



Full wwPDB EM Validation Report ⓘ

Sep 21, 2026 – 01:46 PM JST

PDB ID : 9WXD / pdb_00009wxd
EMDB ID : EMD-66344
Title : Cryo-EM structure of of BetTC cage
Authors : Shi, D.J.; Cheng, X.Q.; Jiang, W.X.; Xing, Q.
Deposited on : 2025-09-25
Resolution : 3.07 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

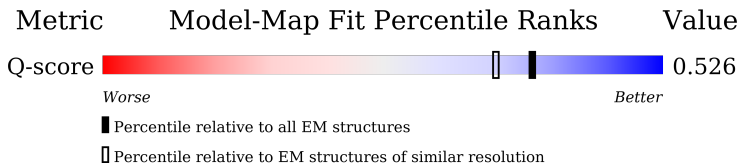
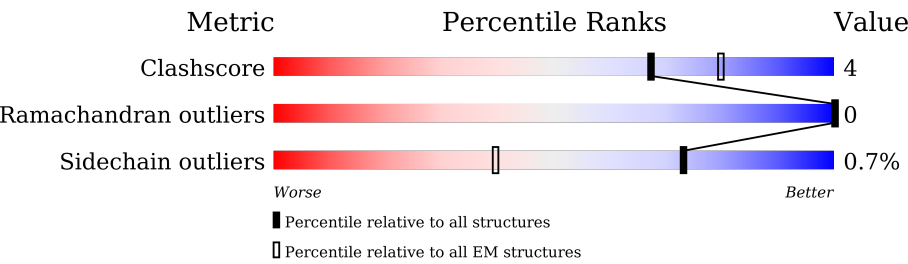
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.07 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.



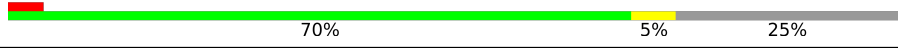
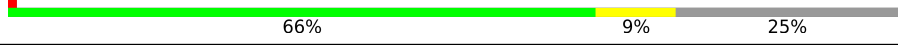
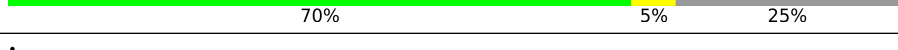
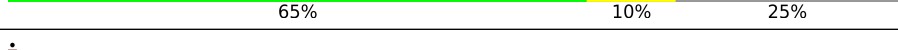
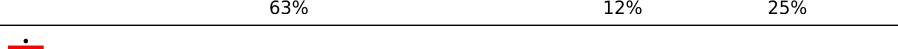
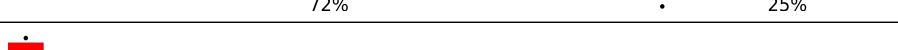
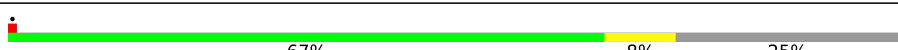
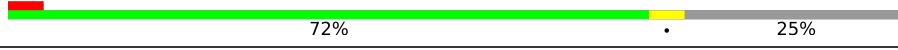
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13977 (2.57 - 3.57)

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	191	60%15%25%
1	AA	191	70%5%25%
1	B	191	70%5%25%
1	BA	191	68%8%25%

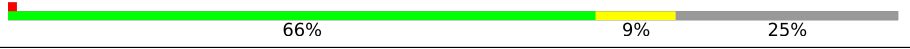
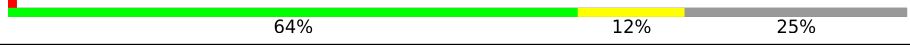
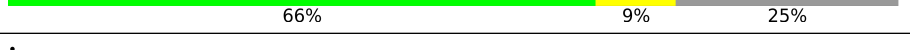
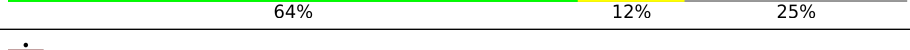
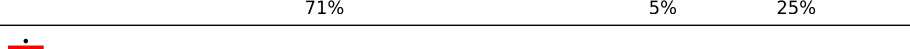
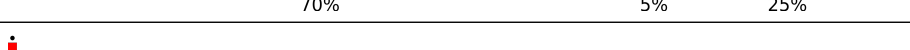
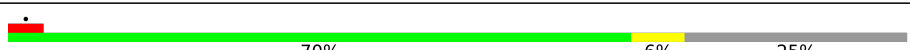
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Mol	Chain	Length	Quality of chain
1	C	191	
1	CA	191	
1	D	191	
1	DA	191	
1	E	191	
1	EA	191	
1	F	191	
1	FA	191	
1	G	191	
1	GA	191	
1	H	191	
1	HA	191	
1	I	191	
1	IA	191	
1	J	191	
1	JA	191	
1	K	191	
1	KA	191	
1	L	191	
1	LA	191	
1	M	191	
1	MA	191	
1	N	191	
1	NA	191	
1	O	191	

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Mol	Chain	Length	Quality of chain
1	OA	191	
1	P	191	
1	PA	191	
1	Q	191	
1	QA	191	
1	R	191	
1	RA	191	
1	S	191	
1	SA	191	
1	T	191	
1	TA	191	
1	UA	191	
1	V	191	
1	VA	191	
1	W	191	
1	WA	191	
1	X	191	
1	Y	191	
1	Z	191	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 57504 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 High-affinity choline transport protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	B	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	C	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	D	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	E	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	F	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	G	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	H	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	I	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	J	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	K	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	L	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	M	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	N	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	O	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	P	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	Q	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	S	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	T	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	V	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	W	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	X	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	Y	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	Z	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	AA	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	BA	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	CA	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	DA	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	EA	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	FA	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	GA	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	HA	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	IA	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	JA	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	KA	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	LA	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	MA	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	NA	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	OA	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	PA	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	QA	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	RA	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	SA	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	TA	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	UA	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		
1	VA	144	Total	C	N	O	S	0	0
			1201	764	207	223	7		
1	WA	144	Total	C	N	O	S	0	0
			1195	761	204	223	7		

