



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 11:34 AM UTC

PDB ID : 6WR2 / pdb_00006wr2
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 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.dev132
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) : 2.49

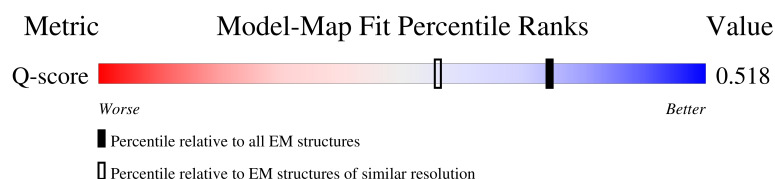
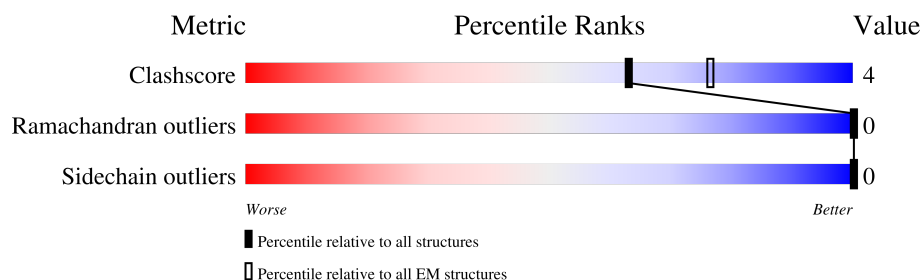
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

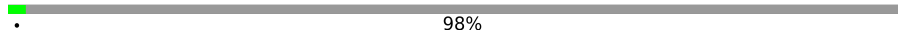
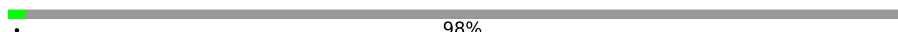
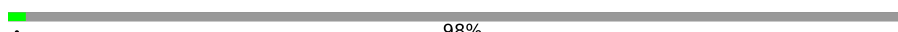
The reported resolution of this entry is 2.88 Å.

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.



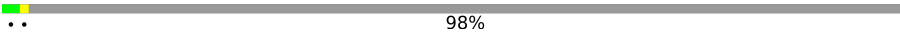
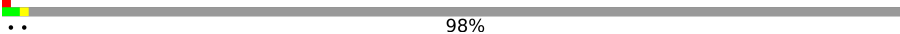
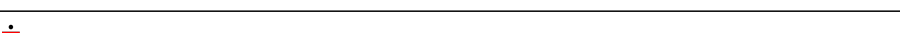
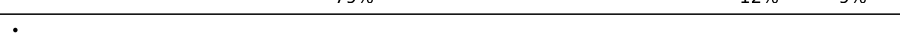
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12111 (2.38 - 3.38)

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%

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Mol	Chain	Length	Quality of chain
1	E	388	 98%
1	F	388	 98%
2	H	207	 83% 10% 7%
2	I	207	 82% 11% 7%
2	J	207	 84% 9% 7%
2	K	207	 87% 5% 7%
2	L	207	 85% 8% 7%
2	M	207	 81% 12% 7%
2	N	207	 5% 86% 9% 5%
2	h	207	 80% 11% 9%
2	i	207	 82% 10% 8%
2	j	207	 84% 7% 9%
2	k	207	 80% 12% 8%
2	l	207	 77% 14% 8%
2	m	207	 79% 12% 9%
2	n	207	 83% 9% 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

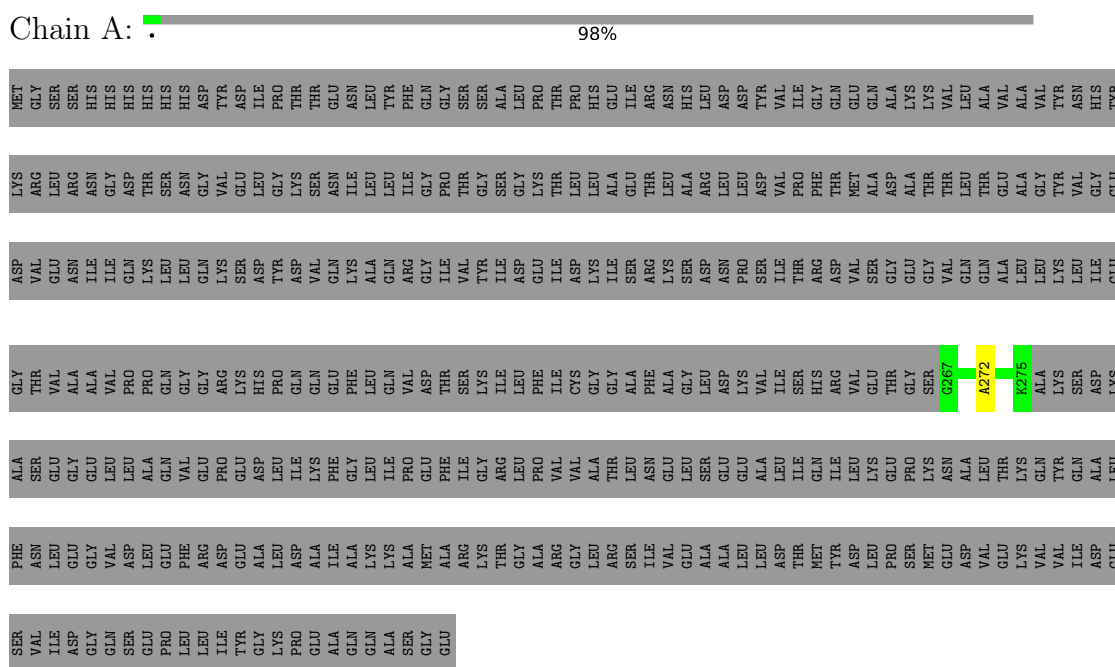
- Molecule 3 is water.

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

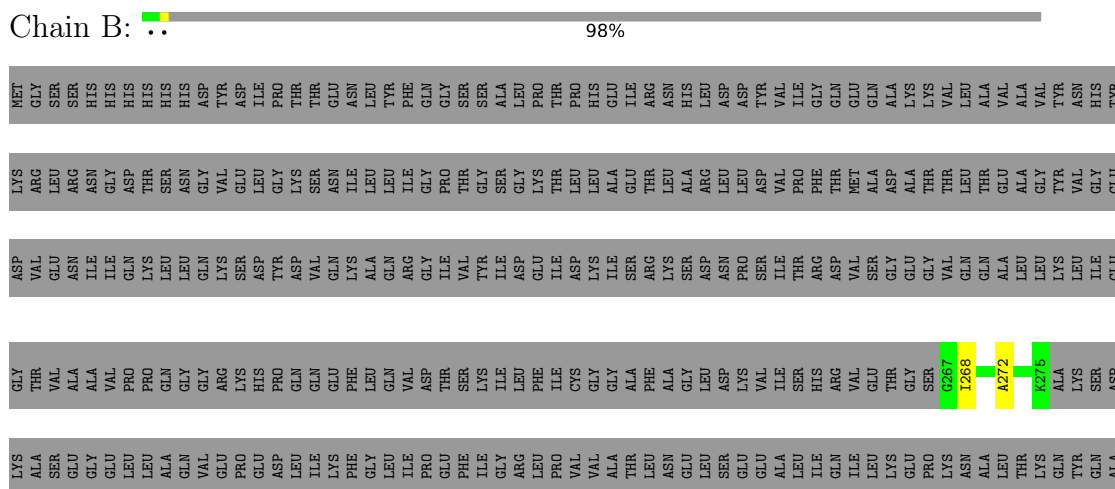
3 Residue-property plots

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: ATP-dependent Clp protease ATP-binding subunit ClpX



