expression tag	UNP P09616
E	310	GLY	-	expression tag	UNP P09616
E	311	PRO	-	expression tag	UNP P09616
E	312	SER	-	expression tag	UNP P09616
E	313	GLY	-	expression tag	UNP P09616
E	314	ASP	-	expression tag	UNP P09616
E	315	MET	-	expression tag	UNP P09616
E	316	THR	-	expression tag	UNP P09616
E	317	THR	-	expression tag	UNP P09616
E	318	GLU	-	expression tag	UNP P09616
E	319	GLU	-	expression tag	UNP P09616
E	320	ASP	-	expression tag	UNP P09616
E	321	SER	-	expression tag	UNP P09616
E	322	ALA	-	expression tag	UNP P09616
E	323	THR	-	expression tag	UNP P09616
E	324	HIS	-	expression tag	UNP P09616
E	325	ILE	-	expression tag	UNP P09616
E	326	LYS	-	expression tag	UNP P09616
E	327	PHE	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
E	328	SER	-	expression tag	UNP P09616
E	329	LYS	-	expression tag	UNP P09616
E	330	ARG	-	expression tag	UNP P09616
E	331	ASP	-	expression tag	UNP P09616
E	332	GLU	-	expression tag	UNP P09616
E	333	ASP	-	expression tag	UNP P09616
E	334	GLY	-	expression tag	UNP P09616
E	335	ARG	-	expression tag	UNP P09616
E	336	GLU	-	expression tag	UNP P09616
E	337	LEU	-	expression tag	UNP P09616
E	338	ALA	-	expression tag	UNP P09616
E	339	GLY	-	expression tag	UNP P09616
E	340	ALA	-	expression tag	UNP P09616
E	341	THR	-	expression tag	UNP P09616
E	342	MET	-	expression tag	UNP P09616
E	343	GLU	-	expression tag	UNP P09616
E	344	LEU	-	expression tag	UNP P09616
E	345	ARG	-	expression tag	UNP P09616
E	346	ASP	-	expression tag	UNP P09616
E	347	SER	-	expression tag	UNP P09616
E	348	SER	-	expression tag	UNP P09616
E	349	GLY	-	expression tag	UNP P09616
E	350	LYS	-	expression tag	UNP P09616
E	351	THR	-	expression tag	UNP P09616
E	352	ILE	-	expression tag	UNP P09616
E	353	SER	-	expression tag	UNP P09616
E	354	THR	-	expression tag	UNP P09616
E	355	TRP	-	expression tag	UNP P09616
E	356	ILE	-	expression tag	UNP P09616
E	357	SER	-	expression tag	UNP P09616
E	358	ASP	-	expression tag	UNP P09616
E	359	GLY	-	expression tag	UNP P09616
E	360	HIS	-	expression tag	UNP P09616
E	361	VAL	-	expression tag	UNP P09616
E	362	LYS	-	expression tag	UNP P09616
E	363	ASP	-	expression tag	UNP P09616
E	364	PHE	-	expression tag	UNP P09616
E	365	TYR	-	expression tag	UNP P09616
E	366	LEU	-	expression tag	UNP P09616
E	367	TYR	-	expression tag	UNP P09616
E	368	PRO	-	expression tag	UNP P09616
E	369	GLY	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
E	370	LYS	-	expression tag	UNP P09616
E	371	TYR	-	expression tag	UNP P09616
E	372	THR	-	expression tag	UNP P09616
E	373	PHE	-	expression tag	UNP P09616
E	374	VAL	-	expression tag	UNP P09616
E	375	GLU	-	expression tag	UNP P09616
E	376	THR	-	expression tag	UNP P09616
E	377	ALA	-	expression tag	UNP P09616
E	378	ALA	-	expression tag	UNP P09616
E	379	PRO	-	expression tag	UNP P09616
E	380	ASP	-	expression tag	UNP P09616
E	381	GLY	-	expression tag	UNP P09616
E	382	TYR	-	expression tag	UNP P09616
E	383	GLU	-	expression tag	UNP P09616
E	384	VAL	-	expression tag	UNP P09616
E	385	ALA	-	expression tag	UNP P09616
E	386	THR	-	expression tag	UNP P09616
E	387	PRO	-	expression tag	UNP P09616
E	388	ILE	-	expression tag	UNP P09616
E	389	GLU	-	expression tag	UNP P09616
E	390	PHE	-	expression tag	UNP P09616
E	391	THR	-	expression tag	UNP P09616
E	392	VAL	-	expression tag	UNP P09616
E	393	ASN	-	expression tag	UNP P09616
E	394	GLU	-	expression tag	UNP P09616
E	395	ASP	-	expression tag	UNP P09616
E	396	GLY	-	expression tag	UNP P09616
E	397	GLN	-	expression tag	UNP P09616
E	398	VAL	-	expression tag	UNP P09616
E	399	THR	-	expression tag	UNP P09616
E	400	VAL	-	expression tag	UNP P09616
E	401	ASP	-	expression tag	UNP P09616
E	402	GLY	-	expression tag	UNP P09616
E	403	GLU	-	expression tag	UNP P09616
E	404	ALA	-	expression tag	UNP P09616
E	405	THR	-	expression tag	UNP P09616
E	406	GLU	-	expression tag	UNP P09616
E	407	GLY	-	expression tag	UNP P09616
E	408	ASP	-	expression tag	UNP P09616
E	409	ALA	-	expression tag	UNP P09616
E	410	HIS	-	expression tag	UNP P09616
E	411	THR	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
E	412	GLY	-	expression tag	UNP P09616
E	413	GLY	-	expression tag	UNP P09616
E	414	SER	-	expression tag	UNP P09616
E	415	HIS	-	expression tag	UNP P09616
E	416	HIS	-	expression tag	UNP P09616
E	417	HIS	-	expression tag	UNP P09616
E	418	HIS	-	expression tag	UNP P09616
E	419	HIS	-	expression tag	UNP P09616
E	420	HIS	-	expression tag	UNP P09616
F	0	MET	-	initiating methionine	UNP P09616
F	122	SER	GLY	engineered mutation	UNP P09616
F	147	ARG	LYS	engineered mutation	UNP P09616
F	237	CYS	LYS	engineered mutation	UNP P09616
F	294	GLY	-	expression tag	UNP P09616
F	295	SER	-	expression tag	UNP P09616
F	296	SER	-	expression tag	UNP P09616
F	297	GLY	-	expression tag	UNP P09616
F	298	SER	-	expression tag	UNP P09616
F	299	VAL	-	expression tag	UNP P09616
F	300	THR	-	expression tag	UNP P09616
F	301	THR	-	expression tag	UNP P09616
F	302	LEU	-	expression tag	UNP P09616
F	303	SER	-	expression tag	UNP P09616
F	304	GLY	-	expression tag	UNP P09616
F	305	LEU	-	expression tag	UNP P09616
F	306	SER	-	expression tag	UNP P09616
F	307	GLY	-	expression tag	UNP P09616
F	308	GLU	-	expression tag	UNP P09616
F	309	GLN	-	expression tag	UNP P09616
F	310	GLY	-	expression tag	UNP P09616
F	311	PRO	-	expression tag	UNP P09616
F	312	SER	-	expression tag	UNP P09616
F	313	GLY	-	expression tag	UNP P09616
F	314	ASP	-	expression tag	UNP P09616
F	315	MET	-	expression tag	UNP P09616
F	316	THR	-	expression tag	UNP P09616
F	317	THR	-	expression tag	UNP P09616
F	318	GLU	-	expression tag	UNP P09616
F	319	GLU	-	expression tag	UNP P09616
F	320	ASP	-	expression tag	UNP P09616
F	321	SER	-	expression tag	UNP P09616
F	322	ALA	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
F	323	THR	-	expression tag	UNP P09616
F	324	HIS	-	expression tag	UNP P09616
F	325	ILE	-	expression tag	UNP P09616
F	326	LYS	-	expression tag	UNP P09616
F	327	PHE	-	expression tag	UNP P09616
F	328	SER	-	expression tag	UNP P09616
F	329	LYS	-	expression tag	UNP P09616
F	330	ARG	-	expression tag	UNP P09616
F	331	ASP	-	expression tag	UNP P09616
F	332	GLU	-	expression tag	UNP P09616
F	333	ASP	-	expression tag	UNP P09616
F	334	GLY	-	expression tag	UNP P09616
F	335	ARG	-	expression tag	UNP P09616
F	336	GLU	-	expression tag	UNP P09616
F	337	LEU	-	expression tag	UNP P09616
F	338	ALA	-	expression tag	UNP P09616
F	339	GLY	-	expression tag	UNP P09616
F	340	ALA	-	expression tag	UNP P09616
F	341	THR	-	expression tag	UNP P09616
F	342	MET	-	expression tag	UNP P09616
F	343	GLU	-	expression tag	UNP P09616
F	344	LEU	-	expression tag	UNP P09616
F	345	ARG	-	expression tag	UNP P09616
F	346	ASP	-	expression tag	UNP P09616
F	347	SER	-	expression tag	UNP P09616
F	348	SER	-	expression tag	UNP P09616
F	349	GLY	-	expression tag	UNP P09616
F	350	LYS	-	expression tag	UNP P09616
F	351	THR	-	expression tag	UNP P09616
F	352	ILE	-	expression tag	UNP P09616
F	353	SER	-	expression tag	UNP P09616
F	354	THR	-	expression tag	UNP P09616
F	355	TRP	-	expression tag	UNP P09616
F	356	ILE	-	expression tag	UNP P09616
F	357	SER	-	expression tag	UNP P09616
F	358	ASP	-	expression tag	UNP P09616
F	359	GLY	-	expression tag	UNP P09616
F	360	HIS	-	expression tag	UNP P09616
F	361	VAL	-	expression tag	UNP P09616
F	362	LYS	-	expression tag	UNP P09616
F	363	ASP	-	expression tag	UNP P09616
F	364	PHE	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
F	365	TYR	-	expression tag	UNP P09616
F	366	LEU	-	expression tag	UNP P09616
F	367	TYR	-	expression tag	UNP P09616
F	368	PRO	-	expression tag	UNP P09616
F	369	GLY	-	expression tag	UNP P09616
F	370	LYS	-	expression tag	UNP P09616
F	371	TYR	-	expression tag	UNP P09616
F	372	THR	-	expression tag	UNP P09616
F	373	PHE	-	expression tag	UNP P09616
F	374	VAL	-	expression tag	UNP P09616
F	375	GLU	-	expression tag	UNP P09616
F	376	THR	-	expression tag	UNP P09616
F	377	ALA	-	expression tag	UNP P09616
F	378	ALA	-	expression tag	UNP P09616
F	379	PRO	-	expression tag	UNP P09616
F	380	ASP	-	expression tag	UNP P09616
F	381	GLY	-	expression tag	UNP P09616
F	382	TYR	-	expression tag	UNP P09616
F	383	GLU	-	expression tag	UNP P09616
F	384	VAL	-	expression tag	UNP P09616
F	385	ALA	-	expression tag	UNP P09616
F	386	THR	-	expression tag	UNP P09616
F	387	PRO	-	expression tag	UNP P09616
F	388	ILE	-	expression tag	UNP P09616
F	389	GLU	-	expression tag	UNP P09616
F	390	PHE	-	expression tag	UNP P09616
F	391	THR	-	expression tag	UNP P09616
F	392	VAL	-	expression tag	UNP P09616
F	393	ASN	-	expression tag	UNP P09616
F	394	GLU	-	expression tag	UNP P09616
F	395	ASP	-	expression tag	UNP P09616
F	396	GLY	-	expression tag	UNP P09616
F	397	GLN	-	expression tag	UNP P09616
F	398	VAL	-	expression tag	UNP P09616
F	399	THR	-	expression tag	UNP P09616
F	400	VAL	-	expression tag	UNP P09616
F	401	ASP	-	expression tag	UNP P09616
F	402	GLY	-	expression tag	UNP P09616
F	403	GLU	-	expression tag	UNP P09616
F	404	ALA	-	expression tag	UNP P09616
F	405	THR	-	expression tag	UNP P09616
F	406	GLU	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
F	407	GLY	-	expression tag	UNP P09616
F	408	ASP	-	expression tag	UNP P09616
F	409	ALA	-	expression tag	UNP P09616
F	410	HIS	-	expression tag	UNP P09616
F	411	THR	-	expression tag	UNP P09616
F	412	GLY	-	expression tag	UNP P09616
F	413	GLY	-	expression tag	UNP P09616
F	414	SER	-	expression tag	UNP P09616
F	415	HIS	-	expression tag	UNP P09616
F	416	HIS	-	expression tag	UNP P09616
F	417	HIS	-	expression tag	UNP P09616
F	418	HIS	-	expression tag	UNP P09616
F	419	HIS	-	expression tag	UNP P09616
F	420	HIS	-	expression tag	UNP P09616
G	0	MET	-	initiating methionine	UNP P09616
G	122	SER	GLY	engineered mutation	UNP P09616
G	147	ARG	LYS	engineered mutation	UNP P09616
G	237	CYS	LYS	engineered mutation	UNP P09616
G	294	GLY	-	expression tag	UNP P09616
G	295	SER	-	expression tag	UNP P09616
G	296	SER	-	expression tag	UNP P09616
G	297	GLY	-	expression tag	UNP P09616
G	298	SER	-	expression tag	UNP P09616
G	299	VAL	-	expression tag	UNP P09616
G	300	THR	-	expression tag	UNP P09616
G	301	THR	-	expression tag	UNP P09616
G	302	LEU	-	expression tag	UNP P09616
G	303	SER	-	expression tag	UNP P09616
G	304	GLY	-	expression tag	UNP P09616
G	305	LEU	-	expression tag	UNP P09616
G	306	SER	-	expression tag	UNP P09616
G	307	GLY	-	expression tag	UNP P09616
G	308	GLU	-	expression tag	UNP P09616
G	309	GLN	-	expression tag	UNP P09616
G	310	GLY	-	expression tag	UNP P09616
G	311	PRO	-	expression tag	UNP P09616
G	312	SER	-	expression tag	UNP P09616
G	313	GLY	-	expression tag	UNP P09616
G	314	ASP	-	expression tag	UNP P09616
G	315	MET	-	expression tag	UNP P09616
G	316	THR	-	expression tag	UNP P09616
G	317	THR	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
G	318	GLU	-	expression tag	UNP P09616
G	319	GLU	-	expression tag	UNP P09616
G	320	ASP	-	expression tag	UNP P09616
G	321	SER	-	expression tag	UNP P09616
G	322	ALA	-	expression tag	UNP P09616
G	323	THR	-	expression tag	UNP P09616
G	324	HIS	-	expression tag	UNP P09616
G	325	ILE	-	expression tag	UNP P09616
G	326	LYS	-	expression tag	UNP P09616
G	327	PHE	-	expression tag	UNP P09616
G	328	SER	-	expression tag	UNP P09616
G	329	LYS	-	expression tag	UNP P09616
G	330	ARG	-	expression tag	UNP P09616
G	331	ASP	-	expression tag	UNP P09616
G	332	GLU	-	expression tag	UNP P09616
G	333	ASP	-	expression tag	UNP P09616
G	334	GLY	-	expression tag	UNP P09616
G	335	ARG	-	expression tag	UNP P09616
G	336	GLU	-	expression tag	UNP P09616
G	337	LEU	-	expression tag	UNP P09616
G	338	ALA	-	expression tag	UNP P09616
G	339	GLY	-	expression tag	UNP P09616
G	340	ALA	-	expression tag	UNP P09616
G	341	THR	-	expression tag	UNP P09616
G	342	MET	-	expression tag	UNP P09616
G	343	GLU	-	expression tag	UNP P09616
G	344	LEU	-	expression tag	UNP P09616
G	345	ARG	-	expression tag	UNP P09616
G	346	ASP	-	expression tag	UNP P09616
G	347	SER	-	expression tag	UNP P09616
G	348	SER	-	expression tag	UNP P09616
G	349	GLY	-	expression tag	UNP P09616
G	350	LYS	-	expression tag	UNP P09616
G	351	THR	-	expression tag	UNP P09616
G	352	ILE	-	expression tag	UNP P09616
G	353	SER	-	expression tag	UNP P09616
G	354	THR	-	expression tag	UNP P09616
G	355	TRP	-	expression tag	UNP P09616
G	356	ILE	-	expression tag	UNP P09616
G	357	SER	-	expression tag	UNP P09616
G	358	ASP	-	expression tag	UNP P09616
G	359	GLY	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
G	360	HIS	-	expression tag	UNP P09616
G	361	VAL	-	expression tag	UNP P09616
G	362	LYS	-	expression tag	UNP P09616
G	363	ASP	-	expression tag	UNP P09616
G	364	PHE	-	expression tag	UNP P09616
G	365	TYR	-	expression tag	UNP P09616
G	366	LEU	-	expression tag	UNP P09616
G	367	TYR	-	expression tag	UNP P09616
G	368	PRO	-	expression tag	UNP P09616
G	369	GLY	-	expression tag	UNP P09616
G	370	LYS	-	expression tag	UNP P09616
G	371	TYR	-	expression tag	UNP P09616
G	372	THR	-	expression tag	UNP P09616
G	373	PHE	-	expression tag	UNP P09616
G	374	VAL	-	expression tag	UNP P09616
G	375	GLU	-	expression tag	UNP P09616
G	376	THR	-	expression tag	UNP P09616
G	377	ALA	-	expression tag	UNP P09616
G	378	ALA	-	expression tag	UNP P09616
G	379	PRO	-	expression tag	UNP P09616
G	380	ASP	-	expression tag	UNP P09616
G	381	GLY	-	expression tag	UNP P09616
G	382	TYR	-	expression tag	UNP P09616
G	383	GLU	-	expression tag	UNP P09616
G	384	VAL	-	expression tag	UNP P09616
G	385	ALA	-	expression tag	UNP P09616
G	386	THR	-	expression tag	UNP P09616
G	387	PRO	-	expression tag	UNP P09616
G	388	ILE	-	expression tag	UNP P09616
G	389	GLU	-	expression tag	UNP P09616
G	390	PHE	-	expression tag	UNP P09616
G	391	THR	-	expression tag	UNP P09616
G	392	VAL	-	expression tag	UNP P09616
G	393	ASN	-	expression tag	UNP P09616
G	394	GLU	-	expression tag	UNP P09616
G	395	ASP	-	expression tag	UNP P09616
G	396	GLY	-	expression tag	UNP P09616
G	397	GLN	-	expression tag	UNP P09616
G	398	VAL	-	expression tag	UNP P09616
G	399	THR	-	expression tag	UNP P09616
G	400	VAL	-	expression tag	UNP P09616
G	401	ASP	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
G	402	GLY	-	expression tag	UNP P09616
G	403	GLU	-	expression tag	UNP P09616
G	404	ALA	-	expression tag	UNP P09616
G	405	THR	-	expression tag	UNP P09616
G	406	GLU	-	expression tag	UNP P09616
G	407	GLY	-	expression tag	UNP P09616
G	408	ASP	-	expression tag	UNP P09616
G	409	ALA	-	expression tag	UNP P09616
G	410	HIS	-	expression tag	UNP P09616
G	411	THR	-	expression tag	UNP P09616
G	412	GLY	-	expression tag	UNP P09616
G	413	GLY	-	expression tag	UNP P09616
G	414	SER	-	expression tag	UNP P09616
G	415	HIS	-	expression tag	UNP P09616
G	416	HIS	-	expression tag	UNP P09616
G	417	HIS	-	expression tag	UNP P09616
G	418	HIS	-	expression tag	UNP P09616
G	419	HIS	-	expression tag	UNP P09616
G	420	HIS	-	expression tag	UNP P09616

