



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 08:34 AM EST

PDB ID : 6WR2
EMDB ID : EMD-21875
Title : ClpP and ClpX IGF loop in ClpX-ClpP complex bound to ssrA tagged GFP
Authors : Fei, X.; Sauer, R.T.
Deposited on : 2020-04-29
Resolution : 2.88 Å(reported)
Based on initial model : 6PPE

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

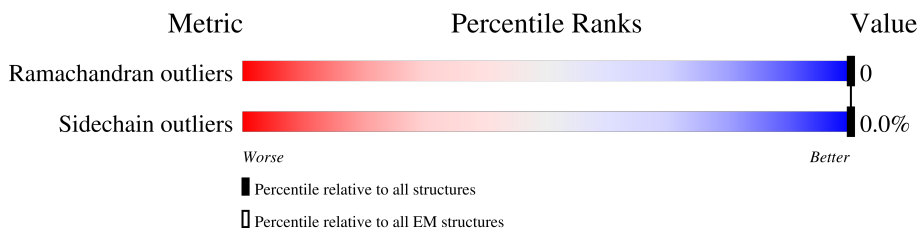
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

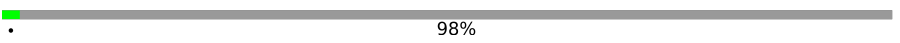
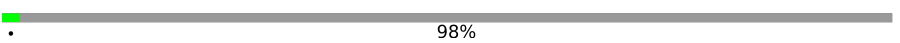
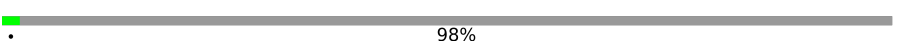
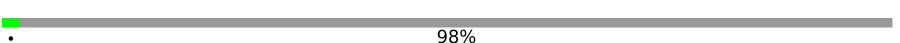

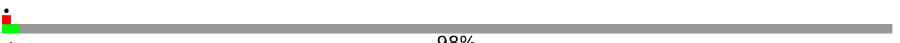



The reported resolution of this entry is 2.88 Å.

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



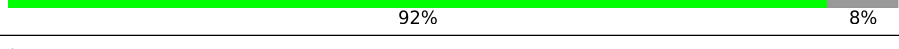
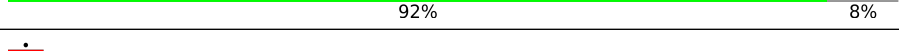
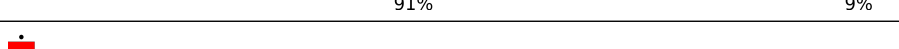
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	388	 98%
1	B	388	 98%
1	C	388	 98%
1	D	388	 98%
1	E	388	 98%
1	F	388	 98%
2	H	207	 92% 7%
2	I	207	 92% 7%
2	J	207	 93% 7%

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Mol	Chain	Length	Quality of chain
2	K	207	 93%7%
2	L	207	 93%7%
2	M	207	 92%7%
2	N	207	 5%95%5%
2	h	207	 91%9%
2	i	207	 92%8%
2	j	207	 91%9%
2	k	207	 92%8%
2	l	207	 92%8%
2	m	207	 91%9%
2	n	207	 92%8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 42671 atoms, of which 21361 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 ATP-dependent Clp protease ATP-binding subunit ClpX.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	9	Total	C	H	N	O	0	0
			106	36	51	9	10		
1	B	9	Total	C	H	N	O	0	0
			106	36	51	9	10		
1	C	9	Total	C	H	N	O	0	0
			106	36	51	9	10		
1	D	9	Total	C	H	N	O	0	0
			106	36	51	9	10		
1	E	9	Total	C	H	N	O	0	0
			106	36	51	9	10		
1	F	9	Total	C	H	N	O	0	0
			106	36	51	9	10		

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	initiating methionine	UNP P0A6H1
A	38	GLY	-	expression tag	UNP P0A6H1
A	39	SER	-	expression tag	UNP P0A6H1
A	40	SER	-	expression tag	UNP P0A6H1
A	41	HIS	-	expression tag	UNP P0A6H1
A	42	HIS	-	expression tag	UNP P0A6H1
A	43	HIS	-	expression tag	UNP P0A6H1
A	44	HIS	-	expression tag	UNP P0A6H1
A	45	HIS	-	expression tag	UNP P0A6H1
A	46	HIS	-	expression tag	UNP P0A6H1
A	47	ASP	-	expression tag	UNP P0A6H1
A	48	TYR	-	expression tag	UNP P0A6H1
A	49	ASP	-	expression tag	UNP P0A6H1
A	50	ILE	-	expression tag	UNP P0A6H1
A	51	PRO	-	expression tag	UNP P0A6H1
A	52	THR	-	expression tag	UNP P0A6H1
A	53	THR	-	expression tag	UNP P0A6H1
A	54	GLU	-	expression tag	UNP P0A6H1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ASN	-	expression tag	UNP P0A6H1
A	56	LEU	-	expression tag	UNP P0A6H1
A	57	TYR	-	expression tag	UNP P0A6H1
A	58	PHE	-	expression tag	UNP P0A6H1
A	59	GLN	-	expression tag	UNP P0A6H1
A	60	GLY	-	expression tag	UNP P0A6H1
A	61	SER	-	expression tag	UNP P0A6H1
A	169	SER	CYS	conflict	UNP P0A6H1
A	408	GLU	LYS	conflict	UNP P0A6H1
B	37	MET	-	initiating methionine	UNP P0A6H1
B	38	GLY	-	expression tag	UNP P0A6H1
B	39	SER	-	expression tag	UNP P0A6H1
B	40	SER	-	expression tag	UNP P0A6H1
B	41	HIS	-	expression tag	UNP P0A6H1
B	42	HIS	-	expression tag	UNP P0A6H1
B	43	HIS	-	expression tag	UNP P0A6H1
B	44	HIS	-	expression tag	UNP P0A6H1
B	45	HIS	-	expression tag	UNP P0A6H1
B	46	HIS	-	expression tag	UNP P0A6H1
B	47	ASP	-	expression tag	UNP P0A6H1
B	48	TYR	-	expression tag	UNP P0A6H1
B	49	ASP	-	expression tag	UNP P0A6H1
B	50	ILE	-	expression tag	UNP P0A6H1
B	51	PRO	-	expression tag	UNP P0A6H1
B	52	THR	-	expression tag	UNP P0A6H1
B	53	THR	-	expression tag	UNP P0A6H1
B	54	GLU	-	expression tag	UNP P0A6H1
B	55	ASN	-	expression tag	UNP P0A6H1
B	56	LEU	-	expression tag	UNP P0A6H1
B	57	TYR	-	expression tag	UNP P0A6H1
B	58	PHE	-	expression tag	UNP P0A6H1
B	59	GLN	-	expression tag	UNP P0A6H1
B	60	GLY	-	expression tag	UNP P0A6H1
B	61	SER	-	expression tag	UNP P0A6H1
B	169	SER	CYS	conflict	UNP P0A6H1
B	408	GLU	LYS	conflict	UNP P0A6H1
C	37	MET	-	initiating methionine	UNP P0A6H1
C	38	GLY	-	expression tag	UNP P0A6H1
C	39	SER	-	expression tag	UNP P0A6H1
C	40	SER	-	expression tag	UNP P0A6H1
C	41	HIS	-	expression tag	UNP P0A6H1
C	42	HIS	-	expression tag	UNP P0A6H1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	43	HIS	-	expression tag	UNP P0A6H1
C	44	HIS	-	expression tag	UNP P0A6H1
C	45	HIS	-	expression tag	UNP P0A6H1
C	46	HIS	-	expression tag	UNP P0A6H1
C	47	ASP	-	expression tag	UNP P0A6H1
C	48	TYR	-	expression tag	UNP P0A6H1
C	49	ASP	-	expression tag	UNP P0A6H1
C	50	ILE	-	expression tag	UNP P0A6H1
C	51	PRO	-	expression tag	UNP P0A6H1
C	52	THR	-	expression tag	UNP P0A6H1
C	53	THR	-	expression tag	UNP P0A6H1
C	54	GLU	-	expression tag	UNP P0A6H1
C	55	ASN	-	expression tag	UNP P0A6H1
C	56	LEU	-	expression tag	UNP P0A6H1
C	57	TYR	-	expression tag	UNP P0A6H1
C	58	PHE	-	expression tag	UNP P0A6H1
C	59	GLN	-	expression tag	UNP P0A6H1
C	60	GLY	-	expression tag	UNP P0A6H1
C	61	SER	-	expression tag	UNP P0A6H1
C	169	SER	CYS	conflict	UNP P0A6H1
C	408	GLU	LYS	conflict	UNP P0A6H1
D	37	MET	-	initiating methionine	UNP P0A6H1
D	38	GLY	-	expression tag	UNP P0A6H1
D	39	SER	-	expression tag	UNP P0A6H1
D	40	SER	-	expression tag	UNP P0A6H1
D	41	HIS	-	expression tag	UNP P0A6H1
D	42	HIS	-	expression tag	UNP P0A6H1
D	43	HIS	-	expression tag	UNP P0A6H1
D	44	HIS	-	expression tag	UNP P0A6H1
D	45	HIS	-	expression tag	UNP P0A6H1
D	46	HIS	-	expression tag	UNP P0A6H1
D	47	ASP	-	expression tag	UNP P0A6H1
D	48	TYR	-	expression tag	UNP P0A6H1
D	49	ASP	-	expression tag	UNP P0A6H1
D	50	ILE	-	expression tag	UNP P0A6H1
D	51	PRO	-	expression tag	UNP P0A6H1
D	52	THR	-	expression tag	UNP P0A6H1
D	53	THR	-	expression tag	UNP P0A6H1
D	54	GLU	-	expression tag	UNP P0A6H1
D	55	ASN	-	expression tag	UNP P0A6H1
D	56	LEU	-	expression tag	UNP P0A6H1
D	57	TYR	-	expression tag	UNP P0A6H1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	58	PHE	-	expression tag	UNP P0A6H1
D	59	GLN	-	expression tag	UNP P0A6H1
D	60	GLY	-	expression tag	UNP P0A6H1
D	61	SER	-	expression tag	UNP P0A6H1
D	169	SER	CYS	conflict	UNP P0A6H1
D	408	GLU	LYS	conflict	UNP P0A6H1
E	37	MET	-	initiating methionine	UNP P0A6H1
E	38	GLY	-	expression tag	UNP P0A6H1
E	39	SER	-	expression tag	UNP P0A6H1
E	40	SER	-	expression tag	UNP P0A6H1
E	41	HIS	-	expression tag	UNP P0A6H1
E	42	HIS	-	expression tag	UNP P0A6H1
E	43	HIS	-	expression tag	UNP P0A6H1
E	44	HIS	-	expression tag	UNP P0A6H1
E	45	HIS	-	expression tag	UNP P0A6H1
E	46	HIS	-	expression tag	UNP P0A6H1
E	47	ASP	-	expression tag	UNP P0A6H1
E	48	TYR	-	expression tag	UNP P0A6H1
E	49	ASP	-	expression tag	UNP P0A6H1
E	50	ILE	-	expression tag	UNP P0A6H1
E	51	PRO	-	expression tag	UNP P0A6H1
E	52	THR	-	expression tag	UNP P0A6H1
E	53	THR	-	expression tag	UNP P0A6H1
E	54	GLU	-	expression tag	UNP P0A6H1
E	55	ASN	-	expression tag	UNP P0A6H1
E	56	LEU	-	expression tag	UNP P0A6H1
E	57	TYR	-	expression tag	UNP P0A6H1
E	58	PHE	-	expression tag	UNP P0A6H1
E	59	GLN	-	expression tag	UNP P0A6H1
E	60	GLY	-	expression tag	UNP P0A6H1
E	61	SER	-	expression tag	UNP P0A6H1
E	169	SER	CYS	conflict	UNP P0A6H1
E	408	GLU	LYS	conflict	UNP P0A6H1
F	37	MET	-	initiating methionine	UNP P0A6H1
F	38	GLY	-	expression tag	UNP P0A6H1
F	39	SER	-	expression tag	UNP P0A6H1
F	40	SER	-	expression tag	UNP P0A6H1
F	41	HIS	-	expression tag	UNP P0A6H1
F	42	HIS	-	expression tag	UNP P0A6H1
F	43	HIS	-	expression tag	UNP P0A6H1
F	44	HIS	-	expression tag	UNP P0A6H1
F	45	HIS	-	expression tag	UNP P0A6H1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	46	HIS	-	expression tag	UNP P0A6H1
F	47	ASP	-	expression tag	UNP P0A6H1
F	48	TYR	-	expression tag	UNP P0A6H1
F	49	ASP	-	expression tag	UNP P0A6H1
F	50	ILE	-	expression tag	UNP P0A6H1
F	51	PRO	-	expression tag	UNP P0A6H1
F	52	THR	-	expression tag	UNP P0A6H1
F	53	THR	-	expression tag	UNP P0A6H1
F	54	GLU	-	expression tag	UNP P0A6H1
F	55	ASN	-	expression tag	UNP P0A6H1
F	56	LEU	-	expression tag	UNP P0A6H1
F	57	TYR	-	expression tag	UNP P0A6H1
F	58	PHE	-	expression tag	UNP P0A6H1
F	59	GLN	-	expression tag	UNP P0A6H1
F	60	GLY	-	expression tag	UNP P0A6H1
F	61	SER	-	expression tag	UNP P0A6H1
F	169	SER	CYS	conflict	UNP P0A6H1
F	408	GLU	LYS	conflict	UNP P0A6H1