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



LEU	PHE	ASN	ASN	LEU	LEU	GLU	GLY	VAL	ASP	ASP	PHE	ARG	ASP	GLU	ALA	ALA	LYS	LYS	LYS	MET	ALA	ARG	LYS	THR	GLY	GLY	ARG	GLY	GLY	ARG	SER	ILE	VAL	GLU	ALA	ALA	ALA	LEU	LEU	TYR	LEU	ASP	THR	THR	TYR	ASP	LEU	PRO	SER	MET	GLY	GLU	VAL	VAL	LYS	GLU	VAL	ILE	ASP
GLU	SER	VAL	ILE	ASP	GLY	GLN	SER	GLU	PRO	LEU	LEU	ILE	THR	GLY	LYS	PRO	GLU	ALA	GLN	GLN	ALA	SER	GLY	GLU	ALA	GLN	GLN	ALA	ALA	ALA	GLY	GLY	GLU	SER	VAL	ASP	GLY	LEU	PRO	THR	THR	TYR	ASP	LEU	PRO	SER	MET	GLY	GLU	VAL	VAL	LYS	GLU	VAL	ILE	ASP			

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

Chain C: 98%

[illegible]

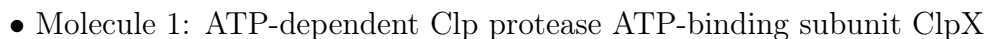
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain D: 98%

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

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

98%



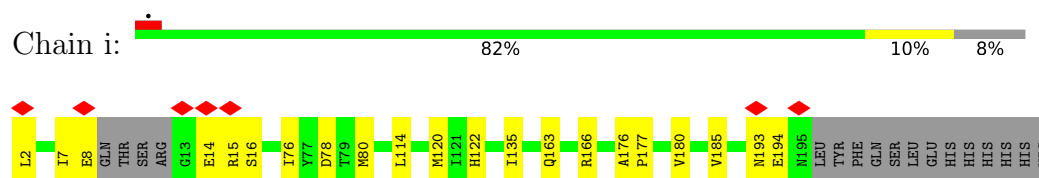
98%



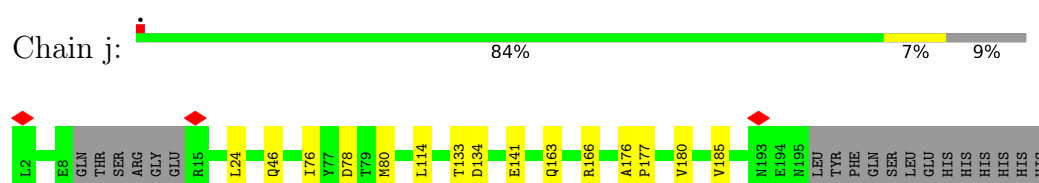
9%



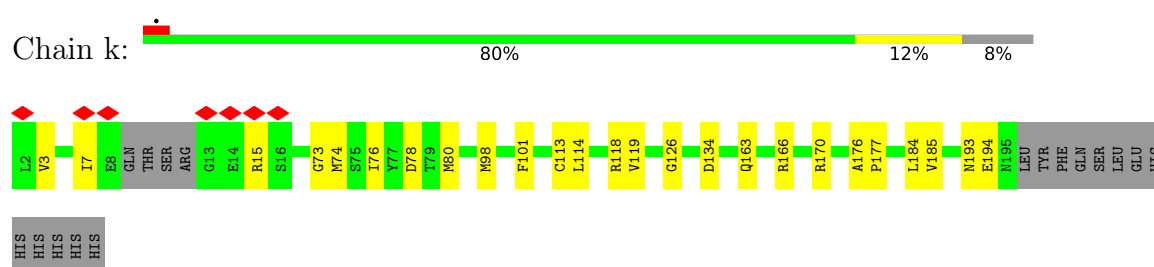
● Molecule 2: ATP-dependent Clp protease proteolytic subunit



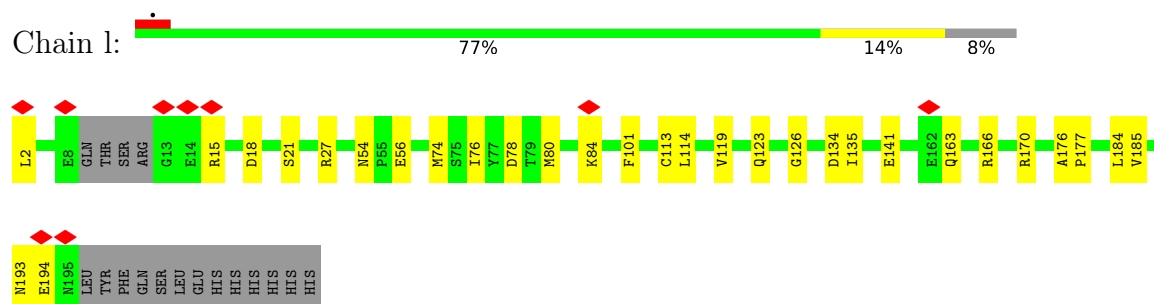
● Molecule 2: ATP-dependent Clp protease proteolytic subunit



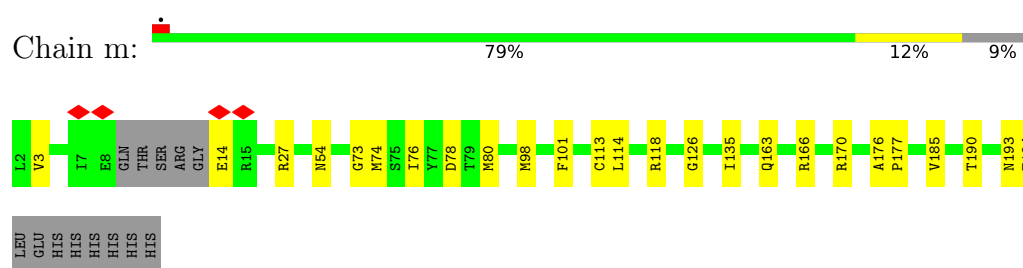
● Molecule 2: ATP-dependent Clp protease proteolytic subunit



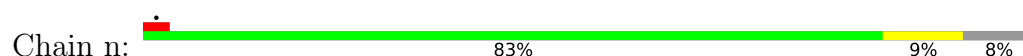
● Molecule 2: ATP-dependent Clp protease proteolytic subunit



● Molecule 2: ATP-dependent Clp protease proteolytic subunit



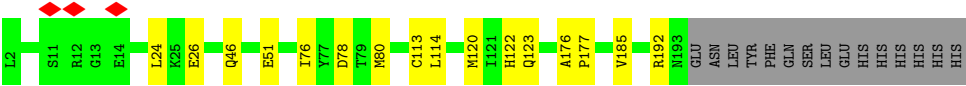
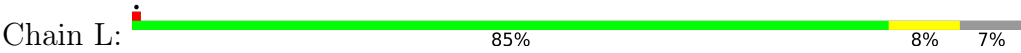
● Molecule 2: ATP-dependent Clp protease proteolytic subunit







- 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	0.36	0/55	0.57	0/73
1	B	0.38	0/55	0.54	0/73
1	C	0.38	0/55	0.49	0/73
1	D	0.38	0/55	0.45	0/73
1	E	0.36	0/55	0.50	0/73
1	F	0.31	0/55	0.44	0/73
2	H	0.59	0/1527	0.50	0/2058
2	I	0.59	0/1527	0.50	0/2058
2	J	0.58	0/1527	0.53	0/2058
2	K	0.58	0/1527	0.51	0/2058
2	L	0.58	0/1527	0.52	0/2058
2	M	0.59	0/1527	0.55	0/2058
2	N	0.58	0/1577	0.52	0/2126
2	h	0.55	0/1497	0.52	0/2017
2	i	0.55	0/1510	0.52	0/2034
2	j	0.56	0/1497	0.49	0/2017
2	k	0.55	0/1510	0.51	0/2034
2	l	0.55	0/1510	0.52	0/2034
2	m	0.55	0/1506	0.52	0/2029
2	n	0.55	0/1530	0.51	0/2062
All	All	0.56	0/21629	0.51	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 ⓘ