- Molecule 2 is a protein called alpha hemolysin fused with spy-tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	293	Total	C	N	O	S	0	0
			2345	1470	402	465	8		
2	I	293	Total	C	N	O	S	0	0
			2345	1470	402	465	8		
2	J	293	Total	C	N	O	S	0	0
			2345	1470	402	465	8		
2	K	293	Total	C	N	O	S	0	0
			2345	1470	402	465	8		
2	L	293	Total	C	N	O	S	0	0
			2345	1470	402	465	8		
2	M	293	Total	C	N	O	S	0	0
			2345	1470	402	465	8		
2	N	293	Total	C	N	O	S	0	0
			2341	1467	401	465	8		

There are 238 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	0	MET	-	initiating methionine	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
H	122	SER	GLY	engineered mutation	UNP P09616
H	147	ARG	LYS	engineered mutation	UNP P09616
H	237	CYS	LYS	engineered mutation	UNP P09616
H	294	GLY	-	expression tag	UNP P09616
H	295	SER	-	expression tag	UNP P09616
H	296	SER	-	expression tag	UNP P09616
H	297	GLY	-	expression tag	UNP P09616
H	298	SER	-	expression tag	UNP P09616
H	299	ARG	-	expression tag	UNP P09616
H	300	GLY	-	expression tag	UNP P09616
H	301	VAL	-	expression tag	UNP P09616
H	302	PRO	-	expression tag	UNP P09616
H	303	HIS	-	expression tag	UNP P09616
H	304	ILE	-	expression tag	UNP P09616
H	305	VAL	-	expression tag	UNP P09616
H	306	MET	-	expression tag	UNP P09616
H	307	VAL	-	expression tag	UNP P09616
H	308	ASP	-	expression tag	UNP P09616
H	309	ALA	-	expression tag	UNP P09616
H	310	TYR	-	expression tag	UNP P09616
H	311	LYS	-	expression tag	UNP P09616
H	312	ARG	-	expression tag	UNP P09616
H	313	TYR	-	expression tag	UNP P09616
H	314	LYS	-	expression tag	UNP P09616
H	315	GLY	-	expression tag	UNP P09616
H	316	GLY	-	expression tag	UNP P09616
H	317	SER	-	expression tag	UNP P09616
H	318	HIS	-	expression tag	UNP P09616
H	319	HIS	-	expression tag	UNP P09616
H	320	HIS	-	expression tag	UNP P09616
H	321	HIS	-	expression tag	UNP P09616
H	322	HIS	-	expression tag	UNP P09616
H	323	HIS	-	expression tag	UNP P09616
I	0	MET	-	initiating methionine	UNP P09616
I	122	SER	GLY	engineered mutation	UNP P09616
I	147	ARG	LYS	engineered mutation	UNP P09616
I	237	CYS	LYS	engineered mutation	UNP P09616
I	294	GLY	-	expression tag	UNP P09616
I	295	SER	-	expression tag	UNP P09616
I	296	SER	-	expression tag	UNP P09616
I	297	GLY	-	expression tag	UNP P09616
I	298	SER	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
I	299	ARG	-	expression tag	UNP P09616
I	300	GLY	-	expression tag	UNP P09616
I	301	VAL	-	expression tag	UNP P09616
I	302	PRO	-	expression tag	UNP P09616
I	303	HIS	-	expression tag	UNP P09616
I	304	ILE	-	expression tag	UNP P09616
I	305	VAL	-	expression tag	UNP P09616
I	306	MET	-	expression tag	UNP P09616
I	307	VAL	-	expression tag	UNP P09616
I	308	ASP	-	expression tag	UNP P09616
I	309	ALA	-	expression tag	UNP P09616
I	310	TYR	-	expression tag	UNP P09616
I	311	LYS	-	expression tag	UNP P09616
I	312	ARG	-	expression tag	UNP P09616
I	313	TYR	-	expression tag	UNP P09616
I	314	LYS	-	expression tag	UNP P09616
I	315	GLY	-	expression tag	UNP P09616
I	316	GLY	-	expression tag	UNP P09616
I	317	SER	-	expression tag	UNP P09616
I	318	HIS	-	expression tag	UNP P09616
I	319	HIS	-	expression tag	UNP P09616
I	320	HIS	-	expression tag	UNP P09616
I	321	HIS	-	expression tag	UNP P09616
I	322	HIS	-	expression tag	UNP P09616
I	323	HIS	-	expression tag	UNP P09616
J	0	MET	-	initiating methionine	UNP P09616
J	122	SER	GLY	engineered mutation	UNP P09616
J	147	ARG	LYS	engineered mutation	UNP P09616
J	237	CYS	LYS	engineered mutation	UNP P09616
J	294	GLY	-	expression tag	UNP P09616
J	295	SER	-	expression tag	UNP P09616
J	296	SER	-	expression tag	UNP P09616
J	297	GLY	-	expression tag	UNP P09616
J	298	SER	-	expression tag	UNP P09616
J	299	ARG	-	expression tag	UNP P09616
J	300	GLY	-	expression tag	UNP P09616
J	301	VAL	-	expression tag	UNP P09616
J	302	PRO	-	expression tag	UNP P09616
J	303	HIS	-	expression tag	UNP P09616
J	304	ILE	-	expression tag	UNP P09616
J	305	VAL	-	expression tag	UNP P09616
J	306	MET	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
J	307	VAL	-	expression tag	UNP P09616
J	308	ASP	-	expression tag	UNP P09616
J	309	ALA	-	expression tag	UNP P09616
J	310	TYR	-	expression tag	UNP P09616
J	311	LYS	-	expression tag	UNP P09616
J	312	ARG	-	expression tag	UNP P09616
J	313	TYR	-	expression tag	UNP P09616
J	314	LYS	-	expression tag	UNP P09616
J	315	GLY	-	expression tag	UNP P09616
J	316	GLY	-	expression tag	UNP P09616
J	317	SER	-	expression tag	UNP P09616
J	318	HIS	-	expression tag	UNP P09616
J	319	HIS	-	expression tag	UNP P09616
J	320	HIS	-	expression tag	UNP P09616
J	321	HIS	-	expression tag	UNP P09616
J	322	HIS	-	expression tag	UNP P09616
J	323	HIS	-	expression tag	UNP P09616
K	0	MET	-	initiating methionine	UNP P09616
K	122	SER	GLY	engineered mutation	UNP P09616
K	147	ARG	LYS	engineered mutation	UNP P09616
K	237	CYS	LYS	engineered mutation	UNP P09616
K	294	GLY	-	expression tag	UNP P09616
K	295	SER	-	expression tag	UNP P09616
K	296	SER	-	expression tag	UNP P09616
K	297	GLY	-	expression tag	UNP P09616
K	298	SER	-	expression tag	UNP P09616
K	299	ARG	-	expression tag	UNP P09616
K	300	GLY	-	expression tag	UNP P09616
K	301	VAL	-	expression tag	UNP P09616
K	302	PRO	-	expression tag	UNP P09616
K	303	HIS	-	expression tag	UNP P09616
K	304	ILE	-	expression tag	UNP P09616
K	305	VAL	-	expression tag	UNP P09616
K	306	MET	-	expression tag	UNP P09616
K	307	VAL	-	expression tag	UNP P09616
K	308	ASP	-	expression tag	UNP P09616
K	309	ALA	-	expression tag	UNP P09616
K	310	TYR	-	expression tag	UNP P09616
K	311	LYS	-	expression tag	UNP P09616
K	312	ARG	-	expression tag	UNP P09616
K	313	TYR	-	expression tag	UNP P09616
K	314	LYS	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
K	315	GLY	-	expression tag	UNP P09616
K	316	GLY	-	expression tag	UNP P09616
K	317	SER	-	expression tag	UNP P09616
K	318	HIS	-	expression tag	UNP P09616
K	319	HIS	-	expression tag	UNP P09616
K	320	HIS	-	expression tag	UNP P09616
K	321	HIS	-	expression tag	UNP P09616
K	322	HIS	-	expression tag	UNP P09616
K	323	HIS	-	expression tag	UNP P09616
L	0	MET	-	initiating methionine	UNP P09616
L	122	SER	GLY	engineered mutation	UNP P09616
L	147	ARG	LYS	engineered mutation	UNP P09616
L	237	CYS	LYS	engineered mutation	UNP P09616
L	294	GLY	-	expression tag	UNP P09616
L	295	SER	-	expression tag	UNP P09616
L	296	SER	-	expression tag	UNP P09616
L	297	GLY	-	expression tag	UNP P09616
L	298	SER	-	expression tag	UNP P09616
L	299	ARG	-	expression tag	UNP P09616
L	300	GLY	-	expression tag	UNP P09616
L	301	VAL	-	expression tag	UNP P09616
L	302	PRO	-	expression tag	UNP P09616
L	303	HIS	-	expression tag	UNP P09616
L	304	ILE	-	expression tag	UNP P09616
L	305	VAL	-	expression tag	UNP P09616
L	306	MET	-	expression tag	UNP P09616
L	307	VAL	-	expression tag	UNP P09616
L	308	ASP	-	expression tag	UNP P09616
L	309	ALA	-	expression tag	UNP P09616
L	310	TYR	-	expression tag	UNP P09616
L	311	LYS	-	expression tag	UNP P09616
L	312	ARG	-	expression tag	UNP P09616
L	313	TYR	-	expression tag	UNP P09616
L	314	LYS	-	expression tag	UNP P09616
L	315	GLY	-	expression tag	UNP P09616
L	316	GLY	-	expression tag	UNP P09616
L	317	SER	-	expression tag	UNP P09616
L	318	HIS	-	expression tag	UNP P09616
L	319	HIS	-	expression tag	UNP P09616
L	320	HIS	-	expression tag	UNP P09616
L	321	HIS	-	expression tag	UNP P09616
L	322	HIS	-	expression tag	UNP P09616