- Molecule 2 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	h	188	Total	C	H	N	O	S	0	0
			2944	931	1470	254	277	12		
2	i	190	Total	C	H	N	O	S	0	0
			2978	938	1491	256	281	12		
2	j	188	Total	C	H	N	O	S	0	0
			2956	931	1482	254	277	12		
2	k	190	Total	C	H	N	O	S	0	0
			2976	938	1489	256	281	12		
2	l	190	Total	C	H	N	O	S	0	0
			2978	938	1491	256	281	12		
2	m	189	Total	C	H	N	O	S	0	0
			2971	936	1488	255	280	12		
2	n	191	Total	C	H	N	O	S	0	0
			3017	955	1512	257	281	12		
2	M	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		
2	N	197	Total	C	H	N	O	S	0	0
			3105	980	1554	267	292	12		
2	H	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	I	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		
2	J	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		
2	K	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		
2	L	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	194	GLU	-	expression tag	UNP P0A6G7
h	195	ASN	-	expression tag	UNP P0A6G7
h	196	LEU	-	expression tag	UNP P0A6G7
h	197	TYR	-	expression tag	UNP P0A6G7
h	198	PHE	-	expression tag	UNP P0A6G7
h	199	GLN	-	expression tag	UNP P0A6G7
h	200	SER	-	expression tag	UNP P0A6G7
h	201	LEU	-	expression tag	UNP P0A6G7
h	202	GLU	-	expression tag	UNP P0A6G7
h	203	HIS	-	expression tag	UNP P0A6G7
h	204	HIS	-	expression tag	UNP P0A6G7
h	205	HIS	-	expression tag	UNP P0A6G7
h	206	HIS	-	expression tag	UNP P0A6G7
h	207	HIS	-	expression tag	UNP P0A6G7
h	208	HIS	-	expression tag	UNP P0A6G7
i	194	GLU	-	expression tag	UNP P0A6G7
i	195	ASN	-	expression tag	UNP P0A6G7
i	196	LEU	-	expression tag	UNP P0A6G7
i	197	TYR	-	expression tag	UNP P0A6G7
i	198	PHE	-	expression tag	UNP P0A6G7
i	199	GLN	-	expression tag	UNP P0A6G7
i	200	SER	-	expression tag	UNP P0A6G7
i	201	LEU	-	expression tag	UNP P0A6G7
i	202	GLU	-	expression tag	UNP P0A6G7
i	203	HIS	-	expression tag	UNP P0A6G7
i	204	HIS	-	expression tag	UNP P0A6G7
i	205	HIS	-	expression tag	UNP P0A6G7
i	206	HIS	-	expression tag	UNP P0A6G7
i	207	HIS	-	expression tag	UNP P0A6G7
i	208	HIS	-	expression tag	UNP P0A6G7
j	194	GLU	-	expression tag	UNP P0A6G7

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Chain	Residue	Modelled	Actual	Comment	Reference
j	195	ASN	-	expression tag	UNP P0A6G7
j	196	LEU	-	expression tag	UNP P0A6G7
j	197	TYR	-	expression tag	UNP P0A6G7
j	198	PHE	-	expression tag	UNP P0A6G7
j	199	GLN	-	expression tag	UNP P0A6G7
j	200	SER	-	expression tag	UNP P0A6G7
j	201	LEU	-	expression tag	UNP P0A6G7
j	202	GLU	-	expression tag	UNP P0A6G7
j	203	HIS	-	expression tag	UNP P0A6G7
j	204	HIS	-	expression tag	UNP P0A6G7
j	205	HIS	-	expression tag	UNP P0A6G7
j	206	HIS	-	expression tag	UNP P0A6G7
j	207	HIS	-	expression tag	UNP P0A6G7
j	208	HIS	-	expression tag	UNP P0A6G7
k	194	GLU	-	expression tag	UNP P0A6G7
k	195	ASN	-	expression tag	UNP P0A6G7
k	196	LEU	-	expression tag	UNP P0A6G7
k	197	TYR	-	expression tag	UNP P0A6G7
k	198	PHE	-	expression tag	UNP P0A6G7
k	199	GLN	-	expression tag	UNP P0A6G7
k	200	SER	-	expression tag	UNP P0A6G7
k	201	LEU	-	expression tag	UNP P0A6G7
k	202	GLU	-	expression tag	UNP P0A6G7
k	203	HIS	-	expression tag	UNP P0A6G7
k	204	HIS	-	expression tag	UNP P0A6G7
k	205	HIS	-	expression tag	UNP P0A6G7
k	206	HIS	-	expression tag	UNP P0A6G7
k	207	HIS	-	expression tag	UNP P0A6G7
k	208	HIS	-	expression tag	UNP P0A6G7
l	194	GLU	-	expression tag	UNP P0A6G7
l	195	ASN	-	expression tag	UNP P0A6G7
l	196	LEU	-	expression tag	UNP P0A6G7
l	197	TYR	-	expression tag	UNP P0A6G7
l	198	PHE	-	expression tag	UNP P0A6G7
l	199	GLN	-	expression tag	UNP P0A6G7
l	200	SER	-	expression tag	UNP P0A6G7
l	201	LEU	-	expression tag	UNP P0A6G7
l	202	GLU	-	expression tag	UNP P0A6G7
l	203	HIS	-	expression tag	UNP P0A6G7
l	204	HIS	-	expression tag	UNP P0A6G7
l	205	HIS	-	expression tag	UNP P0A6G7
l	206	HIS	-	expression tag	UNP P0A6G7