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	55	51	51	1	0
1	B	55	51	51	2	0
1	C	55	51	51	1	0
1	D	55	51	51	1	0
1	E	55	51	51	2	0
1	F	55	51	51	2	0
2	H	1503	1513	1513	20	0
2	I	1503	1513	1513	18	0
2	J	1503	1513	1513	15	0
2	K	1503	1513	1513	9	0
2	L	1503	1513	1513	13	0
2	M	1503	1513	1513	21	0
2	N	1551	1554	1554	17	0
2	h	1474	1470	1482	20	0
2	i	1487	1491	1491	18	0
2	j	1474	1482	1482	12	0
2	k	1487	1489	1491	19	0
2	l	1487	1491	1491	23	0
2	m	1483	1488	1488	19	0
2	n	1505	1512	1511	15	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	h	1	0	0	0	0
3	i	1	0	0	1	0
3	j	1	0	0	0	0
3	k	1	0	0	0	0
3	l	1	0	0	0	0
3	m	1	0	0	0	0
3	n	1	0	0	0	0
All	All	21310	21361	21374	179	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 (179) 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)
2:h:113:CYS:HG	2:h:117:SER:HG	1.08	0.89
2:l:141:GLU:OE2	2:m:118:ARG:NH1	2.22	0.72
2:k:134:ASP:OD1	2:l:170:ARG:NH2	2.24	0.70
2:l:15:ARG:NH1	2:m:14:GLU:OE1	2.24	0.70
2:n:119:VAL:HG11	2:n:184:LEU:HD21	1.73	0.70
2:l:163:GLN:OE1	2:l:166:ARG:NH1	2.25	0.69
2:m:78:ASP:HB3	2:n:114:LEU:HD23	1.75	0.68
2:l:78:ASP:HB3	2:m:114:LEU:HD23	1.76	0.67
2:h:120:MET:HE3	2:h:122:HIS:HD2	1.61	0.66
2:L:113:CYS:SG	2:L:185:VAL:HG11	2.36	0.66
2:h:78:ASP:HB3	2:i:114:LEU:HD23	1.79	0.64
2:H:51:GLU:OE2	2:I:192:ARG:NE	2.29	0.64
2:l:119:VAL:HG11	2:l:184:LEU:HD21	1.80	0.63
2:k:78:ASP:HB3	2:l:114:LEU:HD23	1.81	0.63
2:k:126:GLY:O	2:K:135:ILE:HD11	1.98	0.62
2:m:126:GLY:O	2:I:135:ILE:HD11	1.99	0.62
2:h:126:GLY:O	2:N:135:ILE:HD11	1.99	0.62
2:i:135:ILE:HD11	2:M:126:GLY:O	1.99	0.61
2:m:113:CYS:SG	2:m:185:VAL:HG11	2.41	0.61
2:H:119:VAL:HG11	2:H:184:LEU:HD21	1.82	0.61
2:l:126:GLY:O	2:J:135:ILE:HD11	2.00	0.61
2:l:134:ASP:OD1	2:m:170:ARG:NH2	2.34	0.61
2:m:163:GLN:OE1	2:m:166:ARG:NH1	2.34	0.61
2:i:8:GLU:O	2:i:15:ARG:N	2.29	0.61
2:l:135:ILE:HD11	2:J:126:GLY:O	2.01	0.60
2:m:135:ILE:HD11	2:I:126:GLY:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:163:GLN:OE1	2:j:166:ARG:NH1	2.34	0.60
2:H:78:ASP:CB	2:I:114:LEU:HD23	2.32	0.60
2:h:163:GLN:OE1	2:h:166:ARG:NH1	2.35	0.60
2:M:114:LEU:HD23	2:L:78:ASP:HB2	1.84	0.59
2:M:114:LEU:HD23	2:L:78:ASP:CB	2.32	0.59
2:m:3:VAL:HG21	2:n:2:LEU:HD22	1.84	0.59
2:M:10:THR:OG1	2:M:13:GLY:O	2.20	0.58
2:j:134:ASP:OD1	2:k:170:ARG:NH2	2.36	0.58
2:I:51:GLU:OE2	2:J:192:ARG:NE	2.35	0.58
2:k:119:VAL:HG11	2:k:184:LEU:HD21	1.86	0.57
2:N:113:CYS:SG	2:N:185:VAL:HG11	2.44	0.57
2:N:78:ASP:CB	2:H:114:LEU:HD23	2.34	0.56
2:h:3:VAL:HG21	2:i:2:LEU:HD22	1.87	0.56
2:J:113:CYS:SG	2:J:185:VAL:HG21	2.45	0.56
2:M:163:GLN:OE1	2:M:166:ARG:NH1	2.38	0.56
2:h:78:ASP:CB	2:i:114:LEU:HD23	2.35	0.56
1:B:272:ALA:O	2:I:192:ARG:NH1	2.37	0.56
2:l:113:CYS:SG	2:l:185:VAL:HG11	2.46	0.55
2:M:78:ASP:CB	2:N:114:LEU:HD23	2.37	0.55
2:n:8:GLU:O	2:n:15:ARG:N	2.40	0.55
2:k:113:CYS:SG	2:k:185:VAL:HG11	2.47	0.54
2:H:77:TYR:OH	2:H:152:LEU:HD22	2.08	0.54
2:L:76:ILE:HG22	2:L:80:MET:SD	2.47	0.54
2:H:78:ASP:HB3	2:I:114:LEU:HD23	1.90	0.54
2:H:119:VAL:HG11	2:H:184:LEU:CD2	2.38	0.54
2:h:15:ARG:HG3	2:i:14:GLU:OE1	2.08	0.53
2:k:163:GLN:OE1	2:k:166:ARG:NH1	2.41	0.53
2:h:113:CYS:SG	2:h:117:SER:OG	2.37	0.53
2:J:24:LEU:HD13	2:J:46:GLN:OE1	2.08	0.53
2:m:78:ASP:CB	2:n:114:LEU:HD23	2.39	0.53
2:I:76:ILE:HG22	2:I:80:MET:SD	2.49	0.53
2:i:120:MET:HE3	2:i:122:HIS:HD2	1.74	0.52
2:n:73:GLY:HA3	2:n:98:MET:HE2	1.90	0.52
2:N:78:ASP:HB3	2:H:114:LEU:HD23	1.91	0.52
2:I:24:LEU:HD13	2:I:46:GLN:OE1	2.09	0.52
2:M:78:ASP:HB2	2:N:114:LEU:HD23	1.91	0.52
2:i:76:ILE:HG22	2:i:80:MET:SD	2.50	0.52
2:l:119:VAL:HG11	2:l:184:LEU:CD2	2.40	0.51
2:m:73:GLY:HA3	2:m:98:MET:HE2	1.92	0.51
2:h:76:ILE:HG22	2:h:80:MET:SD	2.51	0.50
2:N:120:MET:HE3	2:N:122:HIS:ND1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:113:CYS:SG	2:K:176:ALA:HB1	2.51	0.50
2:i:193:ASN:OD1	2:i:194:GLU:N	2.43	0.50
2:h:8:GLU:O	2:h:15:ARG:HB2	2.11	0.50
2:l:78:ASP:CB	2:m:114:LEU:HD23	2.40	0.50
2:N:76:ILE:HG22	2:N:80:MET:SD	2.51	0.50
2:H:78:ASP:HB2	2:I:114:LEU:HD23	1.93	0.50
2:K:78:ASP:HB2	2:L:114:LEU:HD23	1.94	0.50
2:h:114:LEU:HD23	2:n:78:ASP:CB	2.41	0.50
2:i:163:GLN:OE1	2:i:166:ARG:NH1	2.44	0.50
2:h:176:ALA:HB3	2:h:177:PRO:HD3	1.94	0.50
2:k:78:ASP:CB	2:l:114:LEU:HD23	2.41	0.49
2:l:56:GLU:OE2	2:l:84:LYS:NZ	2.28	0.49
2:m:74:MET:HE1	2:m:101:PHE:CE2	2.48	0.49
2:J:78:ASP:HB2	2:K:114:LEU:HD23	1.92	0.49
2:M:74:MET:HE1	2:M:101:PHE:CE2	2.47	0.49
2:L:24:LEU:HD13	2:L:46:GLN:OE1	2.12	0.49
2:n:7:ILE:HD13	2:n:16:SER:H	1.78	0.49
2:n:176:ALA:HB3	2:n:177:PRO:HD3	1.95	0.49