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Chain	Residue	Modelled	Actual	Comment	Reference
L	323	HIS	-	expression tag	UNP P09616
M	0	MET	-	initiating methionine	UNP P09616
M	122	SER	GLY	engineered mutation	UNP P09616
M	147	ARG	LYS	engineered mutation	UNP P09616
M	237	CYS	LYS	engineered mutation	UNP P09616
M	294	GLY	-	expression tag	UNP P09616
M	295	SER	-	expression tag	UNP P09616
M	296	SER	-	expression tag	UNP P09616
M	297	GLY	-	expression tag	UNP P09616
M	298	SER	-	expression tag	UNP P09616
M	299	ARG	-	expression tag	UNP P09616
M	300	GLY	-	expression tag	UNP P09616
M	301	VAL	-	expression tag	UNP P09616
M	302	PRO	-	expression tag	UNP P09616
M	303	HIS	-	expression tag	UNP P09616
M	304	ILE	-	expression tag	UNP P09616
M	305	VAL	-	expression tag	UNP P09616
M	306	MET	-	expression tag	UNP P09616
M	307	VAL	-	expression tag	UNP P09616
M	308	ASP	-	expression tag	UNP P09616
M	309	ALA	-	expression tag	UNP P09616
M	310	TYR	-	expression tag	UNP P09616
M	311	LYS	-	expression tag	UNP P09616
M	312	ARG	-	expression tag	UNP P09616
M	313	TYR	-	expression tag	UNP P09616
M	314	LYS	-	expression tag	UNP P09616
M	315	GLY	-	expression tag	UNP P09616
M	316	GLY	-	expression tag	UNP P09616
M	317	SER	-	expression tag	UNP P09616
M	318	HIS	-	expression tag	UNP P09616
M	319	HIS	-	expression tag	UNP P09616
M	320	HIS	-	expression tag	UNP P09616
M	321	HIS	-	expression tag	UNP P09616
M	322	HIS	-	expression tag	UNP P09616
M	323	HIS	-	expression tag	UNP P09616
N	0	MET	-	initiating methionine	UNP P09616
N	122	SER	GLY	engineered mutation	UNP P09616
N	147	ARG	LYS	engineered mutation	UNP P09616
N	237	CYS	LYS	engineered mutation	UNP P09616
N	294	GLY	-	expression tag	UNP P09616
N	295	SER	-	expression tag	UNP P09616
N	296	SER	-	expression tag	UNP P09616

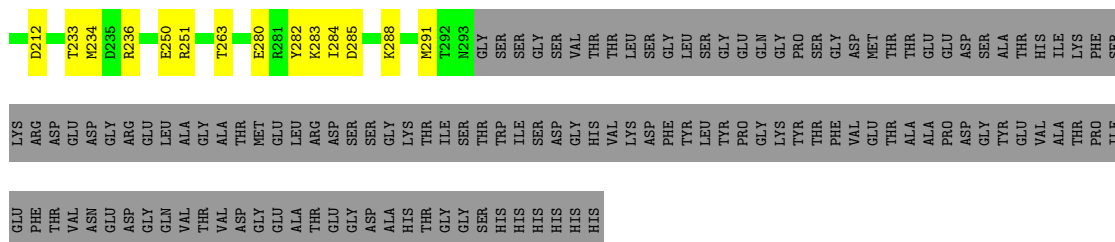
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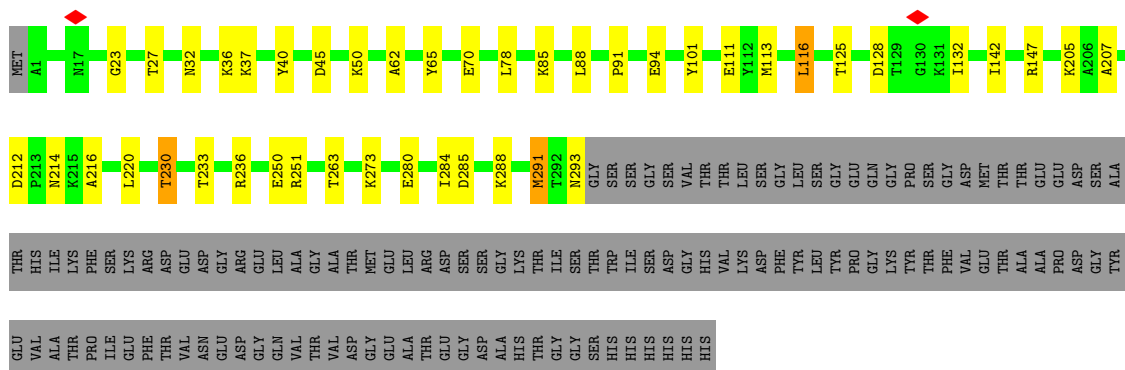
Chain	Residue	Modelled	Actual	Comment	Reference
N	297	GLY	-	expression tag	UNP P09616
N	298	SER	-	expression tag	UNP P09616
N	299	ARG	-	expression tag	UNP P09616
N	300	GLY	-	expression tag	UNP P09616
N	301	VAL	-	expression tag	UNP P09616
N	302	PRO	-	expression tag	UNP P09616
N	303	HIS	-	expression tag	UNP P09616
N	304	ILE	-	expression tag	UNP P09616
N	305	VAL	-	expression tag	UNP P09616
N	306	MET	-	expression tag	UNP P09616
N	307	VAL	-	expression tag	UNP P09616
N	308	ASP	-	expression tag	UNP P09616
N	309	ALA	-	expression tag	UNP P09616
N	310	TYR	-	expression tag	UNP P09616
N	311	LYS	-	expression tag	UNP P09616
N	312	ARG	-	expression tag	UNP P09616
N	313	TYR	-	expression tag	UNP P09616
N	314	LYS	-	expression tag	UNP P09616
N	315	GLY	-	expression tag	UNP P09616
N	316	GLY	-	expression tag	UNP P09616
N	317	SER	-	expression tag	UNP P09616
N	318	HIS	-	expression tag	UNP P09616
N	319	HIS	-	expression tag	UNP P09616
N	320	HIS	-	expression tag	UNP P09616
N	321	HIS	-	expression tag	UNP P09616
N	322	HIS	-	expression tag	UNP P09616
N	323	HIS	-	expression tag	UNP P09616



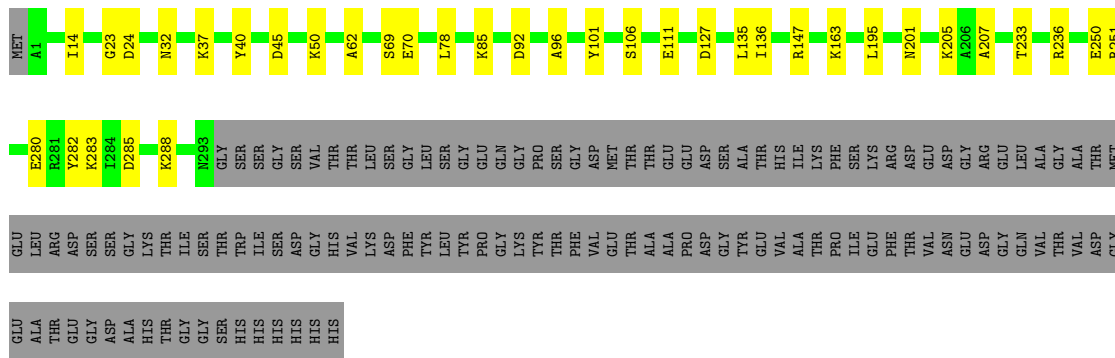




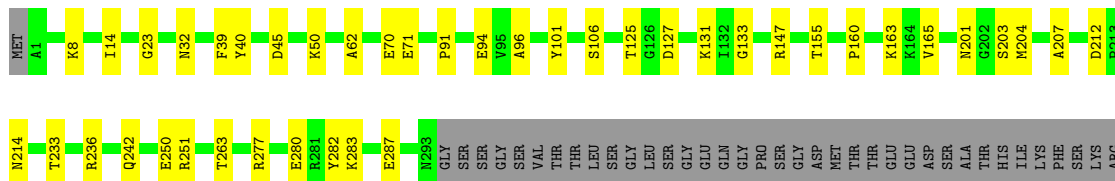
• Molecule 1: alpha hemolysin fused with spy-catcher



• Molecule 1: alpha hemolysin fused with spy-catcher

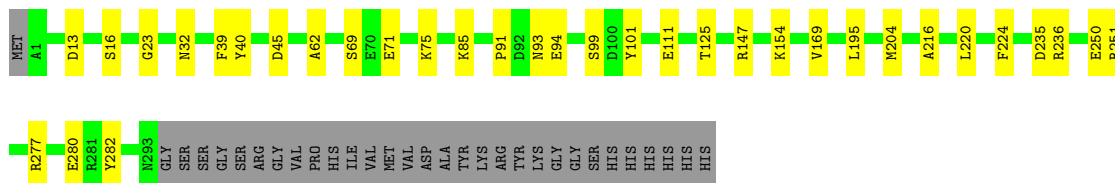
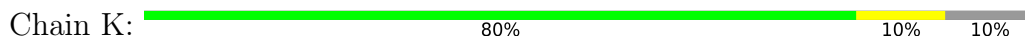


• Molecule 1: alpha hemolysin fused with spy-catcher

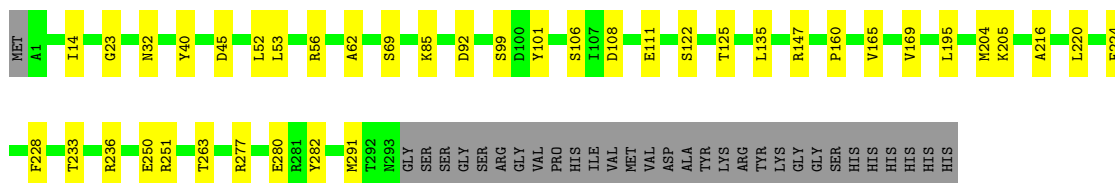
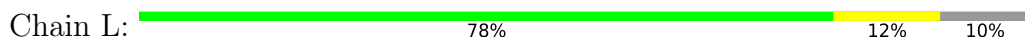




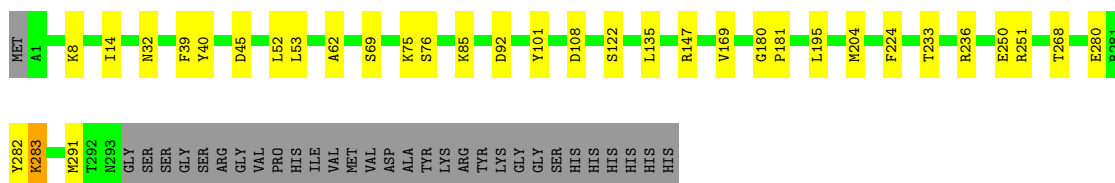
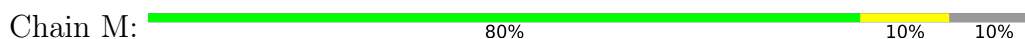
• Molecule 2: alpha hemolysin fused with spy-tag



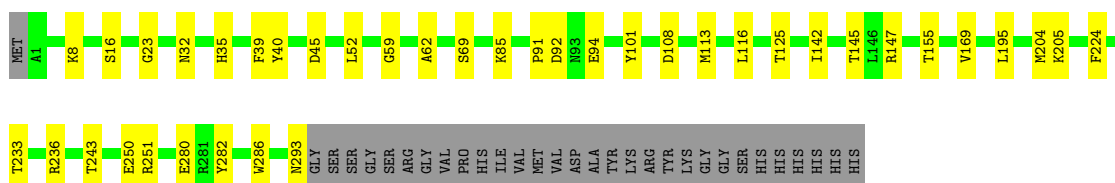
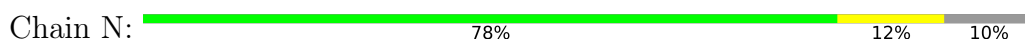
• Molecule 2: alpha hemolysin fused with spy-tag



• Molecule 2: alpha hemolysin fused with spy-tag



• Molecule 2: alpha hemolysin fused with spy-tag



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	349752	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.705	Depositor
Minimum map value	-0.792	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	315.19998, 315.19998, 315.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7879999, 0.7879999, 0.7879999	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.35	0/2397	0.51	0/3246
1	B	0.34	0/2397	0.51	0/3246
1	C	0.34	0/2397	0.51	0/3246
1	D	0.35	0/2397	0.50	0/3246
1	E	0.34	0/2397	0.50	0/3246
1	F	0.34	0/2397	0.50	0/3246
1	G	0.34	0/2397	0.50	0/3246
2	H	0.37	0/2397	0.51	0/3246
2	I	0.37	0/2397	0.51	0/3246
2	J	0.38	0/2397	0.51	0/3246
2	K	0.38	0/2397	0.51	0/3246
2	L	0.38	0/2397	0.50	0/3246
2	M	0.37	0/2397	0.51	0/3246
2	N	0.37	0/2393	0.51	0/3242
All	All	0.36	0/33554	0.51	0/45440

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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	2345	0	2263	20	0
1	B	2345	0	2263	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2345	0	2263	25	0
1	D	2345	0	2263	20	0
1	E	2345	0	2263	19	0
1	F	2345	0	2263	25	0
1	G	2345	0	2263	18	0
2	H	2345	0	2263	17	0
2	I	2345	0	2263	22	0
2	J	2345	0	2263	20	0
2	K	2345	0	2263	20	0
2	L	2345	0	2263	19	0
2	M	2345	0	2263	19	0
2	N	2341	0	2252	21	0
All	All	32826	0	31671	250	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 4.

