



wwPDB EM Validation Summary Report ⓘ

Jul 13, 2026 – 03:36 pm BST

PDB ID : 9HXJ / pdb_00009hxj
EMDB ID : EMD-52479
Title : Bacterial antiviral defense protein Ec3ApeA from Escherichia coli strain KK-NP016
Authors : Sasnauskas, G.; Juozapaitis, J.; Puteikiene, R.; Tamulaitiene, G.
Deposited on : 2025-01-08
Resolution : 3.00 Å(reported)
Based on initial model : .

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

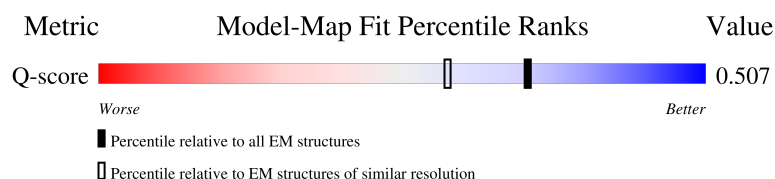
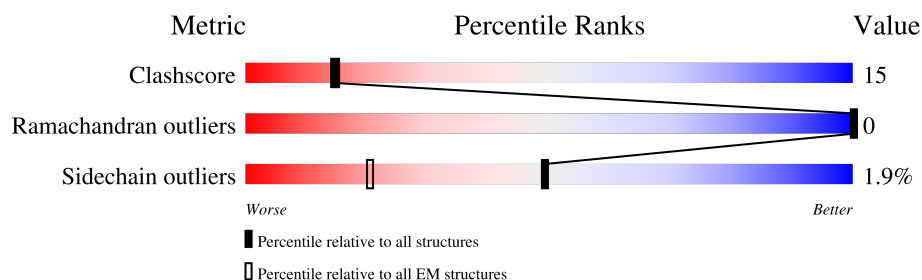
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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.



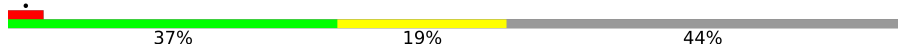
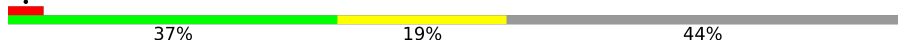
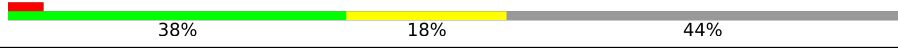
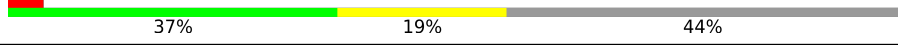
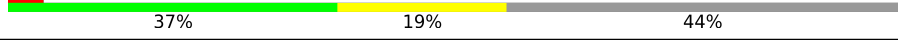
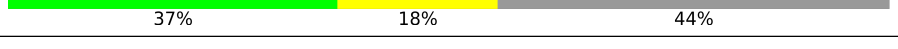
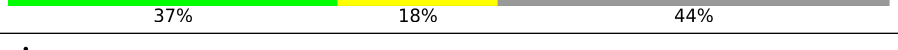
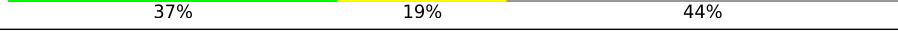
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	1029	37% 19% 44%
1	B	1029	37% 18% 44%
1	C	1029	37% 19% 44%
1	D	1029	37% 19% 44%

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Mol	Chain	Length	Quality of chain
1	E	1029	
1	F	1029	
1	G	1029	
1	H	1029	
1	I	1029	
1	J	1029	
1	K	1029	
1	L	1029	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 53808 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 Maltose/maltodextrin-binding periplasmic protein,Bacterial antiviral defense protein Ec3ApeA from Escherichia coli strain KK-NP016.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	B	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	C	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	D	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	E	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	F	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	G	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	H	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	I	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	J	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	K	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		
1	L	575	Total	C	N	O	S	0	0
			4483	2911	762	797	13		