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Chain	Residue	Modelled	Actual	Comment	Reference
l	207	HIS	-	expression tag	UNP P0A6G7
l	208	HIS	-	expression tag	UNP P0A6G7
m	194	GLU	-	expression tag	UNP P0A6G7
m	195	ASN	-	expression tag	UNP P0A6G7
m	196	LEU	-	expression tag	UNP P0A6G7
m	197	TYR	-	expression tag	UNP P0A6G7
m	198	PHE	-	expression tag	UNP P0A6G7
m	199	GLN	-	expression tag	UNP P0A6G7
m	200	SER	-	expression tag	UNP P0A6G7
m	201	LEU	-	expression tag	UNP P0A6G7
m	202	GLU	-	expression tag	UNP P0A6G7
m	203	HIS	-	expression tag	UNP P0A6G7
m	204	HIS	-	expression tag	UNP P0A6G7
m	205	HIS	-	expression tag	UNP P0A6G7
m	206	HIS	-	expression tag	UNP P0A6G7
m	207	HIS	-	expression tag	UNP P0A6G7
m	208	HIS	-	expression tag	UNP P0A6G7
n	194	GLU	-	expression tag	UNP P0A6G7
n	195	ASN	-	expression tag	UNP P0A6G7
n	196	LEU	-	expression tag	UNP P0A6G7
n	197	TYR	-	expression tag	UNP P0A6G7
n	198	PHE	-	expression tag	UNP P0A6G7
n	199	GLN	-	expression tag	UNP P0A6G7
n	200	SER	-	expression tag	UNP P0A6G7
n	201	LEU	-	expression tag	UNP P0A6G7
n	202	GLU	-	expression tag	UNP P0A6G7
n	203	HIS	-	expression tag	UNP P0A6G7
n	204	HIS	-	expression tag	UNP P0A6G7
n	205	HIS	-	expression tag	UNP P0A6G7
n	206	HIS	-	expression tag	UNP P0A6G7
n	207	HIS	-	expression tag	UNP P0A6G7
n	208	HIS	-	expression tag	UNP P0A6G7
M	194	GLU	-	expression tag	UNP P0A6G7
M	195	ASN	-	expression tag	UNP P0A6G7
M	196	LEU	-	expression tag	UNP P0A6G7
M	197	TYR	-	expression tag	UNP P0A6G7
M	198	PHE	-	expression tag	UNP P0A6G7
M	199	GLN	-	expression tag	UNP P0A6G7
M	200	SER	-	expression tag	UNP P0A6G7
M	201	LEU	-	expression tag	UNP P0A6G7
M	202	GLU	-	expression tag	UNP P0A6G7
M	203	HIS	-	expression tag	UNP P0A6G7

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Chain	Residue	Modelled	Actual	Comment	Reference
M	204	HIS	-	expression tag	UNP P0A6G7
M	205	HIS	-	expression tag	UNP P0A6G7
M	206	HIS	-	expression tag	UNP P0A6G7
M	207	HIS	-	expression tag	UNP P0A6G7
M	208	HIS	-	expression tag	UNP P0A6G7
N	194	GLU	-	expression tag	UNP P0A6G7
N	195	ASN	-	expression tag	UNP P0A6G7
N	196	LEU	-	expression tag	UNP P0A6G7
N	197	TYR	-	expression tag	UNP P0A6G7
N	198	PHE	-	expression tag	UNP P0A6G7
N	199	GLN	-	expression tag	UNP P0A6G7
N	200	SER	-	expression tag	UNP P0A6G7
N	201	LEU	-	expression tag	UNP P0A6G7
N	202	GLU	-	expression tag	UNP P0A6G7
N	203	HIS	-	expression tag	UNP P0A6G7
N	204	HIS	-	expression tag	UNP P0A6G7
N	205	HIS	-	expression tag	UNP P0A6G7
N	206	HIS	-	expression tag	UNP P0A6G7
N	207	HIS	-	expression tag	UNP P0A6G7
N	208	HIS	-	expression tag	UNP P0A6G7
H	194	GLU	-	expression tag	UNP P0A6G7
H	195	ASN	-	expression tag	UNP P0A6G7
H	196	LEU	-	expression tag	UNP P0A6G7
H	197	TYR	-	expression tag	UNP P0A6G7
H	198	PHE	-	expression tag	UNP P0A6G7
H	199	GLN	-	expression tag	UNP P0A6G7
H	200	SER	-	expression tag	UNP P0A6G7
H	201	LEU	-	expression tag	UNP P0A6G7
H	202	GLU	-	expression tag	UNP P0A6G7
H	203	HIS	-	expression tag	UNP P0A6G7
H	204	HIS	-	expression tag	UNP P0A6G7
H	205	HIS	-	expression tag	UNP P0A6G7
H	206	HIS	-	expression tag	UNP P0A6G7
H	207	HIS	-	expression tag	UNP P0A6G7
H	208	HIS	-	expression tag	UNP P0A6G7
I	194	GLU	-	expression tag	UNP P0A6G7
I	195	ASN	-	expression tag	UNP P0A6G7
I	196	LEU	-	expression tag	UNP P0A6G7
I	197	TYR	-	expression tag	UNP P0A6G7
I	198	PHE	-	expression tag	UNP P0A6G7
I	199	GLN	-	expression tag	UNP P0A6G7
I	200	SER	-	expression tag	UNP P0A6G7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	201	LEU	-	expression tag	UNP P0A6G7
I	202	GLU	-	expression tag	UNP P0A6G7
I	203	HIS	-	expression tag	UNP P0A6G7
I	204	HIS	-	expression tag	UNP P0A6G7
I	205	HIS	-	expression tag	UNP P0A6G7
I	206	HIS	-	expression tag	UNP P0A6G7
I	207	HIS	-	expression tag	UNP P0A6G7
I	208	HIS	-	expression tag	UNP P0A6G7
J	194	GLU	-	expression tag	UNP P0A6G7
J	195	ASN	-	expression tag	UNP P0A6G7
J	196	LEU	-	expression tag	UNP P0A6G7
J	197	TYR	-	expression tag	UNP P0A6G7
J	198	PHE	-	expression tag	UNP P0A6G7
J	199	GLN	-	expression tag	UNP P0A6G7
J	200	SER	-	expression tag	UNP P0A6G7
J	201	LEU	-	expression tag	UNP P0A6G7
J	202	GLU	-	expression tag	UNP P0A6G7
J	203	HIS	-	expression tag	UNP P0A6G7
J	204	HIS	-	expression tag	UNP P0A6G7
J	205	HIS	-	expression tag	UNP P0A6G7
J	206	HIS	-	expression tag	UNP P0A6G7
J	207	HIS	-	expression tag	UNP P0A6G7
J	208	HIS	-	expression tag	UNP P0A6G7
K	194	GLU	-	expression tag	UNP P0A6G7
K	195	ASN	-	expression tag	UNP P0A6G7
K	196	LEU	-	expression tag	UNP P0A6G7
K	197	TYR	-	expression tag	UNP P0A6G7
K	198	PHE	-	expression tag	UNP P0A6G7
K	199	GLN	-	expression tag	UNP P0A6G7
K	200	SER	-	expression tag	UNP P0A6G7
K	201	LEU	-	expression tag	UNP P0A6G7
K	202	GLU	-	expression tag	UNP P0A6G7
K	203	HIS	-	expression tag	UNP P0A6G7
K	204	HIS	-	expression tag	UNP P0A6G7
K	205	HIS	-	expression tag	UNP P0A6G7
K	206	HIS	-	expression tag	UNP P0A6G7
K	207	HIS	-	expression tag	UNP P0A6G7
K	208	HIS	-	expression tag	UNP P0A6G7
L	194	GLU	-	expression tag	UNP P0A6G7
L	195	ASN	-	expression tag	UNP P0A6G7
L	196	LEU	-	expression tag	UNP P0A6G7
L	197	TYR	-	expression tag	UNP P0A6G7

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Chain	Residue	Modelled	Actual	Comment	Reference
L	198	PHE	-	expression tag	UNP P0A6G7
L	199	GLN	-	expression tag	UNP P0A6G7
L	200	SER	-	expression tag	UNP P0A6G7
L	201	LEU	-	expression tag	UNP P0A6G7
L	202	GLU	-	expression tag	UNP P0A6G7
L	203	HIS	-	expression tag	UNP P0A6G7
L	204	HIS	-	expression tag	UNP P0A6G7
L	205	HIS	-	expression tag	UNP P0A6G7
L	206	HIS	-	expression tag	UNP P0A6G7
L	207	HIS	-	expression tag	UNP P0A6G7
L	208	HIS	-	expression tag	UNP P0A6G7

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	AltConf
3	h	1	Total O 1 1	0
3	i	1	Total O 1 1	0
3	j	1	Total O 1 1	0
3	k	1	Total O 1 1	0
3	l	1	Total O 1 1	0
3	m	1	Total O 1 1	0
3	n	1	Total O 1 1	0
3	M	1	Total O 1 1	0
3	N	1	Total O 1 1	0
3	H	1	Total O 1 1	0
3	I	1	Total O 1 1	0
3	J	1	Total O 1 1	0
3	K	1	Total O 1 1	0
3	L	1	Total O 1 1	0

[illegible]

- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain C: 98%

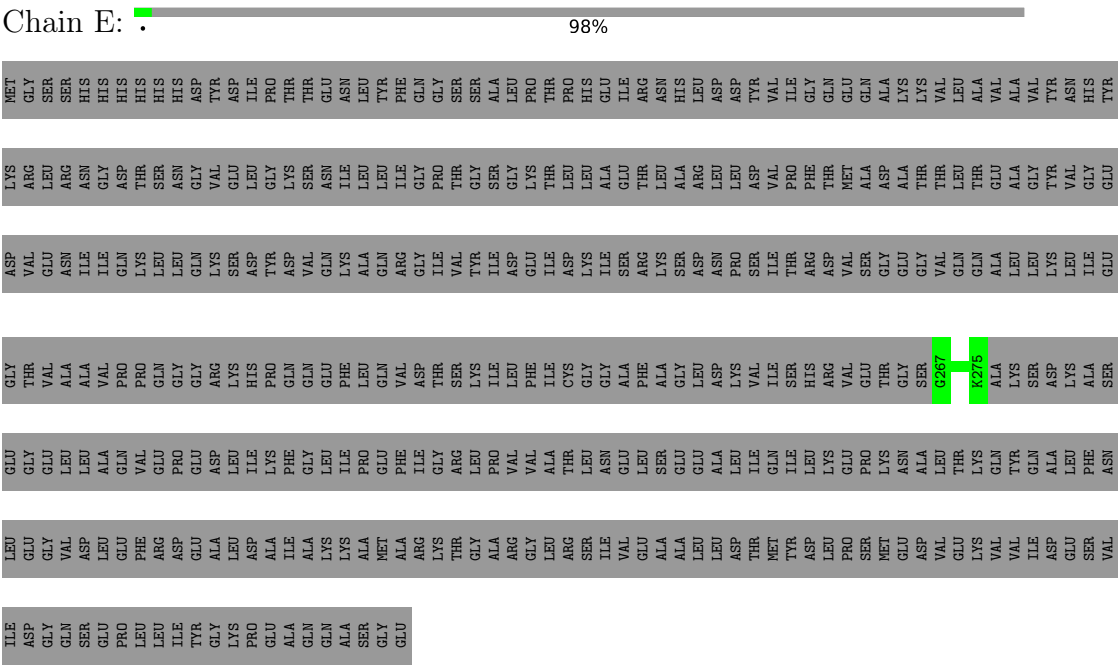
TLE	LEU	GLU	GLY	THR	GLY	ASP	VAL	LYS	GLY	MET
ASP	GLY	GLY	GLU	VAL	VAL	GLU	GLU	ARG	LEU	GLY
GLN	ASP	LEU	LEU	ALA	ASN	ASN	ASN	ARG	ASN	HIS
SER	VAL	LEU	ALA	VAL	ILE	ILE	ILE	GLY	HIS	HIS
GLU	LEU	ALA	GLN	PRO	PRO	PRO	GLN	ASP	HIS	HIS
PRO	PHE	VAL	VAL	THR	GLN	GLN	GLN	THR	ASP	ASP
LEU	ARG	GLU	GLU	GLN	GLN	GLN	GLN	VAL	TYR	TYR
LEU	ASP	PRO	PRO	GLY	GLY	GLY	LEU	ASN	HIS	HIS
ILE	ASP	GLU	GLU	GLY	GLY	GLY	GLN	GLY	ASN	ASN
TYR	GLU	GLU	ASP	ARG	LYS	LYS	LYS	VAL	GLY	GLY
GLY	ALA	LEU	LEU	LYS	LYS	LYS	GLN	GLY	GLY	GLY
LYS	LEU	LEU	ILE	LYS	HIS	LYS	SER	GLU	LEU	ILE
PRO	ASP	ILE	ILE	HIS	PRO	PRO	TYR	ASP	ASP	GLY
GLU	ALA	LYS	PHE	GLN	GLN	GLN	VAL	LYS	GLY	GLY
ALA	ILE	ALA	GLA	GLY	GLY	GLY	VAL	VAL	SER	THR
GLN	LYS	LYS	LEU	GLU	GLU	GLN	GLN	ASN	ASN	ASN
ALA	LYS	ILE	ILE	PHE	PHE	LYS	LYS	ILE	ILE	ASN
ALA	ALA	PRO	PRO	GLU	GLN	ALA	ALA	LEU	LEU	LEU
SER	MET	PHE	PHE	VAL	VAL	ARG	ARG	ILE	ILE	TYR
GLY	ALA	ILE	ILE	ASP	ASP	GLY	GLY	GLY	ILE	PHE
GLU	ARG	GLY	GLY	THR	THR	ILE	ILE	PRO	PRO	GLY
	LYS	GLY	ARG	SER	SER	ILE	VAL	THR	THR	SER
	THR	THR	LEU	GLY	LYS	TYR	VAL	GLY	GLY	SER
	GLY	LEU	LEU	ILE	ILE	ILE	TYR	GLY	LEU	ALA
	ALA	PRO	VAL	LYS	LYS	ASP	ASP	GLY	LEU	ALA
	ARG	VAL	VAL	PHE	PHE	ILE	ILE	GLY	PRO	PRO
	LEU	ALA	ALA	ILE	ILE	ILE	ILE	LYS	THR	THR
	ARG	THR	THR	CYS	ASP	ASP	ASP	LEU	LEU	HIS
	SER	LEU	LEU	GLY	GLY	ILE	ILE	LEU	LEU	LEU
	ILE	ASN	ASN	GLY	ILE	SER	SER	ARG	ASP	ASN
	VAL	GLU	GLU	ALA	ALA	GLU	ARG	THR	LEU	ASN
	GLU	LEU	SER	PHE	ALA	LYS	LYS	LEU	ALA	HIS
	ALA	SER	ALA	GLY	SER	SER	SER	ALA	ASN	ASN
	LEU	GLU	GLU	LEU	LEU	ASN	PRO	LEU	LEU	LEU
	ASP	LEU	ASP	LYS	LYS	PRO	SER	ASP	ASP	ASP
	THR	ILE	THR	VAL	VAL	ILE	ILE	VAL	VAL	THR
	MET	GLN	GLN	ILE	ILE	THR	THR	PRO	PRO	ILE
	TYR	ILE	ILE	SER	HIS	ARG	ARG	THR	GLN	GLY
	ASP	LEU	LYS	HIS	ARG	VAL	VAL	MET	GLN	GLY
	PRO	GLU	GLU	VAL	VAL	GLU	SER	ALA	GLN	GLN
	SER	PRO	LYS	THR	GLY	THR	GLY	ASP	ALA	ALA
	MET	LYS	ASN	GLY	GLY	GLY	GLY	ALA	LYS	LYS
	GLU	ASP	ALA	SER	SER	GLY	VAL	THR	THR	VAL
	VAL	VAL	LEU	GLY	GLY	GLY	GLN	THR	LEU	LEU
	GLY	LYS	LYS	C267	C275	C267	GLN	THR	ALA	ALA
	LYS	LYS	LYS	C275	C275	C275	GLN	THR	GLY	GLY
	VAL	GLN	GLN	ALA	ALA	ALA	ALA	GLU	THR	THR
	VAL	TYR	TYR	LYS	LYS	LEU	LEU	ALA	ALA	ALA
	ILE	GLN	GLN	SER	SER	LEU	LEU	GLY	VAL	VAL
	ASP	ALA	ALA	ASP	ASP	LYS	LYS	TYR	VAL	VAL
	GLU	LEU	LEU	LYS	LYS	ASP	ASP	ASN	ASN	ASN
	SER	PHE	PHE	SER	SER	ILE	ILE	GLY	GLY	GLY
	VAL	ASN	ASN	THR	THR	THR	THR	THR	THR	THR

- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

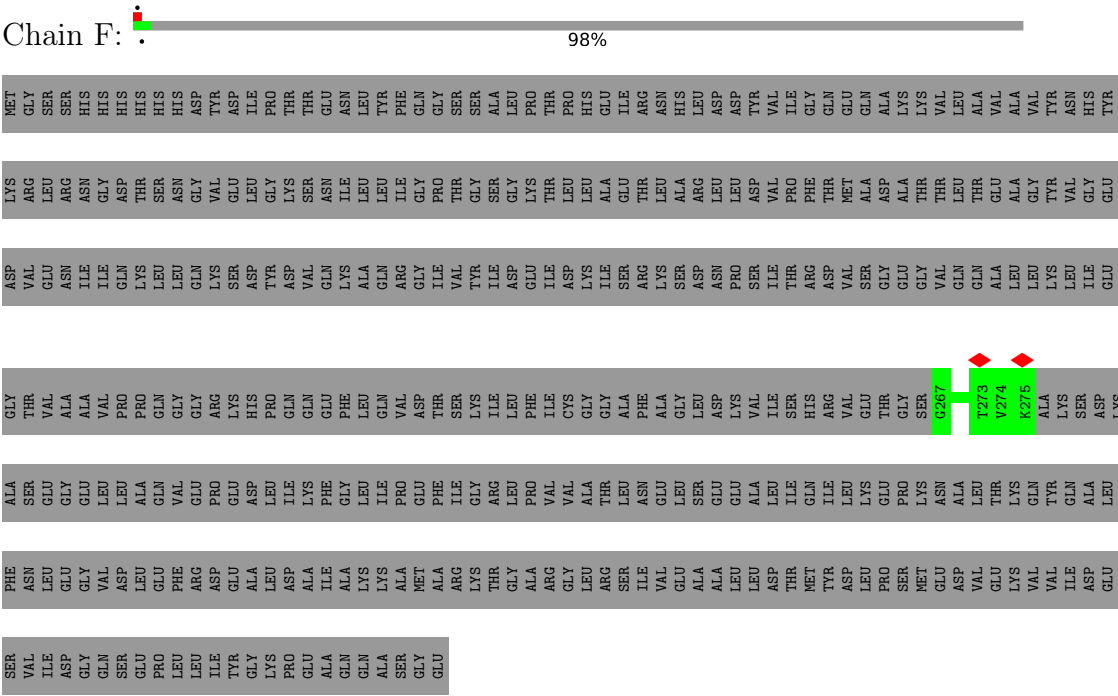
Chain D: 98%

[illegible]