All (250) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:MET:HG3	1:B:147:ARG:HG3	1.55	0.88
1:B:113:MET:HG3	1:C:147:ARG:HG3	1.58	0.85
1:B:8:LYS:HE3	1:C:16:SER:HB3	1.66	0.78
2:L:111:GLU:OE1	2:L:147:ARG:NH1	2.26	0.69
2:J:85:LYS:HB2	2:J:250:GLU:HB3	1.73	0.69
1:C:85:LYS:HB2	1:C:250:GLU:HB3	1.73	0.69
2:I:147:ARG:HH11	2:I:147:ARG:HG2	1.59	0.68
1:G:24:ASP:OD1	1:G:37:LYS:HE2	1.94	0.67
1:E:85:LYS:HB2	1:E:250:GLU:HB3	1.76	0.67
2:H:147:ARG:HG2	2:H:147:ARG:HH11	1.59	0.67
2:L:85:LYS:HB2	2:L:250:GLU:HB3	1.78	0.66
1:G:85:LYS:HB2	1:G:250:GLU:HB3	1.77	0.66
2:M:85:LYS:HB2	2:M:250:GLU:HB2	1.78	0.66
2:M:147:ARG:HG2	2:M:147:ARG:HH11	1.61	0.65
2:K:45:ASP:O	2:K:236:ARG:NH2	2.30	0.65
1:D:85:LYS:HB2	1:D:250:GLU:HB3	1.78	0.64
1:A:45:ASP:O	1:A:236:ARG:NH2	2.30	0.64
1:B:45:ASP:O	1:B:236:ARG:NH2	2.30	0.64
2:N:85:LYS:HB2	2:N:250:GLU:HB2	1.81	0.63
2:H:85:LYS:HB2	2:H:250:GLU:HB3	1.80	0.63
2:I:45:ASP:O	2:I:236:ARG:NH2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:280:GLU:OE1	2:I:293:ASN:ND2	2.33	0.62
1:B:92:ASP:OD1	1:B:92:ASP:N	2.32	0.62
1:G:45:ASP:O	1:G:236:ARG:NH2	2.32	0.62
2:J:45:ASP:O	2:J:236:ARG:NH2	2.33	0.62
2:L:45:ASP:O	2:L:236:ARG:NH2	2.33	0.62
2:K:71:GLU:HB2	2:K:75:LYS:HG3	1.81	0.62
1:D:45:ASP:O	1:D:236:ARG:NH2	2.33	0.62
2:M:45:ASP:O	2:M:236:ARG:NH2	2.33	0.62
1:C:50:LYS:HD3	1:C:233:THR:HB	1.82	0.61
2:I:85:LYS:HB2	2:I:250:GLU:HB3	1.83	0.61
2:H:45:ASP:O	2:H:236:ARG:NH2	2.32	0.61
1:F:62:ALA:O	1:F:251:ARG:NH1	2.34	0.61
1:C:92:ASP:N	1:C:92:ASP:OD1	2.33	0.60
1:A:85:LYS:HB2	1:A:250:GLU:HB3	1.83	0.60
1:C:62:ALA:O	1:C:251:ARG:NH1	2.33	0.60
1:E:92:ASP:N	1:E:92:ASP:OD1	2.35	0.60
1:F:45:ASP:O	1:F:236:ARG:NH2	2.35	0.60
2:L:125:THR:HG22	2:M:135:LEU:HD12	1.82	0.60
1:E:285:ASP:OD2	1:E:288:LYS:HG2	2.01	0.59
2:K:62:ALA:O	2:K:251:ARG:NH1	2.34	0.59
2:N:45:ASP:O	2:N:236:ARG:NH2	2.34	0.59
2:I:62:ALA:O	2:I:251:ARG:NH1	2.33	0.59
1:E:24:ASP:OD1	1:E:37:LYS:HE2	2.02	0.58
1:A:23:GLY:HA3	1:A:40:TYR:CZ	2.39	0.58
1:G:62:ALA:O	1:G:251:ARG:NH1	2.35	0.58
1:B:85:LYS:HB2	1:B:250:GLU:HB3	1.87	0.57
1:E:62:ALA:O	1:E:251:ARG:NH1	2.36	0.57
2:L:108:ASP:OD1	2:L:108:ASP:N	2.36	0.57
1:G:92:ASP:OD1	1:G:92:ASP:N	2.37	0.56
1:E:127:ASP:HA	1:F:133:GLY:HA2	1.87	0.56
1:A:16:SER:HB3	1:G:8:LYS:HE3	1.86	0.56
1:B:62:ALA:O	1:B:251:ARG:NH1	2.37	0.56
1:E:45:ASP:O	1:E:236:ARG:NH2	2.38	0.56
2:N:62:ALA:O	2:N:251:ARG:NH1	2.40	0.55
2:H:125:THR:HG22	2:I:135:LEU:HD12	1.88	0.55
1:B:111:GLU:OE2	1:B:147:ARG:NH1	2.41	0.54
2:K:125:THR:HG22	2:L:135:LEU:HD12	1.88	0.54
2:M:62:ALA:O	2:M:251:ARG:NH1	2.39	0.54
1:B:8:LYS:HG2	1:C:13:ASP:HB3	1.89	0.54
1:D:62:ALA:O	1:D:251:ARG:NH1	2.37	0.54
2:J:283:LYS:NZ	2:J:283:LYS:HB3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:8:LYS:NZ	2:K:16:SER:HB3	2.21	0.53
2:J:32:ASN:O	2:J:251:ARG:NH2	2.30	0.53
1:A:62:ALA:O	1:A:251:ARG:NH1	2.38	0.53
2:N:147:ARG:HH11	2:N:147:ARG:HG2	1.74	0.53
1:D:280:GLU:OE1	1:D:293:ASN:ND2	2.37	0.53
1:A:133:GLY:HA2	1:G:127:ASP:HA	1.90	0.53
1:C:45:ASP:O	1:C:236:ARG:NH2	2.42	0.53
2:K:32:ASN:O	2:K:251:ARG:NH2	2.28	0.53
2:K:147:ARG:HH11	2:K:147:ARG:HG2	1.73	0.52
2:I:32:ASN:O	2:I:251:ARG:NH2	2.30	0.52
1:G:23:GLY:HA3	1:G:40:TYR:CZ	2.45	0.52
2:H:92:ASP:N	2:H:92:ASP:OD1	2.44	0.51
2:K:85:LYS:HB2	2:K:250:GLU:HB3	1.92	0.51
2:I:147:ARG:HG2	2:I:147:ARG:NH1	2.25	0.50
2:N:92:ASP:OD1	2:N:92:ASP:N	2.45	0.50
1:D:285:ASP:OD1	1:D:288:LYS:HD3	2.11	0.50
1:B:27:THR:HG23	1:B:36:LYS:HB2	1.94	0.50
1:C:23:GLY:HA3	1:C:40:TYR:CZ	2.47	0.50
1:D:70:GLU:HG2	1:D:207:ALA:HB2	1.94	0.50
1:F:23:GLY:HA3	1:F:40:TYR:CZ	2.46	0.50
2:J:62:ALA:O	2:J:251:ARG:NH1	2.38	0.50
1:B:23:GLY:HA3	1:B:40:TYR:CZ	2.47	0.50
1:F:250:GLU:HG3	1:F:277:ARG:HG3	1.92	0.50
2:N:32:ASN:O	2:N:251:ARG:NH2	2.30	0.50
1:F:201:ASN:O	1:F:201:ASN:ND2	2.45	0.49
1:F:280:GLU:HG2	1:F:282:TYR:CZ	2.47	0.49
1:A:39:PHE:HE1	1:G:14:ILE:HD11	1.76	0.49
2:J:147:ARG:HG2	2:J:147:ARG:HH11	1.76	0.49
1:A:91:PRO:HD2	1:A:94:GLU:HG3	1.94	0.49
2:H:32:ASN:O	2:H:251:ARG:NH2	2.29	0.49
1:D:23:GLY:HA3	1:D:40:TYR:CZ	2.48	0.49
1:F:127:ASP:HA	1:G:133:GLY:HA2	1.93	0.49
1:E:111:GLU:OE2	1:F:147:ARG:NH1	2.44	0.48
2:M:92:ASP:N	2:M:92:ASP:OD1	2.42	0.48
1:D:113:MET:HG3	1:E:147:ARG:HG3	1.96	0.48
2:M:32:ASN:O	2:M:251:ARG:NH2	2.29	0.48
1:E:14:ILE:HD11	1:F:39:PHE:HE1	1.78	0.48
2:M:108:ASP:OD1	2:M:108:ASP:N	2.42	0.48
1:D:111:GLU:OE1	1:D:147:ARG:NH2	2.39	0.48
1:E:70:GLU:HG2	1:E:207:ALA:HB2	1.96	0.48
2:L:32:ASN:O	2:L:251:ARG:NH2	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:108:ASP:OD1	2:N:108:ASP:N	2.36	0.48
2:N:116:LEU:HD23	2:N:142:ILE:HG12	1.94	0.48
1:F:96:ALA:O	1:F:163:LYS:NZ	2.46	0.48
2:K:111:GLU:OE2	2:K:147:ARG:NH2	2.46	0.48
2:L:62:ALA:O	2:L:251:ARG:NH1	2.41	0.48
2:J:8:LYS:HZ2	2:K:16:SER:HB3	1.78	0.47
1:F:14:ILE:HD11	1:G:39:PHE:HE1	1.79	0.47
1:F:203:SER:O	1:F:203:SER:OG	2.28	0.47
1:B:96:ALA:O	1:B:163:LYS:NZ	2.47	0.47
2:H:62:ALA:O	2:H:251:ARG:NH1	2.44	0.47
1:C:50:LYS:HB2	1:C:234:MET:O	2.14	0.47
2:K:23:GLY:HA3	2:K:40:TYR:CZ	2.50	0.46
1:A:242:GLN:HG2	1:A:283:LYS:HE3	1.97	0.46
1:C:32:ASN:O	1:C:251:ARG:NH2	2.36	0.46
2:I:108:ASP:OD1	2:I:108:ASP:N	2.36	0.46
1:C:31:GLU:CD	1:C:31:GLU:H	2.19	0.46
1:E:96:ALA:O	1:E:163:LYS:NZ	2.47	0.46
1:D:88:LEU:HD22	1:D:230:THR:HG21	1.97	0.46
1:G:88:LEU:HD22	1:G:230:THR:HG21	1.97	0.46
2:I:169:VAL:HG21	2:I:224:PHE:CZ	2.51	0.46
1:A:39:PHE:CE1	1:G:14:ILE:HD11	2.51	0.45
1:C:70:GLU:HG2	1:C:207:ALA:HB2	1.98	0.45
2:K:147:ARG:HG2	2:K:147:ARG:NH1	2.31	0.45
2:M:283:LYS:NZ	2:M:283:LYS:HB3	2.32	0.45
1:F:91:PRO:HD2	1:F:94:GLU:HG3	1.98	0.45
2:L:280:GLU:HG2	2:L:282:TYR:CZ	2.52	0.45
2:N:147:ARG:HG2	2:N:147:ARG:NH1	2.31	0.45
1:F:8:LYS:HE2	1:G:13:ASP:HB2	1.98	0.45
1:A:280:GLU:HG2	1:A:282:TYR:CZ	2.52	0.45
2:H:8:LYS:NZ	2:I:16:SER:HB3	2.32	0.45
1:B:127:ASP:HA	1:C:133:GLY:HA2	1.97	0.45
1:C:284:ILE:HD13	1:C:291:MET:HG3	1.98	0.45
2:M:169:VAL:HG21	2:M:224:PHE:CZ	2.52	0.45
1:A:13:ASP:HB3	1:G:8:LYS:HG2	1.98	0.45
1:A:203:SER:O	1:A:203:SER:OG	2.30	0.45
2:J:8:LYS:HE3	2:K:13:ASP:HB2	1.97	0.44
2:H:23:GLY:HA3	2:H:40:TYR:CZ	2.52	0.44
2:J:113:MET:HB3	2:J:145:THR:HB	1.98	0.44
2:K:169:VAL:HG21	2:K:224:PHE:CZ	2.52	0.44
1:C:128:ASP:OD2	1:D:132:ILE:N	2.42	0.44
1:D:32:ASN:O	1:D:251:ARG:NH2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:280:GLU:HG2	2:N:282:TYR:CZ	2.53	0.44
1:D:91:PRO:HD2	1:D:94:GLU:HG3	1.99	0.44
2:J:147:ARG:HG2	2:J:147:ARG:NH1	2.32	0.44
2:M:8:LYS:NZ	2:N:16:SER:HB3	2.32	0.44
1:A:14:ILE:HD11	1:B:39:PHE:HE1	1.83	0.44
1:E:50:LYS:HD3	1:E:233:THR:HB	2.00	0.44
1:G:65:TYR:CE2	1:G:78:LEU:HD21	2.52	0.44
2:H:147:ARG:HG2	2:H:147:ARG:NH1	2.26	0.44
2:N:23:GLY:HA3	2:N:40:TYR:CZ	2.53	0.44
2:J:14:ILE:HD11	2:K:39:PHE:HE1	1.83	0.44
1:D:284:ILE:HD13	1:D:291:MET:HG3	1.99	0.44
1:F:50:LYS:HD3	1:F:233:THR:HB	2.00	0.43
2:L:169:VAL:HG21	2:L:224:PHE:CZ	2.53	0.43
1:F:70:GLU:HG2	1:F:207:ALA:HB2	2.00	0.43
2:H:216:ALA:HB1	2:H:220:LEU:HD12	2.00	0.43
2:J:216:ALA:HB1	2:J:220:LEU:HD12	1.99	0.43
1:D:27:THR:HG23	1:D:36:LYS:HB2	2.00	0.43
1:E:23:GLY:HA3	1:E:40:TYR:CZ	2.53	0.43
2:I:75:LYS:HB3	2:I:75:LYS:HE3	1.70	0.43
2:L:52:LEU:CD2	2:L:233:THR:HG22	2.49	0.43
2:N:91:PRO:HD2	2:N:94:GLU:HG3	2.01	0.43
1:A:135:LEU:C	1:A:136:ILE:HD13	2.39	0.43
2:L:23:GLY:HA3	2:L:40:TYR:CZ	2.53	0.43
2:M:40:TYR:HB2	2:M:53:LEU:HD11	1.99	0.43
2:I:280:GLU:HG2	2:I:282:TYR:CZ	2.53	0.43
2:J:169:VAL:HG21	2:J:224:PHE:CZ	2.53	0.43
2:N:52:LEU:CD2	2:N:233:THR:HG22	2.48	0.43
1:A:50:LYS:HD3	1:A:233:THR:HB	2.01	0.43
1:F:287:GLU:H	1:F:287:GLU:HG2	1.65	0.43
1:G:280:GLU:HG2	1:G:282:TYR:CZ	2.54	0.43
2:K:154:LYS:O	2:K:169:VAL:HA	2.19	0.43
2:K:280:GLU:HG2	2:K:282:TYR:CZ	2.54	0.43
2:L:92:ASP:OD1	2:L:92:ASP:N	2.51	0.43
2:L:160:PRO:HB3	2:L:165:VAL:HG23	2.01	0.43
1:D:216:ALA:HB1	1:D:220:LEU:HD12	2.01	0.43
1:F:242:GLN:HG2	1:F:283:LYS:HE2	2.00	0.43
1:B:50:LYS:HD3	1:B:233:THR:HB	2.01	0.42
1:B:65:TYR:CE2	1:B:78:LEU:HD21	2.54	0.42
2:I:117:THR:HG23	2:I:141:SER:HB3	2.01	0.42
2:K:216:ALA:HB1	2:K:220:LEU:HD12	2.01	0.42
1:B:280:GLU:HG2	1:B:282:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:52:LEU:CD2	2:I:233:THR:HG22	2.49	0.42
2:M:75:LYS:HE3	2:M:75:LYS:HB3	1.71	0.42
2:H:96:ALA:O	2:H:163:LYS:NZ	2.52	0.42
2:L:14:ILE:HD11	2:M:39:PHE:HE1	1.84	0.42
1:A:14:ILE:HD11	1:B:39:PHE:CE1	2.55	0.42
2:M:280:GLU:HG2	2:M:282:TYR:CZ	2.54	0.42
1:E:14:ILE:HD11	1:F:39:PHE:CE1	2.55	0.42
1:F:32:ASN:O	1:F:251:ARG:NH2	2.37	0.42
2:H:13:ASP:HB2	2:N:8:LYS:HD2	2.00	0.42
2:H:163:LYS:HA	2:H:163:LYS:HD3	1.85	0.42
2:N:205:LYS:HB3	2:N:205:LYS:HE3	1.74	0.42
1:E:135:LEU:C	1:E:136:ILE:HD13	2.40	0.42
1:F:14:ILE:HD11	1:G:39:PHE:CE1	2.55	0.42
1:C:91:PRO:HD2	1:C:94:GLU:HG3	2.01	0.42
1:C:96:ALA:O	1:C:163:LYS:NZ	2.53	0.42
1:B:14:ILE:HD11	1:C:39:PHE:HE1	1.85	0.42
1:C:280:GLU:HG2	1:C:282:TYR:CZ	2.55	0.42
1:C:285:ASP:OD2	1:C:288:LYS:HD3	2.20	0.42
1:E:32:ASN:O	1:E:251:ARG:NH2	2.34	0.42
2:I:40:TYR:HB2	2:I:53:LEU:HD11	2.02	0.42
2:J:280:GLU:HG2	2:J:282:TYR:CZ	2.55	0.42
1:A:284:ILE:HD13	1:A:291:MET:HG3	2.02	0.42
1:B:14:ILE:HD11	1:C:39:PHE:CE1	2.55	0.42
1:E:111:GLU:OE1	1:E:147:ARG:NH1	2.53	0.42
2:K:93:ASN:OD1	2:K:93:ASN:N	2.54	0.41
2:N:169:VAL:HG21	2:N:224:PHE:CZ	2.54	0.41
1:A:160:PRO:HB3	1:A:165:VAL:HG23	2.01	0.41
2:I:216:ALA:HB1	2:I:220:LEU:HD12	2.02	0.41
1:C:135:LEU:C	1:C:136:ILE:HD13	2.40	0.41
2:L:56:ARG:HA	2:L:228:PHE:O	2.20	0.41
2:M:14:ILE:HD11	2:N:39:PHE:HE1	1.84	0.41
2:N:113:MET:HB3	2:N:145:THR:HB	2.03	0.41
1:B:154:LYS:O	1:B:169:VAL:HA	2.21	0.41
1:F:212:ASP:OD2	1:F:214:ASN:HB2	2.20	0.41
2:J:52:LEU:CD2	2:J:233:THR:HG22	2.50	0.41
2:N:243:THR:HG1	2:N:286:TRP:HE1	1.66	0.41
1:E:280:GLU:HG2	1:E:282:TYR:CZ	2.56	0.41
2:H:52:LEU:CD2	2:H:233:THR:HG22	2.50	0.41
2:H:169:VAL:HG21	2:H:224:PHE:CZ	2.56	0.41
2:J:23:GLY:HA3	2:J:40:TYR:CZ	2.55	0.41
2:J:154:LYS:O	2:J:169:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:PRO:HB3	1:F:165:VAL:HG23	2.02	0.41
2:I:240:LYS:HB3	2:I:240:LYS:HE3	1.78	0.41
1:D:116:LEU:HD23	1:D:142:ILE:HG13	2.03	0.41
1:D:212:ASP:OD2	1:D:214:ASN:HB2	2.20	0.41
2:I:14:ILE:HD11	2:J:39:PHE:HE1	1.86	0.41
2:M:52:LEU:CD2	2:M:233:THR:HG22	2.51	0.41
2:I:154:LYS:O	2:I:169:VAL:HA	2.21	0.41
1:C:50:LYS:HE2	1:C:50:LYS:HB3	1.89	0.40
1:C:101:TYR:CZ	1:C:160:PRO:HG2	2.56	0.40
2:J:111:GLU:OE1	2:J:147:ARG:NH2	2.54	0.40
2:K:91:PRO:HD2	2:K:94:GLU:HG3	2.02	0.40
1:D:65:TYR:CE2	1:D:78:LEU:HD21	2.56	0.40
2:I:23:GLY:HA3	2:I:40:TYR:CZ	2.56	0.40
2:L:204:MET:HG2	2:L:205:LYS:O	2.22	0.40
2:M:180:GLY:HA3	2:M:181:PRO:HA	1.98	0.40
1:B:91:PRO:HD2	1:B:94:GLU:HG3	2.04	0.40
1:F:163:LYS:HA	1:F:163:LYS:HD3	1.90	0.40
2:L:40:TYR:HB2	2:L:53:LEU:HD11	2.03	0.40
2:H:154:LYS:O	2:H:169:VAL:HA	2.22	0.40
2:I:101:TYR:CZ	2:I:160:PRO:HG2	2.57	0.40
2:L:216:ALA:HB1	2:L:220:LEU:HD12	2.03	0.40
2:N:35:HIS:O	2:N:59:GLY:HA3	2.21	0.40
1:D:50:LYS:HD3	1:D:233:THR:HB	2.03	0.40
2:M:147:ARG:HG2	2:M:147:ARG:NH1	2.31	0.40