There are 1104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	MET	-	initiating methionine	UNP P0ABC9
A	482	HIS	-	expression tag	UNP P0ABC9
A	483	HIS	-	expression tag	UNP P0ABC9
A	484	HIS	-	expression tag	UNP P0ABC9
A	485	HIS	-	expression tag	UNP P0ABC9
A	486	HIS	-	expression tag	UNP P0ABC9
A	487	HIS	-	expression tag	UNP P0ABC9
A	488	HIS	-	expression tag	UNP P0ABC9
A	489	HIS	-	expression tag	UNP P0ABC9
A	490	HIS	-	expression tag	UNP P0ABC9
A	491	HIS	-	expression tag	UNP P0ABC9
A	492	GLU	-	expression tag	UNP P0ABC9
A	493	ASN	-	expression tag	UNP P0ABC9
A	494	LEU	-	expression tag	UNP P0ABC9
A	495	TYR	-	expression tag	UNP P0ABC9
A	496	PHE	-	expression tag	UNP P0ABC9
A	497	GLN	-	expression tag	UNP P0ABC9
A	498	GLY	-	expression tag	UNP P0ABC9
A	499	GLY	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	500	SER	-	expression tag	UNP P0ABC9
A	669	THR	-	expression tag	UNP P0ABC9
A	670	GLY	-	expression tag	UNP P0ABC9
A	671	CYS	-	expression tag	UNP P0ABC9
B	481	MET	-	initiating methionine	UNP P0ABC9
B	482	HIS	-	expression tag	UNP P0ABC9
B	483	HIS	-	expression tag	UNP P0ABC9
B	484	HIS	-	expression tag	UNP P0ABC9
B	485	HIS	-	expression tag	UNP P0ABC9
B	486	HIS	-	expression tag	UNP P0ABC9
B	487	HIS	-	expression tag	UNP P0ABC9
B	488	HIS	-	expression tag	UNP P0ABC9
B	489	HIS	-	expression tag	UNP P0ABC9
B	490	HIS	-	expression tag	UNP P0ABC9
B	491	HIS	-	expression tag	UNP P0ABC9
B	492	GLU	-	expression tag	UNP P0ABC9
B	493	ASN	-	expression tag	UNP P0ABC9
B	494	LEU	-	expression tag	UNP P0ABC9
B	495	TYR	-	expression tag	UNP P0ABC9
B	496	PHE	-	expression tag	UNP P0ABC9
B	497	GLN	-	expression tag	UNP P0ABC9
B	498	GLY	-	expression tag	UNP P0ABC9
B	499	GLY	-	expression tag	UNP P0ABC9
B	500	SER	-	expression tag	UNP P0ABC9
B	669	THR	-	expression tag	UNP P0ABC9
B	670	GLY	-	expression tag	UNP P0ABC9
B	671	CYS	-	expression tag	UNP P0ABC9
C	481	MET	-	initiating methionine	UNP P0ABC9
C	482	HIS	-	expression tag	UNP P0ABC9
C	483	HIS	-	expression tag	UNP P0ABC9
C	484	HIS	-	expression tag	UNP P0ABC9
C	485	HIS	-	expression tag	UNP P0ABC9
C	486	HIS	-	expression tag	UNP P0ABC9
C	487	HIS	-	expression tag	UNP P0ABC9
C	488	HIS	-	expression tag	UNP P0ABC9
C	489	HIS	-	expression tag	UNP P0ABC9
C	490	HIS	-	expression tag	UNP P0ABC9
C	491	HIS	-	expression tag	UNP P0ABC9
C	492	GLU	-	expression tag	UNP P0ABC9
C	493	ASN	-	expression tag	UNP P0ABC9
C	494	LEU	-	expression tag	UNP P0ABC9
C	495	TYR	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	496	PHE	-	expression tag	UNP P0ABC9
C	497	GLN	-	expression tag	UNP P0ABC9
C	498	GLY	-	expression tag	UNP P0ABC9
C	499	GLY	-	expression tag	UNP P0ABC9
C	500	SER	-	expression tag	UNP P0ABC9
C	669	THR	-	expression tag	UNP P0ABC9
C	670	GLY	-	expression tag	UNP P0ABC9
C	671	CYS	-	expression tag	UNP P0ABC9
D	481	MET	-	initiating methionine	UNP P0ABC9
D	482	HIS	-	expression tag	UNP P0ABC9
D	483	HIS	-	expression tag	UNP P0ABC9
D	484	HIS	-	expression tag	UNP P0ABC9
D	485	HIS	-	expression tag	UNP P0ABC9
D	486	HIS	-	expression tag	UNP P0ABC9
D	487	HIS	-	expression tag	UNP P0ABC9
D	488	HIS	-	expression tag	UNP P0ABC9
D	489	HIS	-	expression tag	UNP P0ABC9
D	490	HIS	-	expression tag	UNP P0ABC9
D	491	HIS	-	expression tag	UNP P0ABC9
D	492	GLU	-	expression tag	UNP P0ABC9
D	493	ASN	-	expression tag	UNP P0ABC9
D	494	LEU	-	expression tag	UNP P0ABC9
D	495	TYR	-	expression tag	UNP P0ABC9
D	496	PHE	-	expression tag	UNP P0ABC9
D	497	GLN	-	expression tag	UNP P0ABC9
D	498	GLY	-	expression tag	UNP P0ABC9
D	499	GLY	-	expression tag	UNP P0ABC9
D	500	SER	-	expression tag	UNP P0ABC9
D	669	THR	-	expression tag	UNP P0ABC9
D	670	GLY	-	expression tag	UNP P0ABC9
D	671	CYS	-	expression tag	UNP P0ABC9
E	481	MET	-	initiating methionine	UNP P0ABC9
E	482	HIS	-	expression tag	UNP P0ABC9
E	483	HIS	-	expression tag	UNP P0ABC9
E	484	HIS	-	expression tag	UNP P0ABC9
E	485	HIS	-	expression tag	UNP P0ABC9
E	486	HIS	-	expression tag	UNP P0ABC9
E	487	HIS	-	expression tag	UNP P0ABC9
E	488	HIS	-	expression tag	UNP P0ABC9
E	489	HIS	-	expression tag	UNP P0ABC9
E	490	HIS	-	expression tag	UNP P0ABC9
E	491	HIS	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	492	GLU	-	expression tag	UNP P0ABC9
E	493	ASN	-	expression tag	UNP P0ABC9
E	494	LEU	-	expression tag	UNP P0ABC9
E	495	TYR	-	expression tag	UNP P0ABC9
E	496	PHE	-	expression tag	UNP P0ABC9
E	497	GLN	-	expression tag	UNP P0ABC9
E	498	GLY	-	expression tag	UNP P0ABC9
E	499	GLY	-	expression tag	UNP P0ABC9
E	500	SER	-	expression tag	UNP P0ABC9
E	669	THR	-	expression tag	UNP P0ABC9
E	670	GLY	-	expression tag	UNP P0ABC9
E	671	CYS	-	expression tag	UNP P0ABC9
F	481	MET	-	initiating methionine	UNP P0ABC9
F	482	HIS	-	expression tag	UNP P0ABC9
F	483	HIS	-	expression tag	UNP P0ABC9
F	484	HIS	-	expression tag	UNP P0ABC9
F	485	HIS	-	expression tag	UNP P0ABC9
F	486	HIS	-	expression tag	UNP P0ABC9
F	487	HIS	-	expression tag	UNP P0ABC9
F	488	HIS	-	expression tag	UNP P0ABC9
F	489	HIS	-	expression tag	UNP P0ABC9
F	490	HIS	-	expression tag	UNP P0ABC9
F	491	HIS	-	expression tag	UNP P0ABC9
F	492	GLU	-	expression tag	UNP P0ABC9
F	493	ASN	-	expression tag	UNP P0ABC9
F	494	LEU	-	expression tag	UNP P0ABC9
F	495	TYR	-	expression tag	UNP P0ABC9
F	496	PHE	-	expression tag	UNP P0ABC9
F	497	GLN	-	expression tag	UNP P0ABC9
F	498	GLY	-	expression tag	UNP P0ABC9
F	499	GLY	-	expression tag	UNP P0ABC9
F	500	SER	-	expression tag	UNP P0ABC9
F	669	THR	-	expression tag	UNP P0ABC9
F	670	GLY	-	expression tag	UNP P0ABC9
F	671	CYS	-	expression tag	UNP P0ABC9
G	481	MET	-	initiating methionine	UNP P0ABC9
G	482	HIS	-	expression tag	UNP P0ABC9
G	483	HIS	-	expression tag	UNP P0ABC9
G	484	HIS	-	expression tag	UNP P0ABC9
G	485	HIS	-	expression tag	UNP P0ABC9
G	486	HIS	-	expression tag	UNP P0ABC9
G	487	HIS	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	488	HIS	-	expression tag	UNP P0ABC9
G	489	HIS	-	expression tag	UNP P0ABC9
G	490	HIS	-	expression tag	UNP P0ABC9
G	491	HIS	-	expression tag	UNP P0ABC9
G	492	GLU	-	expression tag	UNP P0ABC9
G	493	ASN	-	expression tag	UNP P0ABC9
G	494	LEU	-	expression tag	UNP P0ABC9
G	495	TYR	-	expression tag	UNP P0ABC9
G	496	PHE	-	expression tag	UNP P0ABC9
G	497	GLN	-	expression tag	UNP P0ABC9
G	498	GLY	-	expression tag	UNP P0ABC9
G	499	GLY	-	expression tag	UNP P0ABC9
G	500	SER	-	expression tag	UNP P0ABC9
G	669	THR	-	expression tag	UNP P0ABC9
G	670	GLY	-	expression tag	UNP P0ABC9
G	671	CYS	-	expression tag	UNP P0ABC9
H	481	MET	-	initiating methionine	UNP P0ABC9
H	482	HIS	-	expression tag	UNP P0ABC9
H	483	HIS	-	expression tag	UNP P0ABC9
H	484	HIS	-	expression tag	UNP P0ABC9
H	485	HIS	-	expression tag	UNP P0ABC9
H	486	HIS	-	expression tag	UNP P0ABC9
H	487	HIS	-	expression tag	UNP P0ABC9
H	488	HIS	-	expression tag	UNP P0ABC9
H	489	HIS	-	expression tag	UNP P0ABC9
H	490	HIS	-	expression tag	UNP P0ABC9
H	491	HIS	-	expression tag	UNP P0ABC9
H	492	GLU	-	expression tag	UNP P0ABC9
H	493	ASN	-	expression tag	UNP P0ABC9
H	494	LEU	-	expression tag	UNP P0ABC9
H	495	TYR	-	expression tag	UNP P0ABC9
H	496	PHE	-	expression tag	UNP P0ABC9
H	497	GLN	-	expression tag	UNP P0ABC9
H	498	GLY	-	expression tag	UNP P0ABC9
H	499	GLY	-	expression tag	UNP P0ABC9
H	500	SER	-	expression tag	UNP P0ABC9
H	669	THR	-	expression tag	UNP P0ABC9
H	670	GLY	-	expression tag	UNP P0ABC9
H	671	CYS	-	expression tag	UNP P0ABC9
I	481	MET	-	initiating methionine	UNP P0ABC9
I	482	HIS	-	expression tag	UNP P0ABC9
I	483	HIS	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	484	HIS	-	expression tag	UNP P0ABC9
I	485	HIS	-	expression tag	UNP P0ABC9
I	486	HIS	-	expression tag	UNP P0ABC9
I	487	HIS	-	expression tag	UNP P0ABC9
I	488	HIS	-	expression tag	UNP P0ABC9
I	489	HIS	-	expression tag	UNP P0ABC9
I	490	HIS	-	expression tag	UNP P0ABC9
I	491	HIS	-	expression tag	UNP P0ABC9
I	492	GLU	-	expression tag	UNP P0ABC9
I	493	ASN	-	expression tag	UNP P0ABC9
I	494	LEU	-	expression tag	UNP P0ABC9
I	495	TYR	-	expression tag	UNP P0ABC9
I	496	PHE	-	expression tag	UNP P0ABC9
I	497	GLN	-	expression tag	UNP P0ABC9
I	498	GLY	-	expression tag	UNP P0ABC9
I	499	GLY	-	expression tag	UNP P0ABC9
I	500	SER	-	expression tag	UNP P0ABC9
I	669	THR	-	expression tag	UNP P0ABC9
I	670	GLY	-	expression tag	UNP P0ABC9
I	671	CYS	-	expression tag	UNP P0ABC9
J	481	MET	-	initiating methionine	UNP P0ABC9
J	482	HIS	-	expression tag	UNP P0ABC9
J	483	HIS	-	expression tag	UNP P0ABC9
J	484	HIS	-	expression tag	UNP P0ABC9
J	485	HIS	-	expression tag	UNP P0ABC9
J	486	HIS	-	expression tag	UNP P0ABC9
J	487	HIS	-	expression tag	UNP P0ABC9
J	488	HIS	-	expression tag	UNP P0ABC9
J	489	HIS	-	expression tag	UNP P0ABC9
J	490	HIS	-	expression tag	UNP P0ABC9
J	491	HIS	-	expression tag	UNP P0ABC9
J	492	GLU	-	expression tag	UNP P0ABC9
J	493	ASN	-	expression tag	UNP P0ABC9
J	494	LEU	-	expression tag	UNP P0ABC9
J	495	TYR	-	expression tag	UNP P0ABC9
J	496	PHE	-	expression tag	UNP P0ABC9
J	497	GLN	-	expression tag	UNP P0ABC9
J	498	GLY	-	expression tag	UNP P0ABC9
J	499	GLY	-	expression tag	UNP P0ABC9
J	500	SER	-	expression tag	UNP P0ABC9
J	669	THR	-	expression tag	UNP P0ABC9
J	670	GLY	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	671	CYS	-	expression tag	UNP P0ABC9
K	481	MET	-	initiating methionine	UNP P0ABC9
K	482	HIS	-	expression tag	UNP P0ABC9
K	483	HIS	-	expression tag	UNP P0ABC9
K	484	HIS	-	expression tag	UNP P0ABC9
K	485	HIS	-	expression tag	UNP P0ABC9
K	486	HIS	-	expression tag	UNP P0ABC9
K	487	HIS	-	expression tag	UNP P0ABC9
K	488	HIS	-	expression tag	UNP P0ABC9
K	489	HIS	-	expression tag	UNP P0ABC9
K	490	HIS	-	expression tag	UNP P0ABC9
K	491	HIS	-	expression tag	UNP P0ABC9
K	492	GLU	-	expression tag	UNP P0ABC9
K	493	ASN	-	expression tag	UNP P0ABC9
K	494	LEU	-	expression tag	UNP P0ABC9
K	495	TYR	-	expression tag	UNP P0ABC9
K	496	PHE	-	expression tag	UNP P0ABC9
K	497	GLN	-	expression tag	UNP P0ABC9
K	498	GLY	-	expression tag	UNP P0ABC9
K	499	GLY	-	expression tag	UNP P0ABC9
K	500	SER	-	expression tag	UNP P0ABC9
K	669	THR	-	expression tag	UNP P0ABC9
K	670	GLY	-	expression tag	UNP P0ABC9
K	671	CYS	-	expression tag	UNP P0ABC9
L	481	MET	-	initiating methionine	UNP P0ABC9
L	482	HIS	-	expression tag	UNP P0ABC9
L	483	HIS	-	expression tag	UNP P0ABC9
L	484	HIS	-	expression tag	UNP P0ABC9
L	485	HIS	-	expression tag	UNP P0ABC9
L	486	HIS	-	expression tag	UNP P0ABC9
L	487	HIS	-	expression tag	UNP P0ABC9
L	488	HIS	-	expression tag	UNP P0ABC9
L	489	HIS	-	expression tag	UNP P0ABC9
L	490	HIS	-	expression tag	UNP P0ABC9
L	491	HIS	-	expression tag	UNP P0ABC9
L	492	GLU	-	expression tag	UNP P0ABC9
L	493	ASN	-	expression tag	UNP P0ABC9
L	494	LEU	-	expression tag	UNP P0ABC9
L	495	TYR	-	expression tag	UNP P0ABC9
L	496	PHE	-	expression tag	UNP P0ABC9
L	497	GLN	-	expression tag	UNP P0ABC9
L	498	GLY	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
L	499	GLY	-	expression tag	UNP P0ABC9
L	500	SER	-	expression tag	UNP P0ABC9
L	669	THR	-	expression tag	UNP P0ABC9
L	670	GLY	-	expression tag	UNP P0ABC9
L	671	CYS	-	expression tag	UNP P0ABC9
M	481	MET	-	initiating methionine	UNP P0ABC9
M	482	HIS	-	expression tag	UNP P0ABC9
M	483	HIS	-	expression tag	UNP P0ABC9
M	484	HIS	-	expression tag	UNP P0ABC9
M	485	HIS	-	expression tag	UNP P0ABC9
M	486	HIS	-	expression tag	UNP P0ABC9
M	487	HIS	-	expression tag	UNP P0ABC9
M	488	HIS	-	expression tag	UNP P0ABC9
M	489	HIS	-	expression tag	UNP P0ABC9
M	490	HIS	-	expression tag	UNP P0ABC9
M	491	HIS	-	expression tag	UNP P0ABC9
M	492	GLU	-	expression tag	UNP P0ABC9
M	493	ASN	-	expression tag	UNP P0ABC9
M	494	LEU	-	expression tag	UNP P0ABC9
M	495	TYR	-	expression tag	UNP P0ABC9
M	496	PHE	-	expression tag	UNP P0ABC9
M	497	GLN	-	expression tag	UNP P0ABC9
M	498	GLY	-	expression tag	UNP P0ABC9
M	499	GLY	-	expression tag	UNP P0ABC9
M	500	SER	-	expression tag	UNP P0ABC9
M	669	THR	-	expression tag	UNP P0ABC9
M	670	GLY	-	expression tag	UNP P0ABC9
M	671	CYS	-	expression tag	UNP P0ABC9
N	481	MET	-	initiating methionine	UNP P0ABC9
N	482	HIS	-	expression tag	UNP P0ABC9
N	483	HIS	-	expression tag	UNP P0ABC9
N	484	HIS	-	expression tag	UNP P0ABC9
N	485	HIS	-	expression tag	UNP P0ABC9
N	486	HIS	-	expression tag	UNP P0ABC9
N	487	HIS	-	expression tag	UNP P0ABC9
N	488	HIS	-	expression tag	UNP P0ABC9
N	489	HIS	-	expression tag	UNP P0ABC9
N	490	HIS	-	expression tag	UNP P0ABC9
N	491	HIS	-	expression tag	UNP P0ABC9
N	492	GLU	-	expression tag	UNP P0ABC9
N	493	ASN	-	expression tag	UNP P0ABC9
N	494	LEU	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
N	495	TYR	-	expression tag	UNP P0ABC9
N	496	PHE	-	expression tag	UNP P0ABC9
N	497	GLN	-	expression tag	UNP P0ABC9
N	498	GLY	-	expression tag	UNP P0ABC9
N	499	GLY	-	expression tag	UNP P0ABC9
N	500	SER	-	expression tag	UNP P0ABC9
N	669	THR	-	expression tag	UNP P0ABC9
N	670	GLY	-	expression tag	UNP P0ABC9
N	671	CYS	-	expression tag	UNP P0ABC9
O	481	MET	-	initiating methionine	UNP P0ABC9
O	482	HIS	-	expression tag	UNP P0ABC9
O	483	HIS	-	expression tag	UNP P0ABC9
O	484	HIS	-	expression tag	UNP P0ABC9
O	485	HIS	-	expression tag	UNP P0ABC9
O	486	HIS	-	expression tag	UNP P0ABC9
O	487	HIS	-	expression tag	UNP P0ABC9
O	488	HIS	-	expression tag	UNP P0ABC9
O	489	HIS	-	expression tag	UNP P0ABC9
O	490	HIS	-	expression tag	UNP P0ABC9
O	491	HIS	-	expression tag	UNP P0ABC9
O	492	GLU	-	expression tag	UNP P0ABC9
O	493	ASN	-	expression tag	UNP P0ABC9
O	494	LEU	-	expression tag	UNP P0ABC9
O	495	TYR	-	expression tag	UNP P0ABC9
O	496	PHE	-	expression tag	UNP P0ABC9
O	497	GLN	-	expression tag	UNP P0ABC9
O	498	GLY	-	expression tag	UNP P0ABC9
O	499	GLY	-	expression tag	UNP P0ABC9
O	500	SER	-	expression tag	UNP P0ABC9
O	669	THR	-	expression tag	UNP P0ABC9
O	670	GLY	-	expression tag	UNP P0ABC9
O	671	CYS	-	expression tag	UNP P0ABC9
P	481	MET	-	initiating methionine	UNP P0ABC9
P	482	HIS	-	expression tag	UNP P0ABC9
P	483	HIS	-	expression tag	UNP P0ABC9
P	484	HIS	-	expression tag	UNP P0ABC9
P	485	HIS	-	expression tag	UNP P0ABC9
P	486	HIS	-	expression tag	UNP P0ABC9
P	487	HIS	-	expression tag	UNP P0ABC9
P	488	HIS	-	expression tag	UNP P0ABC9
P	489	HIS	-	expression tag	UNP P0ABC9
P	490	HIS	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
P	491	HIS	-	expression tag	UNP P0ABC9
P	492	GLU	-	expression tag	UNP P0ABC9
P	493	ASN	-	expression tag	UNP P0ABC9
P	494	LEU	-	expression tag	UNP P0ABC9
P	495	TYR	-	expression tag	UNP P0ABC9
P	496	PHE	-	expression tag	UNP P0ABC9
P	497	GLN	-	expression tag	UNP P0ABC9
P	498	GLY	-	expression tag	UNP P0ABC9
P	499	GLY	-	expression tag	UNP P0ABC9
P	500	SER	-	expression tag	UNP P0ABC9
P	669	THR	-	expression tag	UNP P0ABC9
P	670	GLY	-	expression tag	UNP P0ABC9
P	671	CYS	-	expression tag	UNP P0ABC9
Q	481	MET	-	initiating methionine	UNP P0ABC9
Q	482	HIS	-	expression tag	UNP P0ABC9
Q	483	HIS	-	expression tag	UNP P0ABC9
Q	484	HIS	-	expression tag	UNP P0ABC9
Q	485	HIS	-	expression tag	UNP P0ABC9
Q	486	HIS	-	expression tag	UNP P0ABC9
Q	487	HIS	-	expression tag	UNP P0ABC9
Q	488	HIS	-	expression tag	UNP P0ABC9
Q	489	HIS	-	expression tag	UNP P0ABC9
Q	490	HIS	-	expression tag	UNP P0ABC9
Q	491	HIS	-	expression tag	UNP P0ABC9
Q	492	GLU	-	expression tag	UNP P0ABC9
Q	493	ASN	-	expression tag	UNP P0ABC9
Q	494	LEU	-	expression tag	UNP P0ABC9
Q	495	TYR	-	expression tag	UNP P0ABC9
Q	496	PHE	-	expression tag	UNP P0ABC9
Q	497	GLN	-	expression tag	UNP P0ABC9
Q	498	GLY	-	expression tag	UNP P0ABC9
Q	499	GLY	-	expression tag	UNP P0ABC9
Q	500	SER	-	expression tag	UNP P0ABC9
Q	669	THR	-	expression tag	UNP P0ABC9
Q	670	GLY	-	expression tag	UNP P0ABC9
Q	671	CYS	-	expression tag	UNP P0ABC9
R	481	MET	-	initiating methionine	UNP P0ABC9
R	482	HIS	-	expression tag	UNP P0ABC9
R	483	HIS	-	expression tag	UNP P0ABC9
R	484	HIS	-	expression tag	UNP P0ABC9
R	485	HIS	-	expression tag	UNP P0ABC9
R	486	HIS	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
R	487	HIS	-	expression tag	UNP P0ABC9
R	488	HIS	-	expression tag	UNP P0ABC9
R	489	HIS	-	expression tag	UNP P0ABC9
R	490	HIS	-	expression tag	UNP P0ABC9
R	491	HIS	-	expression tag	UNP P0ABC9
R	492	GLU	-	expression tag	UNP P0ABC9
R	493	ASN	-	expression tag	UNP P0ABC9
R	494	LEU	-	expression tag	UNP P0ABC9
R	495	TYR	-	expression tag	UNP P0ABC9
R	496	PHE	-	expression tag	UNP P0ABC9
R	497	GLN	-	expression tag	UNP P0ABC9
R	498	GLY	-	expression tag	UNP P0ABC9
R	499	GLY	-	expression tag	UNP P0ABC9
R	500	SER	-	expression tag	UNP P0ABC9
R	669	THR	-	expression tag	UNP P0ABC9
R	670	GLY	-	expression tag	UNP P0ABC9
R	671	CYS	-	expression tag	UNP P0ABC9
S	481	MET	-	initiating methionine	UNP P0ABC9
S	482	HIS	-	expression tag	UNP P0ABC9
S	483	HIS	-	expression tag	UNP P0ABC9
S	484	HIS	-	expression tag	UNP P0ABC9
S	485	HIS	-	expression tag	UNP P0ABC9
S	486	HIS	-	expression tag	UNP P0ABC9
S	487	HIS	-	expression tag	UNP P0ABC9
S	488	HIS	-	expression tag	UNP P0ABC9
S	489	HIS	-	expression tag	UNP P0ABC9
S	490	HIS	-	expression tag	UNP P0ABC9
S	491	HIS	-	expression tag	UNP P0ABC9
S	492	GLU	-	expression tag	UNP P0ABC9
S	493	ASN	-	expression tag	UNP P0ABC9
S	494	LEU	-	expression tag	UNP P0ABC9
S	495	TYR	-	expression tag	UNP P0ABC9
S	496	PHE	-	expression tag	UNP P0ABC9
S	497	GLN	-	expression tag	UNP P0ABC9
S	498	GLY	-	expression tag	UNP P0ABC9
S	499	GLY	-	expression tag	UNP P0ABC9
S	500	SER	-	expression tag	UNP P0ABC9
S	669	THR	-	expression tag	UNP P0ABC9
S	670	GLY	-	expression tag	UNP P0ABC9
S	671	CYS	-	expression tag	UNP P0ABC9
T	481	MET	-	initiating methionine	UNP P0ABC9
T	482	HIS	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
T	483	HIS	-	expression tag	UNP P0ABC9
T	484	HIS	-	expression tag	UNP P0ABC9
T	485	HIS	-	expression tag	UNP P0ABC9
T	486	HIS	-	expression tag	UNP P0ABC9
T	487	HIS	-	expression tag	UNP P0ABC9
T	488	HIS	-	expression tag	UNP P0ABC9
T	489	HIS	-	expression tag	UNP P0ABC9
T	490	HIS	-	expression tag	UNP P0ABC9
T	491	HIS	-	expression tag	UNP P0ABC9
T	492	GLU	-	expression tag	UNP P0ABC9
T	493	ASN	-	expression tag	UNP P0ABC9
T	494	LEU	-	expression tag	UNP P0ABC9
T	495	TYR	-	expression tag	UNP P0ABC9
T	496	PHE	-	expression tag	UNP P0ABC9
T	497	GLN	-	expression tag	UNP P0ABC9
T	498	GLY	-	expression tag	UNP P0ABC9
T	499	GLY	-	expression tag	UNP P0ABC9
T	500	SER	-	expression tag	UNP P0ABC9
T	669	THR	-	expression tag	UNP P0ABC9
T	670	GLY	-	expression tag	UNP P0ABC9
T	671	CYS	-	expression tag	UNP P0ABC9
V	481	MET	-	initiating methionine	UNP P0ABC9
V	482	HIS	-	expression tag	UNP P0ABC9
V	483	HIS	-	expression tag	UNP P0ABC9
V	484	HIS	-	expression tag	UNP P0ABC9
V	485	HIS	-	expression tag	UNP P0ABC9
V	486	HIS	-	expression tag	UNP P0ABC9
V	487	HIS	-	expression tag	UNP P0ABC9
V	488	HIS	-	expression tag	UNP P0ABC9
V	489	HIS	-	expression tag	UNP P0ABC9
V	490	HIS	-	expression tag	UNP P0ABC9
V	491	HIS	-	expression tag	UNP P0ABC9
V	492	GLU	-	expression tag	UNP P0ABC9
V	493	ASN	-	expression tag	UNP P0ABC9
V	494	LEU	-	expression tag	UNP P0ABC9
V	495	TYR	-	expression tag	UNP P0ABC9
V	496	PHE	-	expression tag	UNP P0ABC9
V	497	GLN	-	expression tag	UNP P0ABC9
V	498	GLY	-	expression tag	UNP P0ABC9
V	499	GLY	-	expression tag	UNP P0ABC9
V	500	SER	-	expression tag	UNP P0ABC9
V	669	THR	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
V	670	GLY	-	expression tag	UNP P0ABC9
V	671	CYS	-	expression tag	UNP P0ABC9
W	481	MET	-	initiating methionine	UNP P0ABC9
W	482	HIS	-	expression tag	UNP P0ABC9
W	483	HIS	-	expression tag	UNP P0ABC9
W	484	HIS	-	expression tag	UNP P0ABC9
W	485	HIS	-	expression tag	UNP P0ABC9
W	486	HIS	-	expression tag	UNP P0ABC9
W	487	HIS	-	expression tag	UNP P0ABC9
W	488	HIS	-	expression tag	UNP P0ABC9
W	489	HIS	-	expression tag	UNP P0ABC9
W	490	HIS	-	expression tag	UNP P0ABC9
W	491	HIS	-	expression tag	UNP P0ABC9
W	492	GLU	-	expression tag	UNP P0ABC9
W	493	ASN	-	expression tag	UNP P0ABC9
W	494	LEU	-	expression tag	UNP P0ABC9
W	495	TYR	-	expression tag	UNP P0ABC9
W	496	PHE	-	expression tag	UNP P0ABC9
W	497	GLN	-	expression tag	UNP P0ABC9
W	498	GLY	-	expression tag	UNP P0ABC9
W	499	GLY	-	expression tag	UNP P0ABC9
W	500	SER	-	expression tag	UNP P0ABC9
W	669	THR	-	expression tag	UNP P0ABC9
W	670	GLY	-	expression tag	UNP P0ABC9
W	671	CYS	-	expression tag	UNP P0ABC9
X	481	MET	-	initiating methionine	UNP P0ABC9
X	482	HIS	-	expression tag	UNP P0ABC9
X	483	HIS	-	expression tag	UNP P0ABC9
X	484	HIS	-	expression tag	UNP P0ABC9
X	485	HIS	-	expression tag	UNP P0ABC9
X	486	HIS	-	expression tag	UNP P0ABC9
X	487	HIS	-	expression tag	UNP P0ABC9
X	488	HIS	-	expression tag	UNP P0ABC9
X	489	HIS	-	expression tag	UNP P0ABC9
X	490	HIS	-	expression tag	UNP P0ABC9
X	491	HIS	-	expression tag	UNP P0ABC9
X	492	GLU	-	expression tag	UNP P0ABC9
X	493	ASN	-	expression tag	UNP P0ABC9