There are 1044 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-444	MET	-	initiating methionine	UNP P0AEX9
A	-443	GLY	-	expression tag	UNP P0AEX9
A	-442	GLY	-	expression tag	UNP P0AEX9
A	-441	SER	-	expression tag	UNP P0AEX9
A	-440	ALA	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-439	TRP	-	expression tag	UNP P0AEX9
A	-438	SER	-	expression tag	UNP P0AEX9
A	-437	HIS	-	expression tag	UNP P0AEX9
A	-436	PRO	-	expression tag	UNP P0AEX9
A	-435	GLN	-	expression tag	UNP P0AEX9
A	-434	PHE	-	expression tag	UNP P0AEX9
A	-433	GLU	-	expression tag	UNP P0AEX9
A	-432	LYS	-	expression tag	UNP P0AEX9
A	-431	GLY	-	expression tag	UNP P0AEX9
A	-430	GLY	-	expression tag	UNP P0AEX9
A	-429	GLY	-	expression tag	UNP P0AEX9
A	-428	SER	-	expression tag	UNP P0AEX9
A	-427	GLY	-	expression tag	UNP P0AEX9
A	-426	GLY	-	expression tag	UNP P0AEX9
A	-425	GLY	-	expression tag	UNP P0AEX9
A	-424	SER	-	expression tag	UNP P0AEX9
A	-423	GLY	-	expression tag	UNP P0AEX9
A	-422	GLY	-	expression tag	UNP P0AEX9
A	-421	SER	-	expression tag	UNP P0AEX9
A	-420	ALA	-	expression tag	UNP P0AEX9
A	-419	TRP	-	expression tag	UNP P0AEX9
A	-418	SER	-	expression tag	UNP P0AEX9
A	-417	HIS	-	expression tag	UNP P0AEX9
A	-416	PRO	-	expression tag	UNP P0AEX9
A	-415	GLN	-	expression tag	UNP P0AEX9
A	-414	PHE	-	expression tag	UNP P0AEX9
A	-413	GLU	-	expression tag	UNP P0AEX9
A	-412	LYS	-	expression tag	UNP P0AEX9
A	-411	GLY	-	expression tag	UNP P0AEX9
A	-410	SER	-	expression tag	UNP P0AEX9
A	-409	MET	-	expression tag	UNP P0AEX9
A	-408	GLY	-	expression tag	UNP P0AEX9
A	-407	GLY	-	expression tag	UNP P0AEX9
A	-406	SER	-	expression tag	UNP P0AEX9
A	-405	HIS	-	expression tag	UNP P0AEX9
A	-404	HIS	-	expression tag	UNP P0AEX9
A	-403	HIS	-	expression tag	UNP P0AEX9
A	-402	HIS	-	expression tag	UNP P0AEX9
A	-401	HIS	-	expression tag	UNP P0AEX9
A	-400	HIS	-	expression tag	UNP P0AEX9
A	-399	HIS	-	expression tag	UNP P0AEX9
A	-398	HIS	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-397	HIS	-	expression tag	UNP P0AEX9
A	-396	HIS	-	expression tag	UNP P0AEX9
A	-395	GLY	-	expression tag	UNP P0AEX9
A	-394	MET	-	expression tag	UNP P0AEX9
A	-393	ALA	-	expression tag	UNP P0AEX9
A	-392	SER	-	expression tag	UNP P0AEX9
A	-391	MET	-	expression tag	UNP P0AEX9
A	-24	ASN	-	linker	UNP P0AEX9
A	-23	SER	-	linker	UNP P0AEX9
A	-22	SER	-	linker	UNP P0AEX9
A	-21	SER	-	linker	UNP P0AEX9
A	-20	ASN	-	linker	UNP P0AEX9
A	-19	ASN	-	linker	UNP P0AEX9
A	-18	ASN	-	linker	UNP P0AEX9
A	-17	ASN	-	linker	UNP P0AEX9
A	-16	ASN	-	linker	UNP P0AEX9
A	-15	ASN	-	linker	UNP P0AEX9
A	-14	ASN	-	linker	UNP P0AEX9
A	-13	ASN	-	linker	UNP P0AEX9
A	-12	ASN	-	linker	UNP P0AEX9
A	-11	ASN	-	linker	UNP P0AEX9
A	-10	LEU	-	linker	UNP P0AEX9
A	-9	GLY	-	linker	UNP P0AEX9
A	-8	ILE	-	linker	UNP P0AEX9
A	-7	GLU	-	linker	UNP P0AEX9
A	-6	GLU	-	linker	UNP P0AEX9
A	-5	ASN	-	linker	UNP P0AEX9
A	-4	LEU	-	linker	UNP P0AEX9
A	-3	TYR	-	linker	UNP P0AEX9
A	-2	PHE	-	linker	UNP P0AEX9
A	-1	GLN	-	linker	UNP P0AEX9
A	0	SER	-	linker	UNP P0AEX9
A	1	MET	-	linker	UNP P0AEX9
A	2	LYS	-	linker	UNP P0AEX9
A	3	PHE	-	linker	UNP P0AEX9
A	4	ARG	-	linker	UNP P0AEX9
A	5	SER	-	linker	UNP P0AEX9
A	6	LEU	-	linker	UNP P0AEX9
A	7	TYR	-	linker	UNP P0AEX9
A	8	LYS	-	linker	UNP P0AEX9
B	-444	MET	-	initiating methionine	UNP P0AEX9
B	-443	GLY	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-442	GLY	-	expression tag	UNP P0AEX9
B	-441	SER	-	expression tag	UNP P0AEX9
B	-440	ALA	-	expression tag	UNP P0AEX9
B	-439	TRP	-	expression tag	UNP P0AEX9
B	-438	SER	-	expression tag	UNP P0AEX9
B	-437	HIS	-	expression tag	UNP P0AEX9
B	-436	PRO	-	expression tag	UNP P0AEX9
B	-435	GLN	-	expression tag	UNP P0AEX9
B	-434	PHE	-	expression tag	UNP P0AEX9
B	-433	GLU	-	expression tag	UNP P0AEX9
B	-432	LYS	-	expression tag	UNP P0AEX9
B	-431	GLY	-	expression tag	UNP P0AEX9
B	-430	GLY	-	expression tag	UNP P0AEX9
B	-429	GLY	-	expression tag	UNP P0AEX9
B	-428	SER	-	expression tag	UNP P0AEX9
B	-427	GLY	-	expression tag	UNP P0AEX9
B	-426	GLY	-	expression tag	UNP P0AEX9
B	-425	GLY	-	expression tag	UNP P0AEX9
B	-424	SER	-	expression tag	UNP P0AEX9
B	-423	GLY	-	expression tag	UNP P0AEX9
B	-422	GLY	-	expression tag	UNP P0AEX9
B	-421	SER	-	expression tag	UNP P0AEX9
B	-420	ALA	-	expression tag	UNP P0AEX9
B	-419	TRP	-	expression tag	UNP P0AEX9
B	-418	SER	-	expression tag	UNP P0AEX9
B	-417	HIS	-	expression tag	UNP P0AEX9
B	-416	PRO	-	expression tag	UNP P0AEX9
B	-415	GLN	-	expression tag	UNP P0AEX9
B	-414	PHE	-	expression tag	UNP P0AEX9
B	-413	GLU	-	expression tag	UNP P0AEX9
B	-412	LYS	-	expression tag	UNP P0AEX9
B	-411	GLY	-	expression tag	UNP P0AEX9
B	-410	SER	-	expression tag	UNP P0AEX9
B	-409	MET	-	expression tag	UNP P0AEX9
B	-408	GLY	-	expression tag	UNP P0AEX9
B	-407	GLY	-	expression tag	UNP P0AEX9
B	-406	SER	-	expression tag	UNP P0AEX9
B	-405	HIS	-	expression tag	UNP P0AEX9
B	-404	HIS	-	expression tag	UNP P0AEX9
B	-403	HIS	-	expression tag	UNP P0AEX9
B	-402	HIS	-	expression tag	UNP P0AEX9
B	-401	HIS	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-400	HIS	-	expression tag	UNP P0AEX9
B	-399	HIS	-	expression tag	UNP P0AEX9
B	-398	HIS	-	expression tag	UNP P0AEX9
B	-397	HIS	-	expression tag	UNP P0AEX9
B	-396	HIS	-	expression tag	UNP P0AEX9
B	-395	GLY	-	expression tag	UNP P0AEX9
B	-394	MET	-	expression tag	UNP P0AEX9
B	-393	ALA	-	expression tag	UNP P0AEX9
B	-392	SER	-	expression tag	UNP P0AEX9
B	-391	MET	-	expression tag	UNP P0AEX9
B	-24	ASN	-	linker	UNP P0AEX9
B	-23	SER	-	linker	UNP P0AEX9
B	-22	SER	-	linker	UNP P0AEX9
B	-21	SER	-	linker	UNP P0AEX9
B	-20	ASN	-	linker	UNP P0AEX9
B	-19	ASN	-	linker	UNP P0AEX9
B	-18	ASN	-	linker	UNP P0AEX9
B	-17	ASN	-	linker	UNP P0AEX9
B	-16	ASN	-	linker	UNP P0AEX9
B	-15	ASN	-	linker	UNP P0AEX9
B	-14	ASN	-	linker	UNP P0AEX9
B	-13	ASN	-	linker	UNP P0AEX9
B	-12	ASN	-	linker	UNP P0AEX9
B	-11	ASN	-	linker	UNP P0AEX9
B	-10	LEU	-	linker	UNP P0AEX9
B	-9	GLY	-	linker	UNP P0AEX9
B	-8	ILE	-	linker	UNP P0AEX9
B	-7	GLU	-	linker	UNP P0AEX9
B	-6	GLU	-	linker	UNP P0AEX9
B	-5	ASN	-	linker	UNP P0AEX9
B	-4	LEU	-	linker	UNP P0AEX9
B	-3	TYR	-	linker	UNP P0AEX9
B	-2	PHE	-	linker	UNP P0AEX9
B	-1	GLN	-	linker	UNP P0AEX9
B	0	SER	-	linker	UNP P0AEX9
B	1	MET	-	linker	UNP P0AEX9
B	2	LYS	-	linker	UNP P0AEX9
B	3	PHE	-	linker	UNP P0AEX9
B	4	ARG	-	linker	UNP P0AEX9
B	5	SER	-	linker	UNP P0AEX9
B	6	LEU	-	linker	UNP P0AEX9
B	7	TYR	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	LYS	-	linker	UNP P0AEX9
C	-444	MET	-	initiating methionine	UNP P0AEX9
C	-443	GLY	-	expression tag	UNP P0AEX9
C	-442	GLY	-	expression tag	UNP P0AEX9
C	-441	SER	-	expression tag	UNP P0AEX9
C	-440	ALA	-	expression tag	UNP P0AEX9
C	-439	TRP	-	expression tag	UNP P0AEX9
C	-438	SER	-	expression tag	UNP P0AEX9
C	-437	HIS	-	expression tag	UNP P0AEX9
C	-436	PRO	-	expression tag	UNP P0AEX9
C	-435	GLN	-	expression tag	UNP P0AEX9
C	-434	PHE	-	expression tag	UNP P0AEX9
C	-433	GLU	-	expression tag	UNP P0AEX9
C	-432	LYS	-	expression tag	UNP P0AEX9
C	-431	GLY	-	expression tag	UNP P0AEX9
C	-430	GLY	-	expression tag	UNP P0AEX9
C	-429	GLY	-	expression tag	UNP P0AEX9
C	-428	SER	-	expression tag	UNP P0AEX9
C	-427	GLY	-	expression tag	UNP P0AEX9
C	-426	GLY	-	expression tag	UNP P0AEX9
C	-425	GLY	-	expression tag	UNP P0AEX9
C	-424	SER	-	expression tag	UNP P0AEX9
C	-423	GLY	-	expression tag	UNP P0AEX9
C	-422	GLY	-	expression tag	UNP P0AEX9
C	-421	SER	-	expression tag	UNP P0AEX9
C	-420	ALA	-	expression tag	UNP P0AEX9
C	-419	TRP	-	expression tag	UNP P0AEX9
C	-418	SER	-	expression tag	UNP P0AEX9
C	-417	HIS	-	expression tag	UNP P0AEX9
C	-416	PRO	-	expression tag	UNP P0AEX9
C	-415	GLN	-	expression tag	UNP P0AEX9
C	-414	PHE	-	expression tag	UNP P0AEX9
C	-413	GLU	-	expression tag	UNP P0AEX9
C	-412	LYS	-	expression tag	UNP P0AEX9
C	-411	GLY	-	expression tag	UNP P0AEX9
C	-410	SER	-	expression tag	UNP P0AEX9
C	-409	MET	-	expression tag	UNP P0AEX9
C	-408	GLY	-	expression tag	UNP P0AEX9
C	-407	GLY	-	expression tag	UNP P0AEX9
C	-406	SER	-	expression tag	UNP P0AEX9
C	-405	HIS	-	expression tag	UNP P0AEX9
C	-404	HIS	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-403	HIS	-	expression tag	UNP P0AEX9
C	-402	HIS	-	expression tag	UNP P0AEX9
C	-401	HIS	-	expression tag	UNP P0AEX9
C	-400	HIS	-	expression tag	UNP P0AEX9
C	-399	HIS	-	expression tag	UNP P0AEX9
C	-398	HIS	-	expression tag	UNP P0AEX9
C	-397	HIS	-	expression tag	UNP P0AEX9
C	-396	HIS	-	expression tag	UNP P0AEX9
C	-395	GLY	-	expression tag	UNP P0AEX9
C	-394	MET	-	expression tag	UNP P0AEX9
C	-393	ALA	-	expression tag	UNP P0AEX9
C	-392	SER	-	expression tag	UNP P0AEX9
C	-391	MET	-	expression tag	UNP P0AEX9
C	-24	ASN	-	linker	UNP P0AEX9
C	-23	SER	-	linker	UNP P0AEX9
C	-22	SER	-	linker	UNP P0AEX9
C	-21	SER	-	linker	UNP P0AEX9
C	-20	ASN	-	linker	UNP P0AEX9
C	-19	ASN	-	linker	UNP P0AEX9
C	-18	ASN	-	linker	UNP P0AEX9
C	-17	ASN	-	linker	UNP P0AEX9
C	-16	ASN	-	linker	UNP P0AEX9
C	-15	ASN	-	linker	UNP P0AEX9
C	-14	ASN	-	linker	UNP P0AEX9
C	-13	ASN	-	linker	UNP P0AEX9
C	-12	ASN	-	linker	UNP P0AEX9
C	-11	ASN	-	linker	UNP P0AEX9
C	-10	LEU	-	linker	UNP P0AEX9
C	-9	GLY	-	linker	UNP P0AEX9
C	-8	ILE	-	linker	UNP P0AEX9
C	-7	GLU	-	linker	UNP P0AEX9
C	-6	GLU	-	linker	UNP P0AEX9
C	-5	ASN	-	linker	UNP P0AEX9
C	-4	LEU	-	linker	UNP P0AEX9
C	-3	TYR	-	linker	UNP P0AEX9
C	-2	PHE	-	linker	UNP P0AEX9
C	-1	GLN	-	linker	UNP P0AEX9
C	0	SER	-	linker	UNP P0AEX9
C	1	MET	-	linker	UNP P0AEX9
C	2	LYS	-	linker	UNP P0AEX9
C	3	PHE	-	linker	UNP P0AEX9
C	4	ARG	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	5	SER	-	linker	UNP P0AEX9
C	6	LEU	-	linker	UNP P0AEX9
C	7	TYR	-	linker	UNP P0AEX9
C	8	LYS	-	linker	UNP P0AEX9
D	-444	MET	-	initiating methionine	UNP P0AEX9
D	-443	GLY	-	expression tag	UNP P0AEX9
D	-442	GLY	-	expression tag	UNP P0AEX9
D	-441	SER	-	expression tag	UNP P0AEX9
D	-440	ALA	-	expression tag	UNP P0AEX9
D	-439	TRP	-	expression tag	UNP P0AEX9
D	-438	SER	-	expression tag	UNP P0AEX9
D	-437	HIS	-	expression tag	UNP P0AEX9
D	-436	PRO	-	expression tag	UNP P0AEX9
D	-435	GLN	-	expression tag	UNP P0AEX9
D	-434	PHE	-	expression tag	UNP P0AEX9
D	-433	GLU	-	expression tag	UNP P0AEX9
D	-432	LYS	-	expression tag	UNP P0AEX9
D	-431	GLY	-	expression tag	UNP P0AEX9
D	-430	GLY	-	expression tag	UNP P0AEX9
D	-429	GLY	-	expression tag	UNP P0AEX9
D	-428	SER	-	expression tag	UNP P0AEX9
D	-427	GLY	-	expression tag	UNP P0AEX9
D	-426	GLY	-	expression tag	UNP P0AEX9
D	-425	GLY	-	expression tag	UNP P0AEX9
D	-424	SER	-	expression tag	UNP P0AEX9
D	-423	GLY	-	expression tag	UNP P0AEX9
D	-422	GLY	-	expression tag	UNP P0AEX9
D	-421	SER	-	expression tag	UNP P0AEX9
D	-420	ALA	-	expression tag	UNP P0AEX9
D	-419	TRP	-	expression tag	UNP P0AEX9
D	-418	SER	-	expression tag	UNP P0AEX9
D	-417	HIS	-	expression tag	UNP P0AEX9
D	-416	PRO	-	expression tag	UNP P0AEX9
D	-415	GLN	-	expression tag	UNP P0AEX9
D	-414	PHE	-	expression tag	UNP P0AEX9
D	-413	GLU	-	expression tag	UNP P0AEX9
D	-412	LYS	-	expression tag	UNP P0AEX9
D	-411	GLY	-	expression tag	UNP P0AEX9
D	-410	SER	-	expression tag	UNP P0AEX9
D	-409	MET	-	expression tag	UNP P0AEX9
D	-408	GLY	-	expression tag	UNP P0AEX9
D	-407	GLY	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-406	SER	-	expression tag	UNP P0AEX9
D	-405	HIS	-	expression tag	UNP P0AEX9
D	-404	HIS	-	expression tag	UNP P0AEX9
D	-403	HIS	-	expression tag	UNP P0AEX9
D	-402	HIS	-	expression tag	UNP P0AEX9
D	-401	HIS	-	expression tag	UNP P0AEX9
D	-400	HIS	-	expression tag	UNP P0AEX9
D	-399	HIS	-	expression tag	UNP P0AEX9
D	-398	HIS	-	expression tag	UNP P0AEX9
D	-397	HIS	-	expression tag	UNP P0AEX9
D	-396	HIS	-	expression tag	UNP P0AEX9
D	-395	GLY	-	expression tag	UNP P0AEX9
D	-394	MET	-	expression tag	UNP P0AEX9
D	-393	ALA	-	expression tag	UNP P0AEX9
D	-392	SER	-	expression tag	UNP P0AEX9
D	-391	MET	-	expression tag	UNP P0AEX9
D	-24	ASN	-	linker	UNP P0AEX9
D	-23	SER	-	linker	UNP P0AEX9
D	-22	SER	-	linker	UNP P0AEX9
D	-21	SER	-	linker	UNP P0AEX9
D	-20	ASN	-	linker	UNP P0AEX9
D	-19	ASN	-	linker	UNP P0AEX9
D	-18	ASN	-	linker	UNP P0AEX9
D	-17	ASN	-	linker	UNP P0AEX9
D	-16	ASN	-	linker	UNP P0AEX9
D	-15	ASN	-	linker	UNP P0AEX9
D	-14	ASN	-	linker	UNP P0AEX9
D	-13	ASN	-	linker	UNP P0AEX9
D	-12	ASN	-	linker	UNP P0AEX9
D	-11	ASN	-	linker	UNP P0AEX9
D	-10	LEU	-	linker	UNP P0AEX9
D	-9	GLY	-	linker	UNP P0AEX9
D	-8	ILE	-	linker	UNP P0AEX9
D	-7	GLU	-	linker	UNP P0AEX9
D	-6	GLU	-	linker	UNP P0AEX9
D	-5	ASN	-	linker	UNP P0AEX9
D	-4	LEU	-	linker	UNP P0AEX9
D	-3	TYR	-	linker	UNP P0AEX9
D	-2	PHE	-	linker	UNP P0AEX9
D	-1	GLN	-	linker	UNP P0AEX9
D	0	SER	-	linker	UNP P0AEX9
D	1	MET	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	LYS	-	linker	UNP P0AEX9
D	3	PHE	-	linker	UNP P0AEX9
D	4	ARG	-	linker	UNP P0AEX9
D	5	SER	-	linker	UNP P0AEX9
D	6	LEU	-	linker	UNP P0AEX9
D	7	TYR	-	linker	UNP P0AEX9
D	8	LYS	-	linker	UNP P0AEX9
E	-444	MET	-	initiating methionine	UNP P0AEX9
E	-443	GLY	-	expression tag	UNP P0AEX9
E	-442	GLY	-	expression tag	UNP P0AEX9
E	-441	SER	-	expression tag	UNP P0AEX9
E	-440	ALA	-	expression tag	UNP P0AEX9
E	-439	TRP	-	expression tag	UNP P0AEX9
E	-438	SER	-	expression tag	UNP P0AEX9
E	-437	HIS	-	expression tag	UNP P0AEX9
E	-436	PRO	-	expression tag	UNP P0AEX9
E	-435	GLN	-	expression tag	UNP P0AEX9
E	-434	PHE	-	expression tag	UNP P0AEX9
E	-433	GLU	-	expression tag	UNP P0AEX9
E	-432	LYS	-	expression tag	UNP P0AEX9
E	-431	GLY	-	expression tag	UNP P0AEX9
E	-430	GLY	-	expression tag	UNP P0AEX9
E	-429	GLY	-	expression tag	UNP P0AEX9
E	-428	SER	-	expression tag	UNP P0AEX9
E	-427	GLY	-	expression tag	UNP P0AEX9
E	-426	GLY	-	expression tag	UNP P0AEX9
E	-425	GLY	-	expression tag	UNP P0AEX9
E	-424	SER	-	expression tag	UNP P0AEX9
E	-423	GLY	-	expression tag	UNP P0AEX9
E	-422	GLY	-	expression tag	UNP P0AEX9
E	-421	SER	-	expression tag	UNP P0AEX9
E	-420	ALA	-	expression tag	UNP P0AEX9
E	-419	TRP	-	expression tag	UNP P0AEX9
E	-418	SER	-	expression tag	UNP P0AEX9
E	-417	HIS	-	expression tag	UNP P0AEX9
E	-416	PRO	-	expression tag	UNP P0AEX9
E	-415	GLN	-	expression tag	UNP P0AEX9
E	-414	PHE	-	expression tag	UNP P0AEX9
E	-413	GLU	-	expression tag	UNP P0AEX9
E	-412	LYS	-	expression tag	UNP P0AEX9
E	-411	GLY	-	expression tag	UNP P0AEX9
E	-410	SER	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-409	MET	-	expression tag	UNP P0AEX9
E	-408	GLY	-	expression tag	UNP P0AEX9
E	-407	GLY	-	expression tag	UNP P0AEX9
E	-406	SER	-	expression tag	UNP P0AEX9
E	-405	HIS	-	expression tag	UNP P0AEX9
E	-404	HIS	-	expression tag	UNP P0AEX9
E	-403	HIS	-	expression tag	UNP P0AEX9
E	-402	HIS	-	expression tag	UNP P0AEX9
E	-401	HIS	-	expression tag	UNP P0AEX9
E	-400	HIS	-	expression tag	UNP P0AEX9
E	-399	HIS	-	expression tag	UNP P0AEX9
E	-398	HIS	-	expression tag	UNP P0AEX9
E	-397	HIS	-	expression tag	UNP P0AEX9
E	-396	HIS	-	expression tag	UNP P0AEX9
E	-395	GLY	-	expression tag	UNP P0AEX9
E	-394	MET	-	expression tag	UNP P0AEX9
E	-393	ALA	-	expression tag	UNP P0AEX9
E	-392	SER	-	expression tag	UNP P0AEX9
E	-391	MET	-	expression tag	UNP P0AEX9
E	-24	ASN	-	linker	UNP P0AEX9
E	-23	SER	-	linker	UNP P0AEX9
E	-22	SER	-	linker	UNP P0AEX9
E	-21	SER	-	linker	UNP P0AEX9
E	-20	ASN	-	linker	UNP P0AEX9
E	-19	ASN	-	linker	UNP P0AEX9
E	-18	ASN	-	linker	UNP P0AEX9
E	-17	ASN	-	linker	UNP P0AEX9
E	-16	ASN	-	linker	UNP P0AEX9
E	-15	ASN	-	linker	UNP P0AEX9
E	-14	ASN	-	linker	UNP P0AEX9
E	-13	ASN	-	linker	UNP P0AEX9
E	-12	ASN	-	linker	UNP P0AEX9
E	-11	ASN	-	linker	UNP P0AEX9
E	-10	LEU	-	linker	UNP P0AEX9
E	-9	GLY	-	linker	UNP P0AEX9
E	-8	ILE	-	linker	UNP P0AEX9
E	-7	GLU	-	linker	UNP P0AEX9
E	-6	GLU	-	linker	UNP P0AEX9
E	-5	ASN	-	linker	UNP P0AEX9
E	-4	LEU	-	linker	UNP P0AEX9
E	-3	TYR	-	linker	UNP P0AEX9
E	-2	PHE	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLN	-	linker	UNP P0AEX9
E	0	SER	-	linker	UNP P0AEX9
E	1	MET	-	linker	UNP P0AEX9
E	2	LYS	-	linker	UNP P0AEX9
E	3	PHE	-	linker	UNP P0AEX9
E	4	ARG	-	linker	UNP P0AEX9
E	5	SER	-	linker	UNP P0AEX9
E	6	LEU	-	linker	UNP P0AEX9
E	7	TYR	-	linker	UNP P0AEX9
E	8	LYS	-	linker	UNP P0AEX9
F	-444	MET	-	initiating methionine	UNP P0AEX9
F	-443	GLY	-	expression tag	UNP P0AEX9
F	-442	GLY	-	expression tag	UNP P0AEX9
F	-441	SER	-	expression tag	UNP P0AEX9
F	-440	ALA	-	expression tag	UNP P0AEX9
F	-439	TRP	-	expression tag	UNP P0AEX9
F	-438	SER	-	expression tag	UNP P0AEX9
F	-437	HIS	-	expression tag	UNP P0AEX9
F	-436	PRO	-	expression tag	UNP P0AEX9
F	-435	GLN	-	expression tag	UNP P0AEX9
F	-434	PHE	-	expression tag	UNP P0AEX9
F	-433	GLU	-	expression tag	UNP P0AEX9
F	-432	LYS	-	expression tag	UNP P0AEX9
F	-431	GLY	-	expression tag	UNP P0AEX9
F	-430	GLY	-	expression tag	UNP P0AEX9
F	-429	GLY	-	expression tag	UNP P0AEX9
F	-428	SER	-	expression tag	UNP P0AEX9
F	-427	GLY	-	expression tag	UNP P0AEX9
F	-426	GLY	-	expression tag	UNP P0AEX9
F	-425	GLY	-	expression tag	UNP P0AEX9
F	-424	SER	-	expression tag	UNP P0AEX9
F	-423	GLY	-	expression tag	UNP P0AEX9
F	-422	GLY	-	expression tag	UNP P0AEX9
F	-421	SER	-	expression tag	UNP P0AEX9
F	-420	ALA	-	expression tag	UNP P0AEX9
F	-419	TRP	-	expression tag	UNP P0AEX9
F	-418	SER	-	expression tag	UNP P0AEX9
F	-417	HIS	-	expression tag	UNP P0AEX9
F	-416	PRO	-	expression tag	UNP P0AEX9
F	-415	GLN	-	expression tag	UNP P0AEX9
F	-414	PHE	-	expression tag	UNP P0AEX9
F	-413	GLU	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-412	LYS	-	expression tag	UNP P0AEX9
F	-411	GLY	-	expression tag	UNP P0AEX9
F	-410	SER	-	expression tag	UNP P0AEX9
F	-409	MET	-	expression tag	UNP P0AEX9
F	-408	GLY	-	expression tag	UNP P0AEX9
F	-407	GLY	-	expression tag	UNP P0AEX9
F	-406	SER	-	expression tag	UNP P0AEX9
F	-405	HIS	-	expression tag	UNP P0AEX9
F	-404	HIS	-	expression tag	UNP P0AEX9
F	-403	HIS	-	expression tag	UNP P0AEX9
F	-402	HIS	-	expression tag	UNP P0AEX9
F	-401	HIS	-	expression tag	UNP P0AEX9
F	-400	HIS	-	expression tag	UNP P0AEX9
F	-399	HIS	-	expression tag	UNP P0AEX9
F	-398	HIS	-	expression tag	UNP P0AEX9
F	-397	HIS	-	expression tag	UNP P0AEX9
F	-396	HIS	-	expression tag	UNP P0AEX9
F	-395	GLY	-	expression tag	UNP P0AEX9
F	-394	MET	-	expression tag	UNP P0AEX9
F	-393	ALA	-	expression tag	UNP P0AEX9
F	-392	SER	-	expression tag	UNP P0AEX9
F	-391	MET	-	expression tag	UNP P0AEX9
F	-24	ASN	-	linker	UNP P0AEX9
F	-23	SER	-	linker	UNP P0AEX9
F	-22	SER	-	linker	UNP P0AEX9
F	-21	SER	-	linker	UNP P0AEX9
F	-20	ASN	-	linker	UNP P0AEX9
F	-19	ASN	-	linker	UNP P0AEX9
F	-18	ASN	-	linker	UNP P0AEX9
F	-17	ASN	-	linker	UNP P0AEX9
F	-16	ASN	-	linker	UNP P0AEX9
F	-15	ASN	-	linker	UNP P0AEX9
F	-14	ASN	-	linker	UNP P0AEX9
F	-13	ASN	-	linker	UNP P0AEX9
F	-12	ASN	-	linker	UNP P0AEX9
F	-11	ASN	-	linker	UNP P0AEX9
F	-10	LEU	-	linker	UNP P0AEX9
F	-9	GLY	-	linker	UNP P0AEX9
F	-8	ILE	-	linker	UNP P0AEX9
F	-7	GLU	-	linker	UNP P0AEX9
F	-6	GLU	-	linker	UNP P0AEX9
F	-5	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	LEU	-	linker	UNP P0AEX9
F	-3	TYR	-	linker	UNP P0AEX9
F	-2	PHE	-	linker	UNP P0AEX9
F	-1	GLN	-	linker	UNP P0AEX9
F	0	SER	-	linker	UNP P0AEX9
F	1	MET	-	linker	UNP P0AEX9
F	2	LYS	-	linker	UNP P0AEX9
F	3	PHE	-	linker	UNP P0AEX9
F	4	ARG	-	linker	UNP P0AEX9
F	5	SER	-	linker	UNP P0AEX9
F	6	LEU	-	linker	UNP P0AEX9