There are no symmetry-related clashes.

## 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	291/421 (69%)	285 (98%)	6 (2%)	0	<a href="#">100</a> <a href="#">100</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	291/421 (69%)	283 (97%)	8 (3%)	0	100	100
1	C	291/421 (69%)	286 (98%)	5 (2%)	0	100	100
1	D	291/421 (69%)	287 (99%)	4 (1%)	0	100	100
1	E	291/421 (69%)	287 (99%)	4 (1%)	0	100	100
1	F	291/421 (69%)	285 (98%)	6 (2%)	0	100	100
1	G	291/421 (69%)	285 (98%)	6 (2%)	0	100	100
2	H	291/324 (90%)	285 (98%)	6 (2%)	0	100	100
2	I	291/324 (90%)	284 (98%)	7 (2%)	0	100	100
2	J	291/324 (90%)	286 (98%)	5 (2%)	0	100	100
2	K	291/324 (90%)	285 (98%)	6 (2%)	0	100	100
2	L	291/324 (90%)	284 (98%)	7 (2%)	0	100	100
2	M	291/324 (90%)	287 (99%)	4 (1%)	0	100	100
2	N	291/324 (90%)	286 (98%)	5 (2%)	0	100	100
All	All	4074/5215 (78%)	3995 (98%)	79 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	260/363 (72%)	250 (96%)	10 (4%)	33	42
1	B	260/363 (72%)	249 (96%)	11 (4%)	30	38
1	C	260/363 (72%)	250 (96%)	10 (4%)	33	42
1	D	260/363 (72%)	250 (96%)	10 (4%)	33	42
1	E	260/363 (72%)	252 (97%)	8 (3%)	40	51
1	F	260/363 (72%)	252 (97%)	8 (3%)	40	51
1	G	260/363 (72%)	251 (96%)	9 (4%)	36	46
2	H	260/285 (91%)	249 (96%)	11 (4%)	30	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	260/285 (91%)	252 (97%)	8 (3%)	40	51
2	J	260/285 (91%)	254 (98%)	6 (2%)	50	63
2	K	260/285 (91%)	253 (97%)	7 (3%)	44	57
2	L	260/285 (91%)	251 (96%)	9 (4%)	36	46
2	M	260/285 (91%)	251 (96%)	9 (4%)	36	46
2	N	259/285 (91%)	252 (97%)	7 (3%)	44	57
All	All	3639/4536 (80%)	3516 (97%)	123 (3%)	40	47

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	37	LYS
1	A	69	SER
1	A	78	LEU
1	A	101	TYR
1	A	110	LYS
1	A	114	SER
1	A	131	LYS
1	A	132	ILE
1	A	201	ASN
1	B	17	ASN
1	B	37	LYS
1	B	69	SER
1	B	101	TYR
1	B	115	THR
1	B	174	MET
1	B	201	ASN
1	B	204	MET
1	B	205	LYS
1	B	263	THR
1	B	279	SER
1	C	69	SER
1	C	89	GLN
1	C	92	ASP
1	C	101	TYR
1	C	114	SER
1	C	201	ASN
1	C	205	LYS
1	C	212	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	263	THR
1	C	283	LYS
1	D	37	LYS
1	D	101	TYR
1	D	116	LEU
1	D	125	THR
1	D	128	ASP
1	D	205	LYS
1	D	230	THR
1	D	263	THR
1	D	273	LYS
1	D	291	MET
1	E	69	SER
1	E	78	LEU
1	E	101	TYR
1	E	106	SER
1	E	195	LEU
1	E	201	ASN
1	E	205	LYS
1	E	283	LYS
1	F	71	GLU
1	F	101	TYR
1	F	106	SER
1	F	125	THR
1	F	131	LYS
1	F	155	THR
1	F	204	MET
1	F	263	THR
1	G	24	ASP
1	G	92	ASP
1	G	99	SER
1	G	101	TYR
1	G	106	SER
1	G	131	LYS
1	G	204	MET
1	G	230	THR
1	G	279	SER
2	H	9	THR
2	H	69	SER
2	H	76	SER
2	H	99	SER
2	H	101	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	106	SER
2	H	141	SER
2	H	195	LEU
2	H	204	MET
2	H	234	MET
2	H	293	ASN
2	I	99	SER
2	I	101	TYR
2	I	122	SER
2	I	195	LEU
2	I	204	MET
2	I	235	ASP
2	I	276	ASP
2	I	278	SER
2	J	69	SER
2	J	101	TYR
2	J	109	THR
2	J	203	SER
2	J	204	MET
2	J	263	THR
2	K	69	SER
2	K	99	SER
2	K	101	TYR
2	K	195	LEU
2	K	204	MET
2	K	235	ASP
2	K	277	ARG
2	L	69	SER
2	L	99	SER
2	L	101	TYR
2	L	106	SER
2	L	122	SER
2	L	195	LEU
2	L	263	THR
2	L	277	ARG
2	L	291	MET
2	M	69	SER
2	M	76	SER
2	M	101	TYR
2	M	122	SER
2	M	195	LEU
2	M	204	MET

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Mol	Chain	Res	Type
2	M	268	THR
2	M	283	LYS
2	M	291	MET
2	N	69	SER
2	N	101	TYR
2	N	125	THR
2	N	155	THR
2	N	195	LEU
2	N	204	MET
2	N	293	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	178	ASN
2	H	178	ASN
2	K	178	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no 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

There are no chain breaks in this entry.

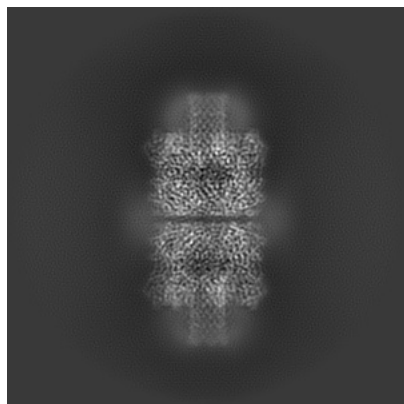
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36689. These allow visual inspection of the internal detail of the map and identification of artifacts.