2:J:76:ILE:HG22	2:J:80:MET:SD	2.53	0.49
1:F:272:ALA:O	2:M:192:ARG:NH1	2.46	0.48
2:m:76:ILE:HG22	2:m:80:MET:SD	2.52	0.48
2:N:10:THR:HG21	2:N:15:ARG:NH2	2.28	0.48
2:L:120:MET:HE3	2:L:122:HIS:HD2	1.78	0.48
2:M:192:ARG:NE	2:L:51:GLU:OE2	2.40	0.48
2:H:113:CYS:SG	2:H:185:VAL:HG21	2.53	0.48
2:N:78:ASP:HB2	2:H:114:LEU:HD23	1.96	0.48
2:M:9:GLN:NE2	2:M:14:GLU:OE2	2.41	0.48
1:E:272:ALA:O	2:L:192:ARG:NH1	2.46	0.48
2:m:190:THR:OG1	2:m:194:GLU:OE1	2.24	0.47
2:m:176:ALA:HB3	2:m:177:PRO:HD3	1.96	0.47
2:M:44:VAL:HG11	2:N:92:MET:HE1	1.97	0.47
2:i:7:ILE:HD13	2:i:16:SER:HA	1.97	0.47
2:j:176:ALA:HB3	2:j:177:PRO:HD3	1.96	0.47
2:J:113:CYS:SG	2:J:176:ALA:HB1	2.55	0.47
2:H:76:ILE:HG22	2:H:80:MET:SD	2.55	0.47
2:k:76:ILE:HG22	2:k:80:MET:SD	2.54	0.47
2:i:78:ASP:CB	2:j:114:LEU:HD23	2.45	0.47
2:j:78:ASP:CB	2:k:114:LEU:HD23	2.45	0.47
2:l:18:ASP:OD1	2:l:21:SER:OG	2.31	0.47
2:n:76:ILE:HG22	2:n:80:MET:SD	2.54	0.47
2:n:74:MET:HE1	2:n:101:PHE:CE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:10:THR:HG21	2:I:15:ARG:NH2	2.30	0.46
2:K:76:ILE:HG22	2:K:80:MET:SD	2.55	0.46
1:E:268:ILE:HD12	2:L:26:GLU:HG3	1.98	0.46
2:K:77:TYR:OH	2:K:152:LEU:HD22	2.14	0.46
2:L:176:ALA:HB3	2:L:177:PRO:HD3	1.96	0.46
2:j:78:ASP:HB3	2:k:114:LEU:HD23	1.97	0.46
2:I:77:TYR:OH	2:I:152:LEU:HD22	2.16	0.46
2:j:24:LEU:HD13	2:j:46:GLN:OE1	2.16	0.46
2:j:76:ILE:HG22	2:j:80:MET:SD	2.56	0.46
2:N:12:ARG:NH1	2:H:9:GLN:OE1	2.48	0.46
2:j:141:GLU:OE2	2:k:118:ARG:NH1	2.49	0.46
2:M:76:ILE:HG22	2:M:80:MET:SD	2.56	0.45
2:M:113:CYS:SG	2:M:185:VAL:HG21	2.56	0.45
2:M:134:ASP:OD1	2:N:170:ARG:NH2	2.49	0.45
2:l:27:ARG:NH1	2:l:54:ASN:O	2.50	0.45
2:i:176:ALA:HB3	2:i:177:PRO:HD3	1.97	0.45
1:D:268:ILE:HD12	2:K:26:GLU:HG3	1.97	0.45
2:i:120:MET:HE3	2:i:122:HIS:CD2	2.51	0.45
2:J:113:CYS:SG	2:J:188:ILE:HG12	2.56	0.45
1:B:268:ILE:HD12	2:I:26:GLU:HG3	1.99	0.45
1:C:268:ILE:HD12	2:J:26:GLU:HG3	1.99	0.45
2:h:74:MET:HE1	2:h:101:PHE:CE2	2.52	0.45
2:M:176:ALA:HB3	2:M:177:PRO:HD3	1.99	0.45
2:H:73:GLY:HA3	2:H:98:MET:HE2	1.98	0.45
2:k:119:VAL:HG11	2:k:184:LEU:CD2	2.46	0.45
2:J:51:GLU:OE1	2:K:192:ARG:NH2	2.50	0.45
2:M:78:ASP:HB3	2:N:114:LEU:HD23	2.00	0.44
2:i:180:VAL:HG22	2:i:185:VAL:HG23	1.99	0.44
2:k:7:ILE:HD12	2:k:15:ARG:O	2.18	0.44
2:h:120:MET:HE3	2:h:122:HIS:CD2	2.48	0.44
2:l:76:ILE:HG22	2:l:80:MET:SD	2.58	0.44
2:M:114:LEU:HD23	2:L:78:ASP:HB3	2.00	0.44
2:N:141:GLU:OE1	2:H:118:ARG:NH2	2.51	0.44
2:h:114:LEU:HD23	2:n:78:ASP:HB3	2.00	0.43
2:j:180:VAL:HG22	2:j:185:VAL:HG23	2.01	0.43
2:h:114:LEU:HD23	2:n:78:ASP:HB2	1.99	0.43
2:N:33:GLY:O	2:N:65:SER:OG	2.36	0.43
1:F:268:ILE:HD12	2:M:26:GLU:HG3	2.00	0.43
2:l:176:ALA:HB3	2:l:177:PRO:HD3	1.99	0.43
2:n:180:VAL:HG22	2:n:185:VAL:HG23	2.01	0.43
2:J:78:ASP:CB	2:K:114:LEU:HD23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:3:VAL:HG21	2:l:2:LEU:HD22	2.01	0.43
1:A:272:ALA:O	2:H:192:ARG:NH1	2.52	0.43
2:H:176:ALA:HB3	2:H:177:PRO:HD3	2.00	0.43
2:H:141:GLU:OE1	2:I:118:ARG:NH1	2.51	0.43
2:k:193:ASN:OD1	2:k:194:GLU:N	2.51	0.42
2:J:10:THR:OG1	2:J:13:GLY:O	2.36	0.42
2:h:15:ARG:HD2	2:i:7:ILE:HD12	2.00	0.42
2:l:123:GLN:NE2	2:J:133:THR:OG1	2.46	0.42
2:N:180:VAL:HG22	2:N:185:VAL:HG23	2.01	0.42
2:i:80:MET:O	3:i:301:HOH:O	2.22	0.42
2:k:73:GLY:HA3	2:k:98:MET:HE2	2.01	0.42
2:I:33:GLY:O	2:I:65:SER:OG	2.33	0.42
2:k:74:MET:HE1	2:k:101:PHE:CE2	2.55	0.42
2:k:176:ALA:HB3	2:k:177:PRO:HD3	2.01	0.42
2:I:113:CYS:SG	2:I:185:VAL:HG21	2.60	0.42
2:l:193:ASN:OD1	2:l:194:GLU:N	2.53	0.42
2:n:119:VAL:HG11	2:n:184:LEU:CD2	2.43	0.42
2:H:180:VAL:HG22	2:H:185:VAL:HG23	2.02	0.42
2:J:176:ALA:HB3	2:J:177:PRO:HD3	2.01	0.42
2:M:114:LEU:O	2:M:117:SER:OG	2.38	0.41
2:I:176:ALA:HB3	2:I:177:PRO:HD3	2.01	0.41
2:i:78:ASP:HB3	2:j:114:LEU:HD23	2.02	0.41
2:M:73:GLY:HA3	2:M:98:MET:HE2	2.01	0.41
2:h:193:ASN:OD1	2:h:194:GLU:N	2.54	0.41
2:H:15:ARG:NH2	2:I:14:GLU:OE2	2.54	0.41
2:j:133:THR:OG1	2:L:123:GLN:NE2	2.49	0.40
2:m:193:ASN:OD1	2:m:194:GLU:N	2.54	0.40
2:m:27:ARG:NH1	2:m:54:ASN:O	2.55	0.40
2:h:73:GLY:HA3	2:h:98:MET:HE2	2.03	0.40
2:l:74:MET:HE1	2:l:101:PHE:CE2	2.56	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	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
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%)	163 (100%)	0	100	100
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
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%)	2297 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	h	191	HIS
2	j	191	HIS
2	M	41	ASN
2	H	38	HIS
2	H	41	ASN
2	H	156	HIS
2	I	41	ASN
2	J	41	ASN
2	K	41	ASN