X	494	LEU	-	expression tag	UNP P0ABC9
X	495	TYR	-	expression tag	UNP P0ABC9
X	496	PHE	-	expression tag	UNP P0ABC9
X	497	GLN	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
X	498	GLY	-	expression tag	UNP P0ABC9
X	499	GLY	-	expression tag	UNP P0ABC9
X	500	SER	-	expression tag	UNP P0ABC9
X	669	THR	-	expression tag	UNP P0ABC9
X	670	GLY	-	expression tag	UNP P0ABC9
X	671	CYS	-	expression tag	UNP P0ABC9
Y	481	MET	-	initiating methionine	UNP P0ABC9
Y	482	HIS	-	expression tag	UNP P0ABC9
Y	483	HIS	-	expression tag	UNP P0ABC9
Y	484	HIS	-	expression tag	UNP P0ABC9
Y	485	HIS	-	expression tag	UNP P0ABC9
Y	486	HIS	-	expression tag	UNP P0ABC9
Y	487	HIS	-	expression tag	UNP P0ABC9
Y	488	HIS	-	expression tag	UNP P0ABC9
Y	489	HIS	-	expression tag	UNP P0ABC9
Y	490	HIS	-	expression tag	UNP P0ABC9
Y	491	HIS	-	expression tag	UNP P0ABC9
Y	492	GLU	-	expression tag	UNP P0ABC9
Y	493	ASN	-	expression tag	UNP P0ABC9
Y	494	LEU	-	expression tag	UNP P0ABC9
Y	495	TYR	-	expression tag	UNP P0ABC9
Y	496	PHE	-	expression tag	UNP P0ABC9
Y	497	GLN	-	expression tag	UNP P0ABC9
Y	498	GLY	-	expression tag	UNP P0ABC9
Y	499	GLY	-	expression tag	UNP P0ABC9
Y	500	SER	-	expression tag	UNP P0ABC9
Y	669	THR	-	expression tag	UNP P0ABC9
Y	670	GLY	-	expression tag	UNP P0ABC9
Y	671	CYS	-	expression tag	UNP P0ABC9
Z	481	MET	-	initiating methionine	UNP P0ABC9
Z	482	HIS	-	expression tag	UNP P0ABC9
Z	483	HIS	-	expression tag	UNP P0ABC9
Z	484	HIS	-	expression tag	UNP P0ABC9
Z	485	HIS	-	expression tag	UNP P0ABC9
Z	486	HIS	-	expression tag	UNP P0ABC9
Z	487	HIS	-	expression tag	UNP P0ABC9
Z	488	HIS	-	expression tag	UNP P0ABC9
Z	489	HIS	-	expression tag	UNP P0ABC9
Z	490	HIS	-	expression tag	UNP P0ABC9
Z	491	HIS	-	expression tag	UNP P0ABC9
Z	492	GLU	-	expression tag	UNP P0ABC9
Z	493	ASN	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	494	LEU	-	expression tag	UNP P0ABC9
Z	495	TYR	-	expression tag	UNP P0ABC9
Z	496	PHE	-	expression tag	UNP P0ABC9
Z	497	GLN	-	expression tag	UNP P0ABC9
Z	498	GLY	-	expression tag	UNP P0ABC9
Z	499	GLY	-	expression tag	UNP P0ABC9
Z	500	SER	-	expression tag	UNP P0ABC9
Z	669	THR	-	expression tag	UNP P0ABC9
Z	670	GLY	-	expression tag	UNP P0ABC9
Z	671	CYS	-	expression tag	UNP P0ABC9
AA	481	MET	-	initiating methionine	UNP P0ABC9
AA	482	HIS	-	expression tag	UNP P0ABC9
AA	483	HIS	-	expression tag	UNP P0ABC9
AA	484	HIS	-	expression tag	UNP P0ABC9
AA	485	HIS	-	expression tag	UNP P0ABC9
AA	486	HIS	-	expression tag	UNP P0ABC9
AA	487	HIS	-	expression tag	UNP P0ABC9
AA	488	HIS	-	expression tag	UNP P0ABC9
AA	489	HIS	-	expression tag	UNP P0ABC9
AA	490	HIS	-	expression tag	UNP P0ABC9
AA	491	HIS	-	expression tag	UNP P0ABC9
AA	492	GLU	-	expression tag	UNP P0ABC9
AA	493	ASN	-	expression tag	UNP P0ABC9
AA	494	LEU	-	expression tag	UNP P0ABC9
AA	495	TYR	-	expression tag	UNP P0ABC9
AA	496	PHE	-	expression tag	UNP P0ABC9
AA	497	GLN	-	expression tag	UNP P0ABC9
AA	498	GLY	-	expression tag	UNP P0ABC9
AA	499	GLY	-	expression tag	UNP P0ABC9
AA	500	SER	-	expression tag	UNP P0ABC9
AA	669	THR	-	expression tag	UNP P0ABC9
AA	670	GLY	-	expression tag	UNP P0ABC9
AA	671	CYS	-	expression tag	UNP P0ABC9
BA	481	MET	-	initiating methionine	UNP P0ABC9
BA	482	HIS	-	expression tag	UNP P0ABC9
BA	483	HIS	-	expression tag	UNP P0ABC9
BA	484	HIS	-	expression tag	UNP P0ABC9
BA	485	HIS	-	expression tag	UNP P0ABC9
BA	486	HIS	-	expression tag	UNP P0ABC9
BA	487	HIS	-	expression tag	UNP P0ABC9
BA	488	HIS	-	expression tag	UNP P0ABC9
BA	489	HIS	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
BA	490	HIS	-	expression tag	UNP P0ABC9
BA	491	HIS	-	expression tag	UNP P0ABC9
BA	492	GLU	-	expression tag	UNP P0ABC9
BA	493	ASN	-	expression tag	UNP P0ABC9
BA	494	LEU	-	expression tag	UNP P0ABC9
BA	495	TYR	-	expression tag	UNP P0ABC9
BA	496	PHE	-	expression tag	UNP P0ABC9
BA	497	GLN	-	expression tag	UNP P0ABC9
BA	498	GLY	-	expression tag	UNP P0ABC9
BA	499	GLY	-	expression tag	UNP P0ABC9
BA	500	SER	-	expression tag	UNP P0ABC9
BA	669	THR	-	expression tag	UNP P0ABC9
BA	670	GLY	-	expression tag	UNP P0ABC9
BA	671	CYS	-	expression tag	UNP P0ABC9
CA	481	MET	-	initiating methionine	UNP P0ABC9
CA	482	HIS	-	expression tag	UNP P0ABC9
CA	483	HIS	-	expression tag	UNP P0ABC9
CA	484	HIS	-	expression tag	UNP P0ABC9
CA	485	HIS	-	expression tag	UNP P0ABC9
CA	486	HIS	-	expression tag	UNP P0ABC9
CA	487	HIS	-	expression tag	UNP P0ABC9
CA	488	HIS	-	expression tag	UNP P0ABC9
CA	489	HIS	-	expression tag	UNP P0ABC9
CA	490	HIS	-	expression tag	UNP P0ABC9
CA	491	HIS	-	expression tag	UNP P0ABC9
CA	492	GLU	-	expression tag	UNP P0ABC9
CA	493	ASN	-	expression tag	UNP P0ABC9
CA	494	LEU	-	expression tag	UNP P0ABC9
CA	495	TYR	-	expression tag	UNP P0ABC9
CA	496	PHE	-	expression tag	UNP P0ABC9
CA	497	GLN	-	expression tag	UNP P0ABC9
CA	498	GLY	-	expression tag	UNP P0ABC9
CA	499	GLY	-	expression tag	UNP P0ABC9
CA	500	SER	-	expression tag	UNP P0ABC9
CA	669	THR	-	expression tag	UNP P0ABC9
CA	670	GLY	-	expression tag	UNP P0ABC9
CA	671	CYS	-	expression tag	UNP P0ABC9
DA	481	MET	-	initiating methionine	UNP P0ABC9
DA	482	HIS	-	expression tag	UNP P0ABC9
DA	483	HIS	-	expression tag	UNP P0ABC9
DA	484	HIS	-	expression tag	UNP P0ABC9
DA	485	HIS	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
DA	486	HIS	-	expression tag	UNP P0ABC9
DA	487	HIS	-	expression tag	UNP P0ABC9
DA	488	HIS	-	expression tag	UNP P0ABC9
DA	489	HIS	-	expression tag	UNP P0ABC9
DA	490	HIS	-	expression tag	UNP P0ABC9
DA	491	HIS	-	expression tag	UNP P0ABC9
DA	492	GLU	-	expression tag	UNP P0ABC9
DA	493	ASN	-	expression tag	UNP P0ABC9
DA	494	LEU	-	expression tag	UNP P0ABC9
DA	495	TYR	-	expression tag	UNP P0ABC9
DA	496	PHE	-	expression tag	UNP P0ABC9
DA	497	GLN	-	expression tag	UNP P0ABC9
DA	498	GLY	-	expression tag	UNP P0ABC9
DA	499	GLY	-	expression tag	UNP P0ABC9
DA	500	SER	-	expression tag	UNP P0ABC9
DA	669	THR	-	expression tag	UNP P0ABC9
DA	670	GLY	-	expression tag	UNP P0ABC9
DA	671	CYS	-	expression tag	UNP P0ABC9
EA	481	MET	-	initiating methionine	UNP P0ABC9
EA	482	HIS	-	expression tag	UNP P0ABC9
EA	483	HIS	-	expression tag	UNP P0ABC9
EA	484	HIS	-	expression tag	UNP P0ABC9
EA	485	HIS	-	expression tag	UNP P0ABC9
EA	486	HIS	-	expression tag	UNP P0ABC9
EA	487	HIS	-	expression tag	UNP P0ABC9
EA	488	HIS	-	expression tag	UNP P0ABC9
EA	489	HIS	-	expression tag	UNP P0ABC9
EA	490	HIS	-	expression tag	UNP P0ABC9
EA	491	HIS	-	expression tag	UNP P0ABC9
EA	492	GLU	-	expression tag	UNP P0ABC9
EA	493	ASN	-	expression tag	UNP P0ABC9
EA	494	LEU	-	expression tag	UNP P0ABC9
EA	495	TYR	-	expression tag	UNP P0ABC9
EA	496	PHE	-	expression tag	UNP P0ABC9
EA	497	GLN	-	expression tag	UNP P0ABC9
EA	498	GLY	-	expression tag	UNP P0ABC9
EA	499	GLY	-	expression tag	UNP P0ABC9
EA	500	SER	-	expression tag	UNP P0ABC9
EA	669	THR	-	expression tag	UNP P0ABC9
EA	670	GLY	-	expression tag	UNP P0ABC9
EA	671	CYS	-	expression tag	UNP P0ABC9
FA	481	MET	-	initiating methionine	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
FA	482	HIS	-	expression tag	UNP P0ABC9
FA	483	HIS	-	expression tag	UNP P0ABC9
FA	484	HIS	-	expression tag	UNP P0ABC9
FA	485	HIS	-	expression tag	UNP P0ABC9
FA	486	HIS	-	expression tag	UNP P0ABC9
FA	487	HIS	-	expression tag	UNP P0ABC9
FA	488	HIS	-	expression tag	UNP P0ABC9
FA	489	HIS	-	expression tag	UNP P0ABC9
FA	490	HIS	-	expression tag	UNP P0ABC9
FA	491	HIS	-	expression tag	UNP P0ABC9
FA	492	GLU	-	expression tag	UNP P0ABC9
FA	493	ASN	-	expression tag	UNP P0ABC9
FA	494	LEU	-	expression tag	UNP P0ABC9
FA	495	TYR	-	expression tag	UNP P0ABC9
FA	496	PHE	-	expression tag	UNP P0ABC9
FA	497	GLN	-	expression tag	UNP P0ABC9
FA	498	GLY	-	expression tag	UNP P0ABC9
FA	499	GLY	-	expression tag	UNP P0ABC9
FA	500	SER	-	expression tag	UNP P0ABC9
FA	669	THR	-	expression tag	UNP P0ABC9
FA	670	GLY	-	expression tag	UNP P0ABC9
FA	671	CYS	-	expression tag	UNP P0ABC9
GA	481	MET	-	initiating methionine	UNP P0ABC9
GA	482	HIS	-	expression tag	UNP P0ABC9
GA	483	HIS	-	expression tag	UNP P0ABC9
GA	484	HIS	-	expression tag	UNP P0ABC9
GA	485	HIS	-	expression tag	UNP P0ABC9
GA	486	HIS	-	expression tag	UNP P0ABC9
GA	487	HIS	-	expression tag	UNP P0ABC9
GA	488	HIS	-	expression tag	UNP P0ABC9
GA	489	HIS	-	expression tag	UNP P0ABC9
GA	490	HIS	-	expression tag	UNP P0ABC9
GA	491	HIS	-	expression tag	UNP P0ABC9
GA	492	GLU	-	expression tag	UNP P0ABC9
GA	493	ASN	-	expression tag	UNP P0ABC9
GA	494	LEU	-	expression tag	UNP P0ABC9
GA	495	TYR	-	expression tag	UNP P0ABC9
GA	496	PHE	-	expression tag	UNP P0ABC9
GA	497	GLN	-	expression tag	UNP P0ABC9
GA	498	GLY	-	expression tag	UNP P0ABC9
GA	499	GLY	-	expression tag	UNP P0ABC9
GA	500	SER	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
GA	669	THR	-	expression tag	UNP P0ABC9
GA	670	GLY	-	expression tag	UNP P0ABC9
GA	671	CYS	-	expression tag	UNP P0ABC9
HA	481	MET	-	initiating methionine	UNP P0ABC9
HA	482	HIS	-	expression tag	UNP P0ABC9
HA	483	HIS	-	expression tag	UNP P0ABC9
HA	484	HIS	-	expression tag	UNP P0ABC9
HA	485	HIS	-	expression tag	UNP P0ABC9
HA	486	HIS	-	expression tag	UNP P0ABC9
HA	487	HIS	-	expression tag	UNP P0ABC9
HA	488	HIS	-	expression tag	UNP P0ABC9
HA	489	HIS	-	expression tag	UNP P0ABC9
HA	490	HIS	-	expression tag	UNP P0ABC9
HA	491	HIS	-	expression tag	UNP P0ABC9
HA	492	GLU	-	expression tag	UNP P0ABC9
HA	493	ASN	-	expression tag	UNP P0ABC9
HA	494	LEU	-	expression tag	UNP P0ABC9
HA	495	TYR	-	expression tag	UNP P0ABC9
HA	496	PHE	-	expression tag	UNP P0ABC9
HA	497	GLN	-	expression tag	UNP P0ABC9
HA	498	GLY	-	expression tag	UNP P0ABC9
HA	499	GLY	-	expression tag	UNP P0ABC9
HA	500	SER	-	expression tag	UNP P0ABC9
HA	669	THR	-	expression tag	UNP P0ABC9
HA	670	GLY	-	expression tag	UNP P0ABC9
HA	671	CYS	-	expression tag	UNP P0ABC9
IA	481	MET	-	initiating methionine	UNP P0ABC9
IA	482	HIS	-	expression tag	UNP P0ABC9
IA	483	HIS	-	expression tag	UNP P0ABC9
IA	484	HIS	-	expression tag	UNP P0ABC9
IA	485	HIS	-	expression tag	UNP P0ABC9
IA	486	HIS	-	expression tag	UNP P0ABC9
IA	487	HIS	-	expression tag	UNP P0ABC9
IA	488	HIS	-	expression tag	UNP P0ABC9
IA	489	HIS	-	expression tag	UNP P0ABC9
IA	490	HIS	-	expression tag	UNP P0ABC9
IA	491	HIS	-	expression tag	UNP P0ABC9
IA	492	GLU	-	expression tag	UNP P0ABC9
IA	493	ASN	-	expression tag	UNP P0ABC9
IA	494	LEU	-	expression tag	UNP P0ABC9
IA	495	TYR	-	expression tag	UNP P0ABC9
IA	496	PHE	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
IA	497	GLN	-	expression tag	UNP P0ABC9
IA	498	GLY	-	expression tag	UNP P0ABC9
IA	499	GLY	-	expression tag	UNP P0ABC9
IA	500	SER	-	expression tag	UNP P0ABC9
IA	669	THR	-	expression tag	UNP P0ABC9
IA	670	GLY	-	expression tag	UNP P0ABC9
IA	671	CYS	-	expression tag	UNP P0ABC9
JA	481	MET	-	initiating methionine	UNP P0ABC9
JA	482	HIS	-	expression tag	UNP P0ABC9
JA	483	HIS	-	expression tag	UNP P0ABC9
JA	484	HIS	-	expression tag	UNP P0ABC9
JA	485	HIS	-	expression tag	UNP P0ABC9
JA	486	HIS	-	expression tag	UNP P0ABC9
JA	487	HIS	-	expression tag	UNP P0ABC9
JA	488	HIS	-	expression tag	UNP P0ABC9
JA	489	HIS	-	expression tag	UNP P0ABC9
JA	490	HIS	-	expression tag	UNP P0ABC9
JA	491	HIS	-	expression tag	UNP P0ABC9
JA	492	GLU	-	expression tag	UNP P0ABC9
JA	493	ASN	-	expression tag	UNP P0ABC9
JA	494	LEU	-	expression tag	UNP P0ABC9
JA	495	TYR	-	expression tag	UNP P0ABC9
JA	496	PHE	-	expression tag	UNP P0ABC9
JA	497	GLN	-	expression tag	UNP P0ABC9
JA	498	GLY	-	expression tag	UNP P0ABC9
JA	499	GLY	-	expression tag	UNP P0ABC9
JA	500	SER	-	expression tag	UNP P0ABC9
JA	669	THR	-	expression tag	UNP P0ABC9
JA	670	GLY	-	expression tag	UNP P0ABC9
JA	671	CYS	-	expression tag	UNP P0ABC9
KA	481	MET	-	initiating methionine	UNP P0ABC9
KA	482	HIS	-	expression tag	UNP P0ABC9
KA	483	HIS	-	expression tag	UNP P0ABC9
KA	484	HIS	-	expression tag	UNP P0ABC9
KA	485	HIS	-	expression tag	UNP P0ABC9
KA	486	HIS	-	expression tag	UNP P0ABC9
KA	487	HIS	-	expression tag	UNP P0ABC9
KA	488	HIS	-	expression tag	UNP P0ABC9
KA	489	HIS	-	expression tag	UNP P0ABC9
KA	490	HIS	-	expression tag	UNP P0ABC9
KA	491	HIS	-	expression tag	UNP P0ABC9
KA	492	GLU	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
KA	493	ASN	-	expression tag	UNP P0ABC9
KA	494	LEU	-	expression tag	UNP P0ABC9
KA	495	TYR	-	expression tag	UNP P0ABC9
KA	496	PHE	-	expression tag	UNP P0ABC9
KA	497	GLN	-	expression tag	UNP P0ABC9
KA	498	GLY	-	expression tag	UNP P0ABC9
KA	499	GLY	-	expression tag	UNP P0ABC9
KA	500	SER	-	expression tag	UNP P0ABC9
KA	669	THR	-	expression tag	UNP P0ABC9
KA	670	GLY	-	expression tag	UNP P0ABC9
KA	671	CYS	-	expression tag	UNP P0ABC9
LA	481	MET	-	initiating methionine	UNP P0ABC9
LA	482	HIS	-	expression tag	UNP P0ABC9
LA	483	HIS	-	expression tag	UNP P0ABC9
LA	484	HIS	-	expression tag	UNP P0ABC9
LA	485	HIS	-	expression tag	UNP P0ABC9
LA	486	HIS	-	expression tag	UNP P0ABC9
LA	487	HIS	-	expression tag	UNP P0ABC9
LA	488	HIS	-	expression tag	UNP P0ABC9
LA	489	HIS	-	expression tag	UNP P0ABC9
LA	490	HIS	-	expression tag	UNP P0ABC9
LA	491	HIS	-	expression tag	UNP P0ABC9
LA	492	GLU	-	expression tag	UNP P0ABC9
LA	493	ASN	-	expression tag	UNP P0ABC9
LA	494	LEU	-	expression tag	UNP P0ABC9
LA	495	TYR	-	expression tag	UNP P0ABC9
LA	496	PHE	-	expression tag	UNP P0ABC9
LA	497	GLN	-	expression tag	UNP P0ABC9
LA	498	GLY	-	expression tag	UNP P0ABC9
LA	499	GLY	-	expression tag	UNP P0ABC9
LA	500	SER	-	expression tag	UNP P0ABC9
LA	669	THR	-	expression tag	UNP P0ABC9
LA	670	GLY	-	expression tag	UNP P0ABC9
LA	671	CYS	-	expression tag	UNP P0ABC9
MA	481	MET	-	initiating methionine	UNP P0ABC9
MA	482	HIS	-	expression tag	UNP P0ABC9
MA	483	HIS	-	expression tag	UNP P0ABC9
MA	484	HIS	-	expression tag	UNP P0ABC9
MA	485	HIS	-	expression tag	UNP P0ABC9
MA	486	HIS	-	expression tag	UNP P0ABC9
MA	487	HIS	-	expression tag	UNP P0ABC9
MA	488	HIS	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
MA	489	HIS	-	expression tag	UNP P0ABC9
MA	490	HIS	-	expression tag	UNP P0ABC9
MA	491	HIS	-	expression tag	UNP P0ABC9
MA	492	GLU	-	expression tag	UNP P0ABC9
MA	493	ASN	-	expression tag	UNP P0ABC9
MA	494	LEU	-	expression tag	UNP P0ABC9
MA	495	TYR	-	expression tag	UNP P0ABC9
MA	496	PHE	-	expression tag	UNP P0ABC9
MA	497	GLN	-	expression tag	UNP P0ABC9
MA	498	GLY	-	expression tag	UNP P0ABC9
MA	499	GLY	-	expression tag	UNP P0ABC9
MA	500	SER	-	expression tag	UNP P0ABC9
MA	669	THR	-	expression tag	UNP P0ABC9
MA	670	GLY	-	expression tag	UNP P0ABC9
MA	671	CYS	-	expression tag	UNP P0ABC9
NA	481	MET	-	initiating methionine	UNP P0ABC9
NA	482	HIS	-	expression tag	UNP P0ABC9
NA	483	HIS	-	expression tag	UNP P0ABC9
NA	484	HIS	-	expression tag	UNP P0ABC9
NA	485	HIS	-	expression tag	UNP P0ABC9
NA	486	HIS	-	expression tag	UNP P0ABC9
NA	487	HIS	-	expression tag	UNP P0ABC9
NA	488	HIS	-	expression tag	UNP P0ABC9
NA	489	HIS	-	expression tag	UNP P0ABC9
NA	490	HIS	-	expression tag	UNP P0ABC9
NA	491	HIS	-	expression tag	UNP P0ABC9
NA	492	GLU	-	expression tag	UNP P0ABC9
NA	493	ASN	-	expression tag	UNP P0ABC9
NA	494	LEU	-	expression tag	UNP P0ABC9
NA	495	TYR	-	expression tag	UNP P0ABC9
NA	496	PHE	-	expression tag	UNP P0ABC9
NA	497	GLN	-	expression tag	UNP P0ABC9
NA	498	GLY	-	expression tag	UNP P0ABC9
NA	499	GLY	-	expression tag	UNP P0ABC9
NA	500	SER	-	expression tag	UNP P0ABC9
NA	669	THR	-	expression tag	UNP P0ABC9
NA	670	GLY	-	expression tag	UNP P0ABC9
NA	671	CYS	-	expression tag	UNP P0ABC9
OA	481	MET	-	initiating methionine	UNP P0ABC9
OA	482	HIS	-	expression tag	UNP P0ABC9
OA	483	HIS	-	expression tag	UNP P0ABC9
OA	484	HIS	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
OA	485	HIS	-	expression tag	UNP P0ABC9
OA	486	HIS	-	expression tag	UNP P0ABC9
OA	487	HIS	-	expression tag	UNP P0ABC9
OA	488	HIS	-	expression tag	UNP P0ABC9
OA	489	HIS	-	expression tag	UNP P0ABC9
OA	490	HIS	-	expression tag	UNP P0ABC9
OA	491	HIS	-	expression tag	UNP P0ABC9
OA	492	GLU	-	expression tag	UNP P0ABC9
OA	493	ASN	-	expression tag	UNP P0ABC9
OA	494	LEU	-	expression tag	UNP P0ABC9
OA	495	TYR	-	expression tag	UNP P0ABC9
OA	496	PHE	-	expression tag	UNP P0ABC9
OA	497	GLN	-	expression tag	UNP P0ABC9
OA	498	GLY	-	expression tag	UNP P0ABC9
OA	499	GLY	-	expression tag	UNP P0ABC9
OA	500	SER	-	expression tag	UNP P0ABC9
OA	669	THR	-	expression tag	UNP P0ABC9
OA	670	GLY	-	expression tag	UNP P0ABC9
OA	671	CYS	-	expression tag	UNP P0ABC9
PA	481	MET	-	initiating methionine	UNP P0ABC9
PA	482	HIS	-	expression tag	UNP P0ABC9
PA	483	HIS	-	expression tag	UNP P0ABC9
PA	484	HIS	-	expression tag	UNP P0ABC9
PA	485	HIS	-	expression tag	UNP P0ABC9
PA	486	HIS	-	expression tag	UNP P0ABC9
PA	487	HIS	-	expression tag	UNP P0ABC9
PA	488	HIS	-	expression tag	UNP P0ABC9
PA	489	HIS	-	expression tag	UNP P0ABC9
PA	490	HIS	-	expression tag	UNP P0ABC9
PA	491	HIS	-	expression tag	UNP P0ABC9
PA	492	GLU	-	expression tag	UNP P0ABC9
PA	493	ASN	-	expression tag	UNP P0ABC9
PA	494	LEU	-	expression tag	UNP P0ABC9
PA	495	TYR	-	expression tag	UNP P0ABC9
PA	496	PHE	-	expression tag	UNP P0ABC9
PA	497	GLN	-	expression tag	UNP P0ABC9
PA	498	GLY	-	expression tag	UNP P0ABC9
PA	499	GLY	-	expression tag	UNP P0ABC9
PA	500	SER	-	expression tag	UNP P0ABC9
PA	669	THR	-	expression tag	UNP P0ABC9
PA	670	GLY	-	expression tag	UNP P0ABC9
PA	671	CYS	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
QA	481	MET	-	initiating methionine	UNP P0ABC9
QA	482	HIS	-	expression tag	UNP P0ABC9
QA	483	HIS	-	expression tag	UNP P0ABC9
QA	484	HIS	-	expression tag	UNP P0ABC9
QA	485	HIS	-	expression tag	UNP P0ABC9
QA	486	HIS	-	expression tag	UNP P0ABC9
QA	487	HIS	-	expression tag	UNP P0ABC9
QA	488	HIS	-	expression tag	UNP P0ABC9
QA	489	HIS	-	expression tag	UNP P0ABC9
QA	490	HIS	-	expression tag	UNP P0ABC9
QA	491	HIS	-	expression tag	UNP P0ABC9
QA	492	GLU	-	expression tag	UNP P0ABC9
QA	493	ASN	-	expression tag	UNP P0ABC9
QA	494	LEU	-	expression tag	UNP P0ABC9
QA	495	TYR	-	expression tag	UNP P0ABC9
QA	496	PHE	-	expression tag	UNP P0ABC9
QA	497	GLN	-	expression tag	UNP P0ABC9
QA	498	GLY	-	expression tag	UNP P0ABC9
QA	499	GLY	-	expression tag	UNP P0ABC9
QA	500	SER	-	expression tag	UNP P0ABC9
QA	669	THR	-	expression tag	UNP P0ABC9
QA	670	GLY	-	expression tag	UNP P0ABC9
QA	671	CYS	-	expression tag	UNP P0ABC9
RA	481	MET	-	initiating methionine	UNP P0ABC9
RA	482	HIS	-	expression tag	UNP P0ABC9
RA	483	HIS	-	expression tag	UNP P0ABC9
RA	484	HIS	-	expression tag	UNP P0ABC9
RA	485	HIS	-	expression tag	UNP P0ABC9
RA	486	HIS	-	expression tag	UNP P0ABC9
RA	487	HIS	-	expression tag	UNP P0ABC9
RA	488	HIS	-	expression tag	UNP P0ABC9
RA	489	HIS	-	expression tag	UNP P0ABC9
RA	490	HIS	-	expression tag	UNP P0ABC9
RA	491	HIS	-	expression tag	UNP P0ABC9
RA	492	GLU	-	expression tag	UNP P0ABC9
RA	493	ASN	-	expression tag	UNP P0ABC9
RA	494	LEU	-	expression tag	UNP P0ABC9
RA	495	TYR	-	expression tag	UNP P0ABC9
RA	496	PHE	-	expression tag	UNP P0ABC9
RA	497	GLN	-	expression tag	UNP P0ABC9
RA	498	GLY	-	expression tag	UNP P0ABC9
RA	499	GLY	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
RA	500	SER	-	expression tag	UNP P0ABC9
RA	669	THR	-	expression tag	UNP P0ABC9
RA	670	GLY	-	expression tag	UNP P0ABC9
RA	671	CYS	-	expression tag	UNP P0ABC9
SA	481	MET	-	initiating methionine	UNP P0ABC9
SA	482	HIS	-	expression tag	UNP P0ABC9
SA	483	HIS	-	expression tag	UNP P0ABC9
SA	484	HIS	-	expression tag	UNP P0ABC9
SA	485	HIS	-	expression tag	UNP P0ABC9
SA	486	HIS	-	expression tag	UNP P0ABC9
SA	487	HIS	-	expression tag	UNP P0ABC9
SA	488	HIS	-	expression tag	UNP P0ABC9
SA	489	HIS	-	expression tag	UNP P0ABC9
SA	490	HIS	-	expression tag	UNP P0ABC9
SA	491	HIS	-	expression tag	UNP P0ABC9
SA	492	GLU	-	expression tag	UNP P0ABC9
SA	493	ASN	-	expression tag	UNP P0ABC9
SA	494	LEU	-	expression tag	UNP P0ABC9
SA	495	TYR	-	expression tag	UNP P0ABC9
SA	496	PHE	-	expression tag	UNP P0ABC9
SA	497	GLN	-	expression tag	UNP P0ABC9
SA	498	GLY	-	expression tag	UNP P0ABC9
SA	499	GLY	-	expression tag	UNP P0ABC9
SA	500	SER	-	expression tag	UNP P0ABC9
SA	669	THR	-	expression tag	UNP P0ABC9
SA	670	GLY	-	expression tag	UNP P0ABC9
SA	671	CYS	-	expression tag	UNP P0ABC9
TA	481	MET	-	initiating methionine	UNP P0ABC9
TA	482	HIS	-	expression tag	UNP P0ABC9
TA	483	HIS	-	expression tag	UNP P0ABC9
TA	484	HIS	-	expression tag	UNP P0ABC9
TA	485	HIS	-	expression tag	UNP P0ABC9
TA	486	HIS	-	expression tag	UNP P0ABC9
TA	487	HIS	-	expression tag	UNP P0ABC9
TA	488	HIS	-	expression tag	UNP P0ABC9
TA	489	HIS	-	expression tag	UNP P0ABC9
TA	490	HIS	-	expression tag	UNP P0ABC9
TA	491	HIS	-	expression tag	UNP P0ABC9
TA	492	GLU	-	expression tag	UNP P0ABC9
TA	493	ASN	-	expression tag	UNP P0ABC9
TA	494	LEU	-	expression tag	UNP P0ABC9
TA	495	TYR	-	expression tag	UNP P0ABC9