F	7	TYR	-	linker	UNP P0AEX9
F	8	LYS	-	linker	UNP P0AEX9
G	-444	MET	-	initiating methionine	UNP P0AEX9
G	-443	GLY	-	expression tag	UNP P0AEX9
G	-442	GLY	-	expression tag	UNP P0AEX9
G	-441	SER	-	expression tag	UNP P0AEX9
G	-440	ALA	-	expression tag	UNP P0AEX9
G	-439	TRP	-	expression tag	UNP P0AEX9
G	-438	SER	-	expression tag	UNP P0AEX9
G	-437	HIS	-	expression tag	UNP P0AEX9
G	-436	PRO	-	expression tag	UNP P0AEX9
G	-435	GLN	-	expression tag	UNP P0AEX9
G	-434	PHE	-	expression tag	UNP P0AEX9
G	-433	GLU	-	expression tag	UNP P0AEX9
G	-432	LYS	-	expression tag	UNP P0AEX9
G	-431	GLY	-	expression tag	UNP P0AEX9
G	-430	GLY	-	expression tag	UNP P0AEX9
G	-429	GLY	-	expression tag	UNP P0AEX9
G	-428	SER	-	expression tag	UNP P0AEX9
G	-427	GLY	-	expression tag	UNP P0AEX9
G	-426	GLY	-	expression tag	UNP P0AEX9
G	-425	GLY	-	expression tag	UNP P0AEX9
G	-424	SER	-	expression tag	UNP P0AEX9
G	-423	GLY	-	expression tag	UNP P0AEX9
G	-422	GLY	-	expression tag	UNP P0AEX9
G	-421	SER	-	expression tag	UNP P0AEX9
G	-420	ALA	-	expression tag	UNP P0AEX9
G	-419	TRP	-	expression tag	UNP P0AEX9
G	-418	SER	-	expression tag	UNP P0AEX9
G	-417	HIS	-	expression tag	UNP P0AEX9
G	-416	PRO	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-415	GLN	-	expression tag	UNP P0AEX9
G	-414	PHE	-	expression tag	UNP P0AEX9
G	-413	GLU	-	expression tag	UNP P0AEX9
G	-412	LYS	-	expression tag	UNP P0AEX9
G	-411	GLY	-	expression tag	UNP P0AEX9
G	-410	SER	-	expression tag	UNP P0AEX9
G	-409	MET	-	expression tag	UNP P0AEX9
G	-408	GLY	-	expression tag	UNP P0AEX9
G	-407	GLY	-	expression tag	UNP P0AEX9
G	-406	SER	-	expression tag	UNP P0AEX9
G	-405	HIS	-	expression tag	UNP P0AEX9
G	-404	HIS	-	expression tag	UNP P0AEX9
G	-403	HIS	-	expression tag	UNP P0AEX9
G	-402	HIS	-	expression tag	UNP P0AEX9
G	-401	HIS	-	expression tag	UNP P0AEX9
G	-400	HIS	-	expression tag	UNP P0AEX9
G	-399	HIS	-	expression tag	UNP P0AEX9
G	-398	HIS	-	expression tag	UNP P0AEX9
G	-397	HIS	-	expression tag	UNP P0AEX9
G	-396	HIS	-	expression tag	UNP P0AEX9
G	-395	GLY	-	expression tag	UNP P0AEX9
G	-394	MET	-	expression tag	UNP P0AEX9
G	-393	ALA	-	expression tag	UNP P0AEX9
G	-392	SER	-	expression tag	UNP P0AEX9
G	-391	MET	-	expression tag	UNP P0AEX9
G	-24	ASN	-	linker	UNP P0AEX9
G	-23	SER	-	linker	UNP P0AEX9
G	-22	SER	-	linker	UNP P0AEX9
G	-21	SER	-	linker	UNP P0AEX9
G	-20	ASN	-	linker	UNP P0AEX9
G	-19	ASN	-	linker	UNP P0AEX9
G	-18	ASN	-	linker	UNP P0AEX9
G	-17	ASN	-	linker	UNP P0AEX9
G	-16	ASN	-	linker	UNP P0AEX9
G	-15	ASN	-	linker	UNP P0AEX9
G	-14	ASN	-	linker	UNP P0AEX9
G	-13	ASN	-	linker	UNP P0AEX9
G	-12	ASN	-	linker	UNP P0AEX9
G	-11	ASN	-	linker	UNP P0AEX9
G	-10	LEU	-	linker	UNP P0AEX9
G	-9	GLY	-	linker	UNP P0AEX9
G	-8	ILE	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLU	-	linker	UNP P0AEX9
G	-6	GLU	-	linker	UNP P0AEX9
G	-5	ASN	-	linker	UNP P0AEX9
G	-4	LEU	-	linker	UNP P0AEX9
G	-3	TYR	-	linker	UNP P0AEX9
G	-2	PHE	-	linker	UNP P0AEX9
G	-1	GLN	-	linker	UNP P0AEX9
G	0	SER	-	linker	UNP P0AEX9
G	1	MET	-	linker	UNP P0AEX9
G	2	LYS	-	linker	UNP P0AEX9
G	3	PHE	-	linker	UNP P0AEX9
G	4	ARG	-	linker	UNP P0AEX9
G	5	SER	-	linker	UNP P0AEX9
G	6	LEU	-	linker	UNP P0AEX9
G	7	TYR	-	linker	UNP P0AEX9
G	8	LYS	-	linker	UNP P0AEX9
H	-444	MET	-	initiating methionine	UNP P0AEX9
H	-443	GLY	-	expression tag	UNP P0AEX9
H	-442	GLY	-	expression tag	UNP P0AEX9
H	-441	SER	-	expression tag	UNP P0AEX9
H	-440	ALA	-	expression tag	UNP P0AEX9
H	-439	TRP	-	expression tag	UNP P0AEX9
H	-438	SER	-	expression tag	UNP P0AEX9
H	-437	HIS	-	expression tag	UNP P0AEX9
H	-436	PRO	-	expression tag	UNP P0AEX9
H	-435	GLN	-	expression tag	UNP P0AEX9
H	-434	PHE	-	expression tag	UNP P0AEX9
H	-433	GLU	-	expression tag	UNP P0AEX9
H	-432	LYS	-	expression tag	UNP P0AEX9
H	-431	GLY	-	expression tag	UNP P0AEX9
H	-430	GLY	-	expression tag	UNP P0AEX9
H	-429	GLY	-	expression tag	UNP P0AEX9
H	-428	SER	-	expression tag	UNP P0AEX9
H	-427	GLY	-	expression tag	UNP P0AEX9
H	-426	GLY	-	expression tag	UNP P0AEX9
H	-425	GLY	-	expression tag	UNP P0AEX9
H	-424	SER	-	expression tag	UNP P0AEX9
H	-423	GLY	-	expression tag	UNP P0AEX9
H	-422	GLY	-	expression tag	UNP P0AEX9
H	-421	SER	-	expression tag	UNP P0AEX9
H	-420	ALA	-	expression tag	UNP P0AEX9
H	-419	TRP	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-418	SER	-	expression tag	UNP P0AEX9
H	-417	HIS	-	expression tag	UNP P0AEX9
H	-416	PRO	-	expression tag	UNP P0AEX9
H	-415	GLN	-	expression tag	UNP P0AEX9
H	-414	PHE	-	expression tag	UNP P0AEX9
H	-413	GLU	-	expression tag	UNP P0AEX9
H	-412	LYS	-	expression tag	UNP P0AEX9
H	-411	GLY	-	expression tag	UNP P0AEX9
H	-410	SER	-	expression tag	UNP P0AEX9
H	-409	MET	-	expression tag	UNP P0AEX9
H	-408	GLY	-	expression tag	UNP P0AEX9
H	-407	GLY	-	expression tag	UNP P0AEX9
H	-406	SER	-	expression tag	UNP P0AEX9
H	-405	HIS	-	expression tag	UNP P0AEX9
H	-404	HIS	-	expression tag	UNP P0AEX9
H	-403	HIS	-	expression tag	UNP P0AEX9
H	-402	HIS	-	expression tag	UNP P0AEX9
H	-401	HIS	-	expression tag	UNP P0AEX9
H	-400	HIS	-	expression tag	UNP P0AEX9
H	-399	HIS	-	expression tag	UNP P0AEX9
H	-398	HIS	-	expression tag	UNP P0AEX9
H	-397	HIS	-	expression tag	UNP P0AEX9
H	-396	HIS	-	expression tag	UNP P0AEX9
H	-395	GLY	-	expression tag	UNP P0AEX9
H	-394	MET	-	expression tag	UNP P0AEX9
H	-393	ALA	-	expression tag	UNP P0AEX9
H	-392	SER	-	expression tag	UNP P0AEX9
H	-391	MET	-	expression tag	UNP P0AEX9
H	-24	ASN	-	linker	UNP P0AEX9
H	-23	SER	-	linker	UNP P0AEX9
H	-22	SER	-	linker	UNP P0AEX9
H	-21	SER	-	linker	UNP P0AEX9
H	-20	ASN	-	linker	UNP P0AEX9
H	-19	ASN	-	linker	UNP P0AEX9
H	-18	ASN	-	linker	UNP P0AEX9
H	-17	ASN	-	linker	UNP P0AEX9
H	-16	ASN	-	linker	UNP P0AEX9
H	-15	ASN	-	linker	UNP P0AEX9
H	-14	ASN	-	linker	UNP P0AEX9
H	-13	ASN	-	linker	UNP P0AEX9
H	-12	ASN	-	linker	UNP P0AEX9
H	-11	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-10	LEU	-	linker	UNP P0AEX9
H	-9	GLY	-	linker	UNP P0AEX9
H	-8	ILE	-	linker	UNP P0AEX9
H	-7	GLU	-	linker	UNP P0AEX9
H	-6	GLU	-	linker	UNP P0AEX9
H	-5	ASN	-	linker	UNP P0AEX9
H	-4	LEU	-	linker	UNP P0AEX9
H	-3	TYR	-	linker	UNP P0AEX9
H	-2	PHE	-	linker	UNP P0AEX9
H	-1	GLN	-	linker	UNP P0AEX9
H	0	SER	-	linker	UNP P0AEX9
H	1	MET	-	linker	UNP P0AEX9
H	2	LYS	-	linker	UNP P0AEX9
H	3	PHE	-	linker	UNP P0AEX9
H	4	ARG	-	linker	UNP P0AEX9
H	5	SER	-	linker	UNP P0AEX9
H	6	LEU	-	linker	UNP P0AEX9
H	7	TYR	-	linker	UNP P0AEX9
H	8	LYS	-	linker	UNP P0AEX9
I	-444	MET	-	initiating methionine	UNP P0AEX9
I	-443	GLY	-	expression tag	UNP P0AEX9
I	-442	GLY	-	expression tag	UNP P0AEX9
I	-441	SER	-	expression tag	UNP P0AEX9
I	-440	ALA	-	expression tag	UNP P0AEX9
I	-439	TRP	-	expression tag	UNP P0AEX9
I	-438	SER	-	expression tag	UNP P0AEX9
I	-437	HIS	-	expression tag	UNP P0AEX9
I	-436	PRO	-	expression tag	UNP P0AEX9
I	-435	GLN	-	expression tag	UNP P0AEX9
I	-434	PHE	-	expression tag	UNP P0AEX9
I	-433	GLU	-	expression tag	UNP P0AEX9
I	-432	LYS	-	expression tag	UNP P0AEX9
I	-431	GLY	-	expression tag	UNP P0AEX9
I	-430	GLY	-	expression tag	UNP P0AEX9
I	-429	GLY	-	expression tag	UNP P0AEX9
I	-428	SER	-	expression tag	UNP P0AEX9
I	-427	GLY	-	expression tag	UNP P0AEX9
I	-426	GLY	-	expression tag	UNP P0AEX9
I	-425	GLY	-	expression tag	UNP P0AEX9
I	-424	SER	-	expression tag	UNP P0AEX9
I	-423	GLY	-	expression tag	UNP P0AEX9
I	-422	GLY	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-421	SER	-	expression tag	UNP P0AEX9
I	-420	ALA	-	expression tag	UNP P0AEX9
I	-419	TRP	-	expression tag	UNP P0AEX9
I	-418	SER	-	expression tag	UNP P0AEX9
I	-417	HIS	-	expression tag	UNP P0AEX9
I	-416	PRO	-	expression tag	UNP P0AEX9
I	-415	GLN	-	expression tag	UNP P0AEX9
I	-414	PHE	-	expression tag	UNP P0AEX9
I	-413	GLU	-	expression tag	UNP P0AEX9
I	-412	LYS	-	expression tag	UNP P0AEX9
I	-411	GLY	-	expression tag	UNP P0AEX9
I	-410	SER	-	expression tag	UNP P0AEX9
I	-409	MET	-	expression tag	UNP P0AEX9
I	-408	GLY	-	expression tag	UNP P0AEX9
I	-407	GLY	-	expression tag	UNP P0AEX9
I	-406	SER	-	expression tag	UNP P0AEX9
I	-405	HIS	-	expression tag	UNP P0AEX9
I	-404	HIS	-	expression tag	UNP P0AEX9
I	-403	HIS	-	expression tag	UNP P0AEX9
I	-402	HIS	-	expression tag	UNP P0AEX9
I	-401	HIS	-	expression tag	UNP P0AEX9
I	-400	HIS	-	expression tag	UNP P0AEX9
I	-399	HIS	-	expression tag	UNP P0AEX9
I	-398	HIS	-	expression tag	UNP P0AEX9
I	-397	HIS	-	expression tag	UNP P0AEX9
I	-396	HIS	-	expression tag	UNP P0AEX9
I	-395	GLY	-	expression tag	UNP P0AEX9
I	-394	MET	-	expression tag	UNP P0AEX9
I	-393	ALA	-	expression tag	UNP P0AEX9
I	-392	SER	-	expression tag	UNP P0AEX9
I	-391	MET	-	expression tag	UNP P0AEX9
I	-24	ASN	-	linker	UNP P0AEX9
I	-23	SER	-	linker	UNP P0AEX9
I	-22	SER	-	linker	UNP P0AEX9
I	-21	SER	-	linker	UNP P0AEX9
I	-20	ASN	-	linker	UNP P0AEX9
I	-19	ASN	-	linker	UNP P0AEX9
I	-18	ASN	-	linker	UNP P0AEX9
I	-17	ASN	-	linker	UNP P0AEX9
I	-16	ASN	-	linker	UNP P0AEX9
I	-15	ASN	-	linker	UNP P0AEX9
I	-14	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-13	ASN	-	linker	UNP P0AEX9
I	-12	ASN	-	linker	UNP P0AEX9
I	-11	ASN	-	linker	UNP P0AEX9
I	-10	LEU	-	linker	UNP P0AEX9
I	-9	GLY	-	linker	UNP P0AEX9
I	-8	ILE	-	linker	UNP P0AEX9
I	-7	GLU	-	linker	UNP P0AEX9
I	-6	GLU	-	linker	UNP P0AEX9
I	-5	ASN	-	linker	UNP P0AEX9
I	-4	LEU	-	linker	UNP P0AEX9
I	-3	TYR	-	linker	UNP P0AEX9
I	-2	PHE	-	linker	UNP P0AEX9
I	-1	GLN	-	linker	UNP P0AEX9
I	0	SER	-	linker	UNP P0AEX9
I	1	MET	-	linker	UNP P0AEX9
I	2	LYS	-	linker	UNP P0AEX9
I	3	PHE	-	linker	UNP P0AEX9
I	4	ARG	-	linker	UNP P0AEX9
I	5	SER	-	linker	UNP P0AEX9
I	6	LEU	-	linker	UNP P0AEX9
I	7	TYR	-	linker	UNP P0AEX9
I	8	LYS	-	linker	UNP P0AEX9
J	-444	MET	-	initiating methionine	UNP P0AEX9
J	-443	GLY	-	expression tag	UNP P0AEX9
J	-442	GLY	-	expression tag	UNP P0AEX9
J	-441	SER	-	expression tag	UNP P0AEX9
J	-440	ALA	-	expression tag	UNP P0AEX9
J	-439	TRP	-	expression tag	UNP P0AEX9
J	-438	SER	-	expression tag	UNP P0AEX9
J	-437	HIS	-	expression tag	UNP P0AEX9
J	-436	PRO	-	expression tag	UNP P0AEX9
J	-435	GLN	-	expression tag	UNP P0AEX9
J	-434	PHE	-	expression tag	UNP P0AEX9
J	-433	GLU	-	expression tag	UNP P0AEX9
J	-432	LYS	-	expression tag	UNP P0AEX9
J	-431	GLY	-	expression tag	UNP P0AEX9
J	-430	GLY	-	expression tag	UNP P0AEX9
J	-429	GLY	-	expression tag	UNP P0AEX9
J	-428	SER	-	expression tag	UNP P0AEX9
J	-427	GLY	-	expression tag	UNP P0AEX9
J	-426	GLY	-	expression tag	UNP P0AEX9
J	-425	GLY	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-424	SER	-	expression tag	UNP P0AEX9
J	-423	GLY	-	expression tag	UNP P0AEX9
J	-422	GLY	-	expression tag	UNP P0AEX9
J	-421	SER	-	expression tag	UNP P0AEX9
J	-420	ALA	-	expression tag	UNP P0AEX9
J	-419	TRP	-	expression tag	UNP P0AEX9
J	-418	SER	-	expression tag	UNP P0AEX9
J	-417	HIS	-	expression tag	UNP P0AEX9
J	-416	PRO	-	expression tag	UNP P0AEX9
J	-415	GLN	-	expression tag	UNP P0AEX9
J	-414	PHE	-	expression tag	UNP P0AEX9
J	-413	GLU	-	expression tag	UNP P0AEX9
J	-412	LYS	-	expression tag	UNP P0AEX9
J	-411	GLY	-	expression tag	UNP P0AEX9
J	-410	SER	-	expression tag	UNP P0AEX9
J	-409	MET	-	expression tag	UNP P0AEX9
J	-408	GLY	-	expression tag	UNP P0AEX9
J	-407	GLY	-	expression tag	UNP P0AEX9
J	-406	SER	-	expression tag	UNP P0AEX9
J	-405	HIS	-	expression tag	UNP P0AEX9
J	-404	HIS	-	expression tag	UNP P0AEX9
J	-403	HIS	-	expression tag	UNP P0AEX9
J	-402	HIS	-	expression tag	UNP P0AEX9
J	-401	HIS	-	expression tag	UNP P0AEX9
J	-400	HIS	-	expression tag	UNP P0AEX9
J	-399	HIS	-	expression tag	UNP P0AEX9
J	-398	HIS	-	expression tag	UNP P0AEX9
J	-397	HIS	-	expression tag	UNP P0AEX9
J	-396	HIS	-	expression tag	UNP P0AEX9
J	-395	GLY	-	expression tag	UNP P0AEX9
J	-394	MET	-	expression tag	UNP P0AEX9
J	-393	ALA	-	expression tag	UNP P0AEX9
J	-392	SER	-	expression tag	UNP P0AEX9
J	-391	MET	-	expression tag	UNP P0AEX9
J	-24	ASN	-	linker	UNP P0AEX9
J	-23	SER	-	linker	UNP P0AEX9
J	-22	SER	-	linker	UNP P0AEX9
J	-21	SER	-	linker	UNP P0AEX9
J	-20	ASN	-	linker	UNP P0AEX9
J	-19	ASN	-	linker	UNP P0AEX9
J	-18	ASN	-	linker	UNP P0AEX9
J	-17	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-16	ASN	-	linker	UNP P0AEX9
J	-15	ASN	-	linker	UNP P0AEX9
J	-14	ASN	-	linker	UNP P0AEX9
J	-13	ASN	-	linker	UNP P0AEX9
J	-12	ASN	-	linker	UNP P0AEX9
J	-11	ASN	-	linker	UNP P0AEX9
J	-10	LEU	-	linker	UNP P0AEX9
J	-9	GLY	-	linker	UNP P0AEX9
J	-8	ILE	-	linker	UNP P0AEX9
J	-7	GLU	-	linker	UNP P0AEX9
J	-6	GLU	-	linker	UNP P0AEX9
J	-5	ASN	-	linker	UNP P0AEX9
J	-4	LEU	-	linker	UNP P0AEX9
J	-3	TYR	-	linker	UNP P0AEX9
J	-2	PHE	-	linker	UNP P0AEX9
J	-1	GLN	-	linker	UNP P0AEX9
J	0	SER	-	linker	UNP P0AEX9
J	1	MET	-	linker	UNP P0AEX9
J	2	LYS	-	linker	UNP P0AEX9
J	3	PHE	-	linker	UNP P0AEX9
J	4	ARG	-	linker	UNP P0AEX9
J	5	SER	-	linker	UNP P0AEX9
J	6	LEU	-	linker	UNP P0AEX9
J	7	TYR	-	linker	UNP P0AEX9
J	8	LYS	-	linker	UNP P0AEX9
K	-444	MET	-	initiating methionine	UNP P0AEX9
K	-443	GLY	-	expression tag	UNP P0AEX9
K	-442	GLY	-	expression tag	UNP P0AEX9
K	-441	SER	-	expression tag	UNP P0AEX9
K	-440	ALA	-	expression tag	UNP P0AEX9
K	-439	TRP	-	expression tag	UNP P0AEX9
K	-438	SER	-	expression tag	UNP P0AEX9
K	-437	HIS	-	expression tag	UNP P0AEX9
K	-436	PRO	-	expression tag	UNP P0AEX9
K	-435	GLN	-	expression tag	UNP P0AEX9
K	-434	PHE	-	expression tag	UNP P0AEX9
K	-433	GLU	-	expression tag	UNP P0AEX9
K	-432	LYS	-	expression tag	UNP P0AEX9
K	-431	GLY	-	expression tag	UNP P0AEX9
K	-430	GLY	-	expression tag	UNP P0AEX9
K	-429	GLY	-	expression tag	UNP P0AEX9
K	-428	SER	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-427	GLY	-	expression tag	UNP P0AEX9
K	-426	GLY	-	expression tag	UNP P0AEX9
K	-425	GLY	-	expression tag	UNP P0AEX9
K	-424	SER	-	expression tag	UNP P0AEX9
K	-423	GLY	-	expression tag	UNP P0AEX9
K	-422	GLY	-	expression tag	UNP P0AEX9
K	-421	SER	-	expression tag	UNP P0AEX9
K	-420	ALA	-	expression tag	UNP P0AEX9
K	-419	TRP	-	expression tag	UNP P0AEX9
K	-418	SER	-	expression tag	UNP P0AEX9
K	-417	HIS	-	expression tag	UNP P0AEX9
K	-416	PRO	-	expression tag	UNP P0AEX9
K	-415	GLN	-	expression tag	UNP P0AEX9
K	-414	PHE	-	expression tag	UNP P0AEX9
K	-413	GLU	-	expression tag	UNP P0AEX9
K	-412	LYS	-	expression tag	UNP P0AEX9
K	-411	GLY	-	expression tag	UNP P0AEX9
K	-410	SER	-	expression tag	UNP P0AEX9
K	-409	MET	-	expression tag	UNP P0AEX9
K	-408	GLY	-	expression tag	UNP P0AEX9
K	-407	GLY	-	expression tag	UNP P0AEX9
K	-406	SER	-	expression tag	UNP P0AEX9
K	-405	HIS	-	expression tag	UNP P0AEX9
K	-404	HIS	-	expression tag	UNP P0AEX9
K	-403	HIS	-	expression tag	UNP P0AEX9
K	-402	HIS	-	expression tag	UNP P0AEX9
K	-401	HIS	-	expression tag	UNP P0AEX9
K	-400	HIS	-	expression tag	UNP P0AEX9
K	-399	HIS	-	expression tag	UNP P0AEX9
K	-398	HIS	-	expression tag	UNP P0AEX9
K	-397	HIS	-	expression tag	UNP P0AEX9
K	-396	HIS	-	expression tag	UNP P0AEX9
K	-395	GLY	-	expression tag	UNP P0AEX9
K	-394	MET	-	expression tag	UNP P0AEX9
K	-393	ALA	-	expression tag	UNP P0AEX9
K	-392	SER	-	expression tag	UNP P0AEX9
K	-391	MET	-	expression tag	UNP P0AEX9
K	-24	ASN	-	linker	UNP P0AEX9
K	-23	SER	-	linker	UNP P0AEX9
K	-22	SER	-	linker	UNP P0AEX9
K	-21	SER	-	linker	UNP P0AEX9
K	-20	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-19	ASN	-	linker	UNP P0AEX9
K	-18	ASN	-	linker	UNP P0AEX9
K	-17	ASN	-	linker	UNP P0AEX9
K	-16	ASN	-	linker	UNP P0AEX9
K	-15	ASN	-	linker	UNP P0AEX9
K	-14	ASN	-	linker	UNP P0AEX9
K	-13	ASN	-	linker	UNP P0AEX9
K	-12	ASN	-	linker	UNP P0AEX9
K	-11	ASN	-	linker	UNP P0AEX9
K	-10	LEU	-	linker	UNP P0AEX9
K	-9	GLY	-	linker	UNP P0AEX9
K	-8	ILE	-	linker	UNP P0AEX9
K	-7	GLU	-	linker	UNP P0AEX9
K	-6	GLU	-	linker	UNP P0AEX9
K	-5	ASN	-	linker	UNP P0AEX9
K	-4	LEU	-	linker	UNP P0AEX9
K	-3	TYR	-	linker	UNP P0AEX9
K	-2	PHE	-	linker	UNP P0AEX9
K	-1	GLN	-	linker	UNP P0AEX9
K	0	SER	-	linker	UNP P0AEX9
K	1	MET	-	linker	UNP P0AEX9
K	2	LYS	-	linker	UNP P0AEX9
K	3	PHE	-	linker	UNP P0AEX9
K	4	ARG	-	linker	UNP P0AEX9
K	5	SER	-	linker	UNP P0AEX9
K	6	LEU	-	linker	UNP P0AEX9
K	7	TYR	-	linker	UNP P0AEX9
K	8	LYS	-	linker	UNP P0AEX9
L	-444	MET	-	initiating methionine	UNP P0AEX9
L	-443	GLY	-	expression tag	UNP P0AEX9
L	-442	GLY	-	expression tag	UNP P0AEX9
L	-441	SER	-	expression tag	UNP P0AEX9
L	-440	ALA	-	expression tag	UNP P0AEX9
L	-439	TRP	-	expression tag	UNP P0AEX9
L	-438	SER	-	expression tag	UNP P0AEX9
L	-437	HIS	-	expression tag	UNP P0AEX9
L	-436	PRO	-	expression tag	UNP P0AEX9
L	-435	GLN	-	expression tag	UNP P0AEX9
L	-434	PHE	-	expression tag	UNP P0AEX9
L	-433	GLU	-	expression tag	UNP P0AEX9
L	-432	LYS	-	expression tag	UNP P0AEX9
L	-431	GLY	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-430	GLY	-	expression tag	UNP P0AEX9
L	-429	GLY	-	expression tag	UNP P0AEX9
L	-428	SER	-	expression tag	UNP P0AEX9
L	-427	GLY	-	expression tag	UNP P0AEX9
L	-426	GLY	-	expression tag	UNP P0AEX9
L	-425	GLY	-	expression tag	UNP P0AEX9
L	-424	SER	-	expression tag	UNP P0AEX9
L	-423	GLY	-	expression tag	UNP P0AEX9
L	-422	GLY	-	expression tag	UNP P0AEX9
L	-421	SER	-	expression tag	UNP P0AEX9
L	-420	ALA	-	expression tag	UNP P0AEX9
L	-419	TRP	-	expression tag	UNP P0AEX9
L	-418	SER	-	expression tag	UNP P0AEX9
L	-417	HIS	-	expression tag	UNP P0AEX9
L	-416	PRO	-	expression tag	UNP P0AEX9
L	-415	GLN	-	expression tag	UNP P0AEX9
L	-414	PHE	-	expression tag	UNP P0AEX9
L	-413	GLU	-	expression tag	UNP P0AEX9
L	-412	LYS	-	expression tag	UNP P0AEX9
L	-411	GLY	-	expression tag	UNP P0AEX9
L	-410	SER	-	expression tag	UNP P0AEX9
L	-409	MET	-	expression tag	UNP P0AEX9
L	-408	GLY	-	expression tag	UNP P0AEX9
L	-407	GLY	-	expression tag	UNP P0AEX9
L	-406	SER	-	expression tag	UNP P0AEX9
L	-405	HIS	-	expression tag	UNP P0AEX9
L	-404	HIS	-	expression tag	UNP P0AEX9
L	-403	HIS	-	expression tag	UNP P0AEX9
L	-402	HIS	-	expression tag	UNP P0AEX9
L	-401	HIS	-	expression tag	UNP P0AEX9
L	-400	HIS	-	expression tag	UNP P0AEX9
L	-399	HIS	-	expression tag	UNP P0AEX9
L	-398	HIS	-	expression tag	UNP P0AEX9
L	-397	HIS	-	expression tag	UNP P0AEX9
L	-396	HIS	-	expression tag	UNP P0AEX9
L	-395	GLY	-	expression tag	UNP P0AEX9
L	-394	MET	-	expression tag	UNP P0AEX9
L	-393	ALA	-	expression tag	UNP P0AEX9
L	-392	SER	-	expression tag	UNP P0AEX9
L	-391	MET	-	expression tag	UNP P0AEX9
L	-24	ASN	-	linker	UNP P0AEX9
L	-23	SER	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-22	SER	-	linker	UNP P0AEX9
L	-21	SER	-	linker	UNP P0AEX9
L	-20	ASN	-	linker	UNP P0AEX9
L	-19	ASN	-	linker	UNP P0AEX9
L	-18	ASN	-	linker	UNP P0AEX9
L	-17	ASN	-	linker	UNP P0AEX9
L	-16	ASN	-	linker	UNP P0AEX9
L	-15	ASN	-	linker	UNP P0AEX9
L	-14	ASN	-	linker	UNP P0AEX9
L	-13	ASN	-	linker	UNP P0AEX9
L	-12	ASN	-	linker	UNP P0AEX9
L	-11	ASN	-	linker	UNP P0AEX9
L	-10	LEU	-	linker	UNP P0AEX9
L	-9	GLY	-	linker	UNP P0AEX9
L	-8	ILE	-	linker	UNP P0AEX9
L	-7	GLU	-	linker	UNP P0AEX9
L	-6	GLU	-	linker	UNP P0AEX9
L	-5	ASN	-	linker	UNP P0AEX9
L	-4	LEU	-	linker	UNP P0AEX9
L	-3	TYR	-	linker	UNP P0AEX9
L	-2	PHE	-	linker	UNP P0AEX9
L	-1	GLN	-	linker	UNP P0AEX9
L	0	SER	-	linker	UNP P0AEX9
L	1	MET	-	linker	UNP P0AEX9
L	2	LYS	-	linker	UNP P0AEX9
L	3	PHE	-	linker	UNP P0AEX9
L	4	ARG	-	linker	UNP P0AEX9
L	5	SER	-	linker	UNP P0AEX9
L	6	LEU	-	linker	UNP P0AEX9
L	7	TYR	-	linker	UNP P0AEX9
L	8	LYS	-	linker	UNP P0AEX9