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Mol	Chain	Res	Type
2	L	41	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

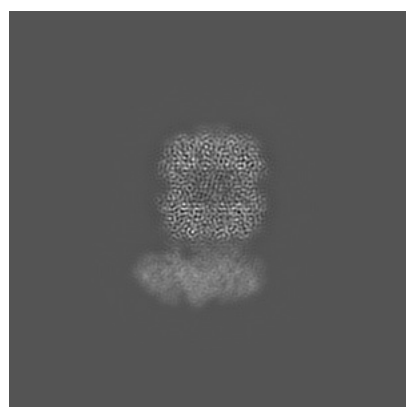
6 Map visualisation [i](#)

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

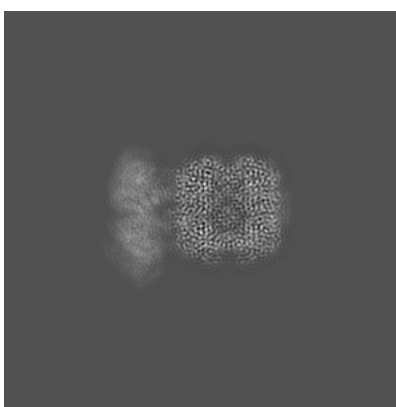
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

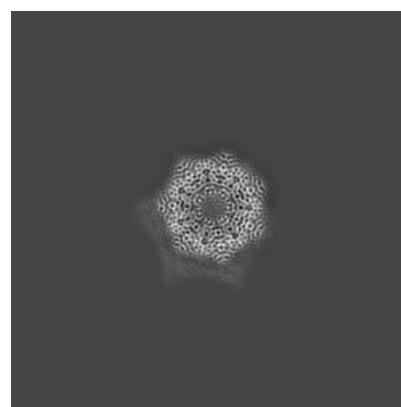
6.1.1 Primary map



X



Y



Z

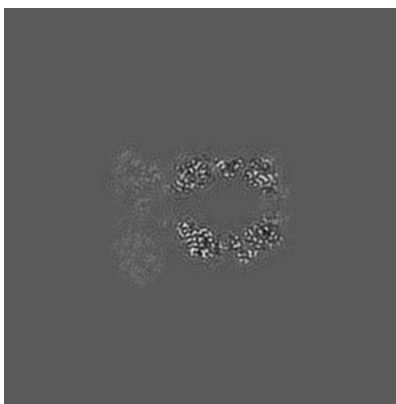
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

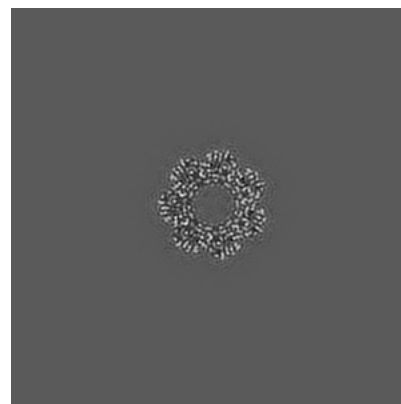
6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

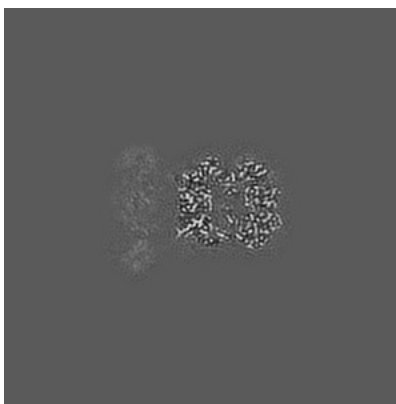
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

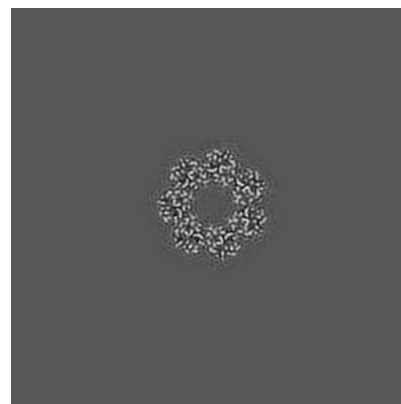
6.3.1 Primary map



X Index: 175



Y Index: 175

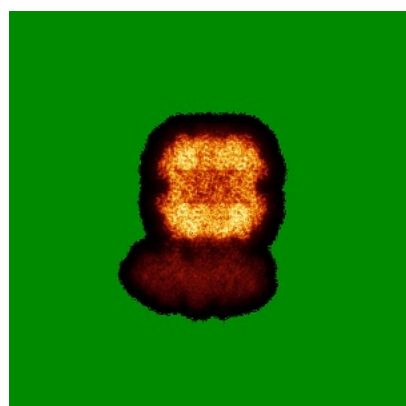


Z Index: 201

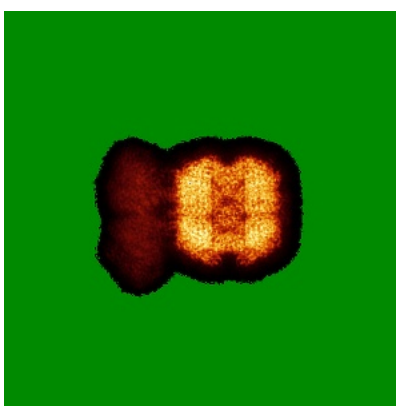
The images above show the largest variance slices of the map in three orthogonal directions.