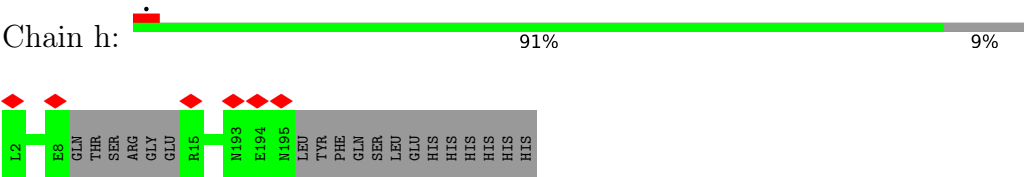
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX



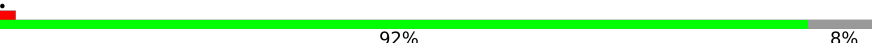
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

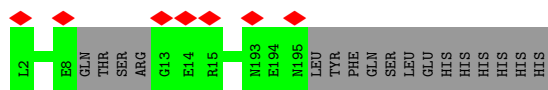


• Molecule 2: ATP-dependent Clp protease proteolytic subunit




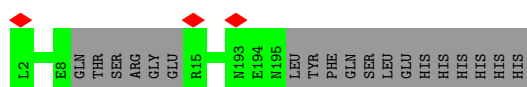
- Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain i:  92% 8%



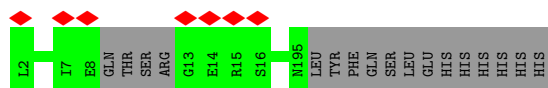
- Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain j:  91% 9%




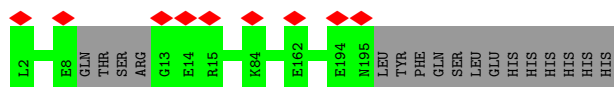
- Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain k:  92% 8%

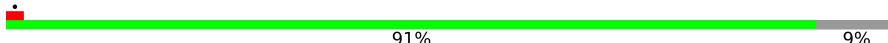


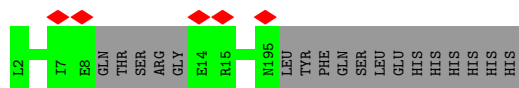
- Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain l:  92% 8%




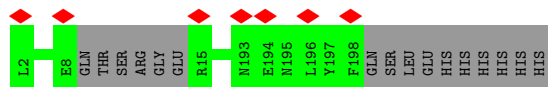
- Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain m:  91% 9%



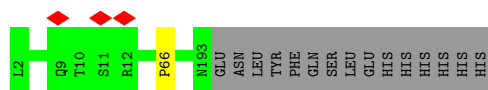
- Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain n:  92% 8%



- Molecule 2: ATP-dependent Clp protease proteolytic subunit

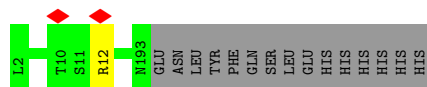
Chain M:  92% 7%



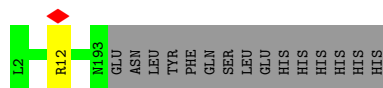
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



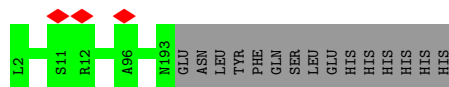
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



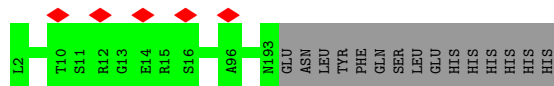
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



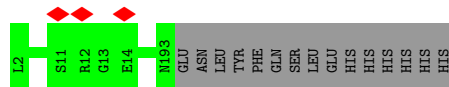
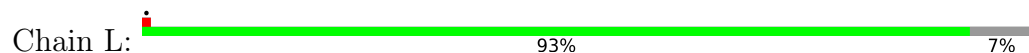
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



- Molecule 2: ATP-dependent Clp protease proteolytic subunit



- Molecule 2: ATP-dependent Clp protease proteolytic subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	334069	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)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	43.423	Depositor
Minimum map value	-28.056	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.07	Depositor
Map size (Å)	348.0, 348.0, 348.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.48	0/55	0.62	0/73
1	B	0.52	0/55	0.63	0/73
1	C	0.51	0/55	0.55	0/73
1	D	0.54	0/55	0.55	0/73
1	E	0.47	0/55	0.62	0/73
1	F	0.44	0/55	0.58	0/73
2	H	0.62	0/1527	0.61	0/2058
2	I	0.62	0/1527	0.60	0/2058
2	J	0.62	0/1527	0.60	0/2058
2	K	0.61	0/1527	0.60	0/2058
2	L	0.61	0/1527	0.59	0/2058
2	M	0.62	0/1527	0.60	0/2058
2	N	0.61	0/1577	0.60	0/2126
2	h	0.58	0/1497	0.59	0/2017
2	i	0.58	0/1510	0.60	0/2034
2	j	0.59	0/1497	0.58	0/2017
2	k	0.58	0/1510	0.60	0/2034
2	l	0.58	0/1510	0.60	0/2034
2	m	0.58	0/1506	0.59	0/2029
2	n	0.58	0/1530	0.60	0/2062
All	All	0.60	0/21629	0.60	0/29139

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	1
2	M	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	12	ARG	Sidechain
2	M	66	PRO	Mainchain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	7/388 (2%)	7 (100%)	0	0	100	100
1	B	7/388 (2%)	7 (100%)	0	0	100	100
1	C	7/388 (2%)	7 (100%)	0	0	100	100
1	D	7/388 (2%)	7 (100%)	0	0	100	100
1	E	7/388 (2%)	7 (100%)	0	0	100	100
1	F	7/388 (2%)	7 (100%)	0	0	100	100
2	H	190/207 (92%)	190 (100%)	0	0	100	100
2	I	190/207 (92%)	190 (100%)	0	0	100	100
2	J	190/207 (92%)	189 (100%)	1 (0%)	0	100	100
2	K	190/207 (92%)	190 (100%)	0	0	100	100
2	L	190/207 (92%)	190 (100%)	0	0	100	100
2	M	190/207 (92%)	189 (100%)	1 (0%)	0	100	100
2	N	195/207 (94%)	195 (100%)	0	0	100	100
2	h	184/207 (89%)	184 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	i	186/207 (90%)	185 (100%)	1 (0%)	0	100	100
2	j	184/207 (89%)	184 (100%)	0	0	100	100
2	k	186/207 (90%)	186 (100%)	0	0	100	100
2	l	186/207 (90%)	186 (100%)	0	0	100	100
2	m	185/207 (89%)	185 (100%)	0	0	100	100
2	n	187/207 (90%)	187 (100%)	0	0	100	100
All	All	2675/5226 (51%)	2672 (100%)	3 (0%)	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	4/322 (1%)	4 (100%)	0	100	100
1	B	4/322 (1%)	4 (100%)	0	100	100
1	C	4/322 (1%)	4 (100%)	0	100	100
1	D	4/322 (1%)	4 (100%)	0	100	100
1	E	4/322 (1%)	4 (100%)	0	100	100
1	F	4/322 (1%)	4 (100%)	0	100	100
2	H	163/178 (92%)	162 (99%)	1 (1%)	86	95
2	I	163/178 (92%)	163 (100%)	0	100	100
2	J	163/178 (92%)	163 (100%)	0	100	100
2	K	163/178 (92%)	163 (100%)	0	100	100
2	L	163/178 (92%)	163 (100%)	0	100	100
2	M	163/178 (92%)	163 (100%)	0	100	100
2	N	168/178 (94%)	168 (100%)	0	100	100
2	h	160/178 (90%)	160 (100%)	0	100	100
2	i	161/178 (90%)	161 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	j	160/178 (90%)	160 (100%)	0	100	100
2	k	161/178 (90%)	161 (100%)	0	100	100
2	l	161/178 (90%)	161 (100%)	0	100	100
2	m	161/178 (90%)	161 (100%)	0	100	100
2	n	163/178 (92%)	163 (100%)	0	100	100
All	All	2297/4424 (52%)	2296 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	12	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	41	ASN
2	L	41	ASN
2	M	41	ASN
2	H	41	ASN
2	I	41	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

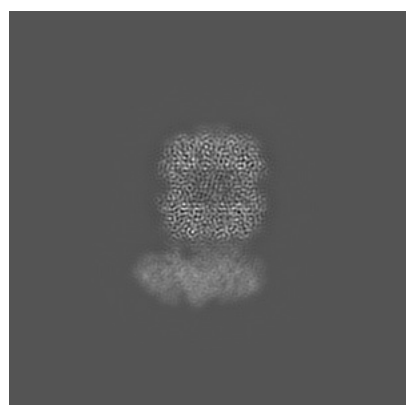
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21875. These allow visual inspection of the internal detail of the map and identification of artifacts.