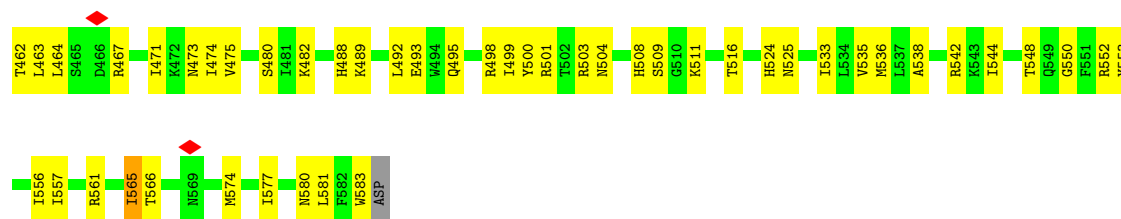
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Zn 1 1	0
2	B	1	Total Zn 1 1	0
2	C	1	Total Zn 1 1	0
2	D	1	Total Zn 1 1	0

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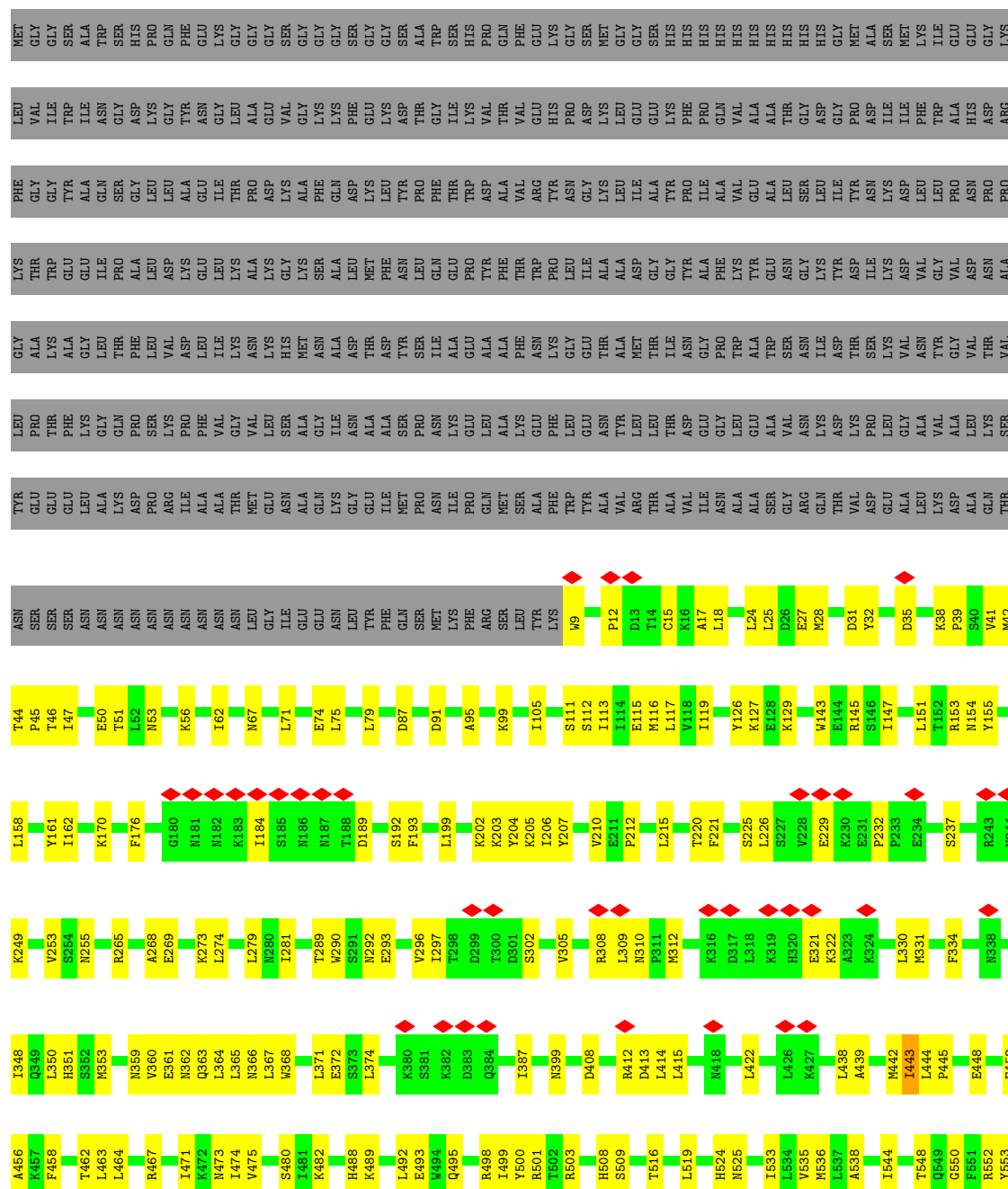
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Mol	Chain	Residues	Atoms		AltConf
2	E	1	Total 1	Zn 1	0
2	F	1	Total 1	Zn 1	0
2	G	1	Total 1	Zn 1	0
2	H	1	Total 1	Zn 1	0
2	I	1	Total 1	Zn 1	0
2	J	1	Total 1	Zn 1	0
2	K	1	Total 1	Zn 1	0
2	L	1	Total 1	Zn 1	0