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Chain	Residue	Modelled	Actual	Comment	Reference
TA	496	PHE	-	expression tag	UNP P0ABC9
TA	497	GLN	-	expression tag	UNP P0ABC9
TA	498	GLY	-	expression tag	UNP P0ABC9
TA	499	GLY	-	expression tag	UNP P0ABC9
TA	500	SER	-	expression tag	UNP P0ABC9
TA	669	THR	-	expression tag	UNP P0ABC9
TA	670	GLY	-	expression tag	UNP P0ABC9
TA	671	CYS	-	expression tag	UNP P0ABC9
UA	481	MET	-	initiating methionine	UNP P0ABC9
UA	482	HIS	-	expression tag	UNP P0ABC9
UA	483	HIS	-	expression tag	UNP P0ABC9
UA	484	HIS	-	expression tag	UNP P0ABC9
UA	485	HIS	-	expression tag	UNP P0ABC9
UA	486	HIS	-	expression tag	UNP P0ABC9
UA	487	HIS	-	expression tag	UNP P0ABC9
UA	488	HIS	-	expression tag	UNP P0ABC9
UA	489	HIS	-	expression tag	UNP P0ABC9
UA	490	HIS	-	expression tag	UNP P0ABC9
UA	491	HIS	-	expression tag	UNP P0ABC9
UA	492	GLU	-	expression tag	UNP P0ABC9
UA	493	ASN	-	expression tag	UNP P0ABC9
UA	494	LEU	-	expression tag	UNP P0ABC9
UA	495	TYR	-	expression tag	UNP P0ABC9
UA	496	PHE	-	expression tag	UNP P0ABC9
UA	497	GLN	-	expression tag	UNP P0ABC9
UA	498	GLY	-	expression tag	UNP P0ABC9
UA	499	GLY	-	expression tag	UNP P0ABC9
UA	500	SER	-	expression tag	UNP P0ABC9
UA	669	THR	-	expression tag	UNP P0ABC9
UA	670	GLY	-	expression tag	UNP P0ABC9
UA	671	CYS	-	expression tag	UNP P0ABC9
VA	481	MET	-	initiating methionine	UNP P0ABC9
VA	482	HIS	-	expression tag	UNP P0ABC9
VA	483	HIS	-	expression tag	UNP P0ABC9
VA	484	HIS	-	expression tag	UNP P0ABC9
VA	485	HIS	-	expression tag	UNP P0ABC9
VA	486	HIS	-	expression tag	UNP P0ABC9
VA	487	HIS	-	expression tag	UNP P0ABC9
VA	488	HIS	-	expression tag	UNP P0ABC9
VA	489	HIS	-	expression tag	UNP P0ABC9
VA	490	HIS	-	expression tag	UNP P0ABC9
VA	491	HIS	-	expression tag	UNP P0ABC9