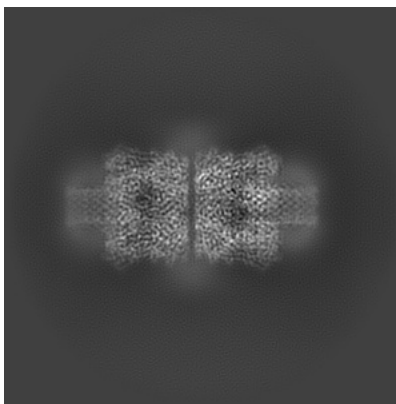
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

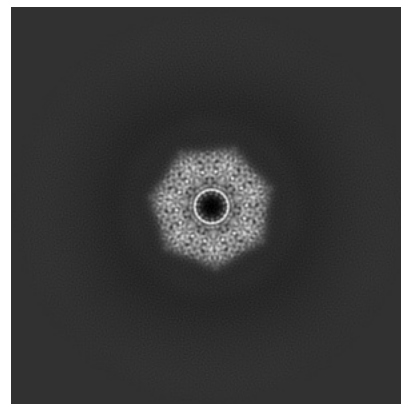
#### 6.1.1 Primary map



X

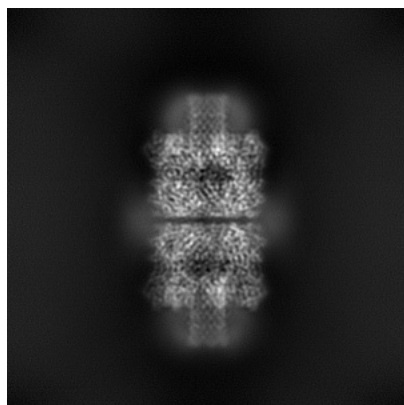


Y

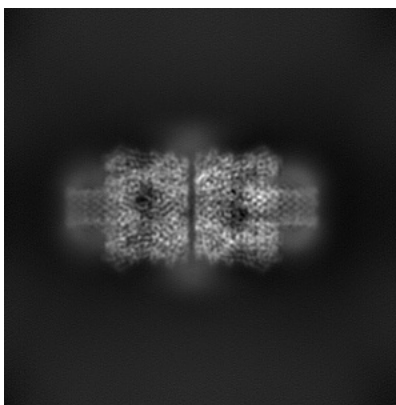


Z

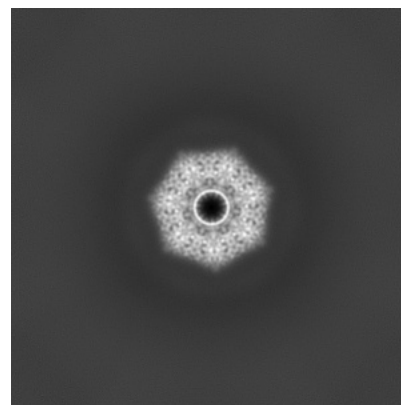
#### 6.1.2 Raw map



X



Y

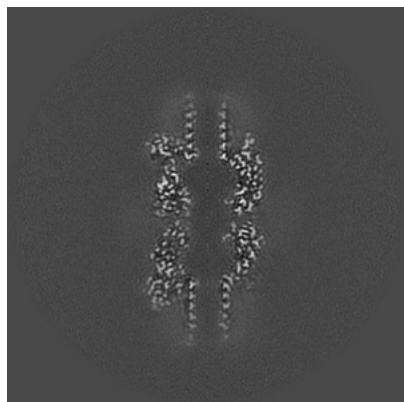


Z

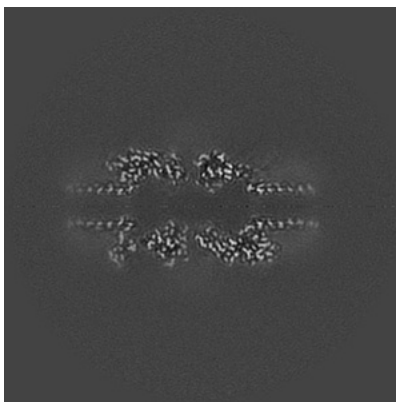
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

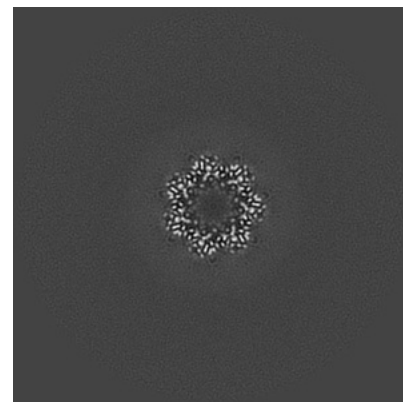
### 6.2.1 Primary map



X Index: 200

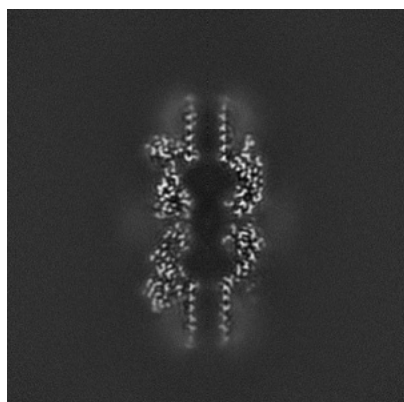


Y Index: 200

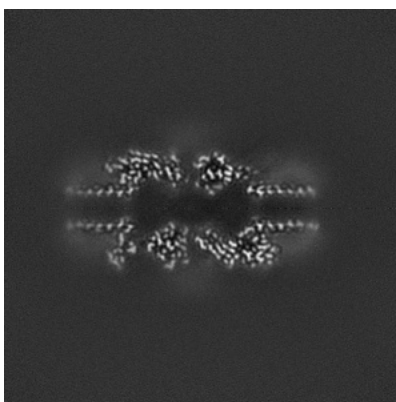


Z Index: 200

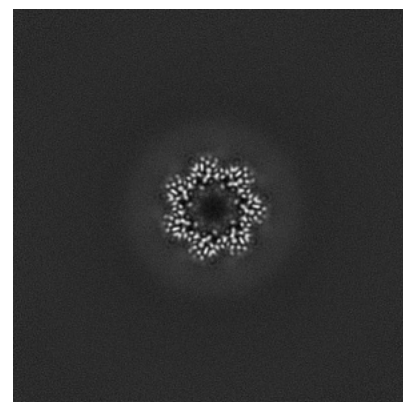
### 6.2.2 Raw map



X Index: 200



Y Index: 200

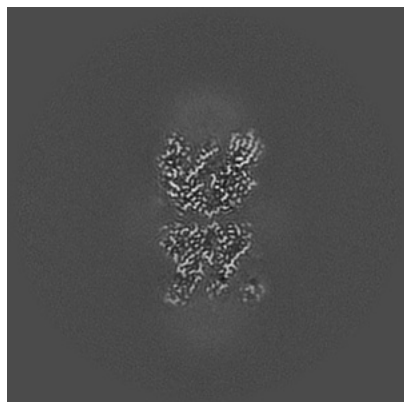


Z Index: 200

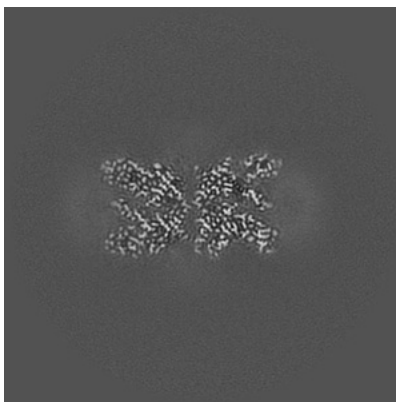
The images above show central slices of the map in three orthogonal directions.