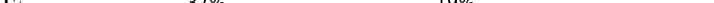


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Bacterial antiviral defense protein Ec3ApeA from Escherichia coli strain KK-NP016

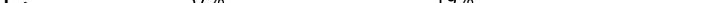
Chain C: 37% 19% 44%





- Chain E:  37% 19% 44%



Chain F:  37% 19% 44%

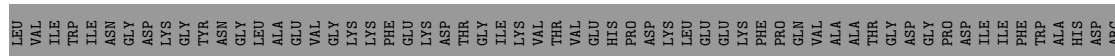
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Bacterial antiviral defense protein Ec3ApeA from *Escherichia coli* strain KK-NP016

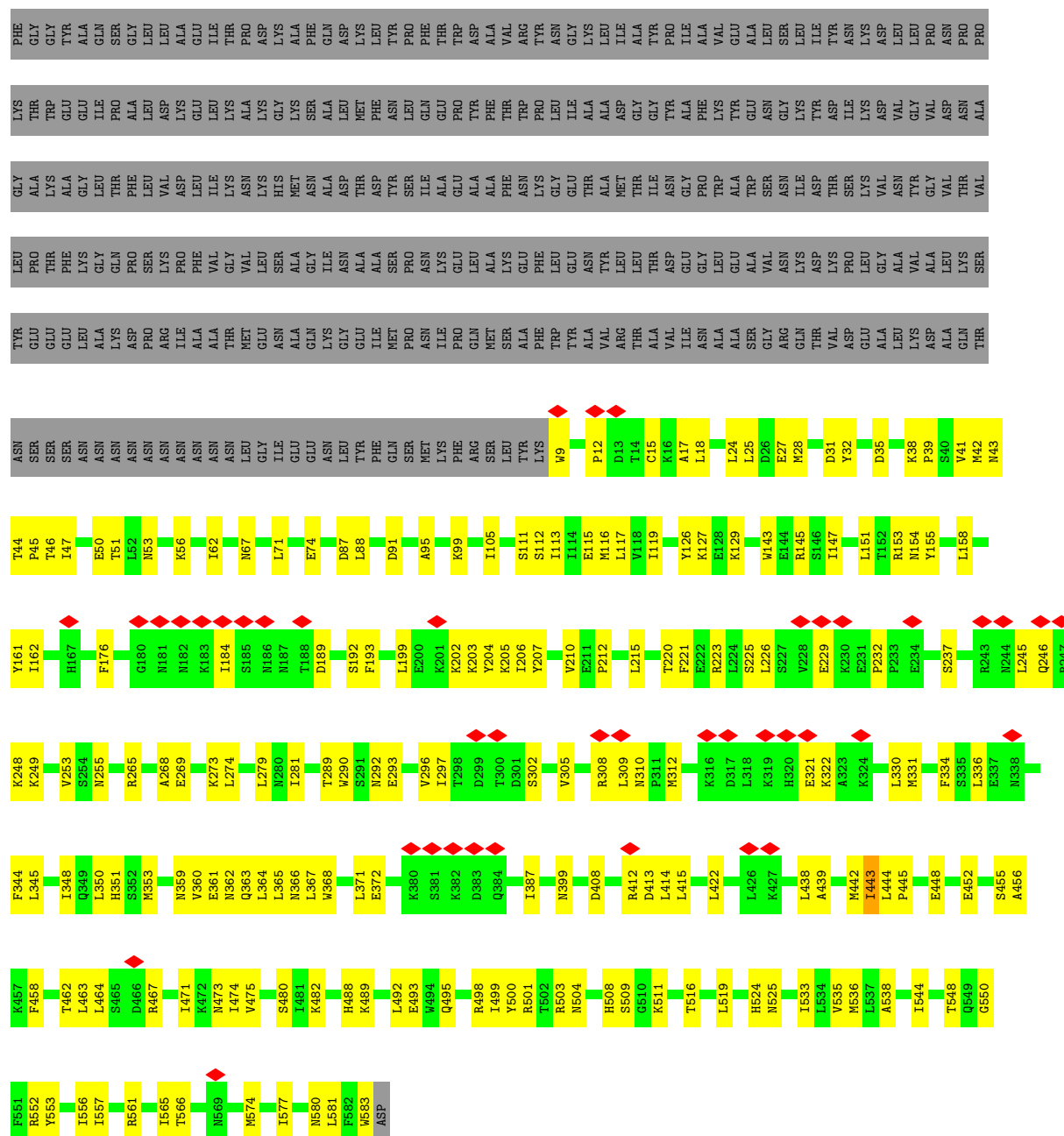
Chain G:  38% 18% 44%

MET	GLY	GLY	SER	ALA	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	GLY	GLY	GLY	SER	SER	ALA	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	GLY	SER	SER	ALA	TRP	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	MET	GLY	GLY	SER	SER	SER	ALA	SER	MET	LYS	ILE	GLU	GLU	GLY	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



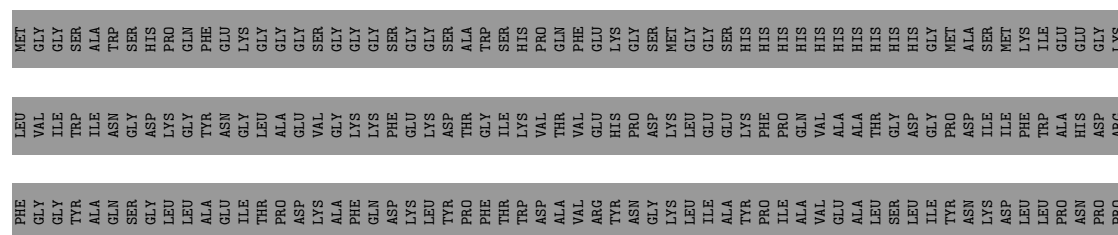
Frequency	Percentage
Daily	37%
Weekly	19%
Monthly	44%



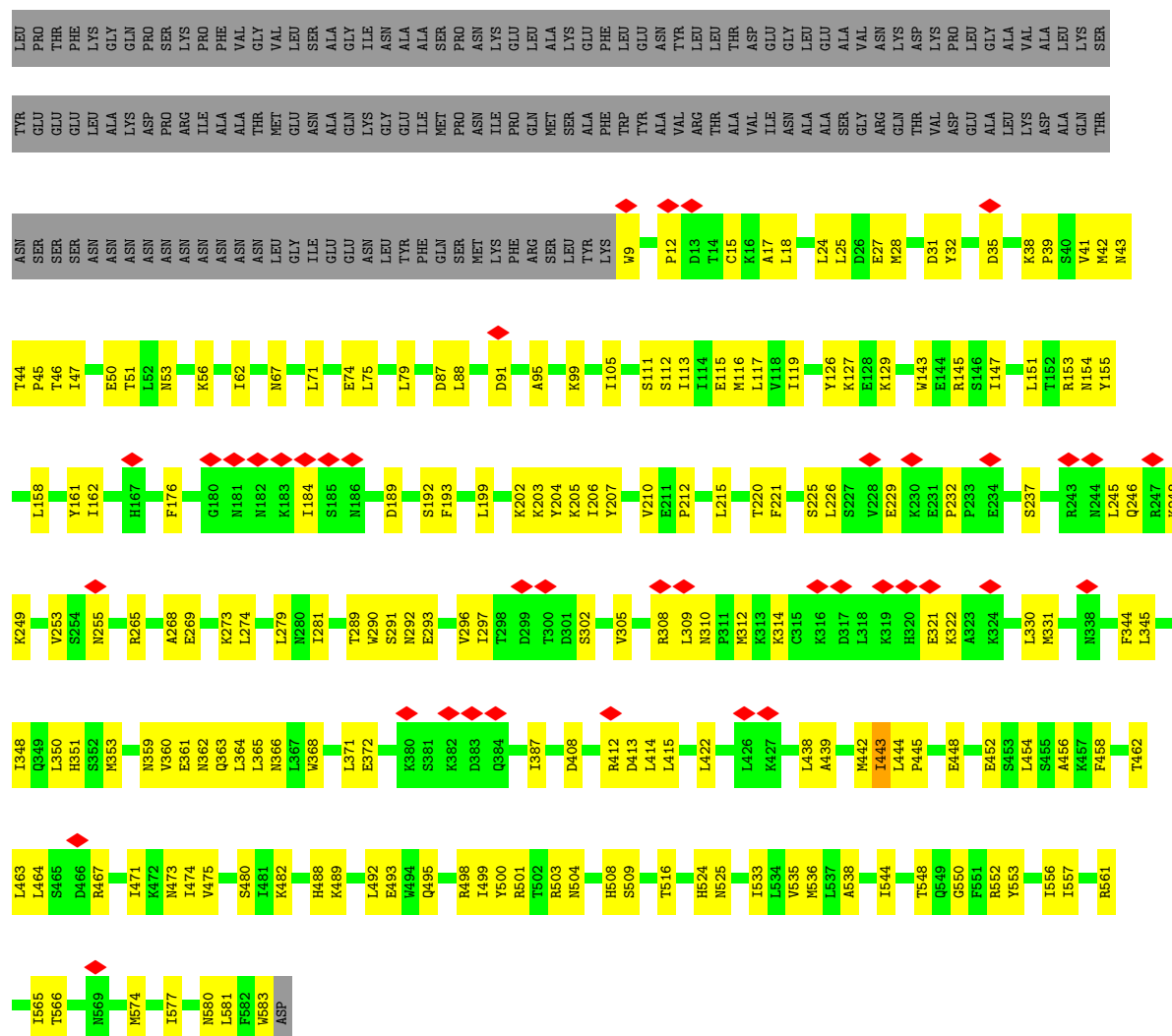


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Bacterial antiviral defense protein Ec3ApeA from Escherichia coli strain KK-NP016

Chain I: 37% 19% 44%

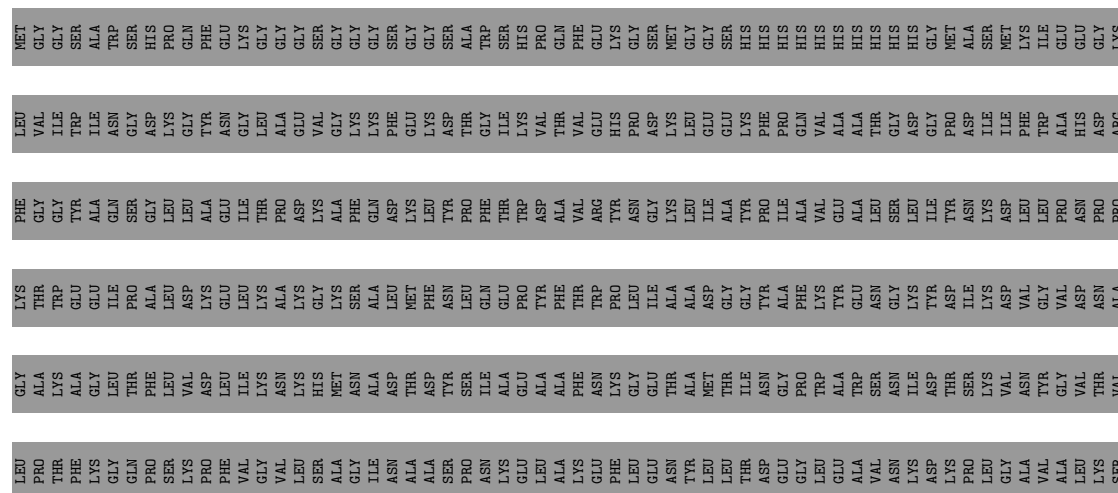


[illegible]



- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Bacterial antiviral defense protein Ec3ApeA from Escherichia coli strain KK-NP016

Chain L: 37% 19% 44%



R552	R457	L345	R247	T44	ASN	TYR
Y553	F458	I348	K248	P45	GLU	GLU
I556	T462	Q349	K249	T46	SER	GLU
I557	L463	L350	V253	I162	SER	GLU
R561	L464	H351	G254	E50	ASN	LEU
I565	R467	M352	N255	T51	ASN	ALA
T566	I471	N359	R265	N53	ASN	LYS
I569	K472	V360	G180	K56	PRO	ASP
M574	M473	E361	M181	L71	ASN	ARG
I577	L474	N362	M182	T62	ASN	ILE
N580	V475	Q363	K183	I67	ASN	ALA
L581	S480	L364	K273	N67	ASN	THR
F582	I481	L365	L274	L75	LEU	MET
W583	K482	N366	L279	L71	GLY	GLU
ASP	K489	W368	I185	L75	ILE	ASN
	L492	E372	M186	L71	GLU	ALA
	E493	S373	N280	E74	GLU	ALA
	Q495	L374	M187	L75	ASN	LYS
	R498	K380	T188	L75	GLY	GLY
	L499	S381	D189	L79	GLU	GLU
Y500	R499	K382	S192	D87	PHE	ILE
R501	Y500	D383	F193	D91	GLN	MET
T502	R501	Q384	L199	D91	SER	ASN
R503	T502	I387	K202	A95	MET	ASN
N504	R503	D408	K203	K99	LYS	ILE
H508	H508	R412	T296	I105	PHE	PRO
S509	S509	D413	T297	I111	ARG	GLN
G510	G510	L414	T298	I113	SER	MET
K511	G511	L414	D299	I114	LEU	SER
T516	M418	N310	T300	E115	ALA	ALA
H524	L422	P311	K205	M16	VAL	VAL
N525	L426	M312	D301	L17	A17	ILE
I533	K427	K316	S302	I119	L18	ASN
V535	L438	D317	V305	Y126	L24	ALA
M536	A439	L318	R308	K127	L25	ALA
L537	M442	K319	L309	E128	D26	SER
A538	M442	H320	N310	K129	E27	GLY
R542	I443	E321	P311	W143	M28	GLN
K543	L444	K322	A217	E144	D31	THR
I544	P445	A323	T220	R145	Y32	VAL
T548	E448	K324	F221	I147	ASP	ASP
Q549	E452	K325	E229	D35	GLU	GLU
G550	S453	K326	E230	L151	ALA	ALA
F551	L454	E333	E231	T152	LEU	LEU
	S455	E333	P232	R153	LYS	LYS
	A456	N338	P233	N154	ASP	ASP
			E234	V41	K38	GLN
			S237	Y155	P39	ALA
			R243		S40	ALA
			N244		V41	GLN
			L245		M42	THR
			F344		M43	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D6	Depositor
Number of particles used	60670	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	34.546	Depositor
Minimum map value	-22.719	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5	Depositor
Map size (Å)	369.6, 369.6, 369.6	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/4582	0.48	0/6227
1	B	0.25	0/4582	0.48	0/6227
1	C	0.25	0/4582	0.48	0/6227
1	D	0.25	0/4582	0.48	0/6227
1	E	0.25	0/4582	0.48	0/6227
1	F	0.25	0/4582	0.48	0/6227
1	G	0.25	0/4582	0.48	0/6227
1	H	0.25	0/4582	0.48	0/6227
1	I	0.25	0/4582	0.48	0/6227
1	J	0.25	0/4582	0.48	0/6227
1	K	0.25	0/4582	0.48	0/6227
1	L	0.25	0/4582	0.48	0/6227
All	All	0.25	0/54984	0.48	0/74724

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	4483	0	4415	146	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4483	0	4415	141	0
1	C	4483	0	4415	143	0
1	D	4483	0	4415	145	0
1	E	4483	0	4415	144	0
1	F	4483	0	4415	141	0
1	G	4483	0	4415	140	0
1	H	4483	0	4415	144	0
1	I	4483	0	4415	143	0
1	J	4483	0	4415	140	0
1	K	4483	0	4415	140	0
1	L	4483	0	4415	142	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
All	All	53808	0	52980	1617	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 15.

The worst 5 of 1617 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:I:87:ASP:HB3	1:I:129:LYS:HE2	1.57	0.87
1:L:87:ASP:HB3	1:L:129:LYS:HE2	1.57	0.86
1:C:87:ASP:HB3	1:C:129:LYS:HE2	1.57	0.86
1:F:87:ASP:HB3	1:F:129:LYS:HE2	1.57	0.86
1:D:87:ASP:HB3	1:D:129:LYS:HE2	1.57	0.86

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	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	B	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	C	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	D	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	E	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	F	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	G	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	H	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	I	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	J	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	K	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
1	L	573/1029 (56%)	564 (98%)	9 (2%)	0	100	100
All	All	6876/12348 (56%)	6768 (98%)	108 (2%)	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	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	B	470/901 (52%)	461 (98%)	9 (2%)	50	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	D	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	E	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	F	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	G	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	H	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	I	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	J	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	K	470/901 (52%)	461 (98%)	9 (2%)	50	76
1	L	470/901 (52%)	461 (98%)	9 (2%)	50	76
All	All	5640/10812 (52%)	5532 (98%)	108 (2%)	49	76

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	279	LEU
1	H	574	MET
1	L	9	TRP
1	G	443	ILE
1	H	246	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	495	GLN
1	K	495	GLN
1	I	580	ASN
1	J	495	GLN
1	L	167	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

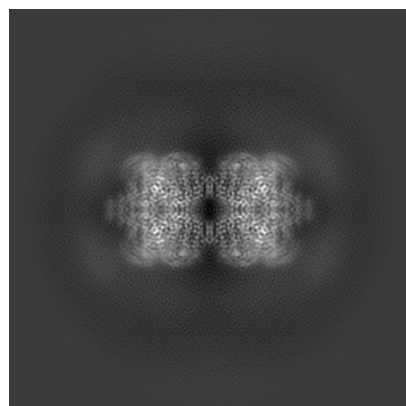
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52479. These allow visual inspection of the internal detail of the map and identification of artifacts.

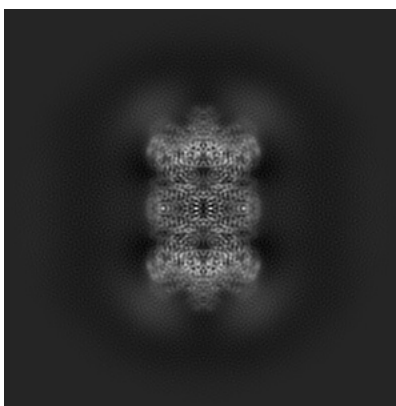
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

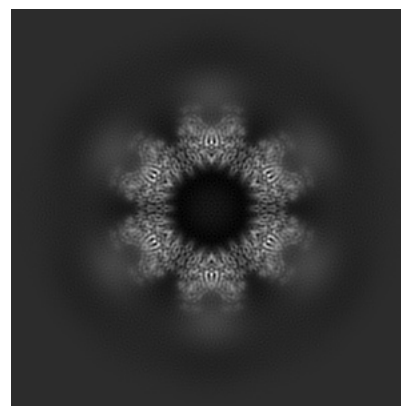
6.1.1 Primary map



X

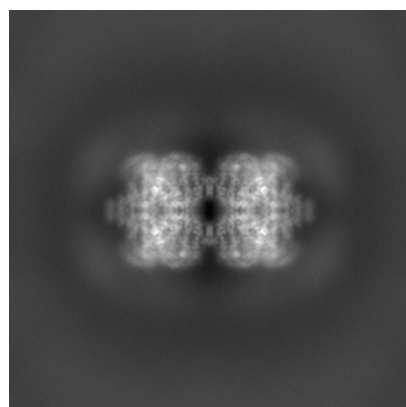


Y

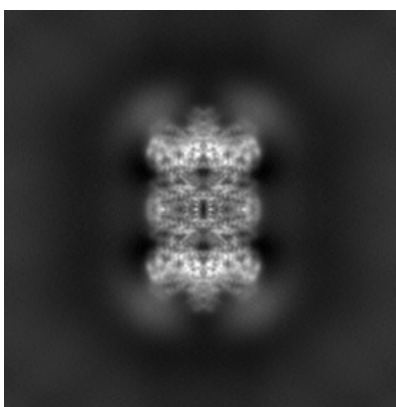


Z

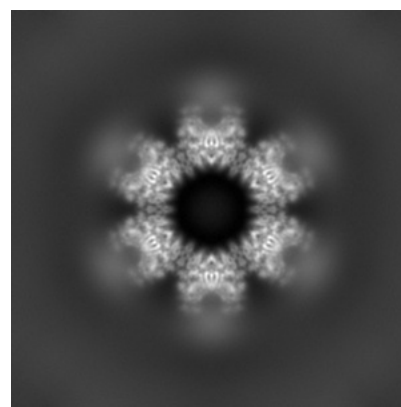
6.1.2 Raw map



X



Y

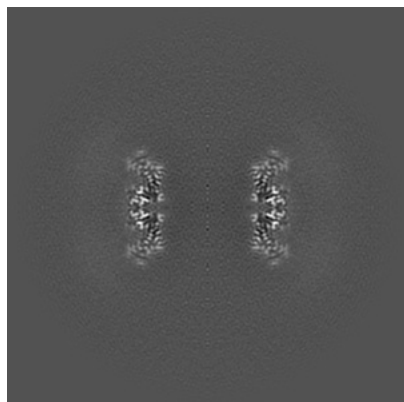


Z

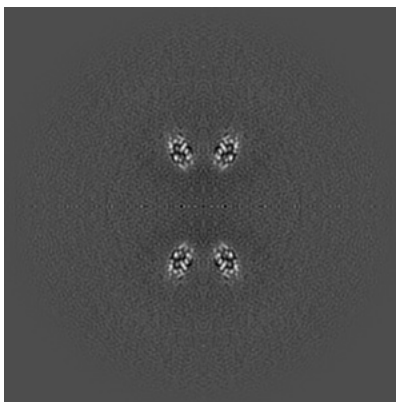
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

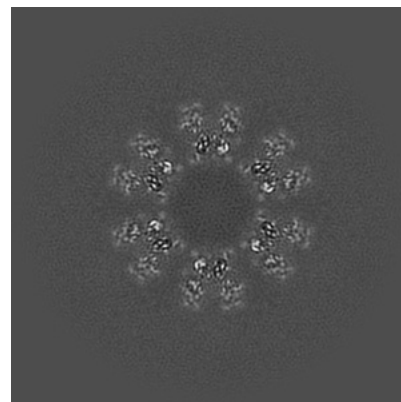
6.2.1 Primary map



X Index: 168

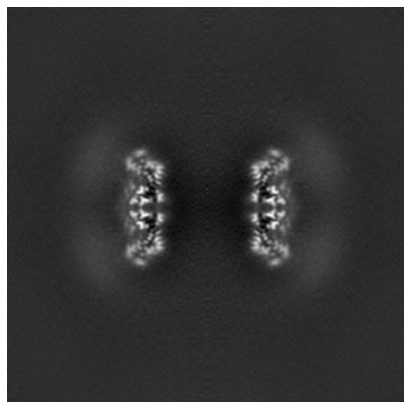


Y Index: 168

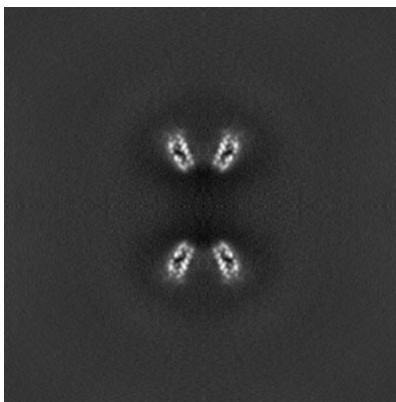


Z Index: 168

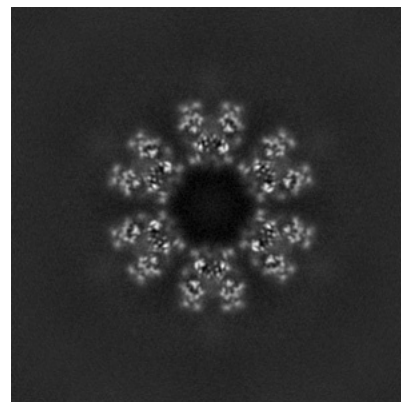
6.2.2 Raw map



X Index: 168



Y Index: 168

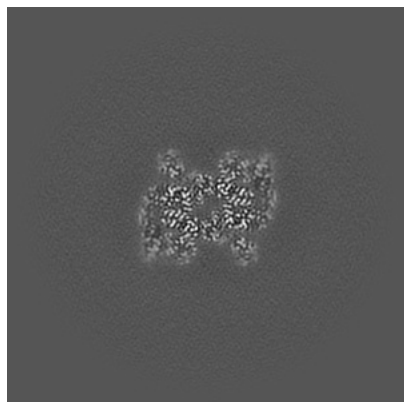


Z Index: 168

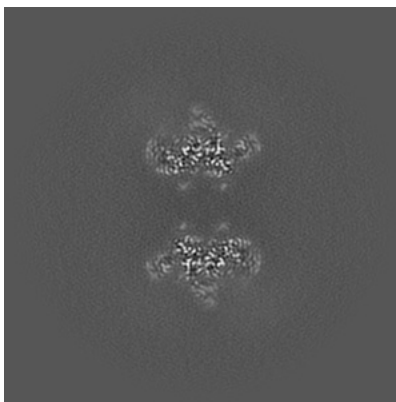
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

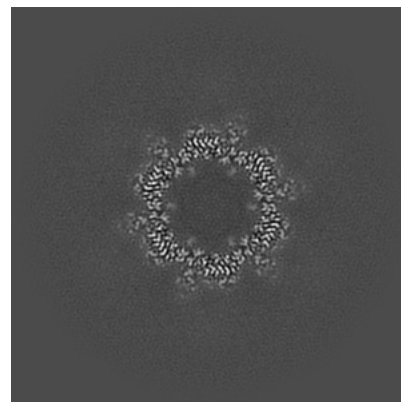
6.3.1 Primary map



X Index: 213

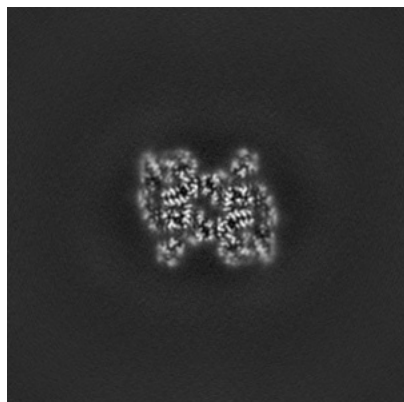


Y Index: 196

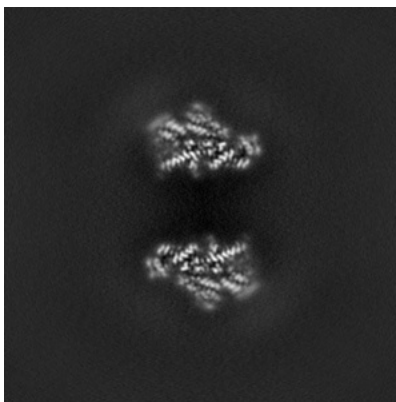


Z Index: 152

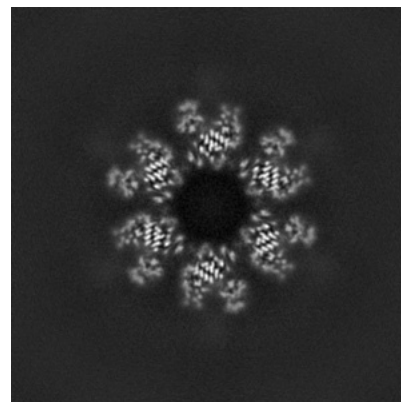
6.3.2 Raw map



X Index: 123



Y Index: 187

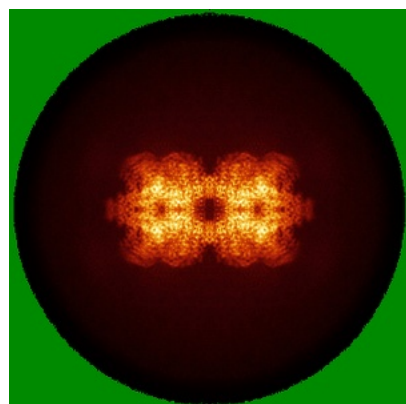


Z Index: 173

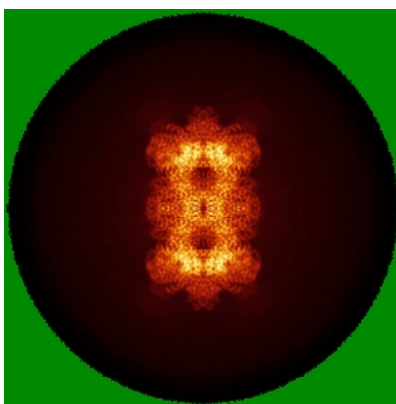
The images above show the largest variance slices of the map in three orthogonal directions.