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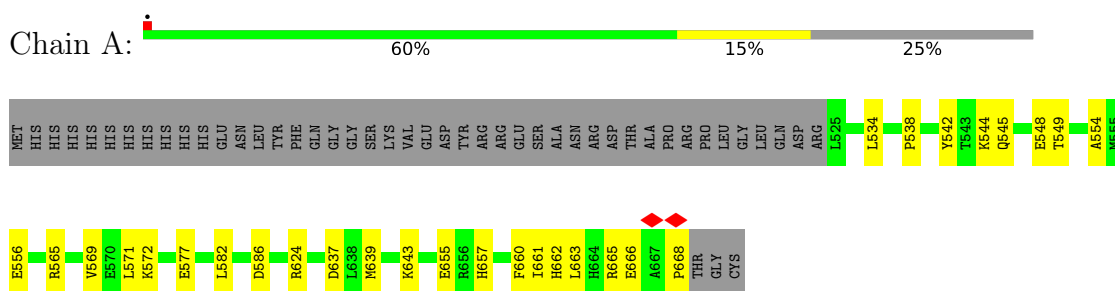
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
VA	492	GLU	-	expression tag	UNP P0ABC9
VA	493	ASN	-	expression tag	UNP P0ABC9
VA	494	LEU	-	expression tag	UNP P0ABC9
VA	495	TYR	-	expression tag	UNP P0ABC9
VA	496	PHE	-	expression tag	UNP P0ABC9
VA	497	GLN	-	expression tag	UNP P0ABC9
VA	498	GLY	-	expression tag	UNP P0ABC9
VA	499	GLY	-	expression tag	UNP P0ABC9
VA	500	SER	-	expression tag	UNP P0ABC9
VA	669	THR	-	expression tag	UNP P0ABC9
VA	670	GLY	-	expression tag	UNP P0ABC9
VA	671	CYS	-	expression tag	UNP P0ABC9
WA	481	MET	-	initiating methionine	UNP P0ABC9
WA	482	HIS	-	expression tag	UNP P0ABC9
WA	483	HIS	-	expression tag	UNP P0ABC9
WA	484	HIS	-	expression tag	UNP P0ABC9
WA	485	HIS	-	expression tag	UNP P0ABC9
WA	486	HIS	-	expression tag	UNP P0ABC9
WA	487	HIS	-	expression tag	UNP P0ABC9
WA	488	HIS	-	expression tag	UNP P0ABC9
WA	489	HIS	-	expression tag	UNP P0ABC9
WA	490	HIS	-	expression tag	UNP P0ABC9
WA	491	HIS	-	expression tag	UNP P0ABC9
WA	492	GLU	-	expression tag	UNP P0ABC9
WA	493	ASN	-	expression tag	UNP P0ABC9
WA	494	LEU	-	expression tag	UNP P0ABC9
WA	495	TYR	-	expression tag	UNP P0ABC9
WA	496	PHE	-	expression tag	UNP P0ABC9
WA	497	GLN	-	expression tag	UNP P0ABC9
WA	498	GLY	-	expression tag	UNP P0ABC9
WA	499	GLY	-	expression tag	UNP P0ABC9
WA	500	SER	-	expression tag	UNP P0ABC9
WA	669	THR	-	expression tag	UNP P0ABC9
WA	670	GLY	-	expression tag	UNP P0ABC9
WA	671	CYS	-	expression tag	UNP P0ABC9

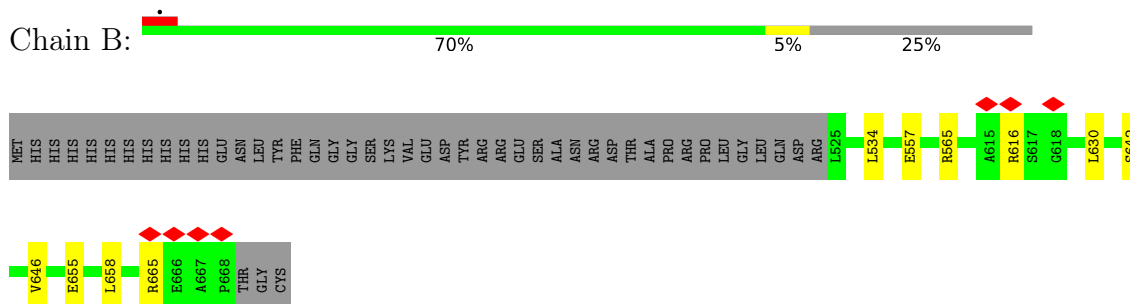
3 Residue-property plots

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

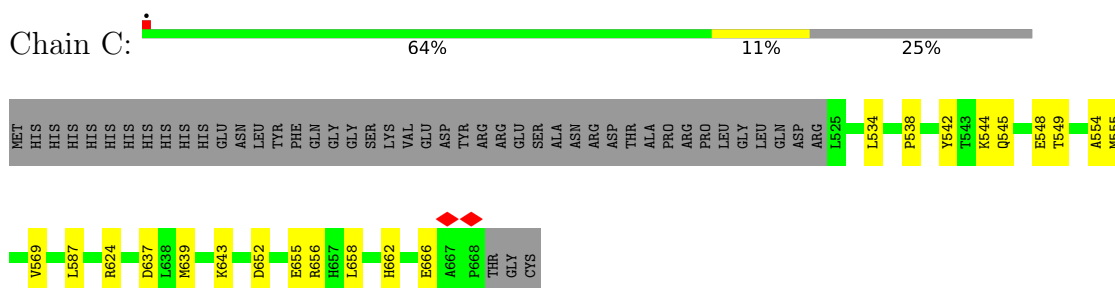
- Molecule 1: High-affinity choline transport protein



- Molecule 1: High-affinity choline transport protein

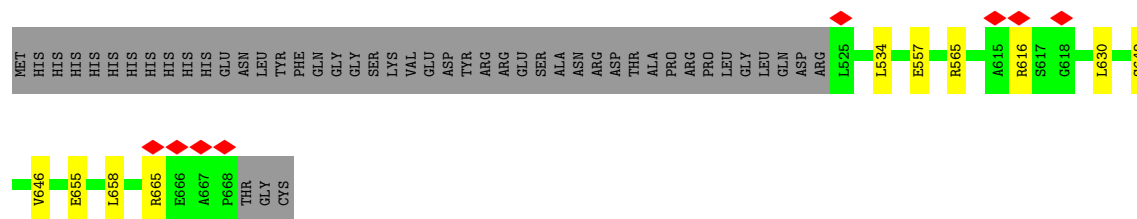


- Molecule 1: High-affinity choline transport protein

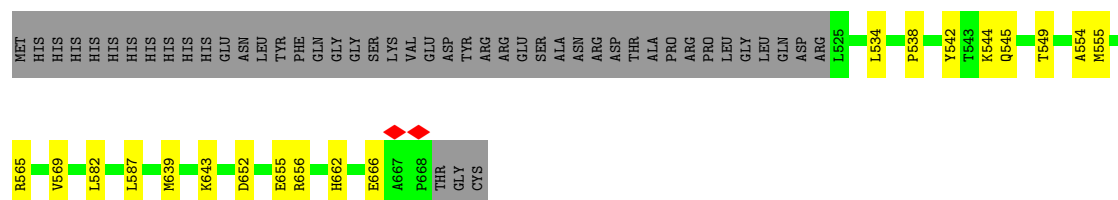


- Molecule 1: High-affinity choline transport protein

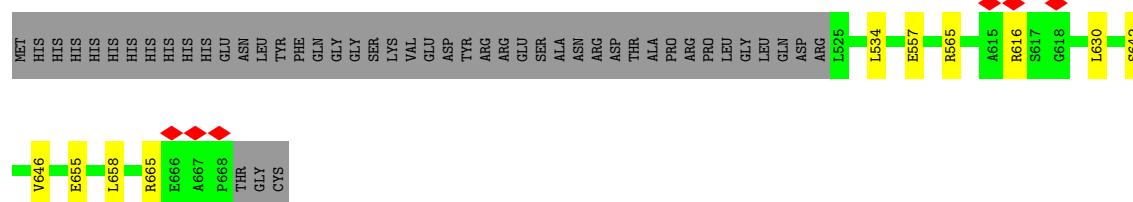




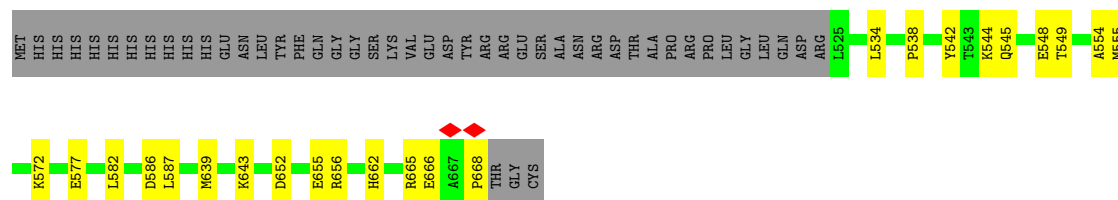
- Molecule 1: High-affinity choline transport protein



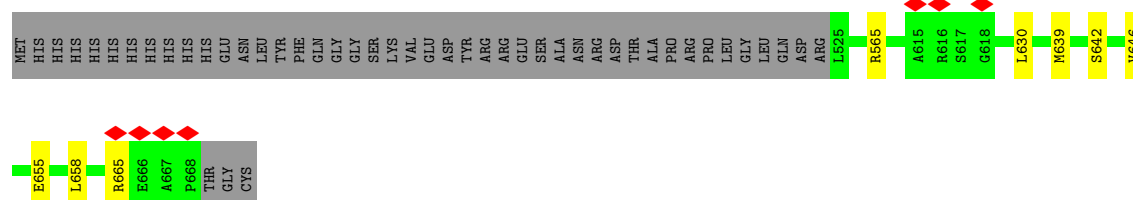
- Molecule 1: High-affinity choline transport protein

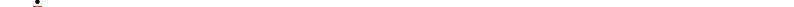


- Molecule 1: High-affinity choline transport protein

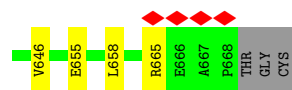


- Molecule 1: High-affinity choline transport protein

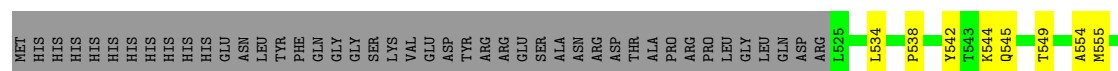


- Chain M: 





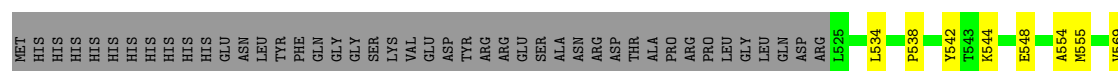
- Molecule 1: High-affinity choline transport protein



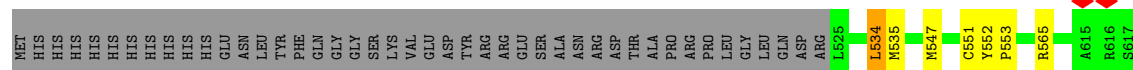
- Molecule 1: High-affinity choline transport protein



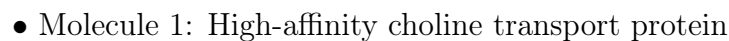
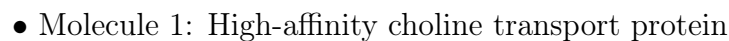
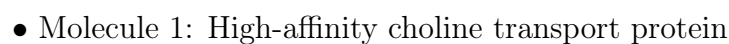
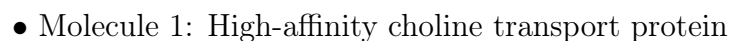
- Molecule 1: High-affinity choline transport protein



- Molecule 1: High-affinity choline transport protein

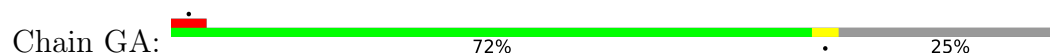


- Molecule 1: High-affinity choline transport protein

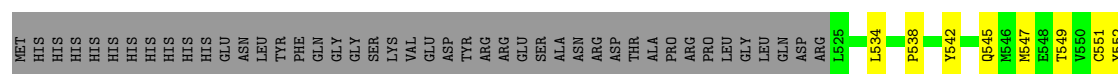




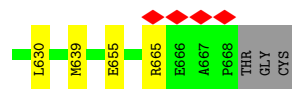
- Molecule 1: High-affinity choline transport protein



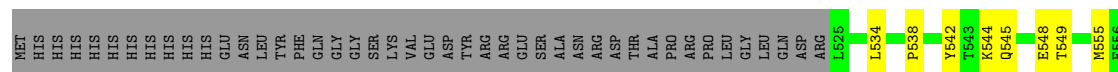
- Molecule 1: High-affinity choline transport protein



- Molecule 1: High-affinity choline transport protein



- Molecule 1: High-affinity choline transport protein



- Molecule 1: High-affinity choline transport protein

Frequency	Percentage
Daily	72%
Weekly	25%
Monthly	3%



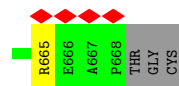
- Molecule 1: High-affinity choline transport protein

Frequency	Percentage
Daily	66%
Weekly	9%
Monthly	25%



- Molecule 1: High-affinity choline transport protein

Frequency	Percentage
Daily	72%
Weekly	25%
Monthly	3%



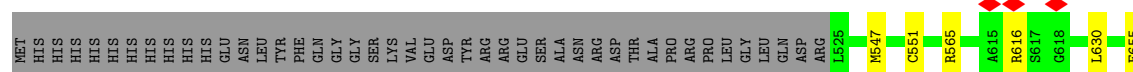
- Molecule 1: High-affinity choline transport protein

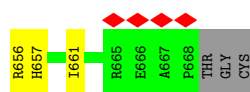
Frequency	Percentage
Daily	65%
Weekly	10%
Monthly	25%



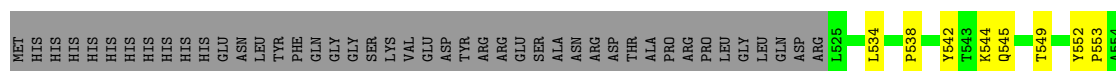
- Molecule 1: High-affinity choline transport protein

Frequency	Percentage
Daily	71%
Weekly	5%
Monthly	25%

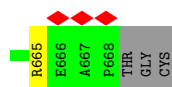
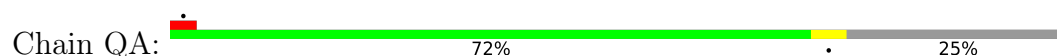




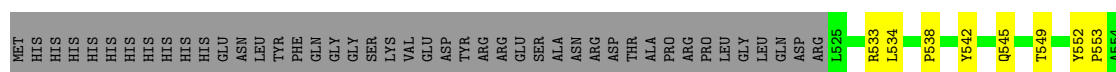
- Molecule 1: High-affinity choline transport protein



- Molecule 1: High-affinity choline transport protein



- Molecule 1: High-affinity choline transport protein

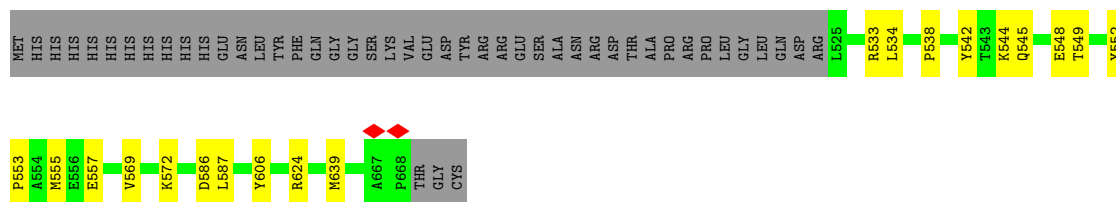


- Molecule 1: High-affinity choline transport protein



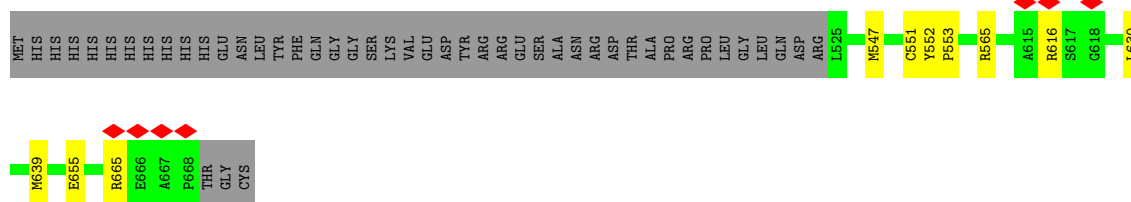
- Molecule 1: High-affinity choline transport protein

Chain TA:  65% 10% 25%



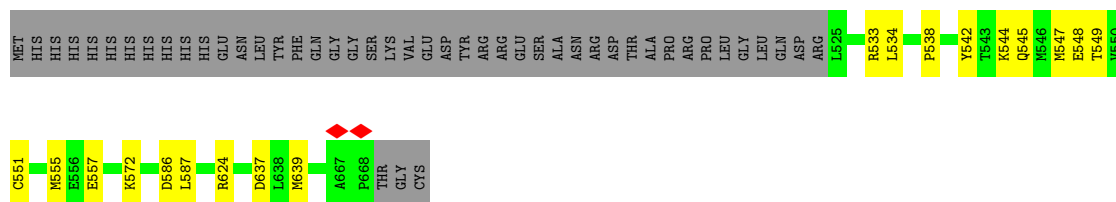
- Molecule 1: High-affinity choline transport protein

Chain UA:  70% 5% 25%



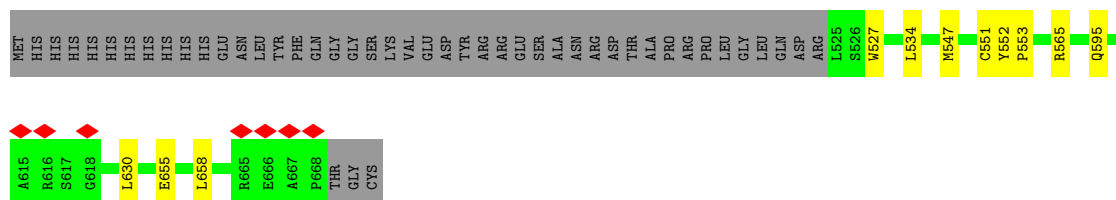
- Molecule 1: High-affinity choline transport protein

Chain VA:  66% 9% 25%



- Molecule 1: High-affinity choline transport protein

Chain WA:  70% 6% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114039	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.502	Depositor
Minimum map value	-0.256	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	317.52, 317.52, 317.52	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.567, 0.567, 0.567	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	0.12	0/1231	0.33	0/1663
1	AA	0.09	0/1225	0.27	0/1656
1	B	0.09	0/1225	0.26	0/1656
1	BA	0.11	0/1231	0.29	0/1663
1	C	0.11	0/1231	0.33	0/1663
1	CA	0.09	0/1225	0.26	0/1656
1	D	0.10	0/1225	0.26	0/1656
1	DA	0.11	0/1231	0.29	0/1663
1	E	0.12	0/1231	0.33	0/1663
1	EA	0.09	0/1225	0.27	0/1656
1	F	0.10	0/1225	0.26	0/1656
1	FA	0.11	0/1231	0.29	0/1663
1	G	0.11	0/1231	0.32	0/1663
1	GA	0.09	0/1225	0.26	0/1656
1	H	0.10	0/1225	0.26	0/1656
1	HA	0.11	0/1231	0.30	0/1663
1	I	0.11	0/1231	0.32	0/1663
1	IA	0.09	0/1225	0.26	0/1656
1	J	0.10	0/1225	0.26	0/1656
1	JA	0.11	0/1231	0.29	0/1663
1	K	0.11	0/1231	0.32	0/1663
1	KA	0.09	0/1225	0.26	0/1656
1	L	0.10	0/1225	0.26	0/1656
1	LA	0.10	0/1231	0.27	0/1663
1	M	0.11	0/1231	0.32	0/1663
1	MA	0.08	0/1225	0.25	0/1656
1	N	0.09	0/1225	0.26	0/1656
1	NA	0.10	0/1231	0.28	0/1663
1	O	0.11	0/1231	0.32	0/1663
1	OA	0.09	0/1225	0.26	0/1656
1	P	0.10	0/1225	0.27	0/1656
1	PA	0.09	0/1231	0.26	0/1663
1	Q	0.11	0/1231	0.32	0/1663
1	QA	0.09	0/1225	0.25	0/1656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	R	0.10	0/1225	0.26	0/1656
1	RA	0.11	0/1231	0.29	0/1663
1	S	0.11	0/1231	0.31	0/1663
1	SA	0.09	0/1225	0.27	0/1656
1	T	0.10	0/1225	0.26	0/1656
1	TA	0.11	0/1231	0.29	0/1663
1	UA	0.09	0/1225	0.25	0/1656
1	V	0.11	0/1231	0.31	0/1663
1	VA	0.10	0/1231	0.27	0/1663
1	W	0.10	0/1225	0.26	0/1656
1	WA	0.09	0/1225	0.26	0/1656
1	X	0.11	0/1231	0.30	0/1663
1	Y	0.10	0/1225	0.26	0/1656
1	Z	0.11	0/1231	0.31	0/1663
All	All	0.10	0/58944	0.28	0/79656