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

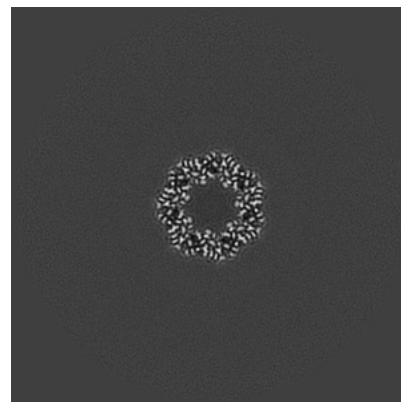
### 6.3.1 Primary map



X Index: 170

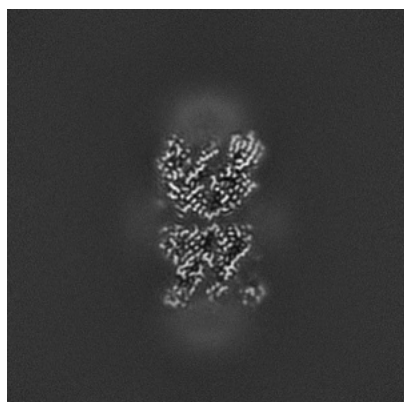


Y Index: 171

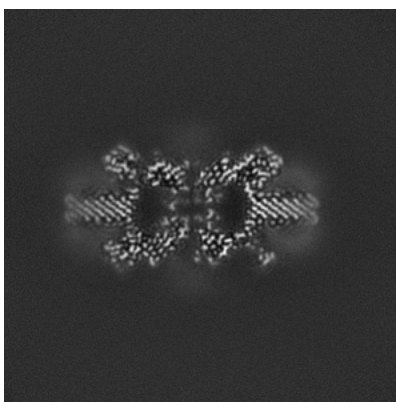


Z Index: 221

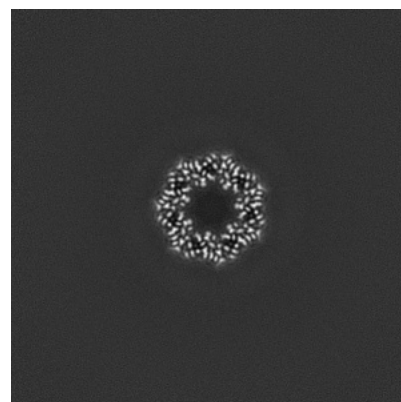
### 6.3.2 Raw map



X Index: 170



Y Index: 216



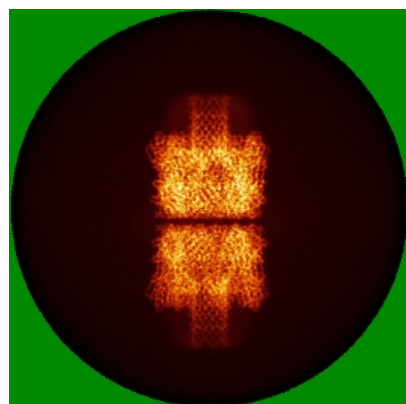
Z Index: 221

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

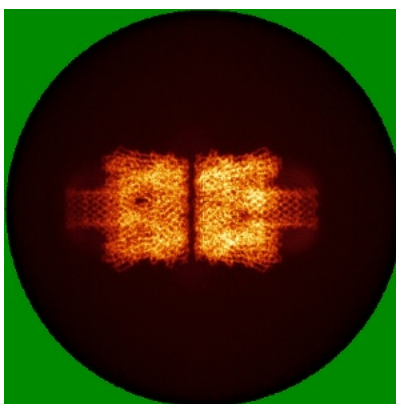


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

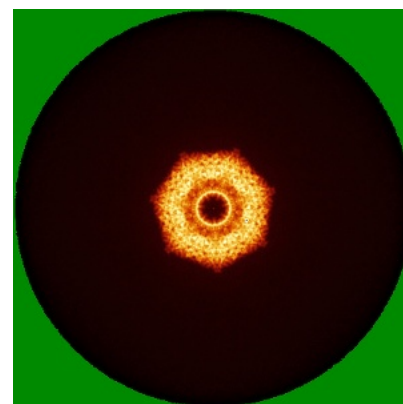
### 6.4.1 Primary map



X

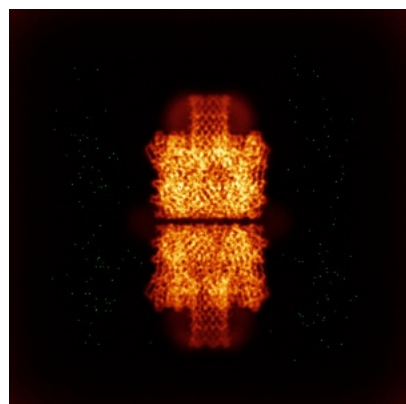


Y

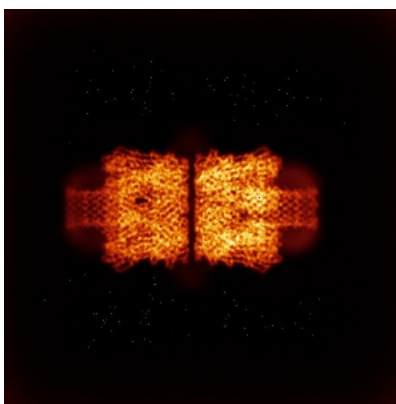


Z

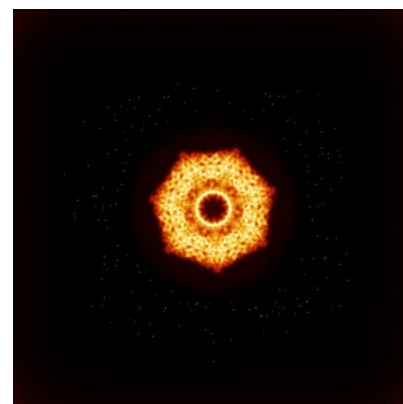
### 6.4.2 Raw map



X



Y

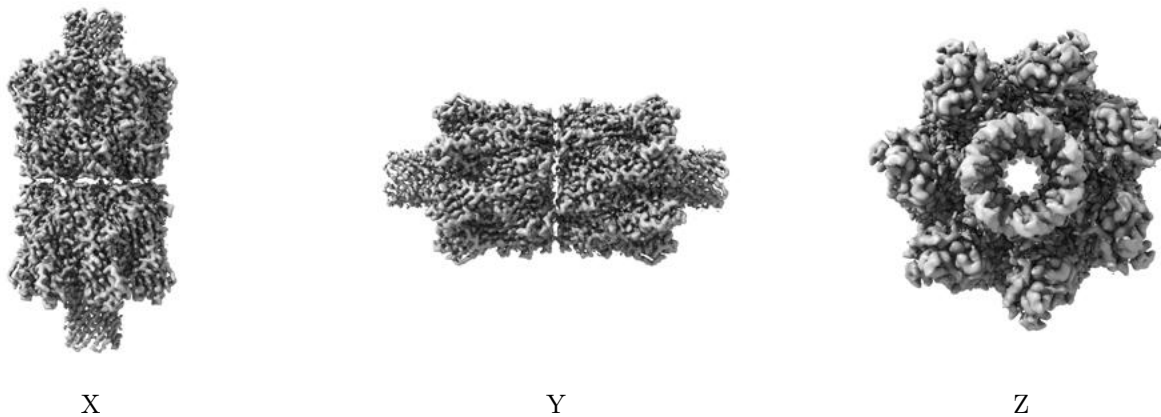


Z

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

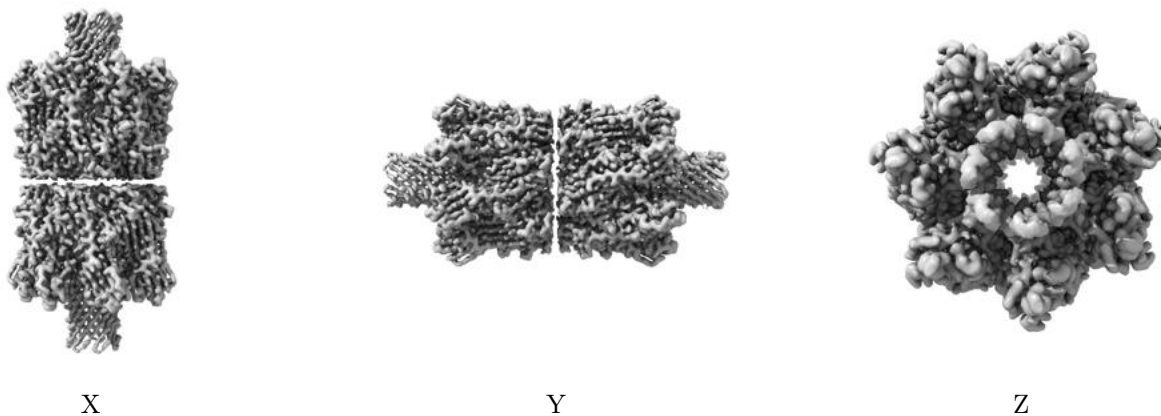
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

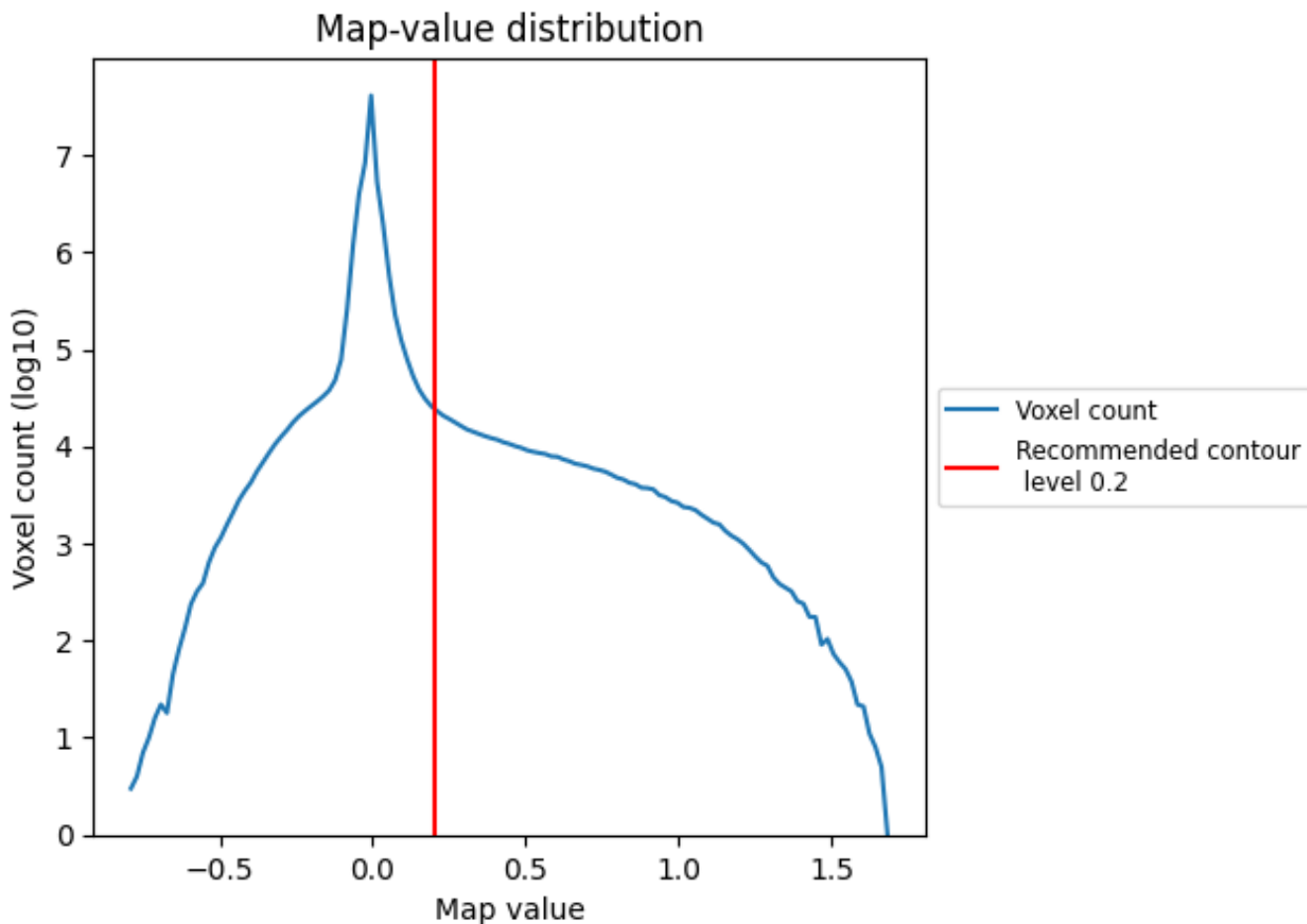
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

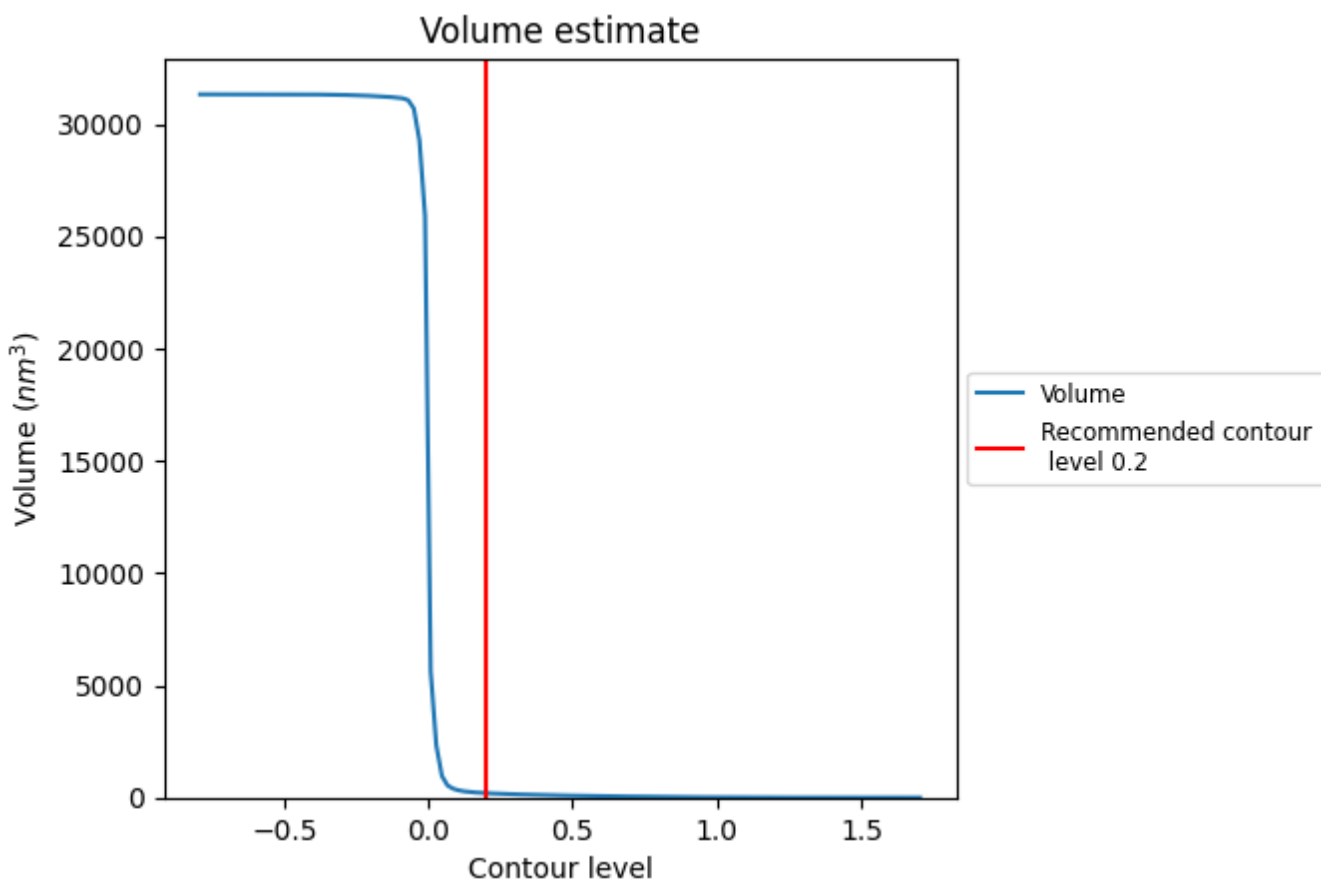
This section contains the results of statistical analysis of the map.

### 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.

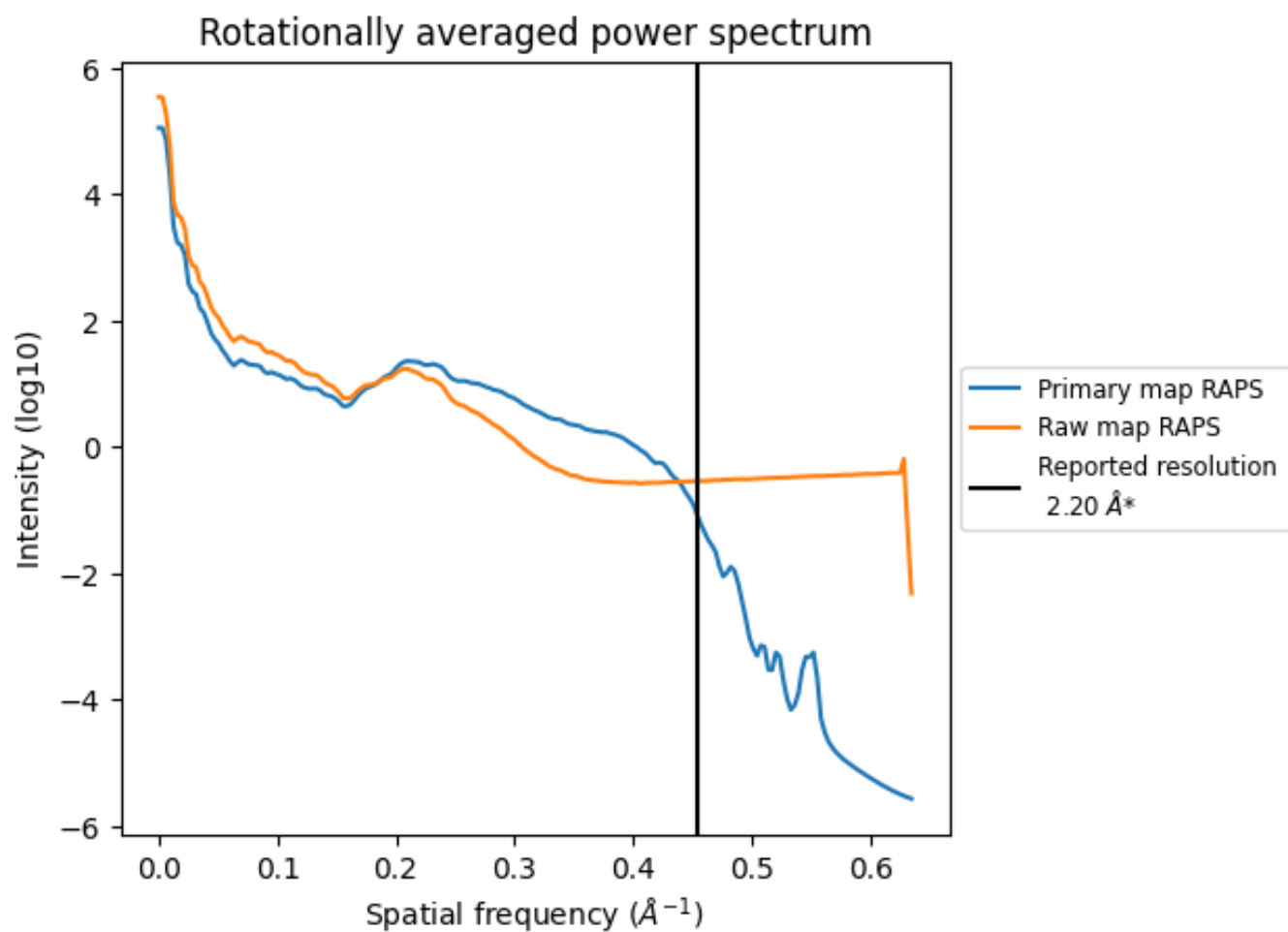
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm<sup>3</sup>; this corresponds to an approximate mass of 178 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