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

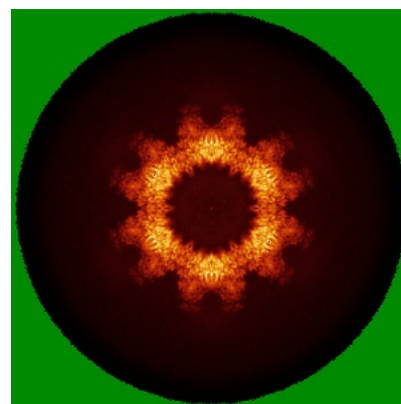
6.4.1 Primary map



X

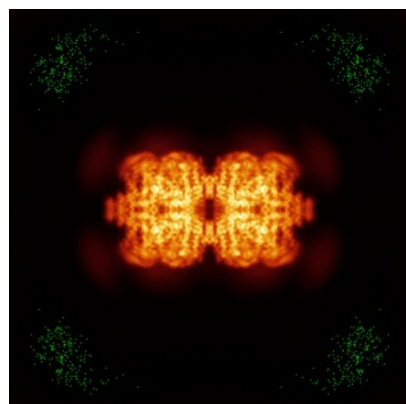


Y

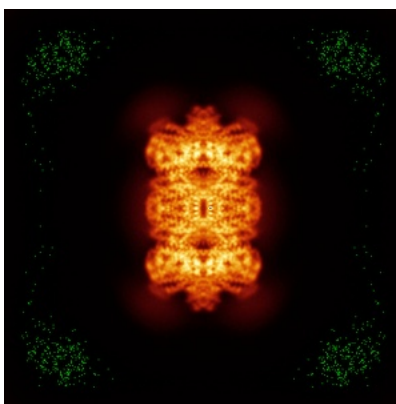


Z

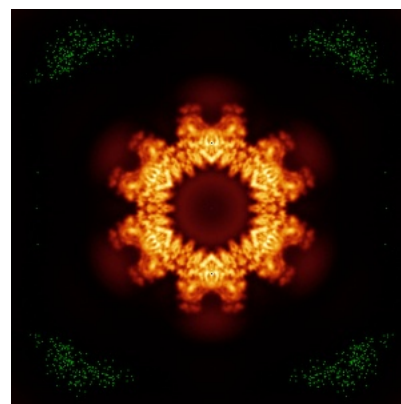
6.4.2 Raw map



X



Y

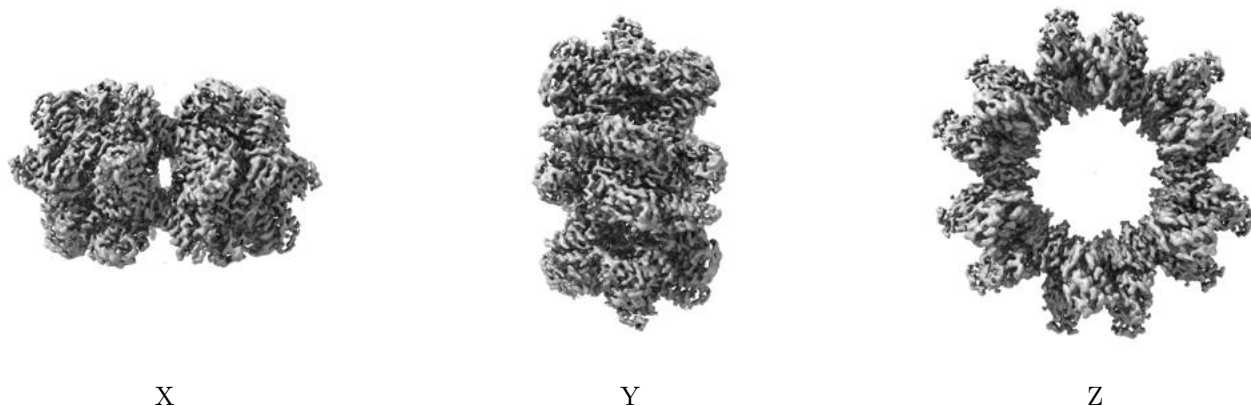


Z

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.

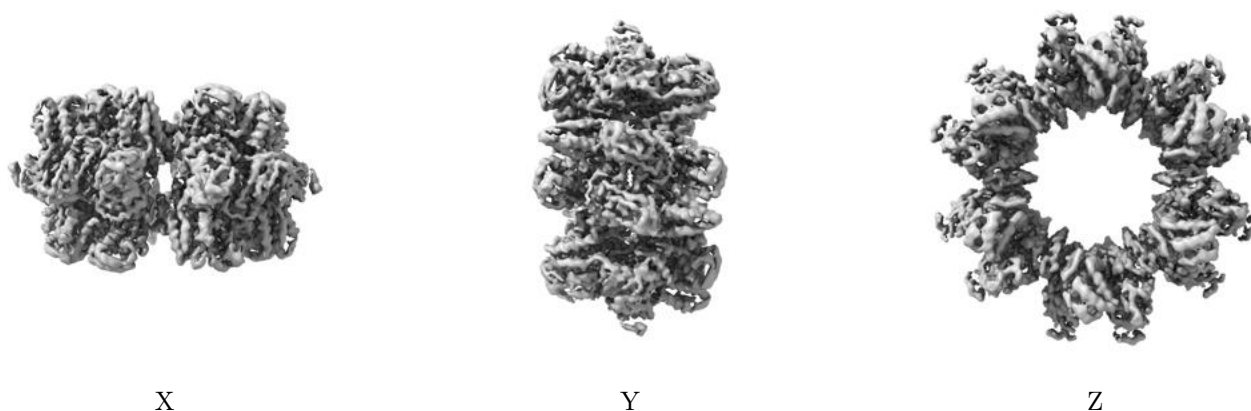
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. 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.

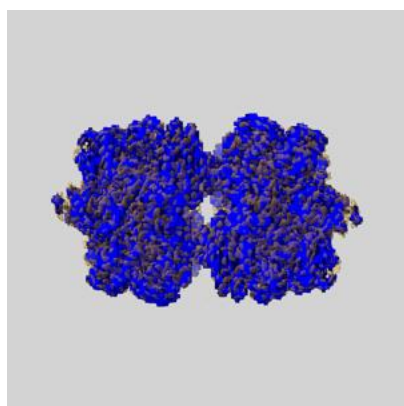
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

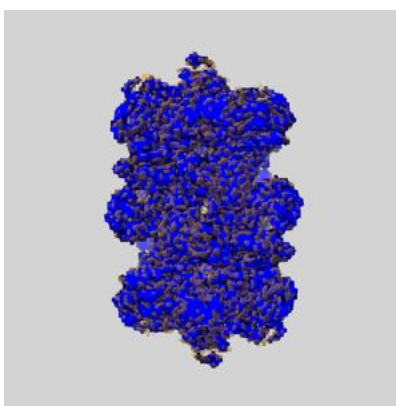
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

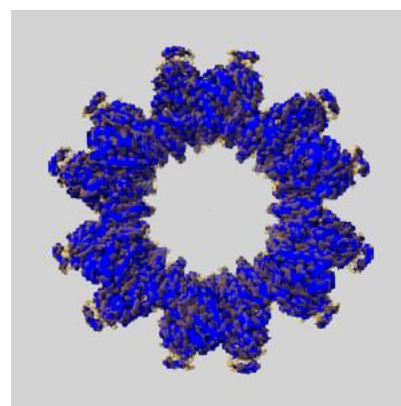
6.6.1 emd_52479_msk_1.map [i](#)



X



Y

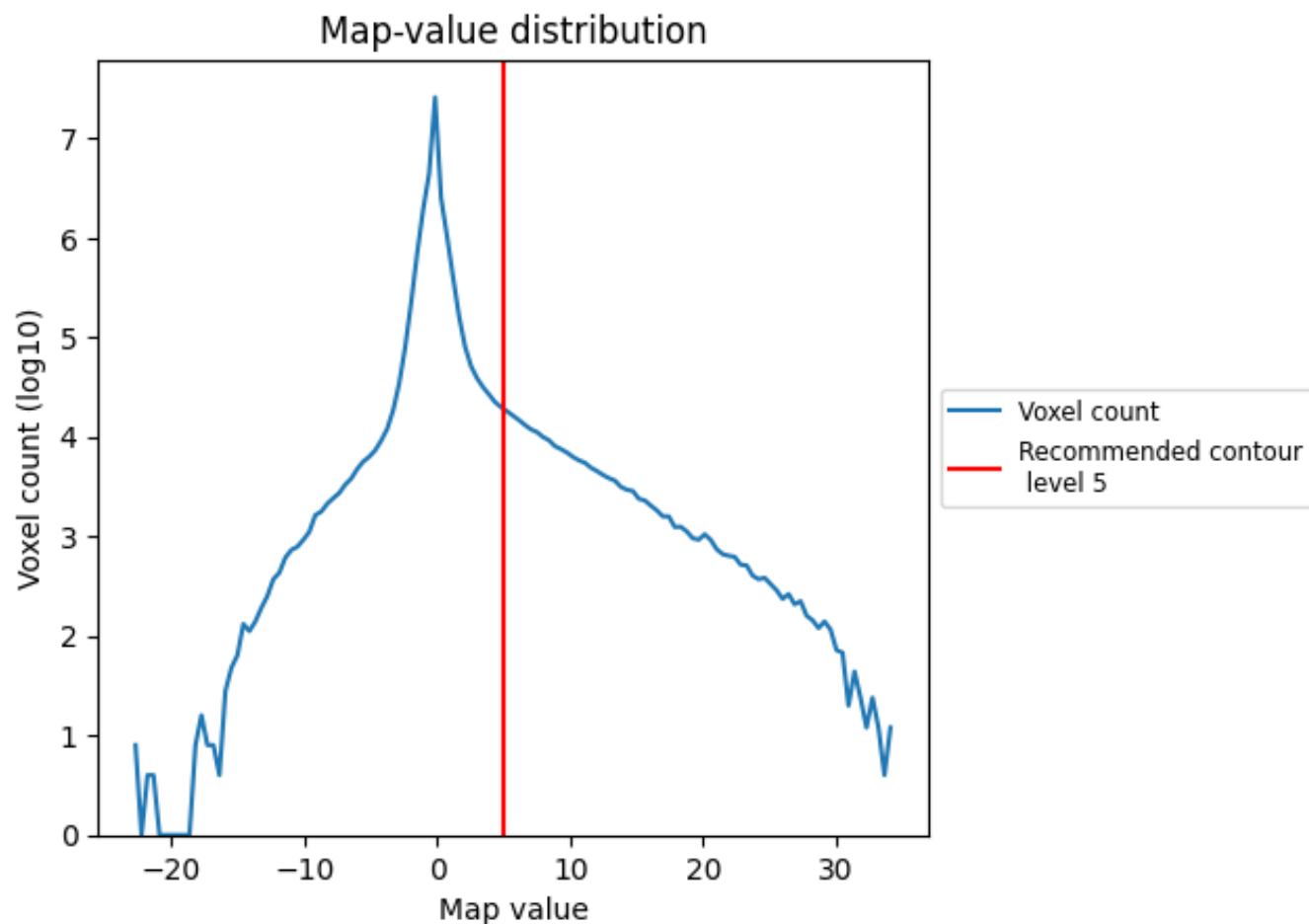


Z

7 Map analysis [i](#)

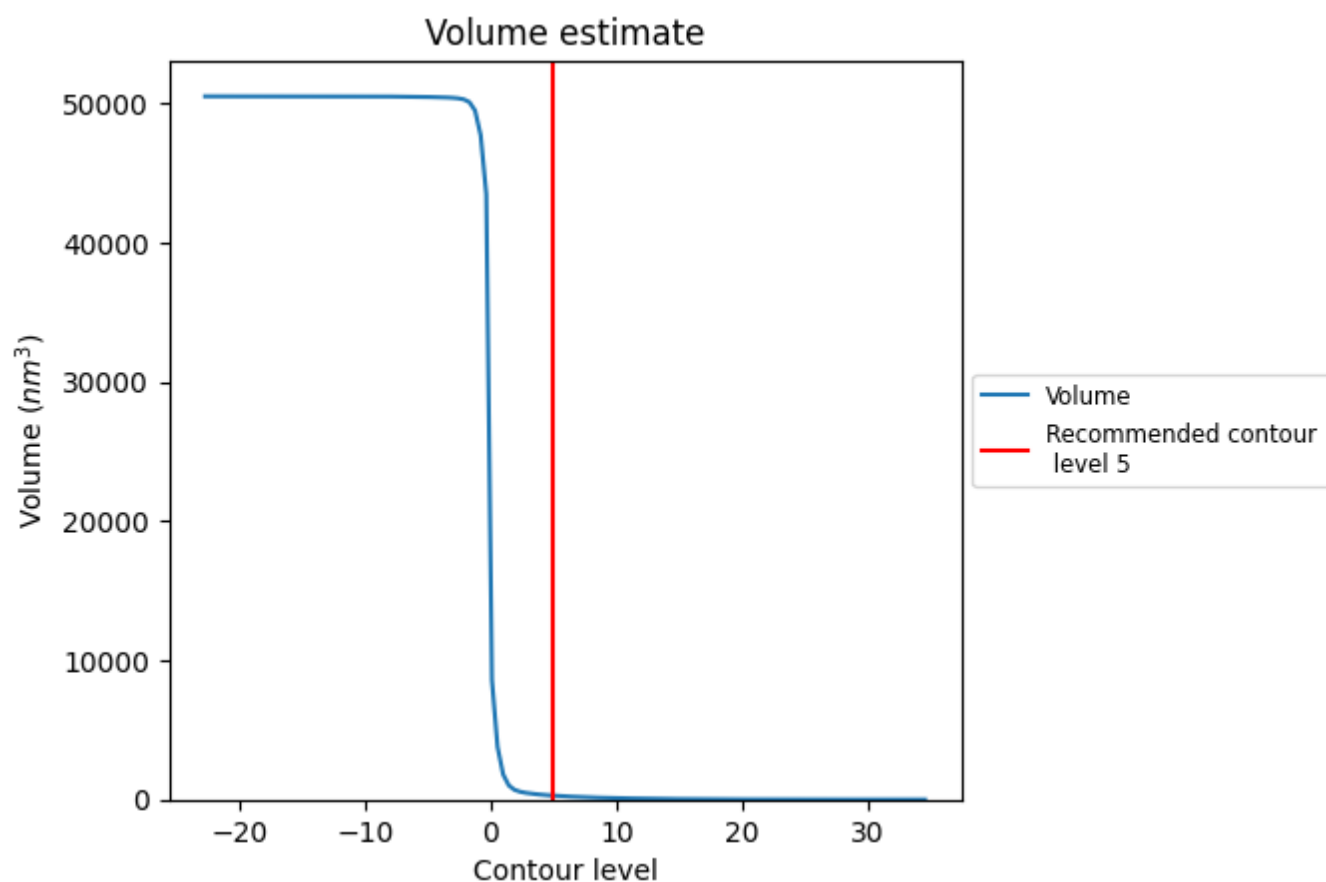
This section contains the results of statistical analysis of the map.

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.