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 ⓘ

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	1201	0	1167	17	0
1	AA	1195	0	1156	9	0
1	B	1195	0	1156	9	0
1	BA	1201	0	1167	10	0
1	C	1201	0	1167	13	0
1	CA	1195	0	1156	6	0
1	D	1195	0	1156	9	0
1	DA	1201	0	1167	11	0
1	E	1201	0	1167	12	0
1	EA	1195	0	1156	9	0
1	F	1195	0	1156	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FA	1201	0	1167	11	0
1	G	1201	0	1167	15	0
1	GA	1195	0	1156	6	0
1	H	1195	0	1156	8	0
1	HA	1201	0	1167	10	0
1	I	1201	0	1167	11	0
1	IA	1195	0	1156	10	0
1	J	1195	0	1156	7	0
1	JA	1201	0	1167	11	0
1	K	1201	0	1167	13	0
1	KA	1195	0	1156	7	0
1	L	1195	0	1156	10	0
1	LA	1201	0	1167	9	0
1	M	1201	0	1167	12	0
1	MA	1195	0	1156	7	0
1	N	1195	0	1156	8	0
1	NA	1201	0	1167	10	0
1	O	1201	0	1167	17	0
1	OA	1195	0	1156	8	0
1	P	1195	0	1156	8	0
1	PA	1201	0	1167	10	0
1	Q	1201	0	1167	14	0
1	QA	1195	0	1156	7	0
1	R	1195	0	1156	9	0
1	RA	1201	0	1167	10	0
1	S	1201	0	1167	13	0
1	SA	1195	0	1156	8	0
1	T	1195	0	1156	9	0
1	TA	1201	0	1167	11	0
1	UA	1195	0	1156	9	0
1	V	1201	0	1167	12	0
1	VA	1201	0	1167	10	0
1	W	1195	0	1156	9	0
1	WA	1195	0	1156	9	0
1	X	1201	0	1167	11	0
1	Y	1195	0	1156	7	0
1	Z	1201	0	1167	14	0
All	All	57504	0	55752	432	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 (432) 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:E:662:HIS:O	1:E:666:GLU:HB3	1.57	1.02
1:Q:662:HIS:O	1:Q:666:GLU:HB3	1.58	1.02
1:K:662:HIS:O	1:K:666:GLU:HB3	1.57	1.01
1:Z:662:HIS:O	1:Z:666:GLU:HB3	1.59	1.00
1:A:662:HIS:O	1:A:666:GLU:HB3	1.62	0.99
1:M:662:HIS:O	1:M:666:GLU:HB3	1.64	0.96
1:I:662:HIS:O	1:I:666:GLU:HB3	1.64	0.96
1:X:662:HIS:O	1:X:666:GLU:HB3	1.65	0.96
1:C:662:HIS:O	1:C:666:GLU:HB3	1.65	0.96
1:S:662:HIS:O	1:S:666:GLU:HB3	1.64	0.96
1:O:662:HIS:O	1:O:666:GLU:HB3	1.66	0.95
1:V:662:HIS:O	1:V:666:GLU:HB3	1.65	0.95
1:G:662:HIS:O	1:G:666:GLU:HB3	1.66	0.94
1:M:534:LEU:HD21	1:R:655:GLU:HG2	1.73	0.71
1:C:534:LEU:HD21	1:W:655:GLU:HG2	1.73	0.70
1:L:655:GLU:HG2	1:Z:534:LEU:HD21	1.73	0.69
1:F:655:GLU:HG2	1:BA:534:LEU:HD21	1.76	0.68
1:SA:547:MET:HA	1:SA:551:CYS:HB2	1.75	0.68
1:WA:547:MET:HA	1:WA:551:CYS:HB2	1.76	0.68
1:H:655:GLU:HG2	1:FA:534:LEU:HD21	1.75	0.68
1:T:655:GLU:HG2	1:TA:534:LEU:HD21	1.76	0.68
1:OA:547:MET:HA	1:OA:551:CYS:HB2	1.75	0.68
1:UA:547:MET:HA	1:UA:551:CYS:HB2	1.76	0.68
1:B:655:GLU:HG2	1:DA:534:LEU:HD21	1.76	0.68
1:P:655:GLU:HG2	1:HA:534:LEU:HD21	1.76	0.67
1:AA:547:MET:HA	1:AA:551:CYS:HB2	1.75	0.67
1:MA:547:MET:HA	1:MA:551:CYS:HB2	1.75	0.67
1:IA:547:MET:HA	1:IA:551:CYS:HB2	1.76	0.67
1:GA:547:MET:HA	1:GA:551:CYS:HB2	1.77	0.66
1:EA:547:MET:HA	1:EA:551:CYS:HB2	1.76	0.66
1:CA:547:MET:HA	1:CA:551:CYS:HB2	1.75	0.66
1:J:655:GLU:HG2	1:O:534:LEU:HD21	1.78	0.66
1:QA:547:MET:HA	1:QA:551:CYS:HB2	1.76	0.66
1:KA:547:MET:HA	1:KA:551:CYS:HB2	1.77	0.66
1:S:534:LEU:HD21	1:MA:655:GLU:HG2	1.78	0.66
1:E:538:PRO:HB3	1:E:542:TYR:HD2	1.61	0.65
1:V:534:LEU:HD21	1:SA:655:GLU:HG2	1.78	0.65
1:D:655:GLU:HG2	1:RA:534:LEU:HD21	1.78	0.65
1:FA:538:PRO:HB3	1:FA:542:TYR:HD2	1.62	0.65
1:G:538:PRO:HB3	1:G:542:TYR:HD2	1.62	0.65
1:N:655:GLU:HG2	1:JA:534:LEU:HD21	1.77	0.65
1:RA:538:PRO:HB3	1:RA:542:TYR:HD2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:LEU:HD21	1:Y:655:GLU:HG2	1.78	0.65
1:I:534:LEU:HD21	1:IA:655:GLU:HG2	1.78	0.65
1:JA:538:PRO:HB3	1:JA:542:TYR:HD2	1.62	0.65
1:I:538:PRO:HB3	1:I:542:TYR:HD2	1.62	0.64
1:BA:538:PRO:HB3	1:BA:542:TYR:HD2	1.62	0.64
1:X:538:PRO:HB3	1:X:542:TYR:HD2	1.62	0.64
1:LA:538:PRO:HB3	1:LA:542:TYR:HD2	1.63	0.64
1:C:538:PRO:HB3	1:C:542:TYR:HD2	1.62	0.64
1:DA:538:PRO:HB3	1:DA:542:TYR:HD2	1.62	0.64
1:PA:538:PRO:HB3	1:PA:542:TYR:HD2	1.63	0.64
1:VA:538:PRO:HB3	1:VA:542:TYR:HD2	1.63	0.64
1:M:538:PRO:HB3	1:M:542:TYR:HD2	1.63	0.64
1:V:538:PRO:HB3	1:V:542:TYR:HD2	1.63	0.64
1:NA:538:PRO:HB3	1:NA:542:TYR:HD2	1.63	0.64
1:HA:538:PRO:HB3	1:HA:542:TYR:HD2	1.63	0.64
1:A:538:PRO:HB3	1:A:542:TYR:HD2	1.62	0.63
1:TA:538:PRO:HB3	1:TA:542:TYR:HD2	1.62	0.63
1:C:545:GLN:O	1:C:549:THR:HG22	1.99	0.63
1:Q:538:PRO:HB3	1:Q:542:TYR:HD2	1.62	0.63
1:Z:538:PRO:HB3	1:Z:542:TYR:HD2	1.64	0.63
1:A:545:GLN:O	1:A:549:THR:HG22	1.99	0.63
1:I:545:GLN:O	1:I:549:THR:HG22	1.99	0.63
1:O:538:PRO:HB3	1:O:542:TYR:HD2	1.63	0.63
1:S:538:PRO:HB3	1:S:542:TYR:HD2	1.63	0.63
1:G:545:GLN:O	1:G:549:THR:HG22	1.99	0.63
1:A:554:ALA:HB2	1:A:643:LYS:HG3	1.81	0.62
1:E:545:GLN:O	1:E:549:THR:HG22	2.00	0.62
1:S:545:GLN:O	1:S:549:THR:HG22	1.99	0.62
1:Q:545:GLN:O	1:Q:549:THR:HG22	2.00	0.62
1:O:545:GLN:O	1:O:549:THR:HG22	1.99	0.62
1:K:538:PRO:HB3	1:K:542:TYR:HD2	1.63	0.61
1:K:545:GLN:O	1:K:549:THR:HG22	1.99	0.61
1:G:534:LEU:HD21	1:OA:655:GLU:HG2	1.81	0.61
1:C:554:ALA:HB2	1:C:643:LYS:HG3	1.83	0.61
1:M:545:GLN:O	1:M:549:THR:HG22	2.00	0.61
1:X:554:ALA:HB2	1:X:643:LYS:HG3	1.83	0.61
1:E:554:ALA:HB2	1:E:643:LYS:HG3	1.83	0.61
1:CA:655:GLU:HG2	1:VA:534:LEU:HD21	1.83	0.61
1:Z:554:ALA:HB2	1:Z:643:LYS:HG3	1.83	0.60
1:O:554:ALA:HB2	1:O:643:LYS:HG3	1.83	0.60
1:Q:554:ALA:HB2	1:Q:643:LYS:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:534:LEU:HD21	1:WA:655:GLU:HG2	1.83	0.60
1:V:554:ALA:HB2	1:V:643:LYS:HG3	1.83	0.60
1:K:534:LEU:HD21	1:QA:655:GLU:HG2	1.84	0.60
1:M:554:ALA:HB2	1:M:643:LYS:HG3	1.84	0.60
1:A:665:ARG:HH22	1:A:668:PRO:HD3	1.67	0.60
1:K:554:ALA:HB2	1:K:643:LYS:HG3	1.83	0.59
1:G:555:MET:HE2	1:G:587:LEU:HB2	1.85	0.59
1:X:545:GLN:O	1:X:549:THR:HG22	2.02	0.59
1:S:544:LYS:O	1:S:548:GLU:HG2	2.03	0.59
1:G:554:ALA:HB2	1:G:643:LYS:HG3	1.83	0.59
1:Q:534:LEU:HD21	1:KA:655:GLU:HG2	1.85	0.58
1:QA:630:LEU:HD12	1:QA:630:LEU:H	1.69	0.58
1:P:630:LEU:HD12	1:P:630:LEU:H	1.69	0.58
1:X:534:LEU:HD21	1:EA:655:GLU:HG2	1.85	0.58
1:HA:555:MET:HE2	1:HA:587:LEU:HB2	1.86	0.58
1:H:630:LEU:HD12	1:H:630:LEU:H	1.69	0.58
1:S:554:ALA:HB2	1:S:643:LYS:HG3	1.84	0.58
1:M:544:LYS:O	1:M:548:GLU:HG2	2.03	0.58
1:Q:544:LYS:O	1:Q:548:GLU:HG2	2.03	0.58
1:L:630:LEU:HD12	1:L:630:LEU:H	1.69	0.58
1:GA:655:GLU:HG2	1:NA:534:LEU:HD21	1.84	0.58
1:KA:630:LEU:HD12	1:KA:630:LEU:H	1.69	0.58
1:W:630:LEU:HD12	1:W:630:LEU:H	1.69	0.58
1:I:554:ALA:HB2	1:I:643:LYS:HG3	1.86	0.58
1:T:630:LEU:HD12	1:T:630:LEU:H	1.69	0.58
1:WA:630:LEU:HD12	1:WA:630:LEU:H	1.69	0.58
1:O:555:MET:HE2	1:O:587:LEU:HB2	1.86	0.58
1:C:555:MET:HE2	1:C:587:LEU:HB2	1.85	0.57
1:RA:555:MET:HE2	1:RA:587:LEU:HB2	1.86	0.57
1:SA:630:LEU:H	1:SA:630:LEU:HD12	1.69	0.57
1:F:630:LEU:HD12	1:F:630:LEU:H	1.69	0.57
1:GA:630:LEU:HD12	1:GA:630:LEU:H	1.69	0.57
1:AA:630:LEU:HD12	1:AA:630:LEU:H	1.69	0.57
1:LA:534:LEU:HD21	1:UA:655:GLU:HG2	1.85	0.57
1:Q:555:MET:HE2	1:Q:587:LEU:HB2	1.87	0.57
1:R:630:LEU:HD12	1:R:630:LEU:H	1.69	0.57
1:BA:555:MET:HE2	1:BA:587:LEU:HB2	1.87	0.56
1:FA:555:MET:HE2	1:FA:587:LEU:HB2	1.86	0.56
1:LA:555:MET:HE2	1:LA:587:LEU:HB2	1.87	0.56
1:DA:555:MET:HE2	1:DA:587:LEU:HB2	1.88	0.56
1:E:555:MET:HE2	1:E:587:LEU:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:533:ARG:HH21	1:RA:637:ASP:HB3	1.70	0.56
1:AA:655:GLU:HG2	1:PA:534:LEU:HD21	1.87	0.56
1:PA:555:MET:HE2	1:PA:587:LEU:HB2	1.87	0.55
1:K:555:MET:HE2	1:K:587:LEU:HB2	1.88	0.55
1:M:555:MET:HE2	1:M:587:LEU:HB2	1.87	0.55
1:Z:555:MET:HE2	1:Z:587:LEU:HB2	1.88	0.55
1:NA:555:MET:HE2	1:NA:587:LEU:HB2	1.88	0.55
1:JA:555:MET:HE2	1:JA:587:LEU:HB2	1.89	0.54
1:VA:555:MET:HE2	1:VA:587:LEU:HB2	1.89	0.54
1:EA:630:LEU:HD12	1:EA:630:LEU:H	1.73	0.54
1:S:555:MET:HE2	1:S:587:LEU:HB2	1.90	0.53
1:Y:630:LEU:HD12	1:Y:630:LEU:H	1.73	0.53
1:TA:555:MET:HE2	1:TA:587:LEU:HB2	1.89	0.53
1:MA:630:LEU:HD12	1:MA:630:LEU:H	1.73	0.52
1:A:556:GLU:HA	1:A:571:LEU:HD11	1.91	0.52
1:A:544:LYS:O	1:A:548:GLU:HG2	2.09	0.52
1:A:572:LYS:HB2	1:A:586:ASP:HB3	1.92	0.52
1:O:544:LYS:O	1:O:548:GLU:HG2	2.10	0.52
1:G:544:LYS:O	1:G:548:GLU:HG2	2.11	0.51
1:G:572:LYS:HB2	1:G:586:ASP:HB3	1.93	0.51
1:O:538:PRO:HG2	1:O:639:MET:HE3	1.93	0.51
1:M:538:PRO:HG2	1:M:639:MET:HE3	1.94	0.50
1:G:655:GLU:HB2	1:P:534:LEU:HD11	1.94	0.50
1:I:544:LYS:O	1:I:548:GLU:HG2	2.11	0.50
1:K:544:LYS:O	1:K:548:GLU:HG2	2.11	0.50
1:C:544:LYS:O	1:C:548:GLU:HG2	2.11	0.50
1:V:538:PRO:HG2	1:V:639:MET:HE3	1.94	0.50
1:V:555:MET:HE2	1:V:587:LEU:HB2	1.93	0.50
1:Q:538:PRO:HG2	1:Q:639:MET:HE3	1.94	0.49
1:C:655:GLU:HB2	1:CA:534:LEU:HD11	1.95	0.49
1:S:538:PRO:HG2	1:S:639:MET:HE3	1.94	0.49
1:X:555:MET:HE2	1:X:587:LEU:HB2	1.93	0.49
1:T:565:ARG:HG3	1:T:565:ARG:HH11	1.78	0.49
1:Z:538:PRO:HG2	1:Z:639:MET:HE3	1.94	0.49
1:H:565:ARG:HG3	1:H:565:ARG:HH11	1.78	0.49
1:X:538:PRO:HG2	1:X:639:MET:HE3	1.95	0.49
1:A:655:GLU:HB2	1:SA:534:LEU:HD11	1.94	0.49
1:P:565:ARG:HG3	1:P:565:ARG:HH11	1.78	0.49
1:B:565:ARG:HG3	1:B:565:ARG:HH11	1.78	0.49
1:M:655:GLU:HB2	1:AA:534:LEU:HD11	1.95	0.49
1:F:565:ARG:HG3	1:F:565:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GA:565:ARG:HG3	1:GA:565:ARG:HH11	1.78	0.48
1:CA:565:ARG:HG3	1:CA:565:ARG:HH11	1.78	0.48
1:WA:565:ARG:HG3	1:WA:565:ARG:HH11	1.78	0.48
1:K:538:PRO:HG2	1:K:639:MET:HE3	1.94	0.48
1:V:655:GLU:HB2	1:Y:534:LEU:HD11	1.94	0.48
1:OA:657:HIS:O	1:OA:661:ILE:HG22	2.13	0.48
1:J:658:LEU:HD12	1:O:534:LEU:HD22	1.95	0.48
1:E:655:GLU:HB2	1:IA:534:LEU:HD11	1.96	0.48
1:N:565:ARG:HG3	1:N:565:ARG:HH11	1.78	0.48
1:G:538:PRO:HG2	1:G:639:MET:HE3	1.95	0.48
1:Y:565:ARG:HG3	1:Y:565:ARG:HH11	1.78	0.48
1:C:538:PRO:HG2	1:C:639:MET:HE3	1.94	0.48
1:D:565:ARG:HH11	1:D:565:ARG:HG3	1.78	0.48
1:W:565:ARG:HG3	1:W:565:ARG:HH11	1.78	0.48
1:Z:655:GLU:HB2	1:GA:534:LEU:HD11	1.95	0.47
1:I:538:PRO:HG2	1:I:639:MET:HE3	1.97	0.47
1:AA:565:ARG:HG3	1:AA:565:ARG:HH11	1.78	0.47
1:HA:572:LYS:HB2	1:HA:586:ASP:HB3	1.97	0.47
1:A:538:PRO:HG2	1:A:639:MET:HE3	1.95	0.47
1:A:565:ARG:HG2	1:A:565:ARG:HH11	1.80	0.47
1:KA:565:ARG:HH11	1:KA:565:ARG:HG3	1.80	0.47
1:E:538:PRO:HG2	1:E:639:MET:HE3	1.96	0.47
1:Z:544:LYS:O	1:Z:548:GLU:HG2	2.14	0.47
1:SA:565:ARG:HG3	1:SA:565:ARG:HH11	1.80	0.47
1:F:534:LEU:HD11	1:K:655:GLU:HB2	1.97	0.47
1:L:565:ARG:HG3	1:L:565:ARG:HH11	1.80	0.47
1:FA:572:LYS:HB2	1:FA:586:ASP:HB3	1.97	0.47
1:IA:565:ARG:HG3	1:IA:565:ARG:HH11	1.80	0.47
1:OA:565:ARG:HG3	1:OA:565:ARG:HH11	1.80	0.47
1:V:544:LYS:O	1:V:548:GLU:HG2	2.15	0.47
1:QA:565:ARG:HG3	1:QA:565:ARG:HH11	1.80	0.47
1:J:534:LEU:HD11	1:X:655:GLU:HB2	1.97	0.46
1:TA:572:LYS:HB2	1:TA:586:ASP:HB3	1.97	0.46
1:P:616:ARG:HA	1:P:616:ARG:HD2	1.70	0.46
1:R:565:ARG:HG3	1:R:565:ARG:HH11	1.80	0.46
1:FA:538:PRO:HG2	1:FA:639:MET:HE3	1.97	0.46
1:RA:538:PRO:HG2	1:RA:639:MET:HE3	1.97	0.46
1:UA:565:ARG:HH11	1:UA:565:ARG:HG3	1.80	0.46
1:E:565:ARG:HH11	1:E:565:ARG:HG2	1.80	0.46
1:K:535:MET:HE3	1:K:535:MET:HB2	1.76	0.46
1:EA:565:ARG:HG3	1:EA:565:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:534:LEU:HD11	1:Q:655:GLU:HB2	1.98	0.46
1:HA:538:PRO:HG2	1:HA:639:MET:HE3	1.97	0.46
1:DA:572:LYS:HB2	1:DA:586:ASP:HB3	1.98	0.46
1:M:534:LEU:HD22	1:R:658:LEU:HD12	1.98	0.46
1:BA:572:LYS:HB2	1:BA:586:ASP:HB3	1.98	0.46
1:H:658:LEU:HD12	1:FA:534:LEU:HD22	1.98	0.46
1:MA:565:ARG:HG3	1:MA:565:ARG:HH11	1.80	0.46
1:BA:538:PRO:HG2	1:BA:639:MET:HE3	1.97	0.46
1:DA:538:PRO:HG2	1:DA:639:MET:HE3	1.98	0.46
1:EA:598:VAL:HB	1:EA:630:LEU:HG	1.98	0.46
1:B:534:LEU:HD11	1:S:655:GLU:HB2	1.98	0.45
1:F:658:LEU:HD12	1:BA:534:LEU:HD22	1.98	0.45
1:VA:572:LYS:HB2	1:VA:586:ASP:HB3	1.99	0.45
1:L:658:LEU:HD12	1:Z:534:LEU:HD22	1.98	0.45
1:RA:572:LYS:HB2	1:RA:586:ASP:HB3	1.98	0.45
1:UA:630:LEU:HD12	1:UA:630:LEU:H	1.81	0.45
1:L:639:MET:HE2	1:L:639:MET:HB2	1.92	0.45
1:HA:545:GLN:O	1:HA:549:THR:HG22	2.17	0.45
1:HA:624:ARG:HG2	1:HA:637:ASP:OD2	2.17	0.45
1:TA:538:PRO:HG2	1:TA:639:MET:HE3	1.98	0.45
1:BA:624:ARG:HG2	1:BA:637:ASP:OD2	2.17	0.45
1:IA:639:MET:HE2	1:IA:639:MET:HB2	1.92	0.45
1:JA:572:LYS:HB2	1:JA:586:ASP:HB3	1.99	0.45
1:DA:533:ARG:HA	1:DA:533:ARG:HD3	1.81	0.45
1:RA:545:GLN:O	1:RA:549:THR:HG22	2.17	0.45
1:T:658:LEU:HD12	1:TA:534:LEU:HD22	1.99	0.45
1:MA:616:ARG:HD2	1:MA:616:ARG:HA	1.72	0.45
1:PA:538:PRO:HG2	1:PA:639:MET:HE3	1.99	0.45
1:JA:545:GLN:O	1:JA:549:THR:HG22	2.17	0.44
1:NA:572:LYS:HB2	1:NA:586:ASP:HB3	1.99	0.44
1:TA:545:GLN:O	1:TA:549:THR:HG22	2.17	0.44
1:I:655:GLU:HB2	1:WA:534:LEU:HD11	2.00	0.44
1:J:630:LEU:HD12	1:J:630:LEU:H	1.83	0.44
1:S:535:MET:HE3	1:S:535:MET:HB2	1.77	0.44
1:LA:538:PRO:HG2	1:LA:639:MET:HE3	1.99	0.44
1:PA:572:LYS:HB2	1:PA:586:ASP:HB3	1.98	0.44
1:N:639:MET:HE2	1:N:639:MET:HB2	1.92	0.44
1:FA:624:ARG:HG2	1:FA:637:ASP:OD2	2.17	0.44
1:LA:545:GLN:O	1:LA:549:THR:HG22	2.17	0.44
1:B:630:LEU:H	1:B:630:LEU:HD12	1.82	0.44
1:B:658:LEU:HD12	1:DA:534:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:534:LEU:HD22	1:W:658:LEU:HD12	1.99	0.44
1:P:658:LEU:HD12	1:HA:534:LEU:HD22	1.99	0.44
1:Y:639:MET:HE2	1:Y:639:MET:HB2	1.92	0.44
1:LA:572:LYS:HB2	1:LA:586:ASP:HB3	1.98	0.44
1:N:658:LEU:HD12	1:JA:534:LEU:HD22	2.00	0.44
1:W:639:MET:HE2	1:W:639:MET:HB2	1.92	0.44
1:OA:630:LEU:HD12	1:OA:630:LEU:H	1.82	0.44
1:RA:624:ARG:HG2	1:RA:637:ASP:OD2	2.17	0.44
1:UA:639:MET:HE2	1:UA:639:MET:HB2	1.92	0.44
1:VA:538:PRO:HG2	1:VA:639:MET:HE3	1.99	0.44
1:FA:533:ARG:HA	1:FA:533:ARG:HD3	1.81	0.44
1:L:665:ARG:HA	1:L:665:ARG:HD2	1.82	0.44
1:N:630:LEU:HD12	1:N:630:LEU:H	1.82	0.44
1:O:624:ARG:HG2	1:O:637:ASP:OD1	2.18	0.44
1:JA:538:PRO:HG2	1:JA:639:MET:HE3	1.98	0.44
1:A:624:ARG:HG2	1:A:637:ASP:OD1	2.18	0.44
1:K:544:LYS:HB3	1:K:544:LYS:HE2	1.84	0.44
1:V:624:ARG:HG2	1:V:637:ASP:OD2	2.18	0.44
1:Z:624:ARG:HG2	1:Z:637:ASP:OD2	2.18	0.44
1:FA:545:GLN:O	1:FA:549:THR:HG22	2.17	0.44
1:IA:630:LEU:H	1:IA:630:LEU:HD12	1.83	0.44
1:NA:545:GLN:O	1:NA:549:THR:HG22	2.17	0.44
1:PA:545:GLN:O	1:PA:549:THR:HG22	2.18	0.44
1:B:616:ARG:HA	1:B:616:ARG:HD2	1.79	0.43
1:NA:538:PRO:HG2	1:NA:639:MET:HE3	1.99	0.43
1:D:630:LEU:HD12	1:D:630:LEU:H	1.83	0.43
1:Q:624:ARG:HG2	1:Q:637:ASP:OD2	2.18	0.43
1:QA:665:ARG:HA	1:QA:665:ARG:HD2	1.82	0.43
1:A:657:HIS:O	1:A:661:ILE:HG23	2.18	0.43
1:C:624:ARG:HG2	1:C:637:ASP:OD2	2.18	0.43
1:G:665:ARG:HH22	1:G:668:PRO:HD3	1.83	0.43
1:J:639:MET:HE2	1:J:639:MET:HB2	1.92	0.43
1:S:624:ARG:HG2	1:S:637:ASP:OD2	2.18	0.43
1:AA:639:MET:HE2	1:AA:639:MET:HB2	1.92	0.43
1:BA:545:GLN:O	1:BA:549:THR:HG22	2.18	0.43
1:O:652:ASP:O	1:O:656:ARG:HG3	2.19	0.43
1:DA:545:GLN:O	1:DA:549:THR:HG22	2.17	0.43
1:JA:624:ARG:HG2	1:JA:637:ASP:OD1	2.19	0.43
1:VA:545:GLN:O	1:VA:549:THR:HG22	2.18	0.43
1:B:565:ARG:HG3	1:B:565:ARG:NH1	2.34	0.43
1:Y:665:ARG:HA	1:Y:665:ARG:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NA:544:LYS:O	1:NA:548:GLU:HG2	2.19	0.43
1:K:624:ARG:HG2	1:K:637:ASP:OD1	2.19	0.43
1:Q:652:ASP:O	1:Q:656:ARG:HG3	2.18	0.43
1:W:565:ARG:HG3	1:W:565:ARG:NH1	2.34	0.43
1:Z:652:ASP:O	1:Z:656:ARG:HG3	2.19	0.43
1:LA:624:ARG:HG2	1:LA:637:ASP:OD1	2.19	0.43
1:WA:565:ARG:HG3	1:WA:565:ARG:NH1	2.34	0.43
1:D:665:ARG:HA	1:D:665:ARG:HD2	1.82	0.43
1:I:652:ASP:O	1:I:656:ARG:HG3	2.19	0.43
1:O:655:GLU:HB2	1:EA:534:LEU:HD11	1.99	0.43
1:GA:565:ARG:HG3	1:GA:565:ARG:NH1	2.34	0.43
1:OA:656:ARG:HH11	1:OA:656:ARG:HB3	1.84	0.43
1:O:665:ARG:NH2	1:O:668:PRO:HD3	2.34	0.43
1:AA:658:LEU:HD12	1:PA:534:LEU:HD22	1.99	0.43
1:NA:624:ARG:HG2	1:NA:637:ASP:OD1	2.19	0.43
1:QA:616:ARG:HA	1:QA:616:ARG:HD2	1.79	0.43
1:I:561:GLU:HG3	1:WA:527:TRP:CH2	2.54	0.42
1:EA:639:MET:HE2	1:EA:639:MET:HB2	1.92	0.42
1:C:652:ASP:O	1:C:656:ARG:HG3	2.19	0.42
1:F:565:ARG:HG3	1:F:565:ARG:NH1	2.34	0.42
1:N:565:ARG:HG3	1:N:565:ARG:NH1	2.34	0.42
1:V:652:ASP:O	1:V:656:ARG:HG3	2.19	0.42
1:W:616:ARG:HD2	1:W:616:ARG:HA	1.79	0.42
1:UA:616:ARG:HD2	1:UA:616:ARG:HA	1.79	0.42
1:P:565:ARG:HG3	1:P:565:ARG:NH1	2.34	0.42
1:S:652:ASP:O	1:S:656:ARG:HG3	2.19	0.42
1:V:665:ARG:NH2	1:V:668:PRO:HD3	2.34	0.42
1:TA:544:LYS:O	1:TA:548:GLU:HG2	2.19	0.42
1:M:652:ASP:O	1:M:656:ARG:HG3	2.19	0.42
1:FA:544:LYS:O	1:FA:548:GLU:HG2	2.19	0.42
1:JA:544:LYS:O	1:JA:548:GLU:HG2	2.19	0.42
1:D:642:SER:O	1:D:646:VAL:HG23	2.20	0.42
1:M:624:ARG:HG2	1:M:637:ASP:OD2	2.19	0.42
1:N:665:ARG:HA	1:N:665:ARG:HD2	1.82	0.42
1:X:652:ASP:O	1:X:656:ARG:HG3	2.19	0.42
1:O:544:LYS:HB2	1:O:582:LEU:HD21	2.02	0.42
1:T:642:SER:O	1:T:646:VAL:HG23	2.20	0.42
1:W:642:SER:O	1:W:646:VAL:HG23	2.20	0.42
1:SA:616:ARG:HA	1:SA:616:ARG:HD2	1.80	0.42
1:D:616:ARG:HA	1:D:616:ARG:HD2	1.79	0.42
1:K:652:ASP:O	1:K:656:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:624:ARG:HG2	1:X:637:ASP:OD2	2.19	0.42
1:BA:533:ARG:HA	1:BA:533:ARG:HD3	1.80	0.42
1:VA:624:ARG:HG2	1:VA:637:ASP:OD1	2.19	0.42
1:B:642:SER:O	1:B:646:VAL:HG23	2.20	0.42
1:G:544:LYS:HB2	1:G:582:LEU:HD21	2.02	0.42
1:H:642:SER:O	1:H:646:VAL:HG23	2.20	0.42
1:R:642:SER:O	1:R:646:VAL:HG23	2.20	0.42
1:V:665:ARG:HH22	1:V:668:PRO:HD3	1.84	0.42
1:AA:565:ARG:HG3	1:AA:565:ARG:NH1	2.34	0.42
1:DA:624:ARG:HG2	1:DA:637:ASP:OD1	2.19	0.42
1:LA:533:ARG:HA	1:LA:533:ARG:HD3	1.80	0.42
1:B:665:ARG:HD2	1:B:665:ARG:HA	1.82	0.42
1:H:565:ARG:HG3	1:H:565:ARG:NH1	2.34	0.42
1:D:565:ARG:HG3	1:D:565:ARG:NH1	2.34	0.42
1:G:652:ASP:O	1:G:656:ARG:HG3	2.18	0.42
1:Q:544:LYS:HB3	1:Q:544:LYS:HE2	1.83	0.42
1:Q:665:ARG:HH22	1:Q:668:PRO:HD3	1.85	0.42
1:R:565:ARG:HG3	1:R:565:ARG:NH1	2.35	0.42
1:R:639:MET:HE2	1:R:639:MET:HB2	1.92	0.42
1:UA:665:ARG:HD2	1:UA:665:ARG:HA	1.83	0.42
1:A:660:PHE:CD1	1:A:660:PHE:C	2.98	0.41
1:J:616:ARG:HA	1:J:616:ARG:HD2	1.79	0.41
1:L:565:ARG:HG3	1:L:565:ARG:NH1	2.35	0.41
1:L:642:SER:O	1:L:646:VAL:HG23	2.20	0.41
1:O:658:LEU:HD23	1:O:658:LEU:HA	1.91	0.41
1:O:665:ARG:HH22	1:O:668:PRO:HD3	1.85	0.41
1:R:642:SER:HG	1:R:645:GLN:HG3	1.85	0.41
1:Z:665:ARG:HH22	1:Z:668:PRO:HD3	1.85	0.41
1:JA:544:LYS:HB3	1:JA:544:LYS:HE2	1.83	0.41
1:D:658:LEU:HD12	1:RA:534:LEU:HD22	2.00	0.41
1:I:544:LYS:HB2	1:I:582:LEU:HD21	2.02	0.41
1:T:616:ARG:HA	1:T:616:ARG:HD2	1.79	0.41
1:W:665:ARG:HD2	1:W:665:ARG:HA	1.82	0.41
1:CA:565:ARG:HG3	1:CA:565:ARG:NH1	2.34	0.41
1:IA:616:ARG:HA	1:IA:616:ARG:HD2	1.79	0.41
1:PA:624:ARG:HG2	1:PA:637:ASP:OD1	2.19	0.41
1:J:642:SER:O	1:J:646:VAL:HG23	2.19	0.41
1:DA:544:LYS:O	1:DA:548:GLU:HG2	2.19	0.41
1:IA:565:ARG:HG3	1:IA:565:ARG:NH1	2.36	0.41
1:KA:565:ARG:HG3	1:KA:565:ARG:NH1	2.35	0.41
1:OA:565:ARG:HG3	1:OA:565:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:616:ARG:HA	1:L:616:ARG:HD2	1.79	0.41
1:O:535:MET:HB2	1:O:535:MET:HE3	1.83	0.41
1:Y:642:SER:O	1:Y:646:VAL:HG23	2.20	0.41
1:HA:552:TYR:HB3	1:HA:553:PRO:HD3	2.03	0.41
1:IA:665:ARG:HA	1:IA:665:ARG:HD2	1.83	0.41
1:VA:547:MET:HA	1:VA:551:CYS:HB2	2.03	0.41
1:C:658:LEU:HD23	1:C:658:LEU:HA	1.91	0.41
1:E:652:ASP:O	1:E:656:ARG:HG3	2.19	0.41
1:F:642:SER:O	1:F:646:VAL:HG23	2.20	0.41
1:N:642:SER:O	1:N:646:VAL:HG23	2.20	0.41
1:LA:544:LYS:O	1:LA:548:GLU:HG2	2.19	0.41
1:QA:565:ARG:HG3	1:QA:565:ARG:NH1	2.36	0.41
1:RA:552:TYR:HB3	1:RA:553:PRO:HD3	2.03	0.41
1:VA:533:ARG:HA	1:VA:533:ARG:HD3	1.80	0.41
1:VA:544:LYS:O	1:VA:548:GLU:HG2	2.20	0.41
1:A:544:LYS:HB2	1:A:582:LEU:HD21	2.02	0.41
1:G:665:ARG:NH2	1:G:668:PRO:HD3	2.35	0.41
1:X:544:LYS:HB2	1:X:582:LEU:HD21	2.02	0.41
1:KA:665:ARG:HD2	1:KA:665:ARG:HA	1.83	0.41
1:SA:665:ARG:HD2	1:SA:665:ARG:HA	1.83	0.41
1:MA:565:ARG:HG3	1:MA:565:ARG:NH1	2.36	0.41
1:UA:565:ARG:HG3	1:UA:565:ARG:NH1	2.36	0.41
1:E:534:LEU:HD22	1:WA:658:LEU:HD12	2.03	0.41
1:F:616:ARG:HA	1:F:616:ARG:HD2	1.79	0.41
1:T:665:ARG:HD2	1:T:665:ARG:HA	1.82	0.41
1:Z:658:LEU:HD23	1:Z:658:LEU:HA	1.91	0.41
1:E:544:LYS:HB2	1:E:582:LEU:HD21	2.02	0.41
1:T:639:MET:HE2	1:T:639:MET:HB2	1.92	0.41
1:EA:616:ARG:HA	1:EA:616:ARG:HD2	1.72	0.41
1:SA:639:MET:HE2	1:SA:639:MET:HB2	1.92	0.41
1:TA:533:ARG:HA	1:TA:533:ARG:HD3	1.81	0.41
1:TA:552:TYR:HB3	1:TA:553:PRO:HD3	2.03	0.41
1:P:642:SER:O	1:P:646:VAL:HG23	2.20	0.41
1:JA:577:GLU:H	1:JA:577:GLU:CD	2.29	0.41
1:G:577:GLU:CD	1:G:577:GLU:H	2.30	0.40
1:Q:534:LEU:HD22	1:KA:658:LEU:HD12	2.02	0.40
1:R:665:ARG:HD2	1:R:665:ARG:HA	1.82	0.40
1:T:565:ARG:HG3	1:T:565:ARG:NH1	2.34	0.40
1:A:577:GLU:H	1:A:577:GLU:CD	2.30	0.40
1:S:544:LYS:HB2	1:S:582:LEU:HD21	2.03	0.40
1:Z:665:ARG:NH2	1:Z:668:PRO:HD3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:577:GLU:CD	1:BA:577:GLU:H	2.30	0.40
1:HA:547:MET:HA	1:HA:551:CYS:HB2	2.04	0.40
1:IA:552:TYR:HB3	1:IA:553:PRO:HD3	2.04	0.40
1:MA:665:ARG:HA	1:MA:665:ARG:HD2	1.84	0.40
1:TA:606:TYR:HD2	1:TA:624:ARG:HD3	1.87	0.40
1:H:639:MET:HE2	1:H:639:MET:HB2	1.92	0.40
1:OA:616:ARG:HA	1:OA:616:ARG:HD2	1.79	0.40
1:PA:552:TYR:HB3	1:PA:553:PRO:HD3	2.03	0.40
1:WA:552:TYR:HB3	1:WA:553:PRO:HD3	2.04	0.40
1:AA:552:TYR:HB3	1:AA:553:PRO:HD3	2.04	0.40
1:EA:552:TYR:HB3	1:EA:553:PRO:HD3	2.04	0.40
1:UA:552:TYR:HB3	1:UA:553:PRO:HD3	2.04	0.40
1:F:665:ARG:HD2	1:F:665:ARG:HA	1.82	0.40
1:H:665:ARG:HD2	1:H:665:ARG:HA	1.82	0.40
1:L:564:LEU:HD12	1:L:564:LEU:HA	1.88	0.40
1:CA:639:MET:HE2	1:CA:639:MET:HB2	1.92	0.40
1:DA:552:TYR:HB3	1:DA:553:PRO:HD3	2.03	0.40
1:FA:552:TYR:HB3	1:FA:553:PRO:HD3	2.03	0.40
1:NA:577:GLU:CD	1:NA:577:GLU:H	2.30	0.40
1:NA:652:ASP:O	1:NA:656:ARG:HG3	2.22	0.40
1:PA:544:LYS:HB2	1:PA:582:LEU:HD21	2.04	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	142/191 (74%)	142 (100%)	0	0	100	100
1	AA	142/191 (74%)	138 (97%)	4 (3%)	0	100	100
1	B	142/191 (74%)	140 (99%)	2 (1%)	0	100	100
1	BA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	142/191 (74%)	142 (100%)	0	0	100	100
1	CA	142/191 (74%)	138 (97%)	4 (3%)	0	100	100
1	D	142/191 (74%)	140 (99%)	2 (1%)	0	100	100
1	DA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100
1	E	142/191 (74%)	142 (100%)	0	0	100	100
1	EA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100
1	F	142/191 (74%)	140 (99%)	2 (1%)	0	100	100
1	FA	142/191 (74%)	138 (97%)	4 (3%)	0	100	100
1	G	142/191 (74%)	142 (100%)	0	0	100	100
1	GA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100
1	H	142/191 (74%)	140 (99%)	2 (1%)	0	100	100
1	HA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100
1	I	142/191 (74%)	142 (100%)	0	0	100	100
1	IA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100
1	J	142/191 (74%)	140 (99%)	2 (1%)	0	100	100
1	JA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100
1	K	142/191 (74%)	142 (100%)	0	0	100	100
1	KA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100
1	L	142/191 (74%)	140 (99%)	2 (1%)	0	100	100
1	LA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100
1	M	142/191 (74%)	142 (100%)	0	0	100	100
1	MA	142/191 (74%)	140 (99%)	2 (1%)	0	100	100
1	N	142/191 (74%)	140 (99%)	2 (1%)	0	100	100
1	NA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100
1	O	142/191 (74%)	142 (100%)	0	0	100	100
1	OA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100
1	P	142/191 (74%)	140 (99%)	2 (1%)	0	100	100
1	PA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100
1	Q	142/191 (74%)	142 (100%)	0	0	100	100
1	QA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100
1	R	142/191 (74%)	139 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	RA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100
1	S	142/191 (74%)	142 (100%)	0	0	100	100
1	SA	142/191 (74%)	138 (97%)	4 (3%)	0	100	100
1	T	142/191 (74%)	140 (99%)	2 (1%)	0	100	100
1	TA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100
1	UA	142/191 (74%)	138 (97%)	4 (3%)	0	100	100
1	V	142/191 (74%)	142 (100%)	0	0	100	100
1	VA	142/191 (74%)	138 (97%)	4 (3%)	0	100	100
1	W	142/191 (74%)	140 (99%)	2 (1%)	0	100	100
1	WA	142/191 (74%)	139 (98%)	3 (2%)	0	100	100
1	X	142/191 (74%)	142 (100%)	0	0	100	100
1	Y	142/191 (74%)	140 (99%)	2 (1%)	0	100	100
1	Z	142/191 (74%)	142 (100%)	0	0	100	100
All	All	6816/9168 (74%)	6717 (98%)	99 (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	130/171 (76%)	128 (98%)	2 (2%)	57	73
1	AA	129/171 (75%)	127 (98%)	2 (2%)	55	72
1	B	129/171 (75%)	128 (99%)	1 (1%)	73	79
1	BA	130/171 (76%)	129 (99%)	1 (1%)	73	79
1	C	130/171 (76%)	129 (99%)	1 (1%)	73	79
1	CA	129/171 (75%)	128 (99%)	1 (1%)	73	79
1	D	129/171 (75%)	128 (99%)	1 (1%)	73	79
1	DA	130/171 (76%)	129 (99%)	1 (1%)	73	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	130/171 (76%)	129 (99%)	1 (1%)	73	79
1	EA	129/171 (75%)	129 (100%)	0	100	100
1	F	129/171 (75%)	128 (99%)	1 (1%)	73	79
1	FA	130/171 (76%)	128 (98%)	2 (2%)	57	73
1	G	130/171 (76%)	130 (100%)	0	100	100
1	GA	129/171 (75%)	129 (100%)	0	100	100
1	H	129/171 (75%)	129 (100%)	0	100	100
1	HA	130/171 (76%)	128 (98%)	2 (2%)	57	73
1	I	130/171 (76%)	129 (99%)	1 (1%)	73	79
1	IA	129/171 (75%)	129 (100%)	0	100	100
1	J	129/171 (75%)	128 (99%)	1 (1%)	73	79
1	JA	130/171 (76%)	129 (99%)	1 (1%)	73	79
1	K	130/171 (76%)	129 (99%)	1 (1%)	73	79
1	KA	129/171 (75%)	129 (100%)	0	100	100
1	L	129/171 (75%)	128 (99%)	1 (1%)	73	79
1	LA	130/171 (76%)	128 (98%)	2 (2%)	57	73
1	M	130/171 (76%)	129 (99%)	1 (1%)	73	79
1	MA	129/171 (75%)	129 (100%)	0	100	100
1	N	129/171 (75%)	128 (99%)	1 (1%)	73	79
1	NA	130/171 (76%)	128 (98%)	2 (2%)	57	73
1	O	130/171 (76%)	129 (99%)	1 (1%)	73	79
1	OA	129/171 (75%)	129 (100%)	0	100	100
1	P	129/171 (75%)	128 (99%)	1 (1%)	73	79
1	PA	130/171 (76%)	128 (98%)	2 (2%)	57	73
1	Q	130/171 (76%)	129 (99%)	1 (1%)	73	79
1	QA	129/171 (75%)	129 (100%)	0	100	100
1	R	129/171 (75%)	128 (99%)	1 (1%)	73	79
1	RA	130/171 (76%)	128 (98%)	2 (2%)	57	73
1	S	130/171 (76%)	129 (99%)	1 (1%)	73	79
1	SA	129/171 (75%)	129 (100%)	0	100	100
1	T	129/171 (75%)	128 (99%)	1 (1%)	73	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	TA	130/171 (76%)	128 (98%)	2 (2%)	57	73
1	UA	129/171 (75%)	129 (100%)	0	100	100
1	V	130/171 (76%)	129 (99%)	1 (1%)	73	79
1	VA	130/171 (76%)	129 (99%)	1 (1%)	73	79
1	W	129/171 (75%)	128 (99%)	1 (1%)	73	79
1	WA	129/171 (75%)	128 (99%)	1 (1%)	73	79
1	X	130/171 (76%)	129 (99%)	1 (1%)	73	79
1	Y	129/171 (75%)	129 (100%)	0	100	100
1	Z	130/171 (76%)	129 (99%)	1 (1%)	73	79
All	All	6216/8208 (76%)	6171 (99%)	45 (1%)	73	80

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	569	VAL
1	A	663	LEU
1	B	557	GLU
1	C	569	VAL
1	D	557	GLU
1	E	569	VAL
1	F	557	GLU
1	I	569	VAL
1	J	557	GLU
1	K	569	VAL
1	L	557	GLU
1	M	569	VAL
1	N	557	GLU
1	O	569	VAL
1	P	557	GLU
1	Q	569	VAL
1	R	557	GLU
1	S	569	VAL
1	T	557	GLU
1	V	569	VAL
1	W	557	GLU
1	X	569	VAL
1	Z	569	VAL
1	AA	534	LEU
1	AA	535	MET

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Mol	Chain	Res	Type
1	BA	557	GLU
1	CA	534	LEU
1	DA	557	GLU
1	FA	557	GLU
1	FA	569	VAL
1	HA	557	GLU
1	HA	569	VAL
1	JA	557	GLU
1	LA	557	GLU
1	LA	569	VAL
1	NA	557	GLU
1	NA	569	VAL
1	PA	557	GLU
1	PA	569	VAL
1	RA	557	GLU
1	RA	569	VAL
1	TA	557	GLU
1	TA	569	VAL
1	VA	557	GLU
1	WA	595	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	657	HIS
1	C	605	GLN
1	D	604	GLN
1	E	605	GLN
1	F	604	GLN
1	H	604	GLN
1	I	605	GLN
1	J	604	GLN
1	K	580	GLN
1	K	605	GLN
1	L	604	GLN
1	M	580	GLN
1	M	604	GLN
1	M	605	GLN
1	N	604	GLN
1	O	605	GLN
1	Q	605	GLN
1	Q	664	HIS

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Mol	Chain	Res	Type
1	S	605	GLN
1	T	604	GLN
1	V	580	GLN
1	V	605	GLN
1	X	580	GLN
1	X	605	GLN
1	Z	580	GLN
1	Z	604	GLN
1	Z	605	GLN
1	AA	604	GLN
1	AA	657	HIS
1	BA	604	GLN
1	BA	605	GLN
1	CA	604	GLN
1	DA	604	GLN
1	EA	604	GLN
1	EA	657	HIS
1	FA	560	GLN
1	FA	604	GLN
1	GA	604	GLN
1	HA	560	GLN
1	HA	604	GLN
1	IA	604	GLN
1	JA	604	GLN
1	KA	604	GLN
1	LA	605	GLN
1	MA	604	GLN
1	NA	604	GLN
1	NA	605	GLN
1	NA	664	HIS
1	OA	604	GLN
1	PA	605	GLN
1	QA	604	GLN
1	RA	604	GLN
1	SA	604	GLN
1	TA	604	GLN
1	UA	604	GLN
1	WA	604	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

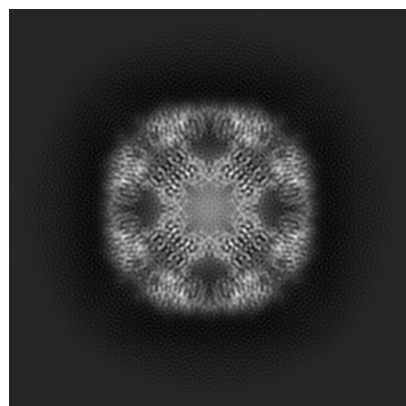
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66344. These allow visual inspection of the internal detail of the map and identification of artifacts.