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

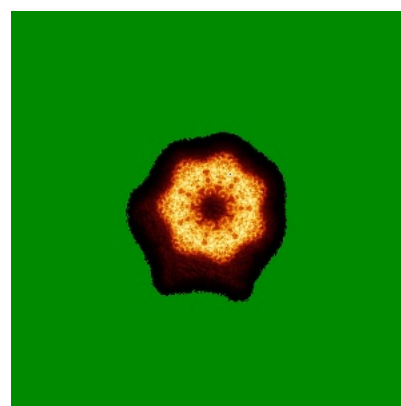
6.4.1 Primary map



X



Y

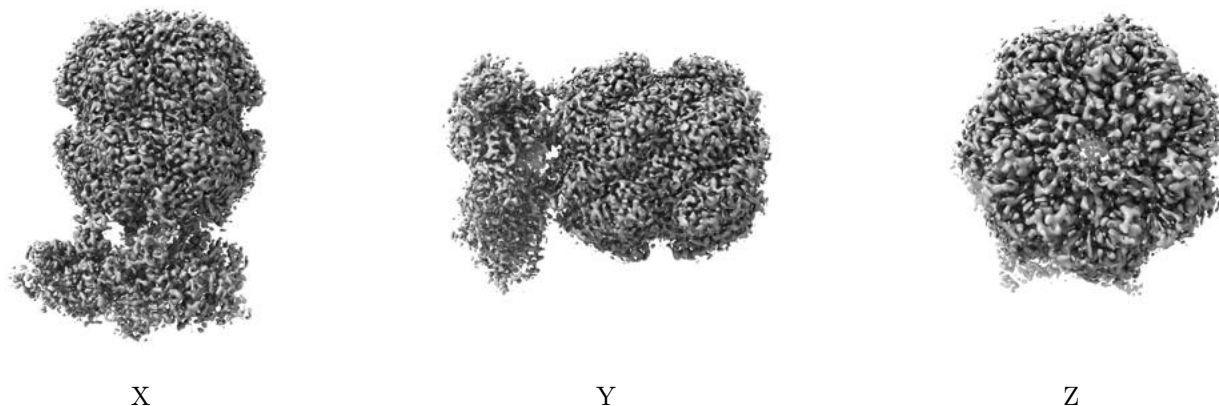


Z

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 4.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

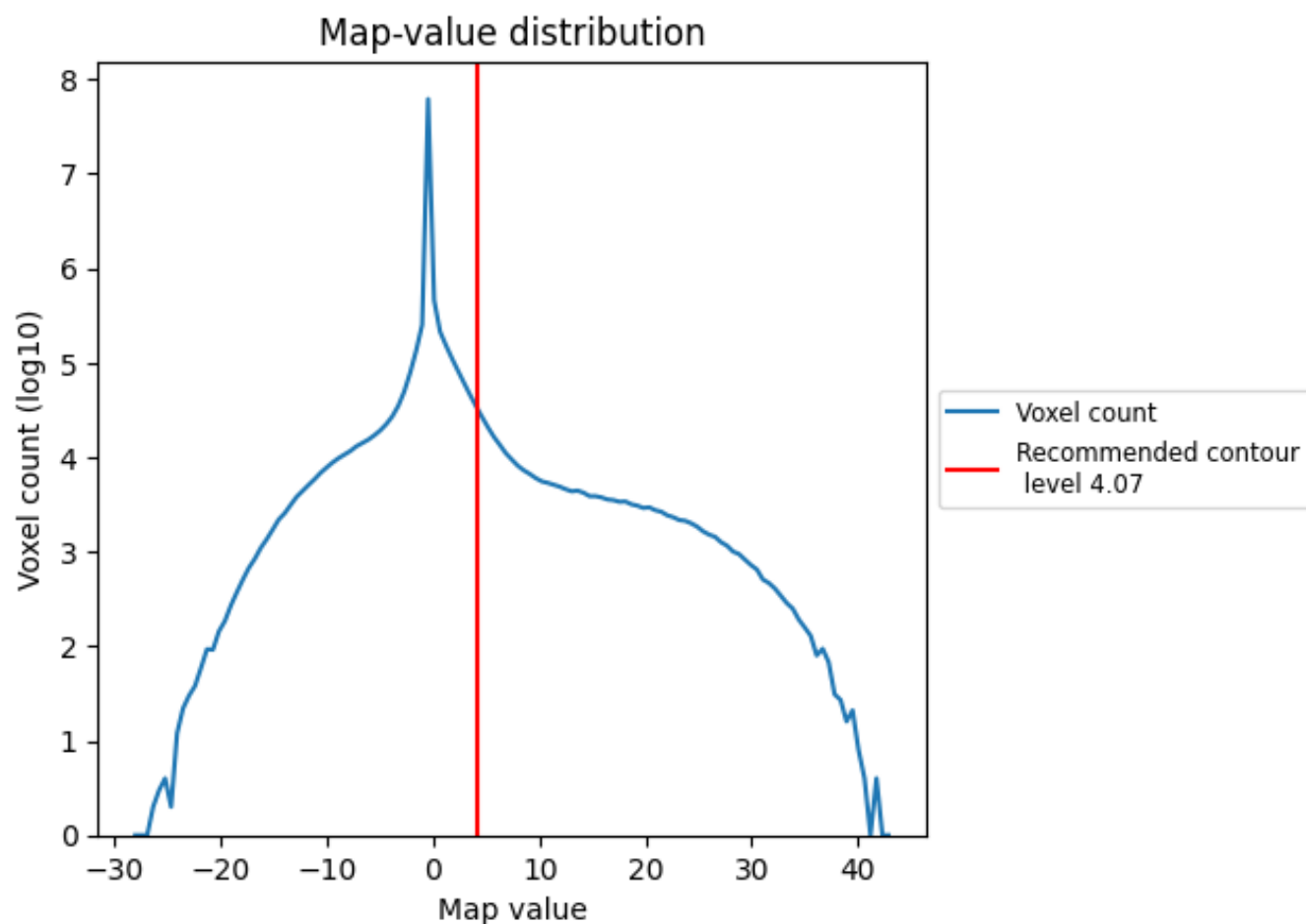
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