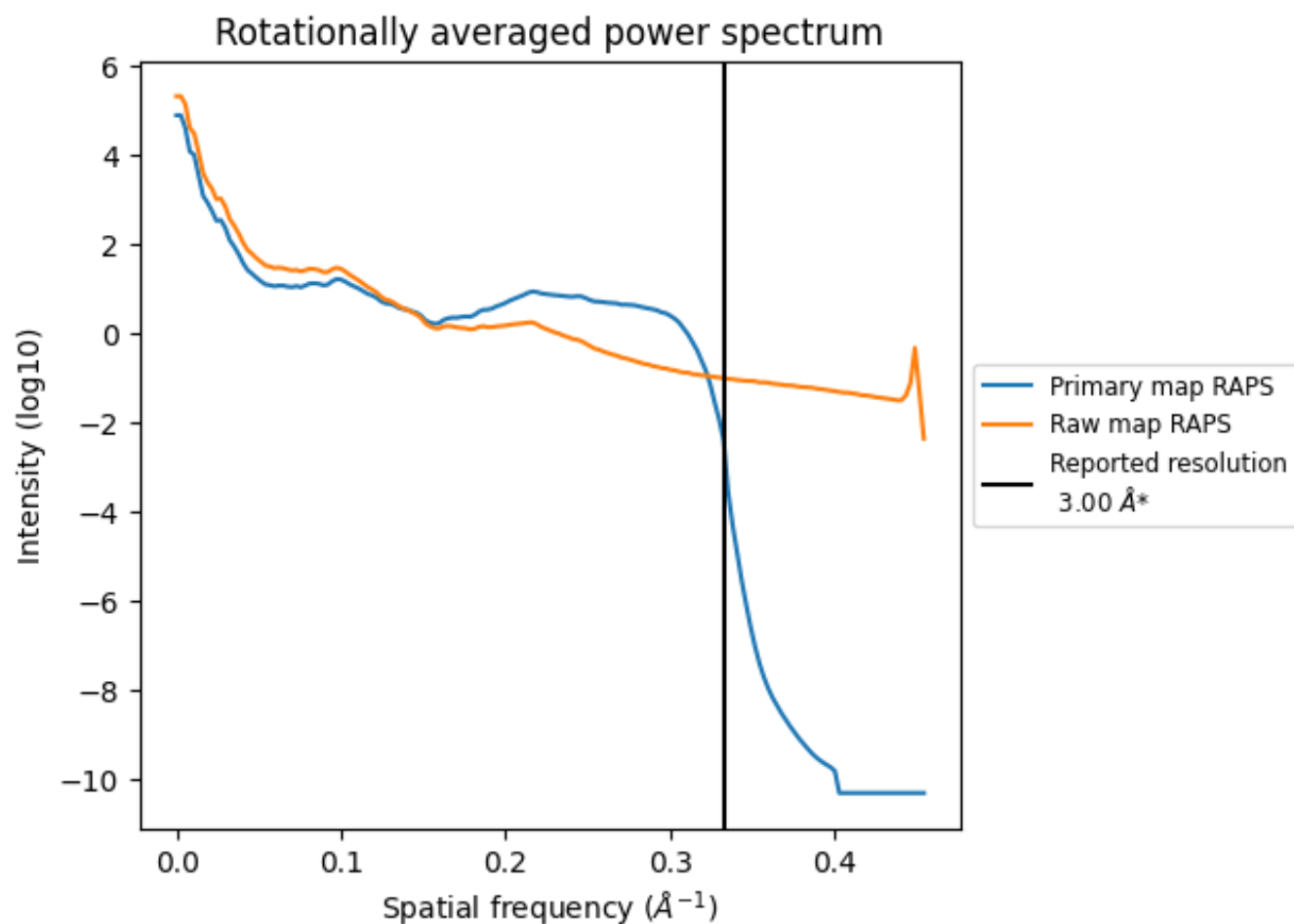
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 282 nm^3 ; this corresponds to an approximate mass of 255 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 ⓘ

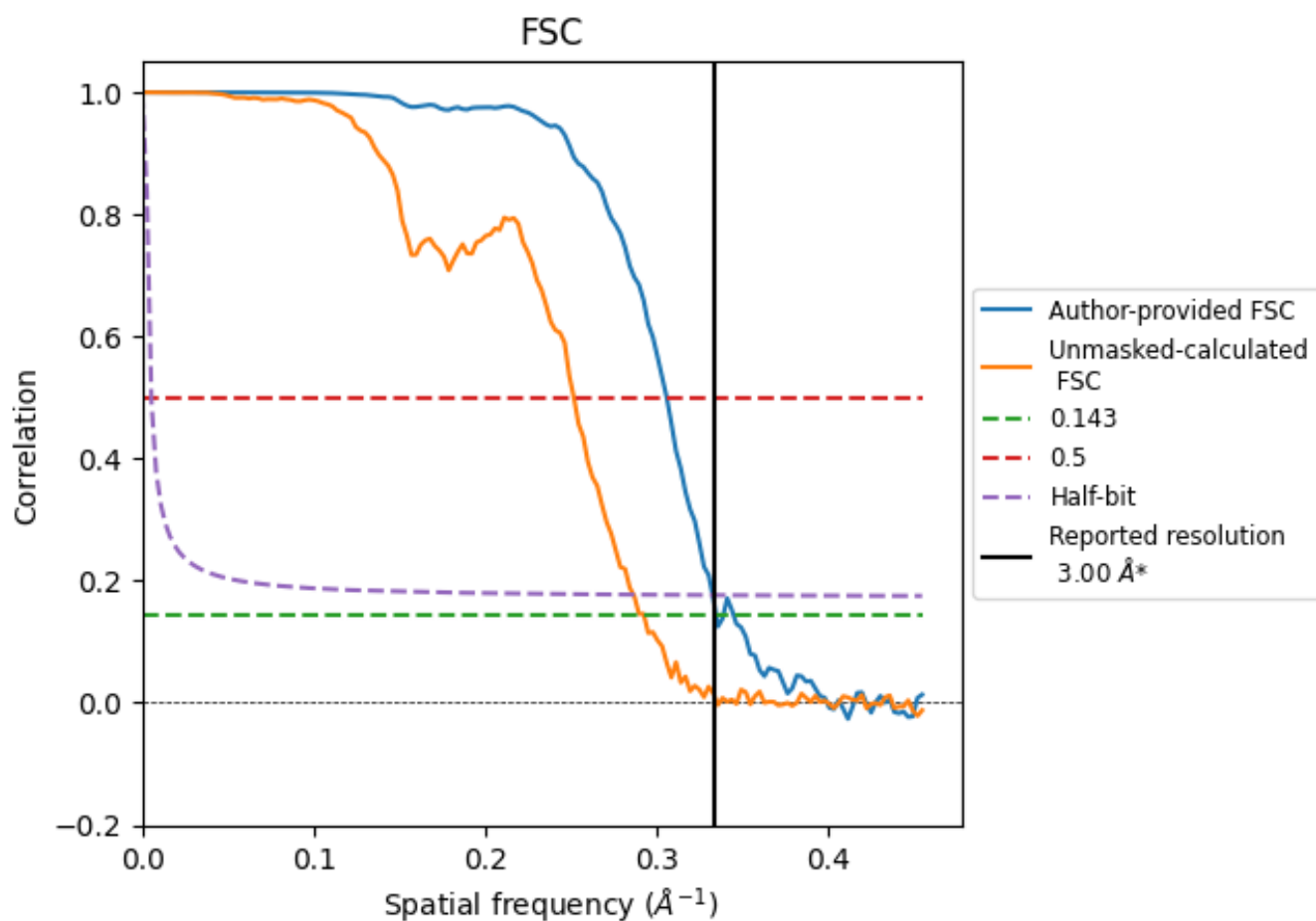


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 $0.333 \text{ \AA}^{-1}$

8.2 Resolution estimates

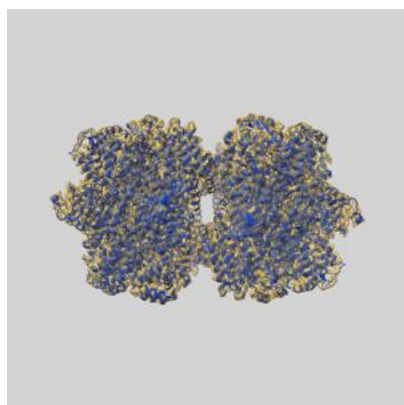
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.27	3.01
Unmasked-calculated*	3.42	3.97	3.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 3.0 by more than 10 %

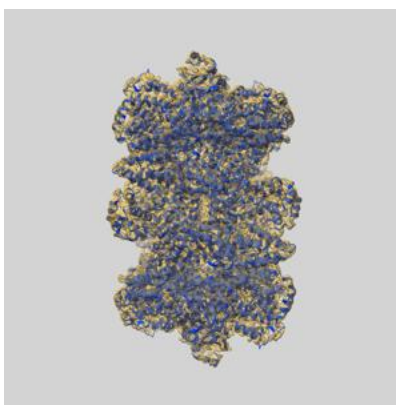
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52479 and PDB model 9HXJ. Per-residue inclusion information can be found in [section 3](#) on [page 31](#).

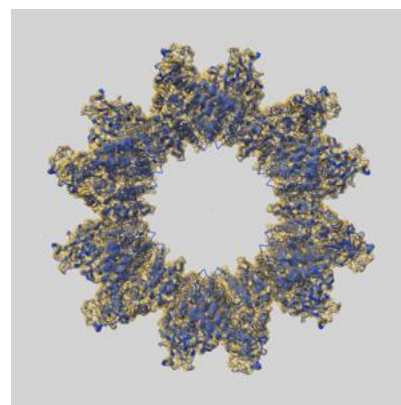
9.1 Map-model overlay [i](#)



X



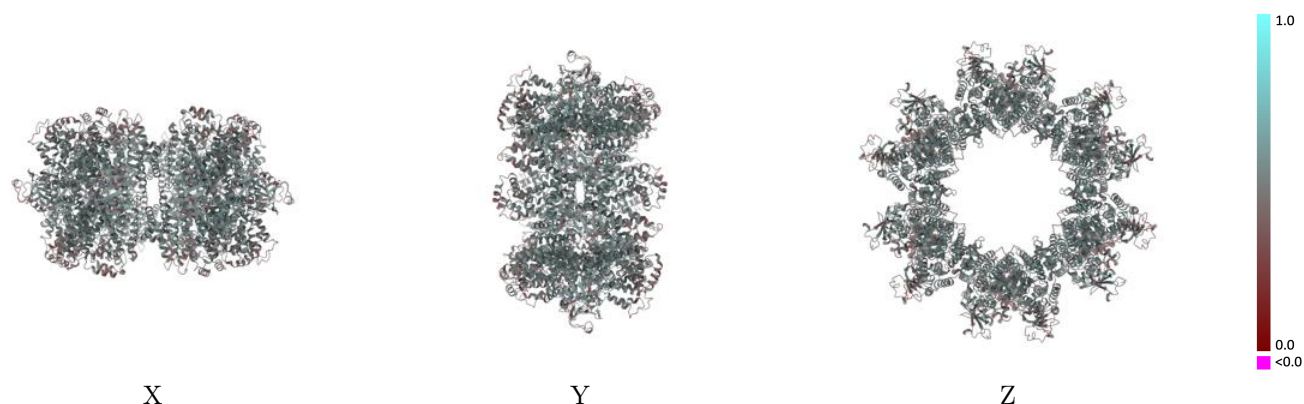
Y



Z

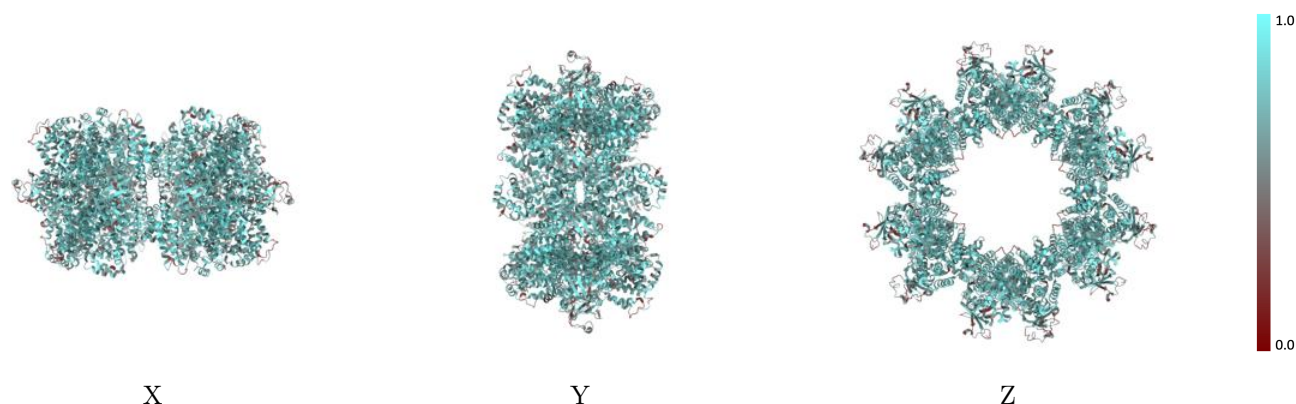
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



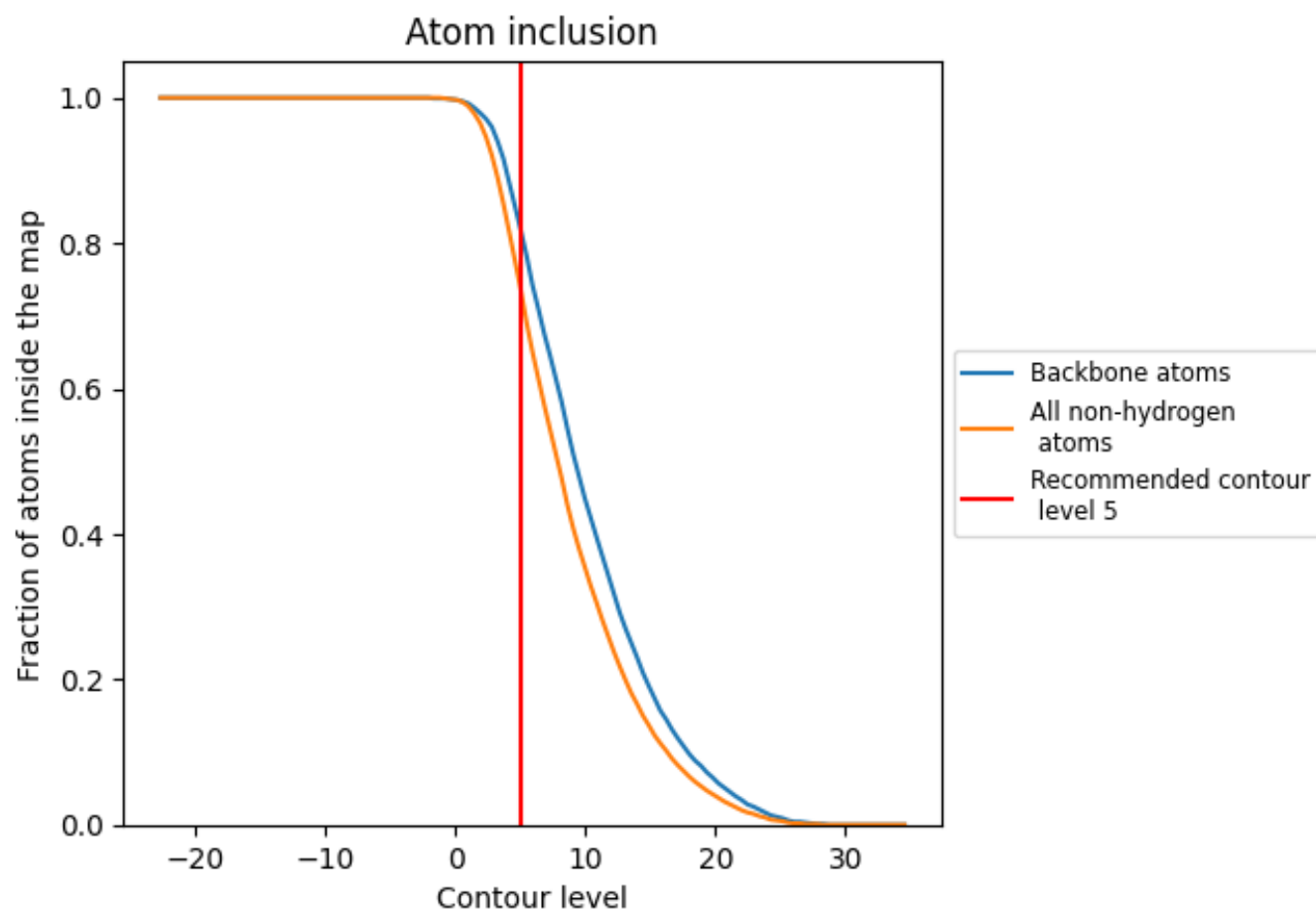
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7360	0.5070
A	0.7350	0.5070
B	0.7340	0.5060
C	0.7380	0.5080
D	0.7380	0.5060
E	0.7370	0.5070
F	0.7370	0.5080
G	0.7360	0.5080
H	0.7350	0.5070
I	0.7370	0.5080
J	0.7370	0.5070
K	0.7360	0.5060
L	0.7370	0.5070

1.0

0.0

<0.0