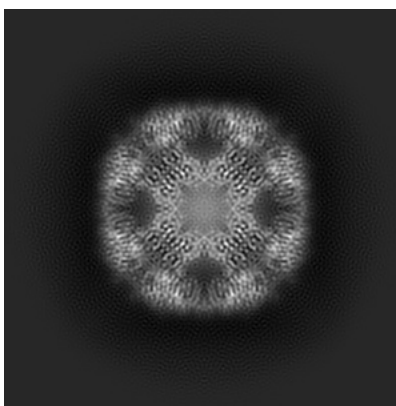
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

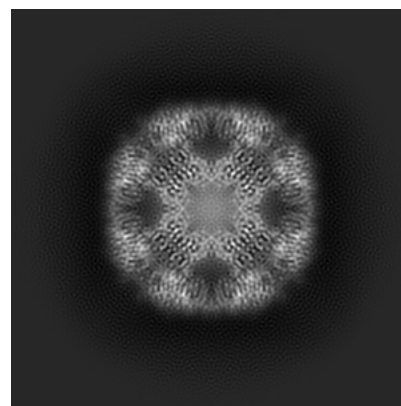
6.1.1 Primary map



X

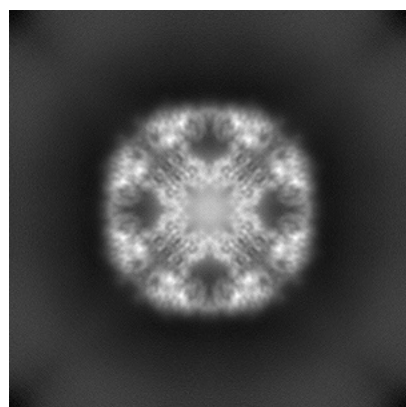


Y

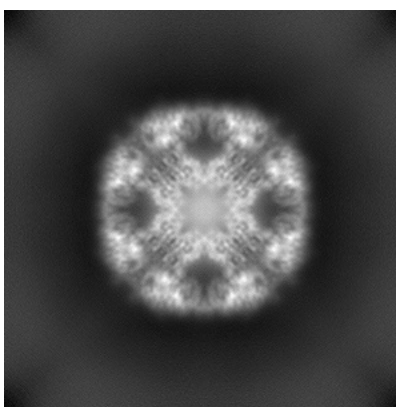


Z

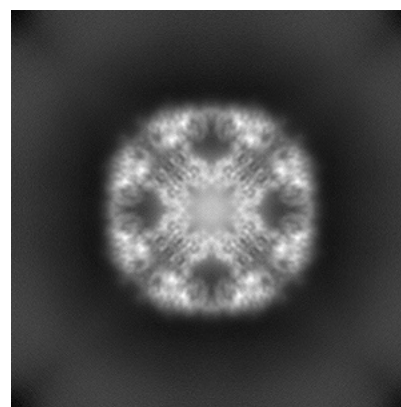
6.1.2 Raw map



X



Y

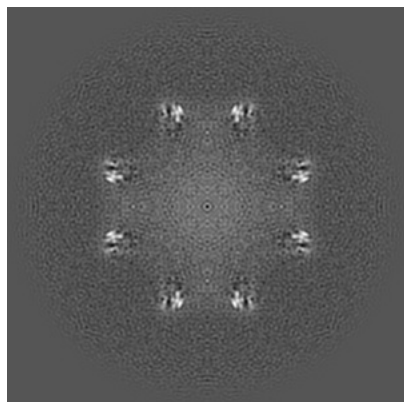


Z

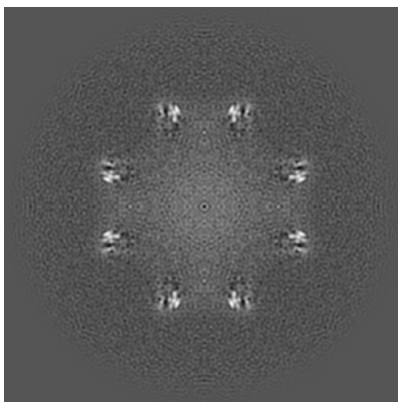
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

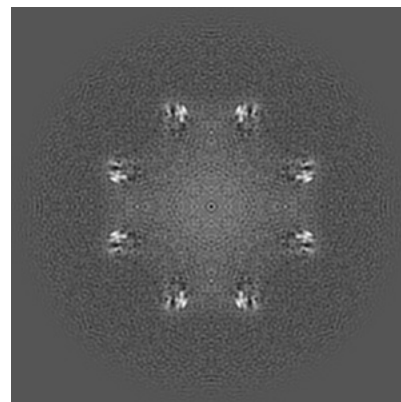
6.2.1 Primary map



X Index: 280

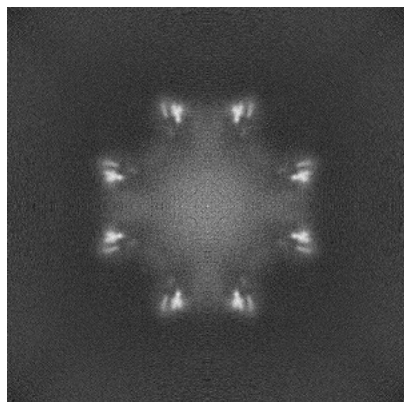


Y Index: 280

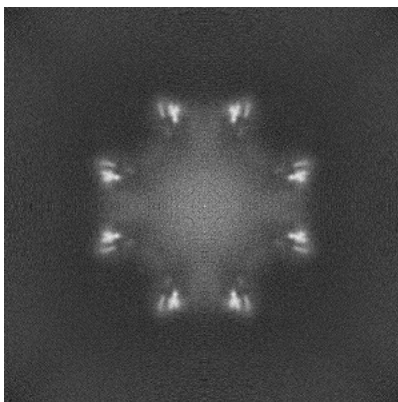


Z Index: 280

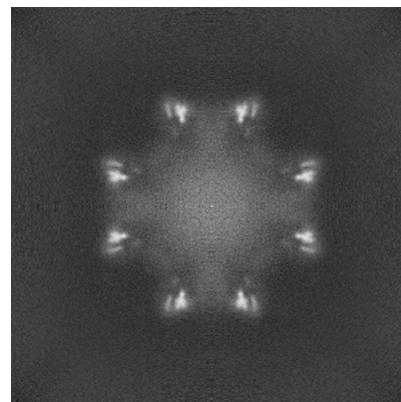
6.2.2 Raw map



X Index: 280



Y Index: 280

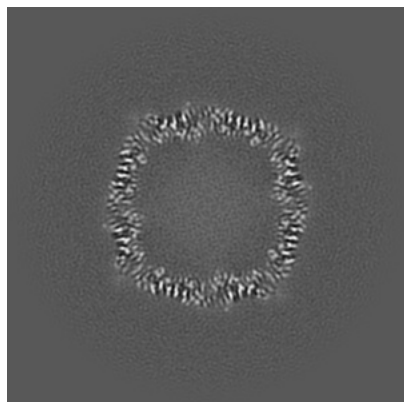


Z Index: 280

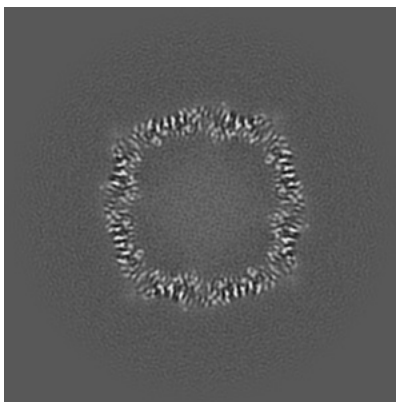
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

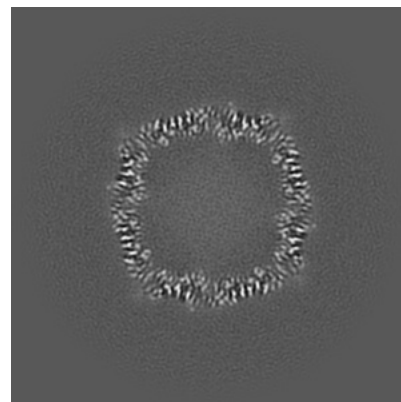
6.3.1 Primary map



X Index: 229

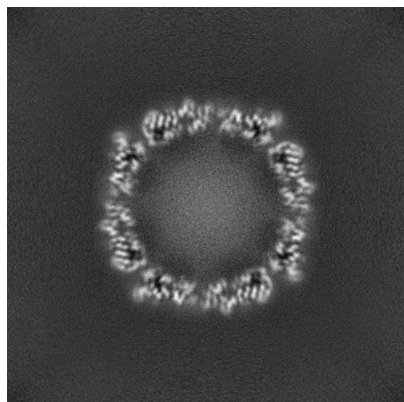


Y Index: 331

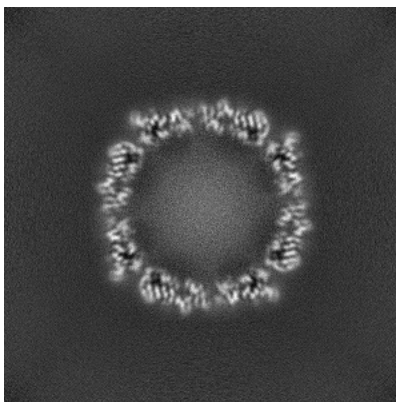


Z Index: 331

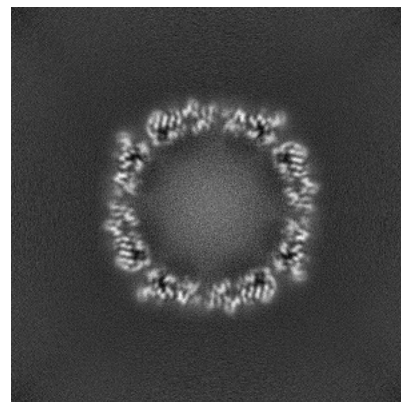
6.3.2 Raw map



X Index: 318



Y Index: 242

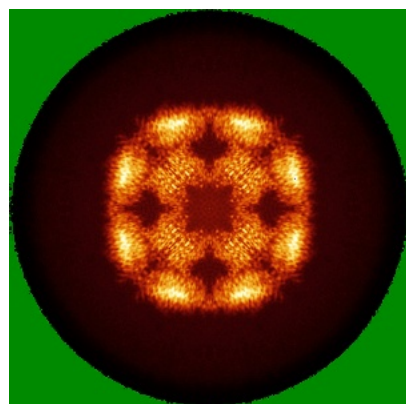


Z Index: 318

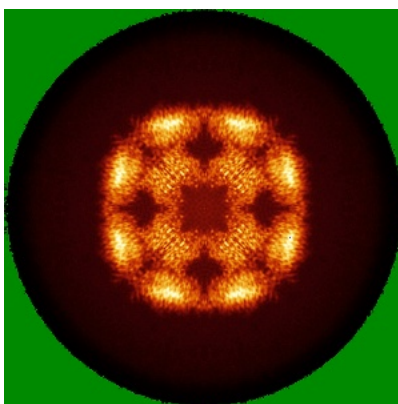
The images above show the largest variance slices of the map in three orthogonal directions.

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

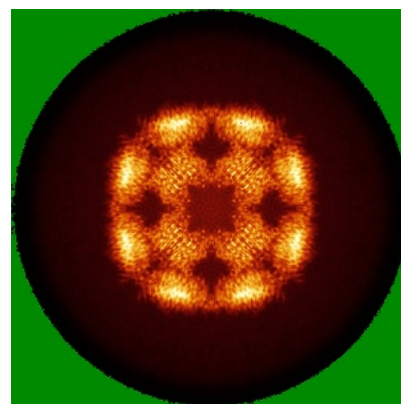
6.4.1 Primary map



X

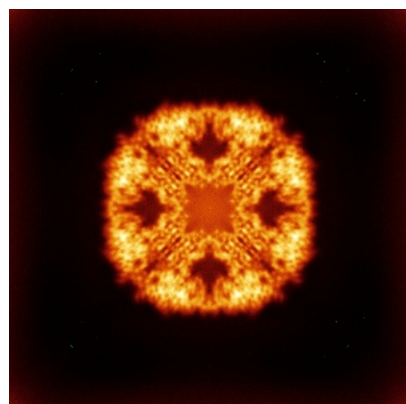


Y

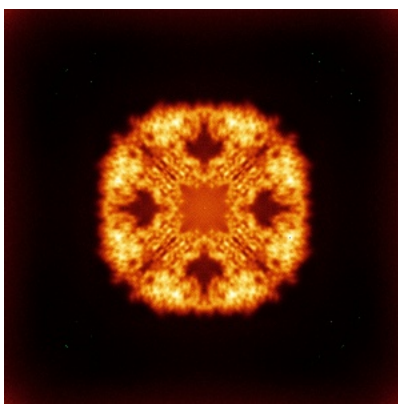


Z

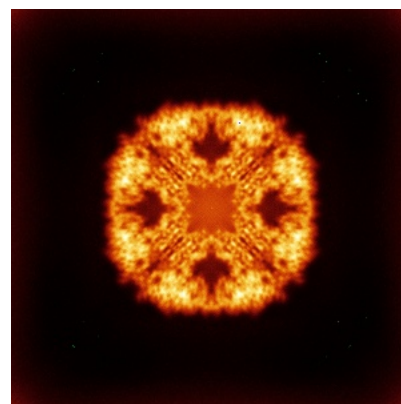
6.4.2 Raw map



X



Y

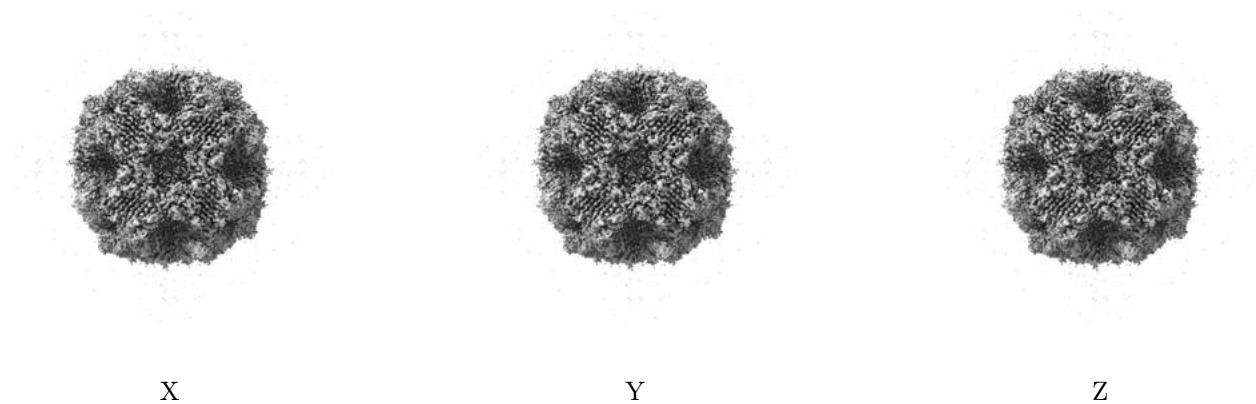


Z

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.

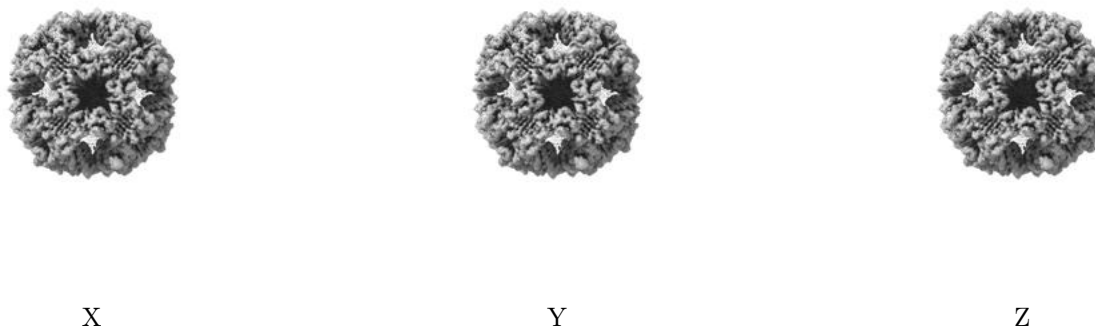
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

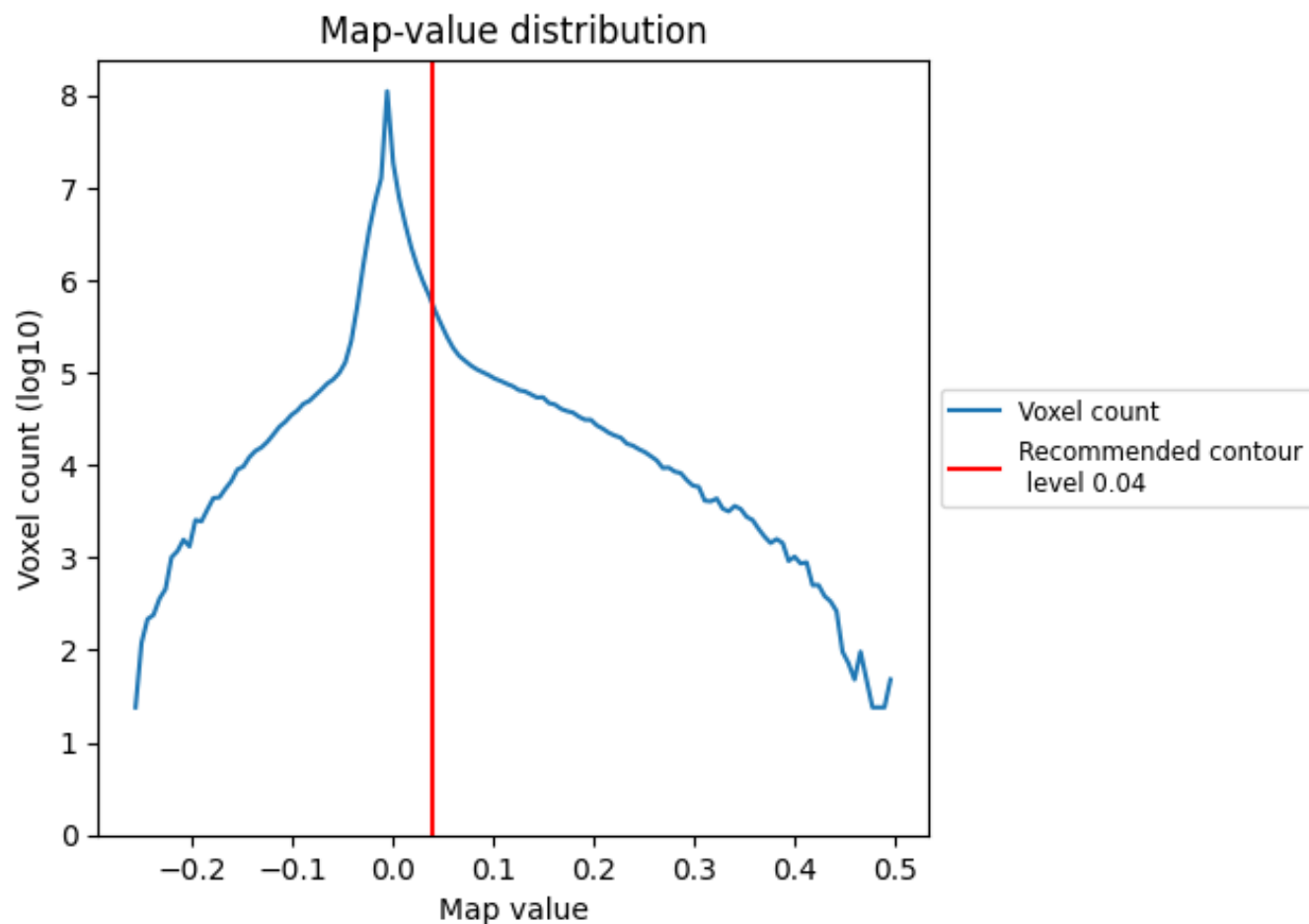
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