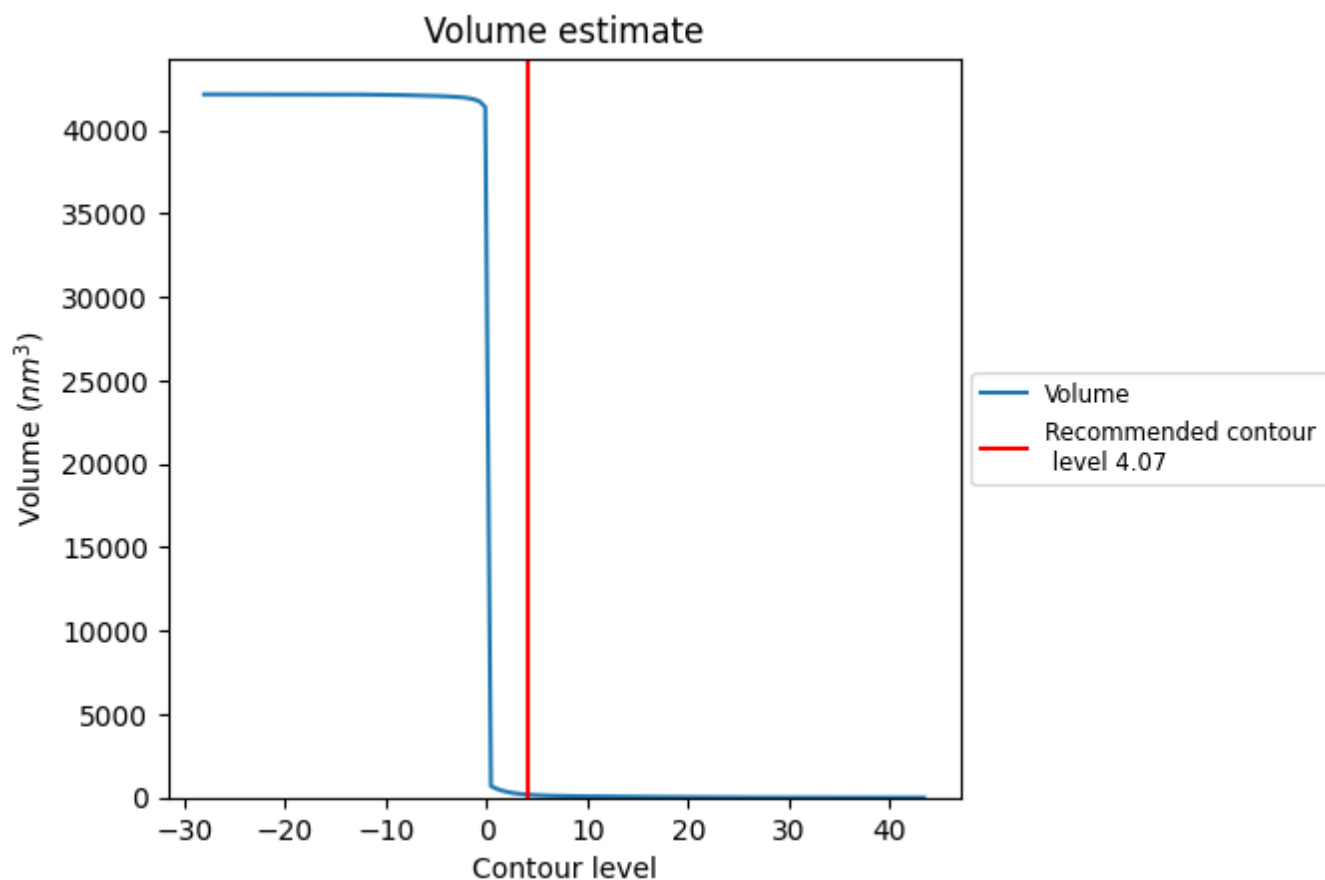
This section contains the results of statistical analysis of the map.

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.

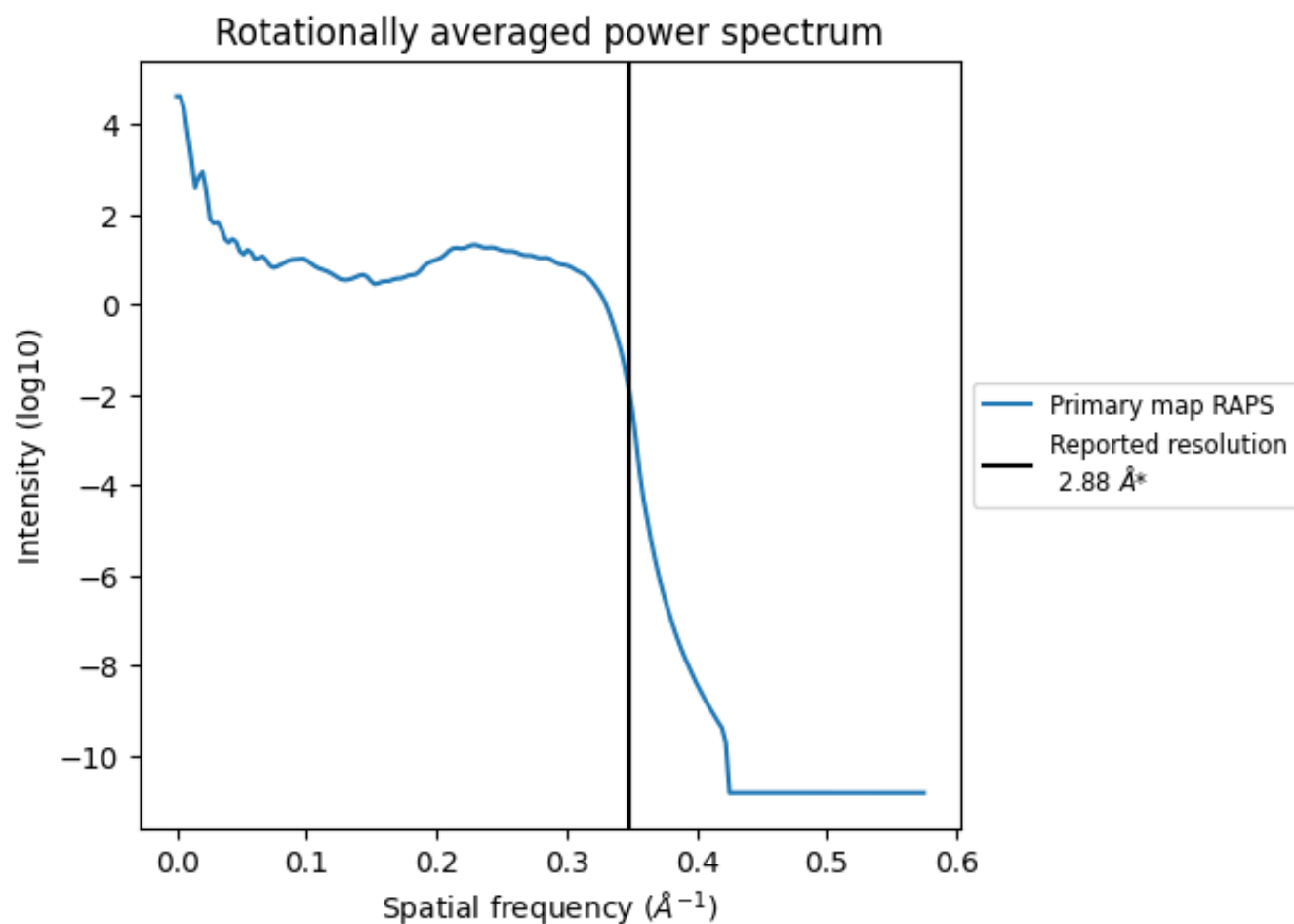
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