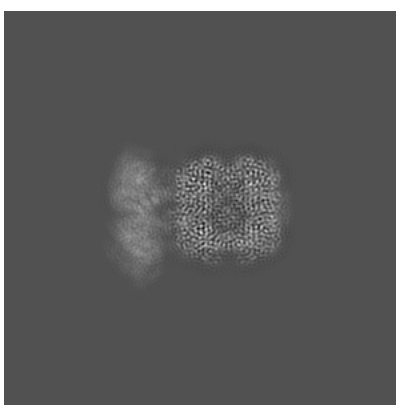
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

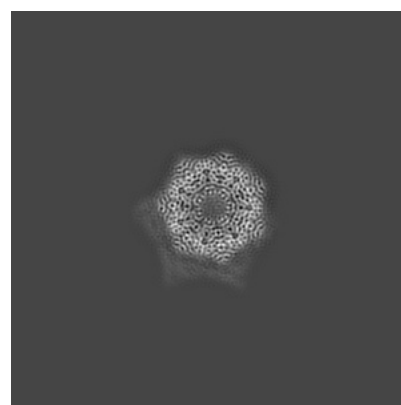
6.1.1 Primary map



X



Y



Z

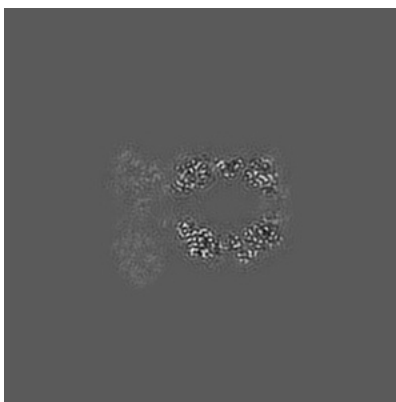
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

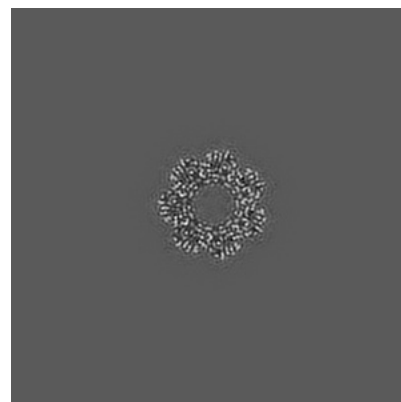
6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

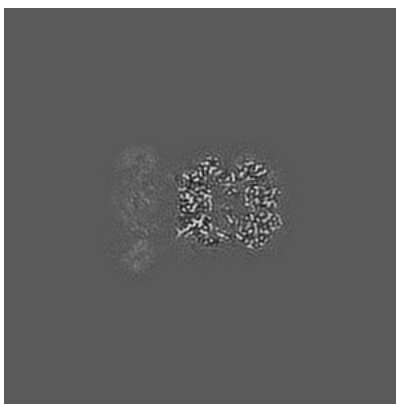
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

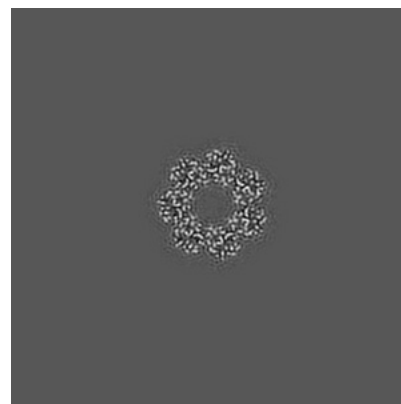
6.3.1 Primary map



X Index: 175



Y Index: 175

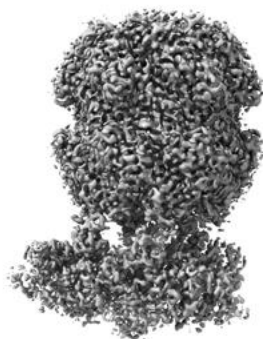


Z Index: 201

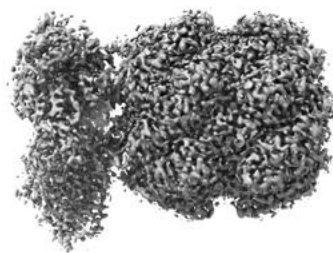
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

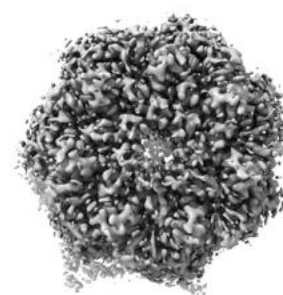
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

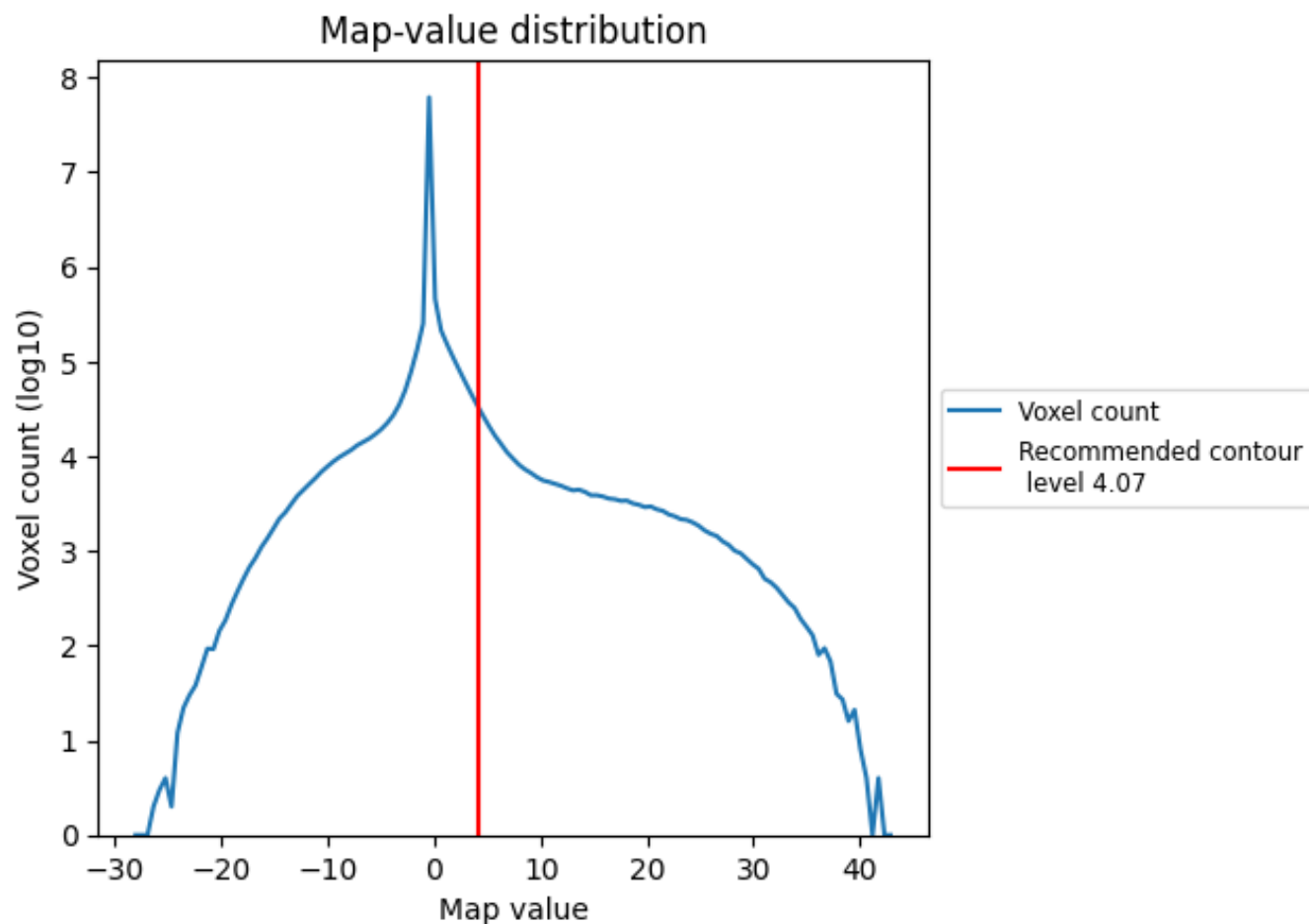
6.5 Mask visualisation

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

7 Map analysis [i](#)

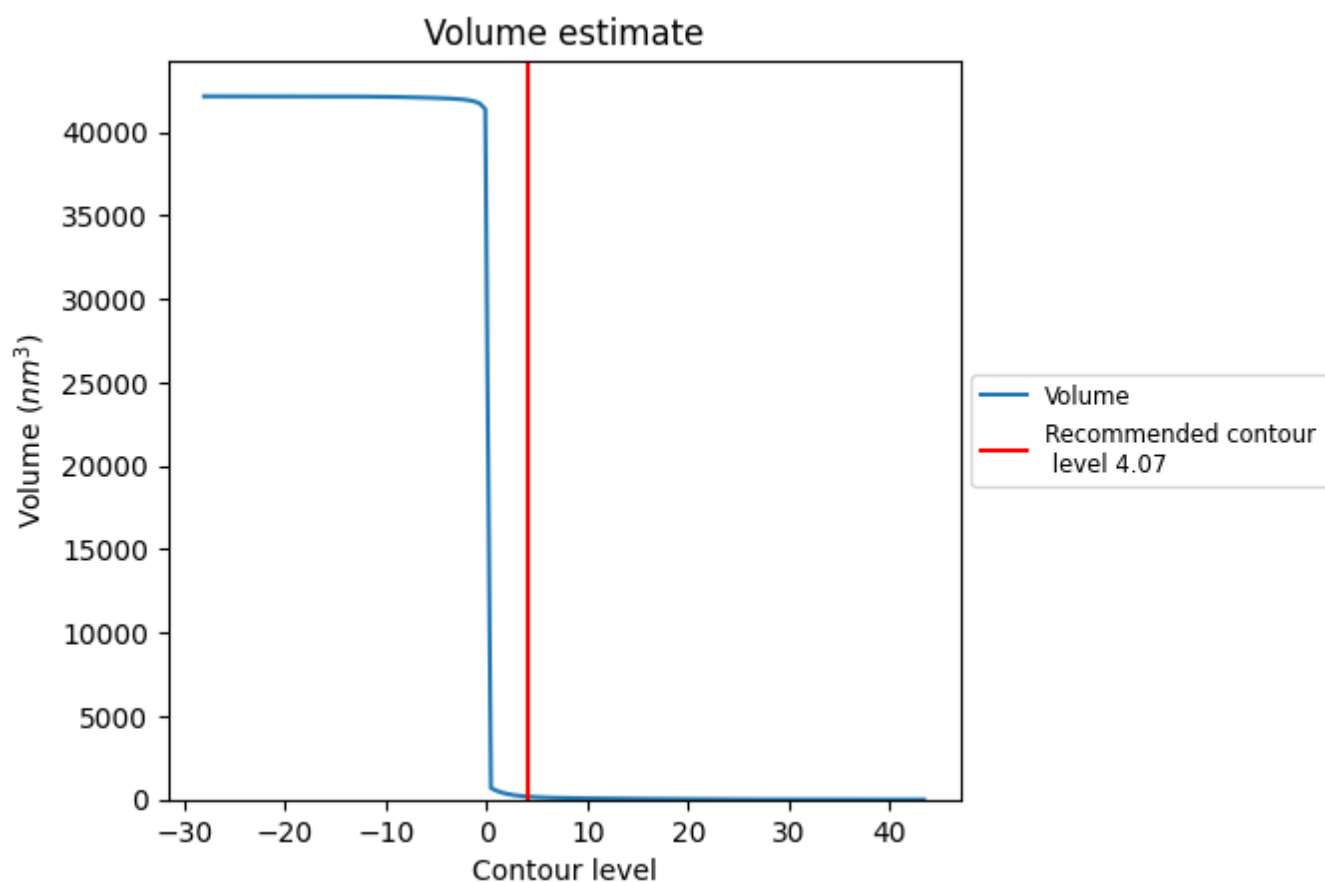
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