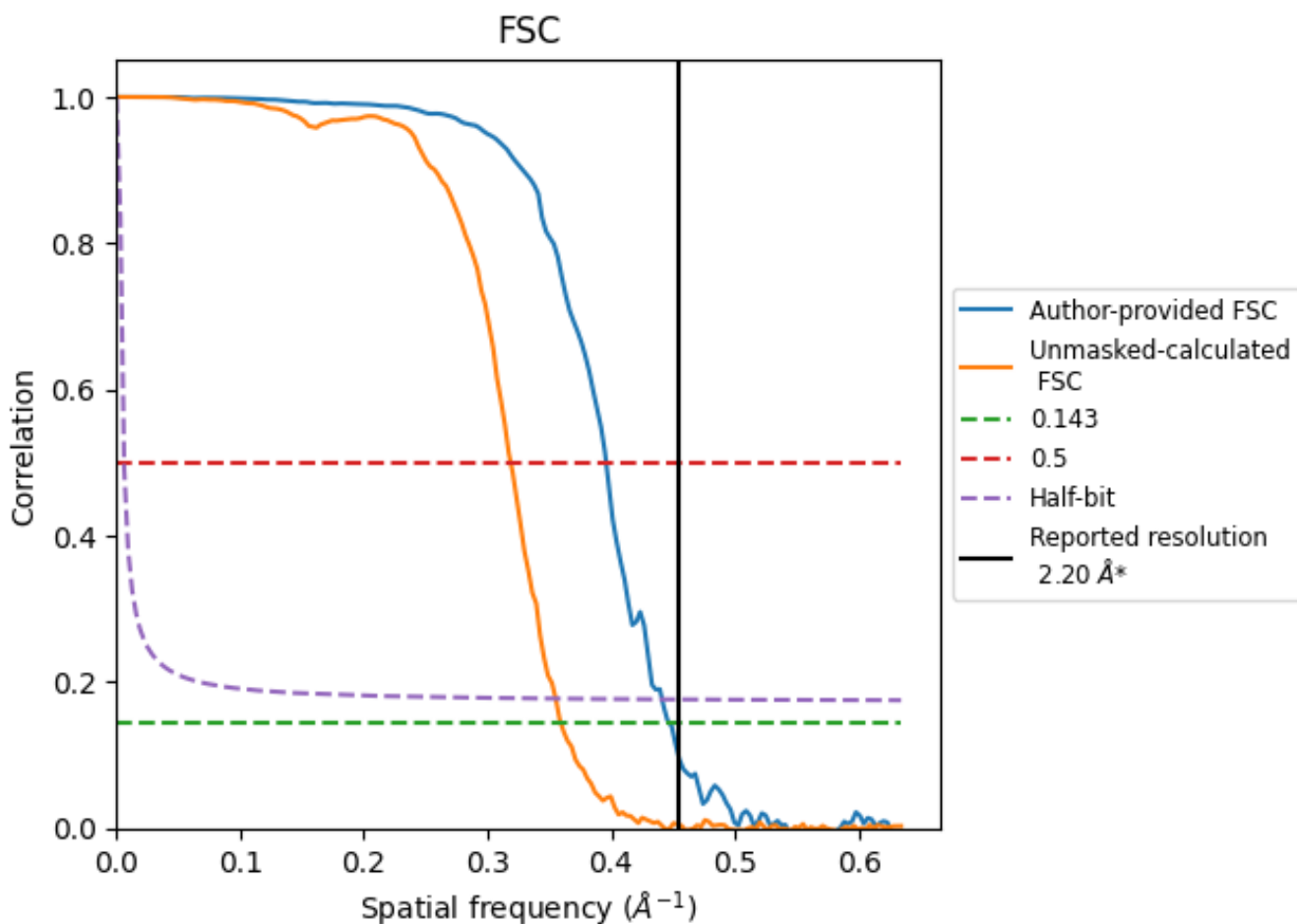


\*Reported resolution corresponds to spatial frequency of  $0.455 \text{ \AA}^{-1}$

## 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 0.455 Å<sup>-1</sup>

## 8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.24	2.53	2.27
Unmasked-calculated*	2.78	3.14	2.81

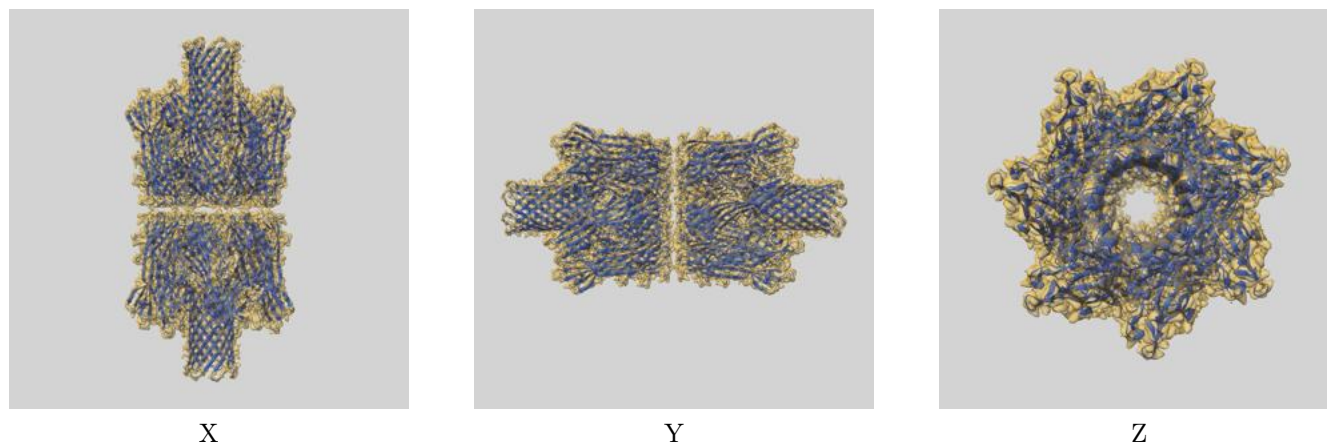
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.78 differs from the reported value 2.2 by more than 10 %



## 9 Map-model fit [i](#)

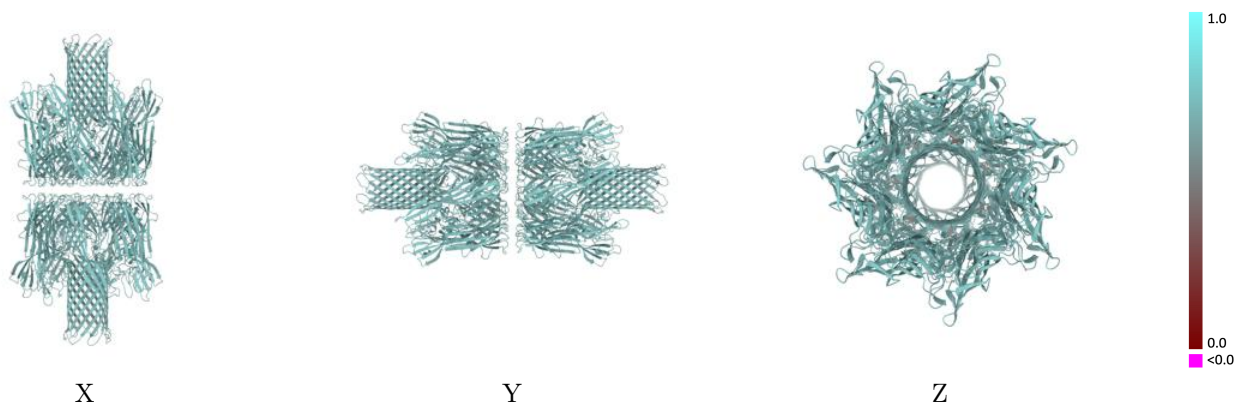
This section contains information regarding the fit between EMDB map EMD-36689 and PDB model 8JX3. Per-residue inclusion information can be found in section 3 on page 33.

### 9.1 Map-model overlay [i](#)



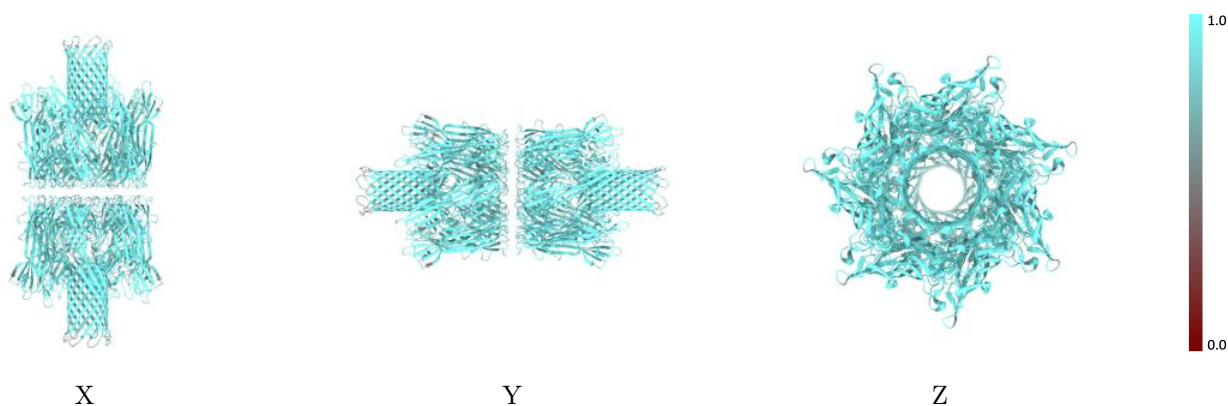
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



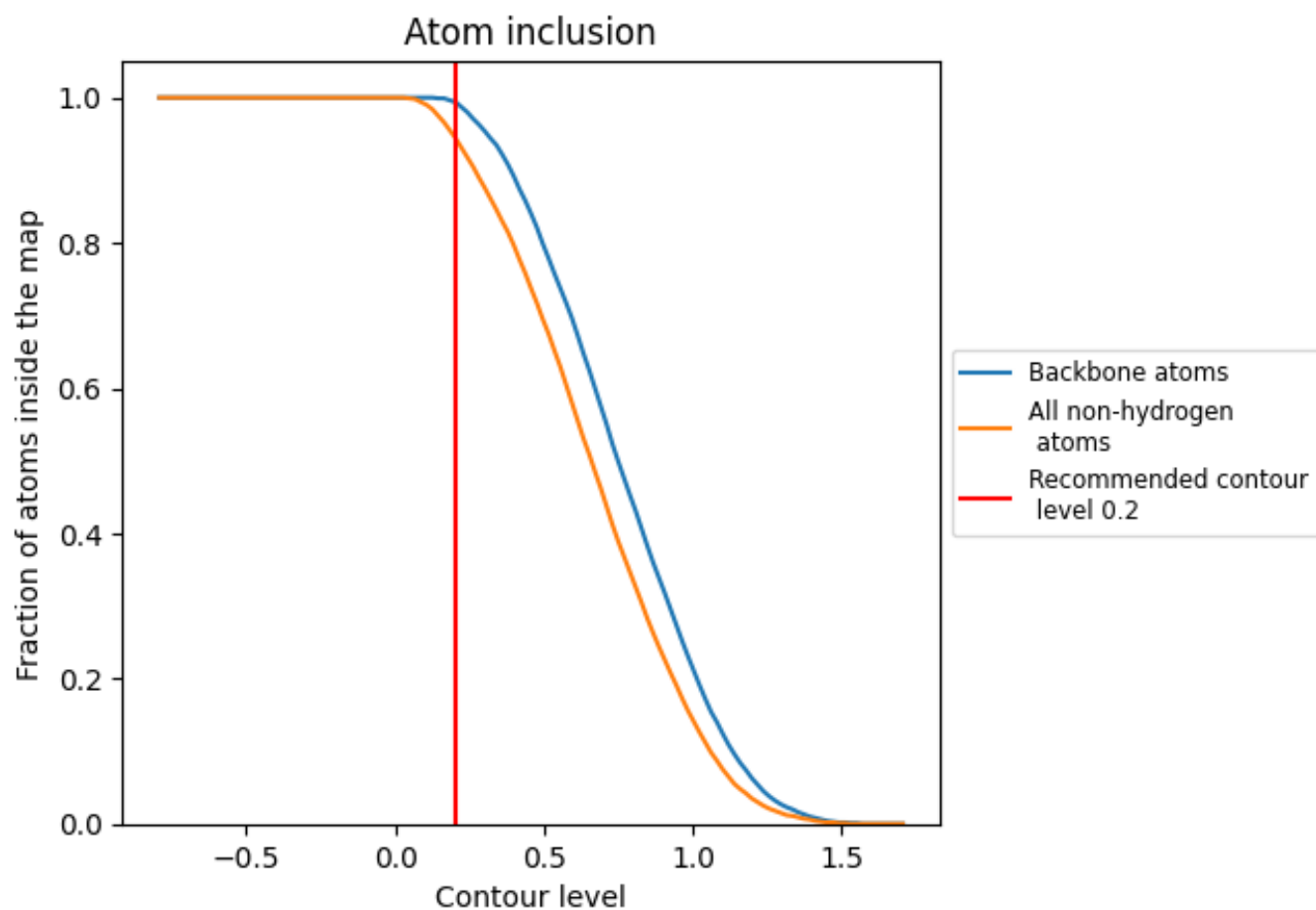
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 95% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9460	 0.6810
A	 0.9350	 0.6780
B	 0.9360	 0.6770
C	 0.9350	 0.6790
D	 0.9340	 0.6800
E	 0.9390	 0.6780
F	 0.9370	 0.6780
G	 0.9370	 0.6780
H	 0.9560	 0.6840
I	 0.9540	 0.6830
J	 0.9560	 0.6840
K	 0.9530	 0.6830
L	 0.9560	 0.6830
M	 0.9570	 0.6840
N	 0.9550	 0.6840