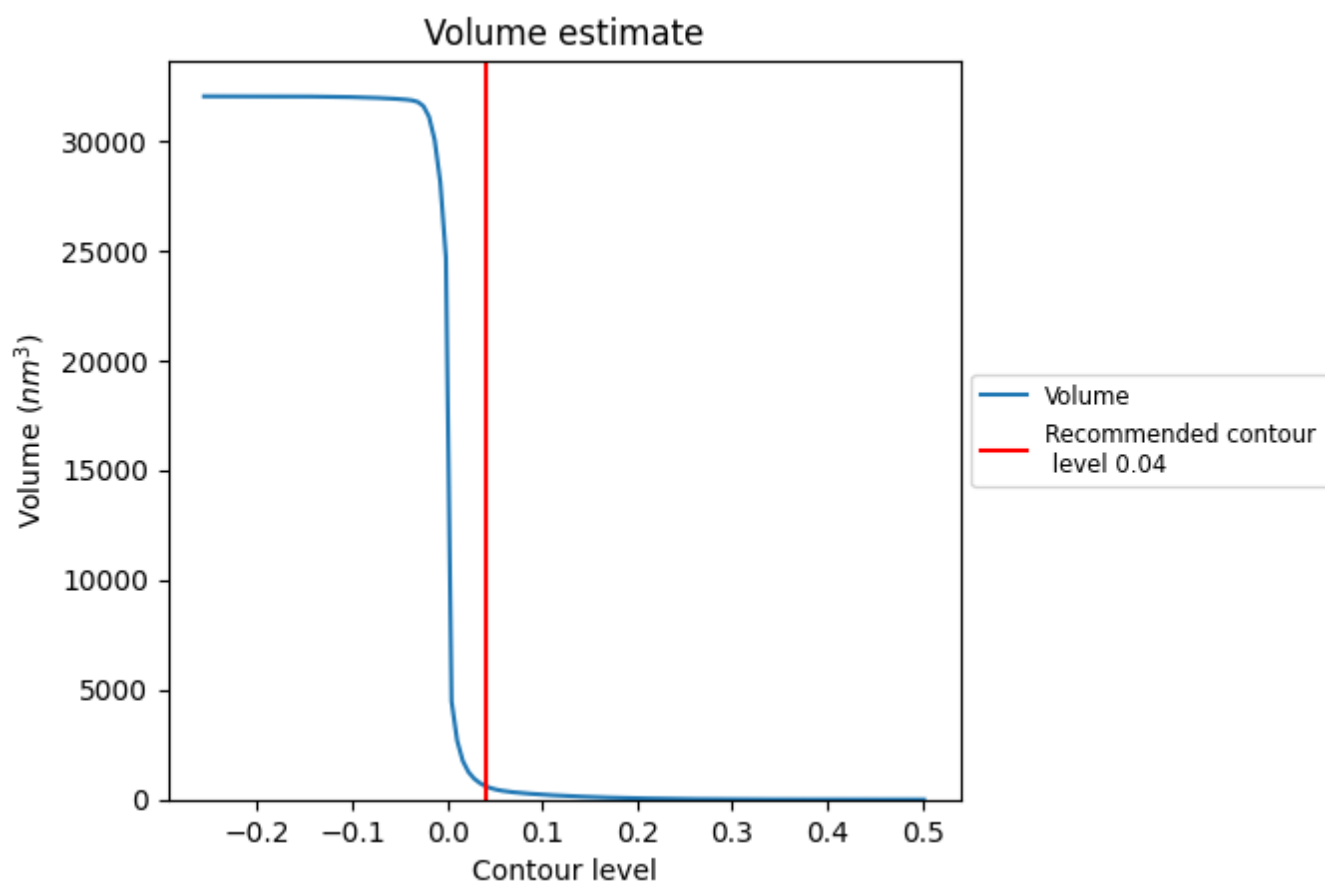
This section contains the results of statistical analysis of the map.

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.

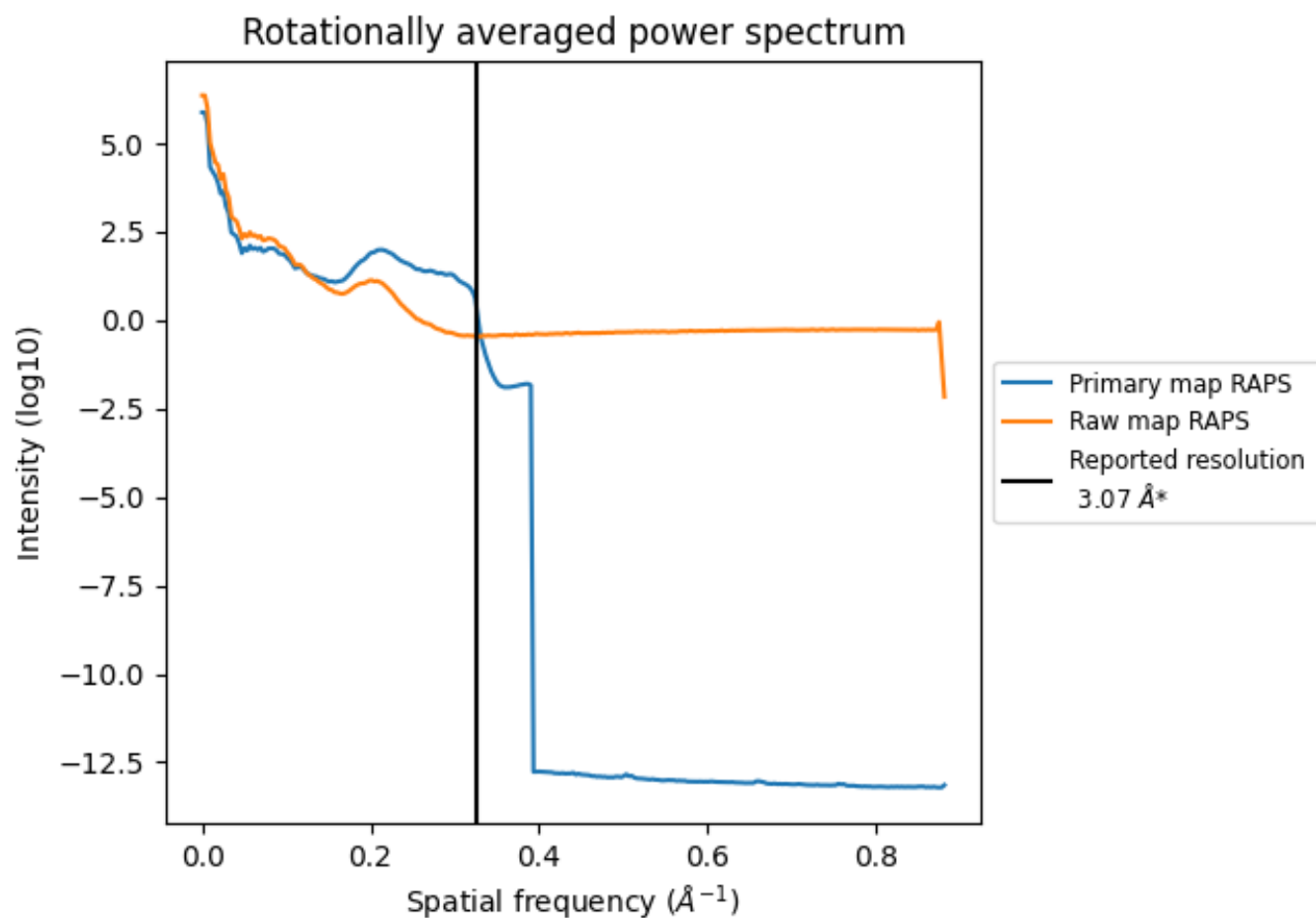
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 618 nm³; this corresponds to an approximate mass of 559 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 ⓘ

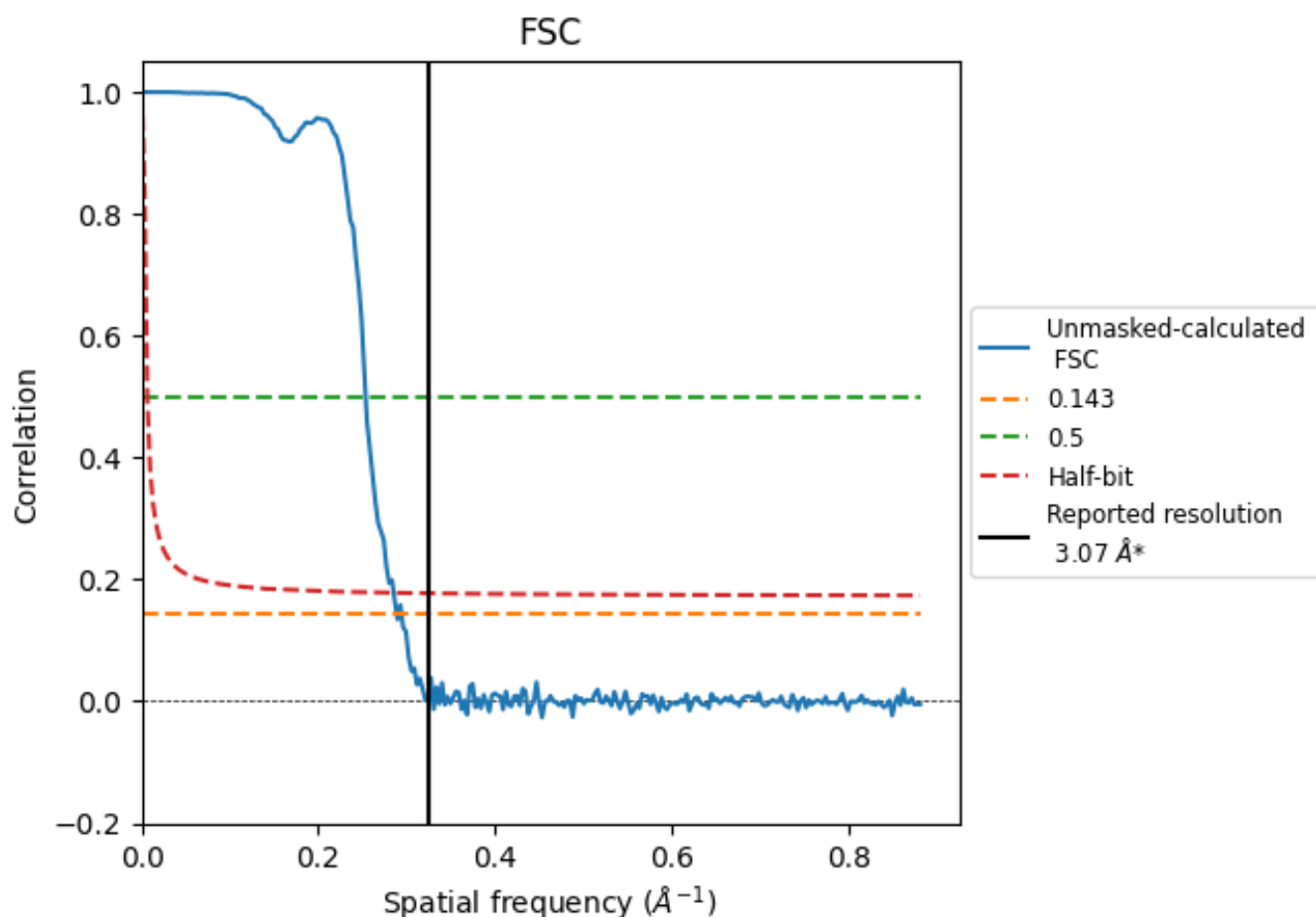


*Reported resolution corresponds to spatial frequency of 0.326 Å⁻¹

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 $0.326 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

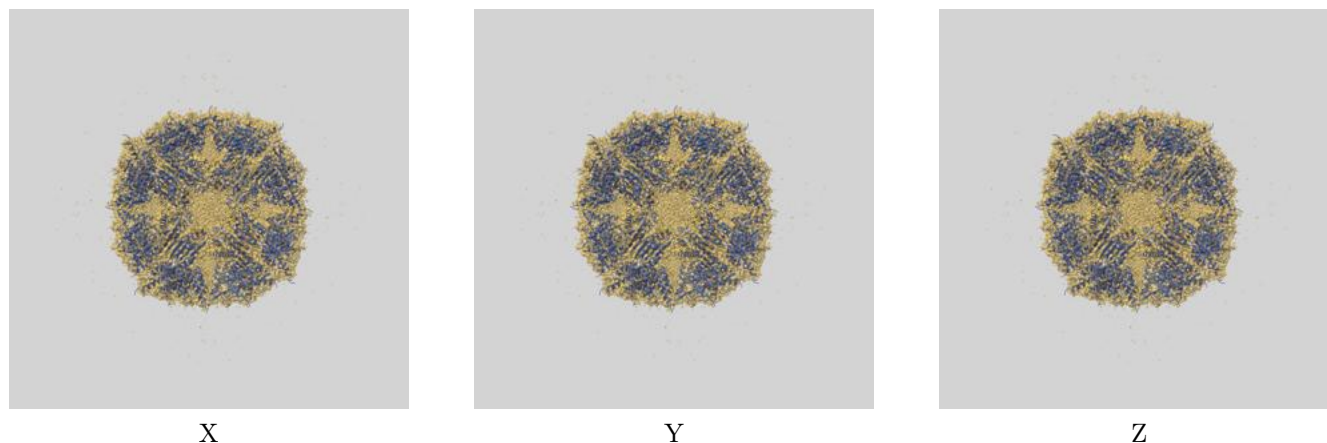
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.46	3.94	3.51

*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 3.46 differs from the reported value 3.07 by more than 10 %

9 Map-model fit [i](#)

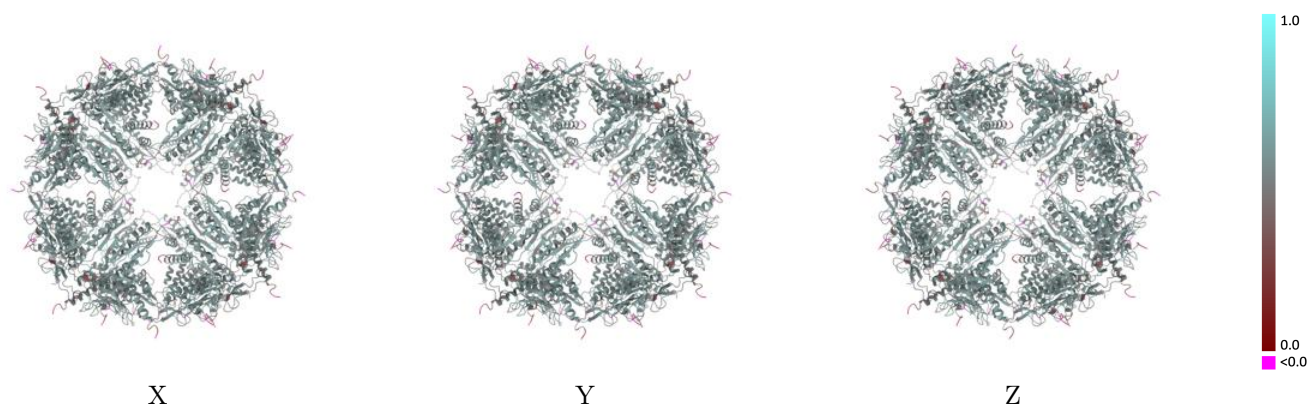
This section contains information regarding the fit between EMDB map EMD-66344 and PDB model 9WXD. Per-residue inclusion information can be found in [section 3](#) on [page 34](#).

9.1 Map-model overlay [i](#)



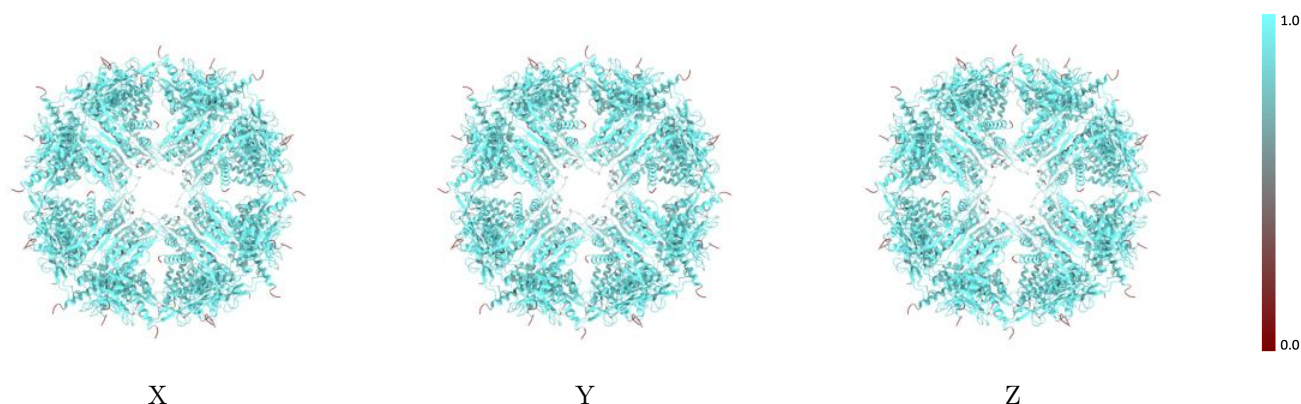
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



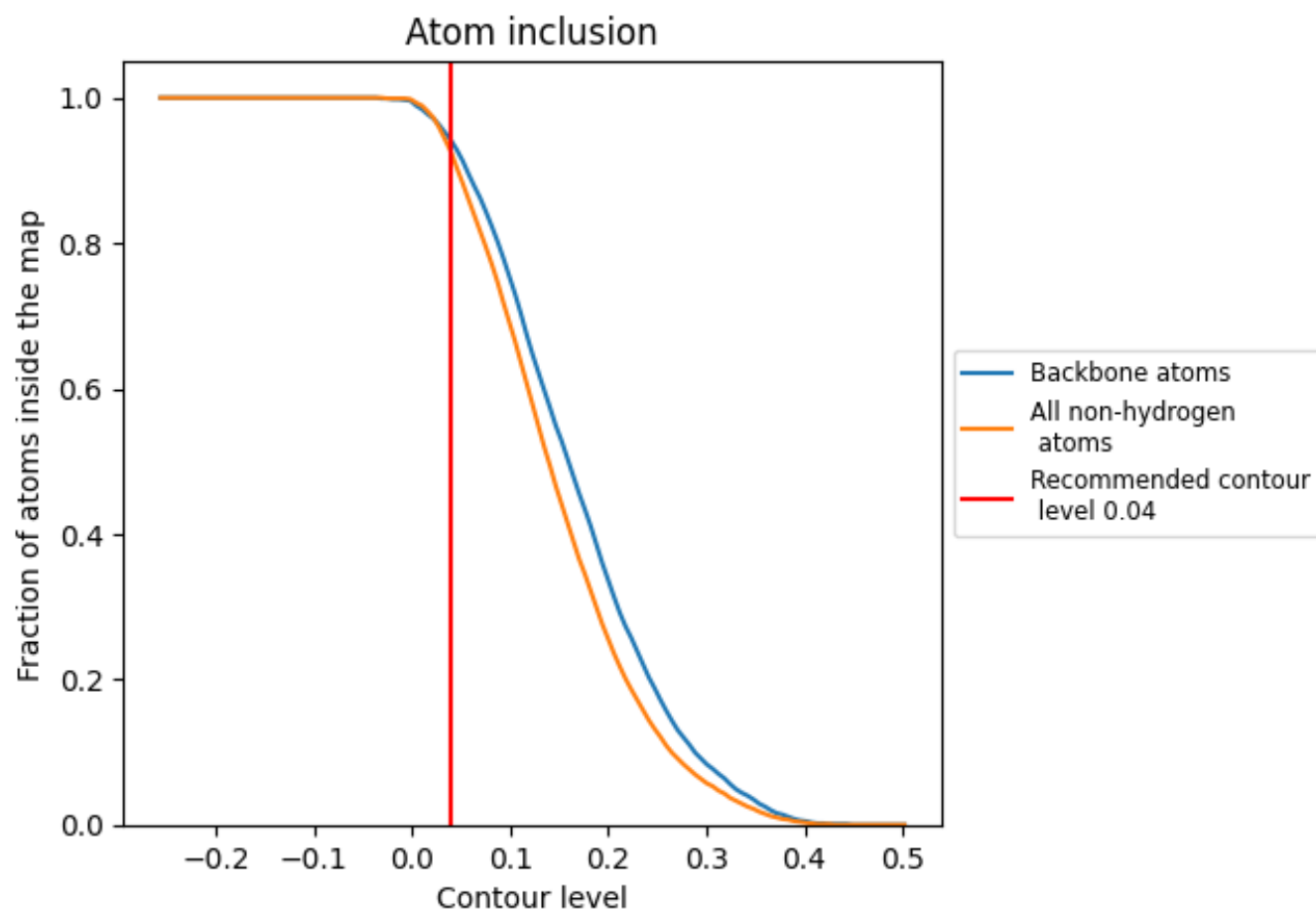
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9250	 0.5260
A	 0.9230	 0.5270
AA	 0.9280	 0.5230
B	 0.9220	 0.5250
BA	 0.9320	 0.5330
C	 0.9310	 0.5240
CA	 0.9170	 0.5270
D	 0.9170	 0.5220
DA	 0.9360	 0.5380
E	 0.9220	 0.5260
EA	 0.9220	 0.5260
F	 0.9220	 0.5240
FA	 0.9290	 0.5280
G	 0.9190	 0.5240
GA	 0.9230	 0.5240
H	 0.9280	 0.5230
HA	 0.9330	 0.5370
I	 0.9260	 0.5210
IA	 0.9160	 0.5280
J	 0.9190	 0.5240
JA	 0.9290	 0.5330
K	 0.9230	 0.5270
KA	 0.9230	 0.5280
L	 0.9250	 0.5240
LA	 0.9330	 0.5330
M	 0.9340	 0.5220
MA	 0.9250	 0.5270
N	 0.9190	 0.5200
NA	 0.9320	 0.5310
O	 0.9220	 0.5300
OA	 0.9190	 0.5260
P	 0.9230	 0.5240
PA	 0.9280	 0.5300
Q	 0.9270	 0.5270
QA	 0.9270	 0.5290



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Chain	Atom inclusion	Q-score
R	 0.9230	 0.5220
RA	 0.9330	 0.5320
S	 0.9230	 0.5280
SA	 0.9240	 0.5260
T	 0.9220	 0.5240
TA	 0.9360	 0.5320
UA	 0.9190	 0.5230
V	 0.9230	 0.5260
VA	 0.9250	 0.5290
W	 0.9230	 0.5200
WA	 0.9270	 0.5240
X	 0.9290	 0.5260
Y	 0.9220	 0.5230
Z	 0.9240	 0.5210