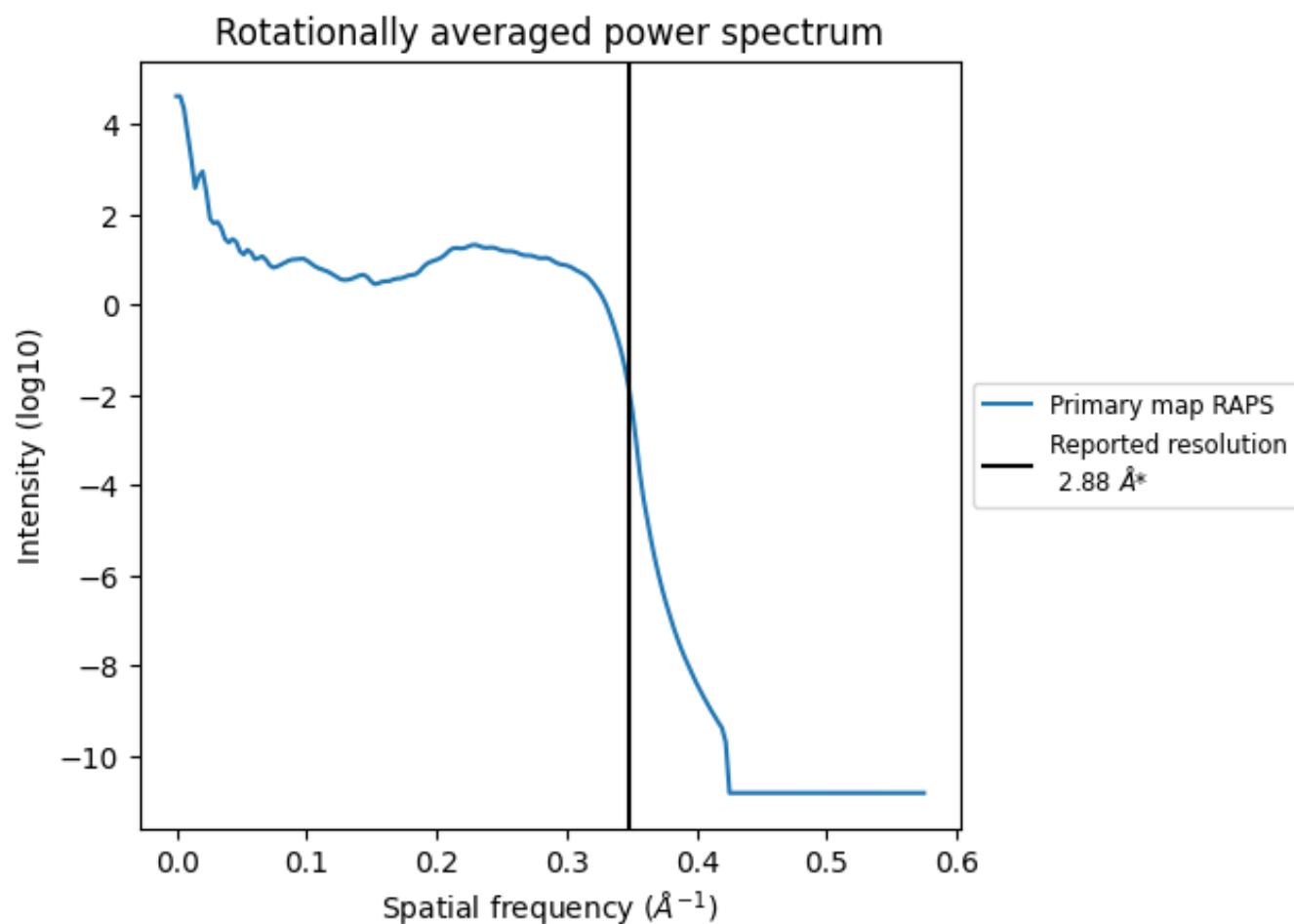
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176 nm^3 ; this corresponds to an approximate mass of 159 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 ⓘ

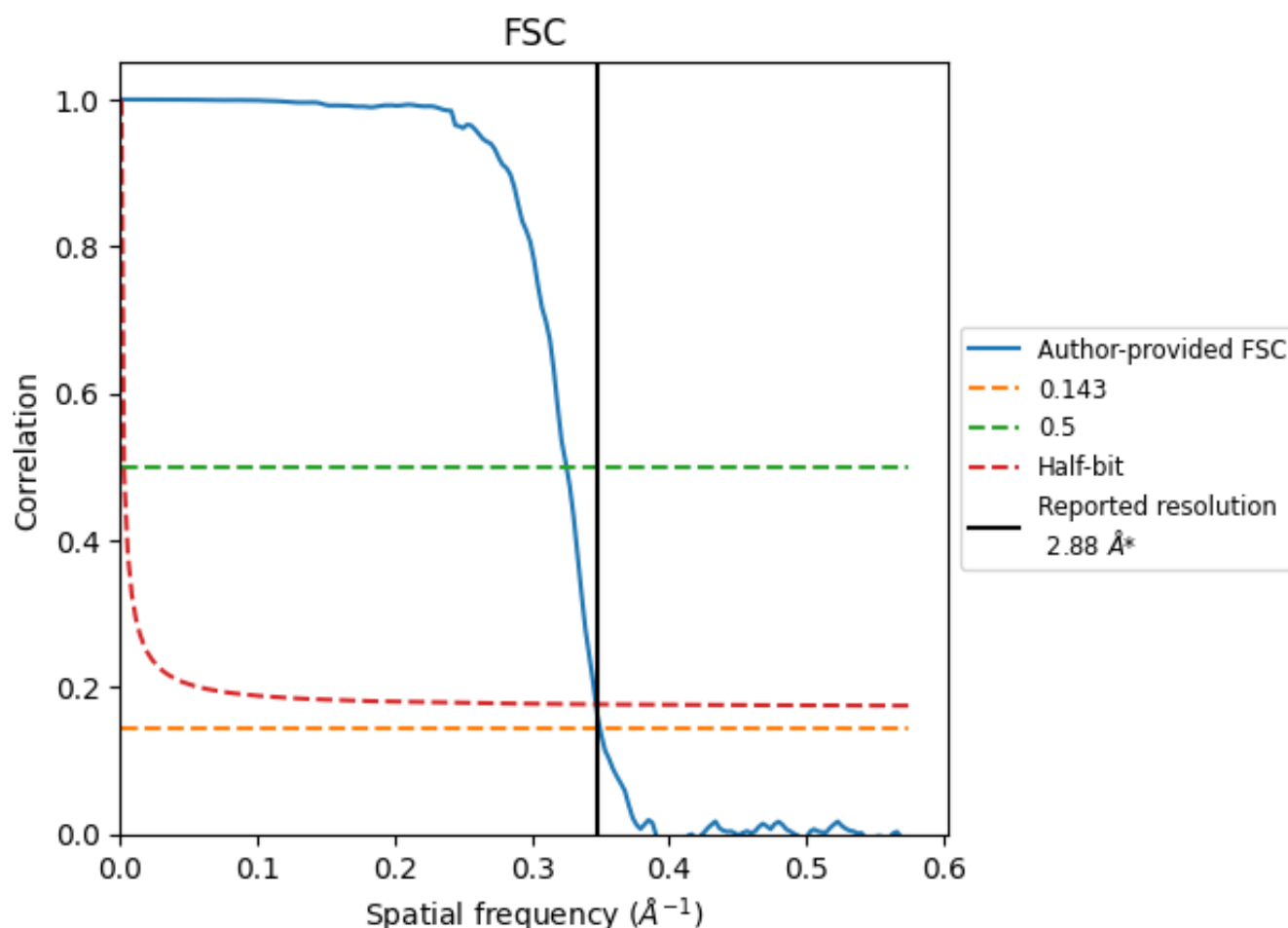


*Reported resolution corresponds to spatial frequency of 0.347 Å⁻¹

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 0.347 Å⁻¹

8.2 Resolution estimates [i](#)

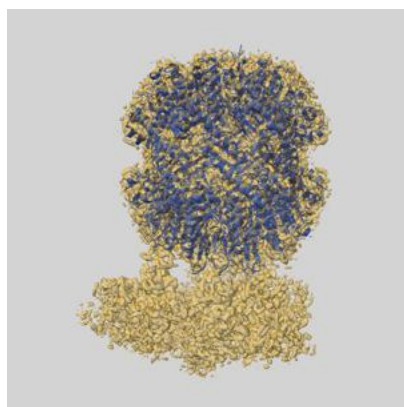
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.86	3.07	2.88
Unmasked-calculated*	-	-	-

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

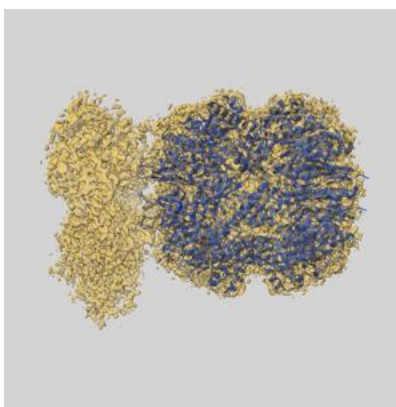
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21875 and PDB model 6WR2. Per-residue inclusion information can be found in section [3](#) on page [15](#).

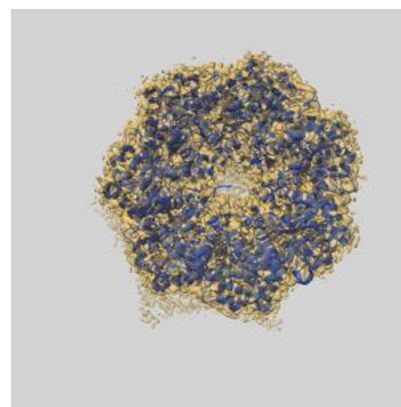
9.1 Map-model overlay [i](#)



X



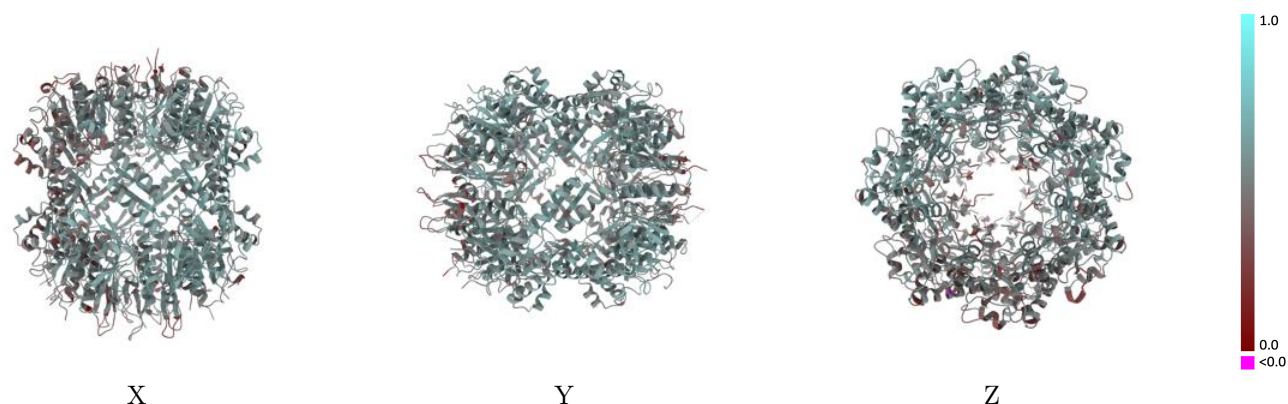
Y



Z

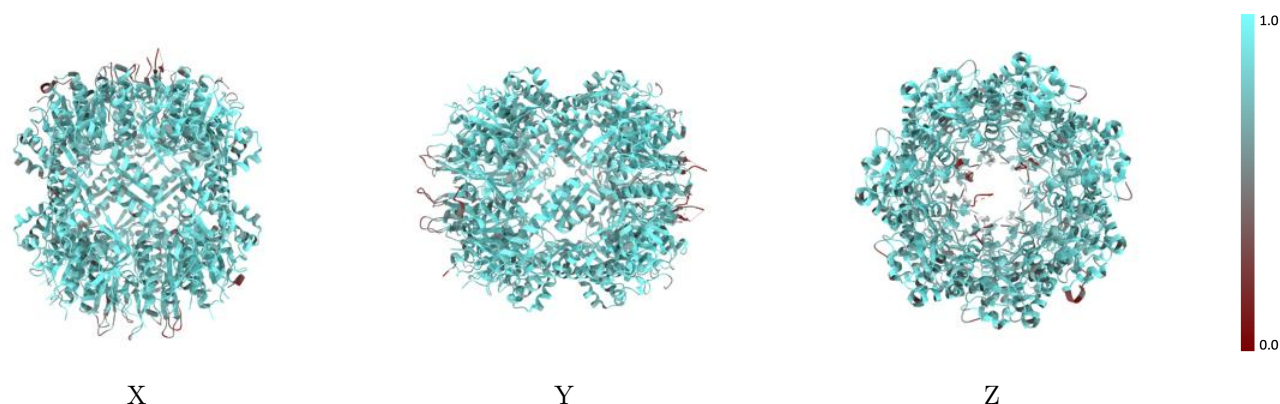
The images above show the 3D surface view of the map at the recommended contour level 4.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



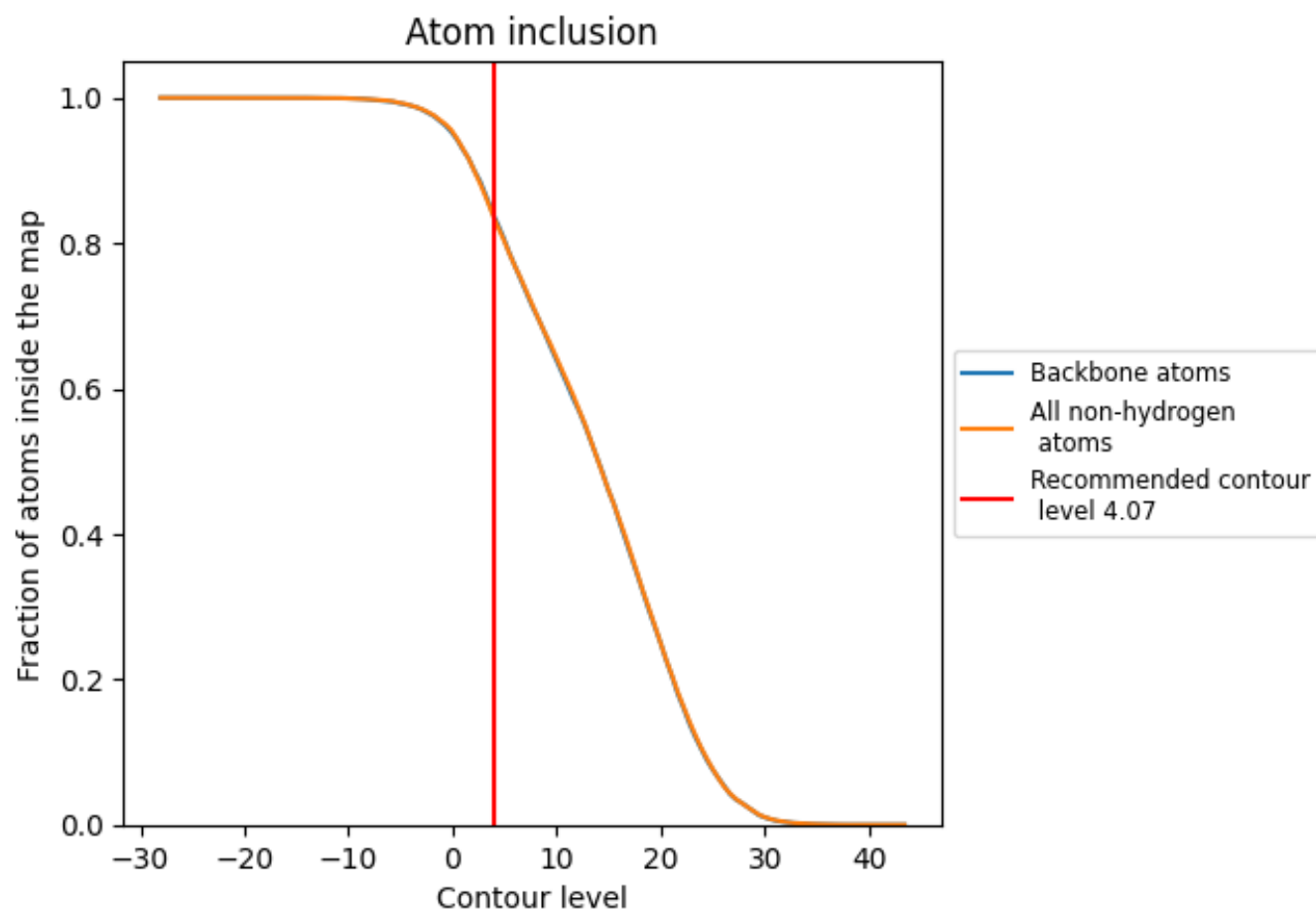
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.07).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (4.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8316	 0.5180
A	 0.8364	 0.4900
B	 0.8909	 0.4930
C	 0.8182	 0.4500
D	 0.7818	 0.3780
E	 0.8000	 0.4290
F	 0.6545	 0.4140
H	 0.8540	 0.5640
I	 0.8635	 0.5380
J	 0.8384	 0.4810
K	 0.8208	 0.4790
L	 0.8486	 0.5340
M	 0.8568	 0.5500
N	 0.8276	 0.5390
h	 0.8527	 0.5330
i	 0.8485	 0.5380
j	 0.8658	 0.5650
k	 0.8417	 0.5320
l	 0.7999	 0.4700
m	 0.7890	 0.4490
n	 0.8157	 0.4960