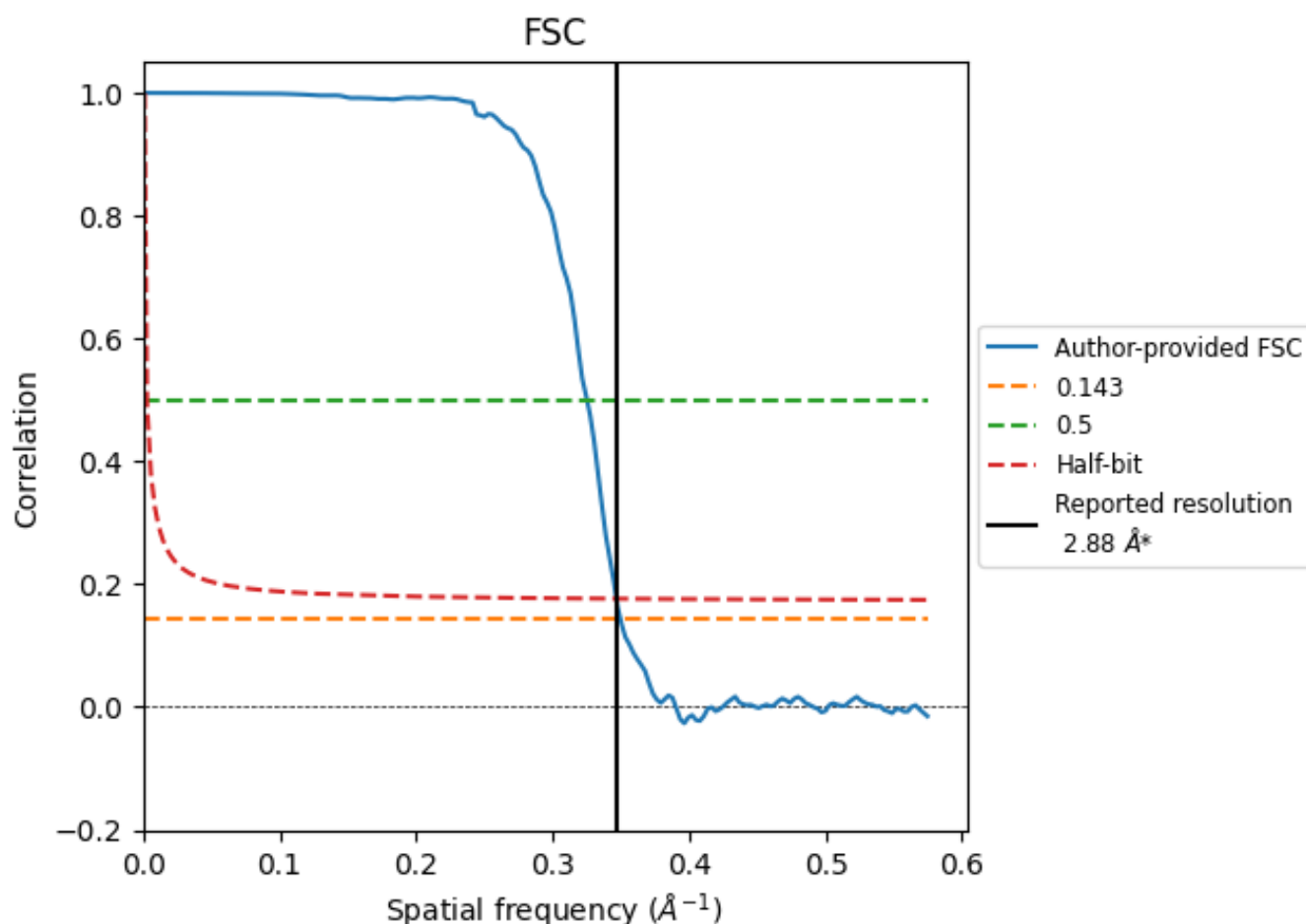


*Reported resolution corresponds to spatial frequency of 0.347 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.347 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

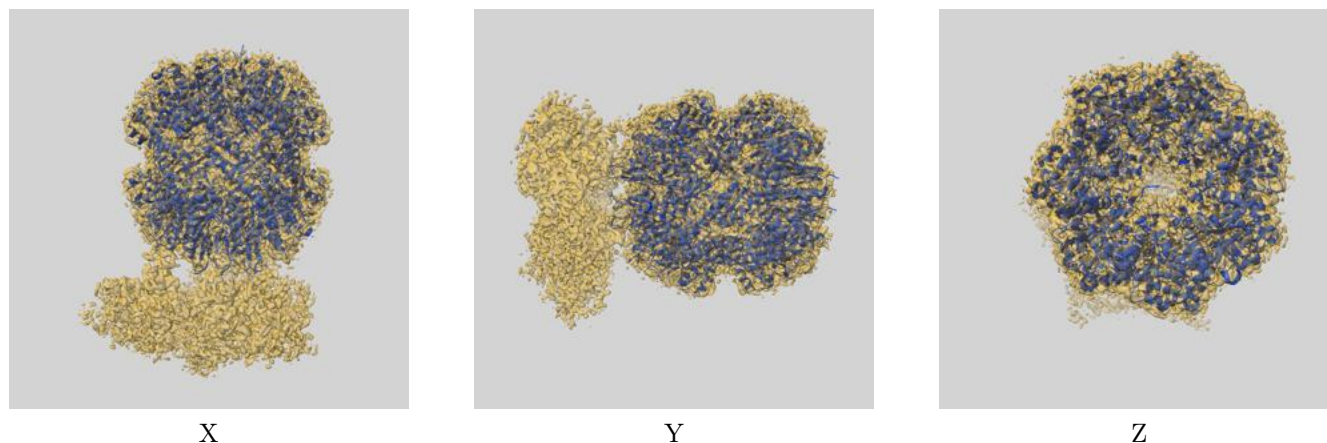
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.86	3.07	2.88
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

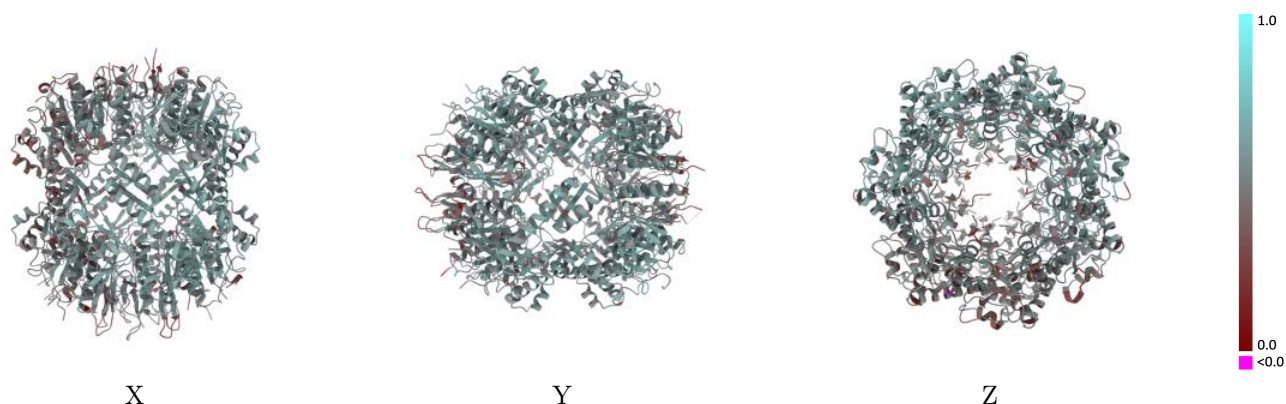
This section contains information regarding the fit between EMDB map EMD-21875 and PDB model 6WR2. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



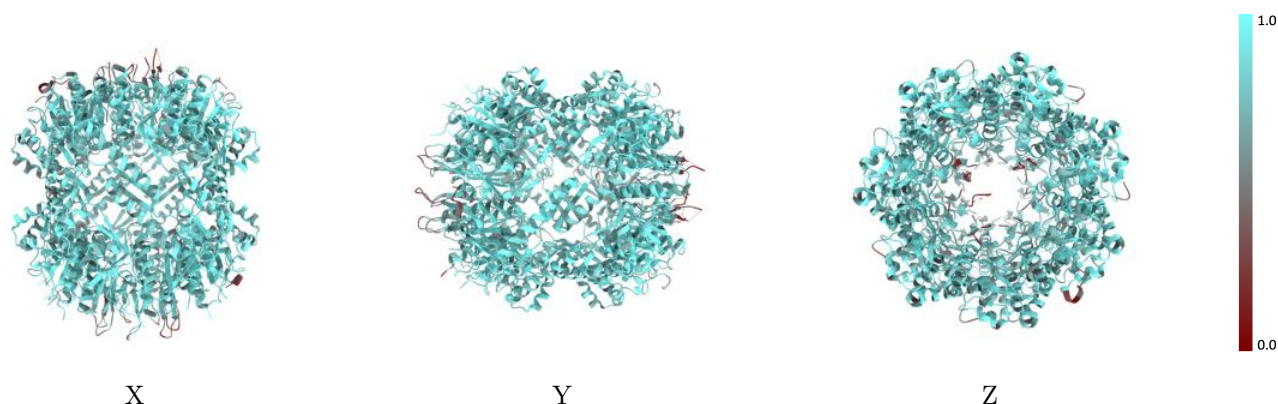
The images above show the 3D surface view of the map at the recommended contour level 4.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



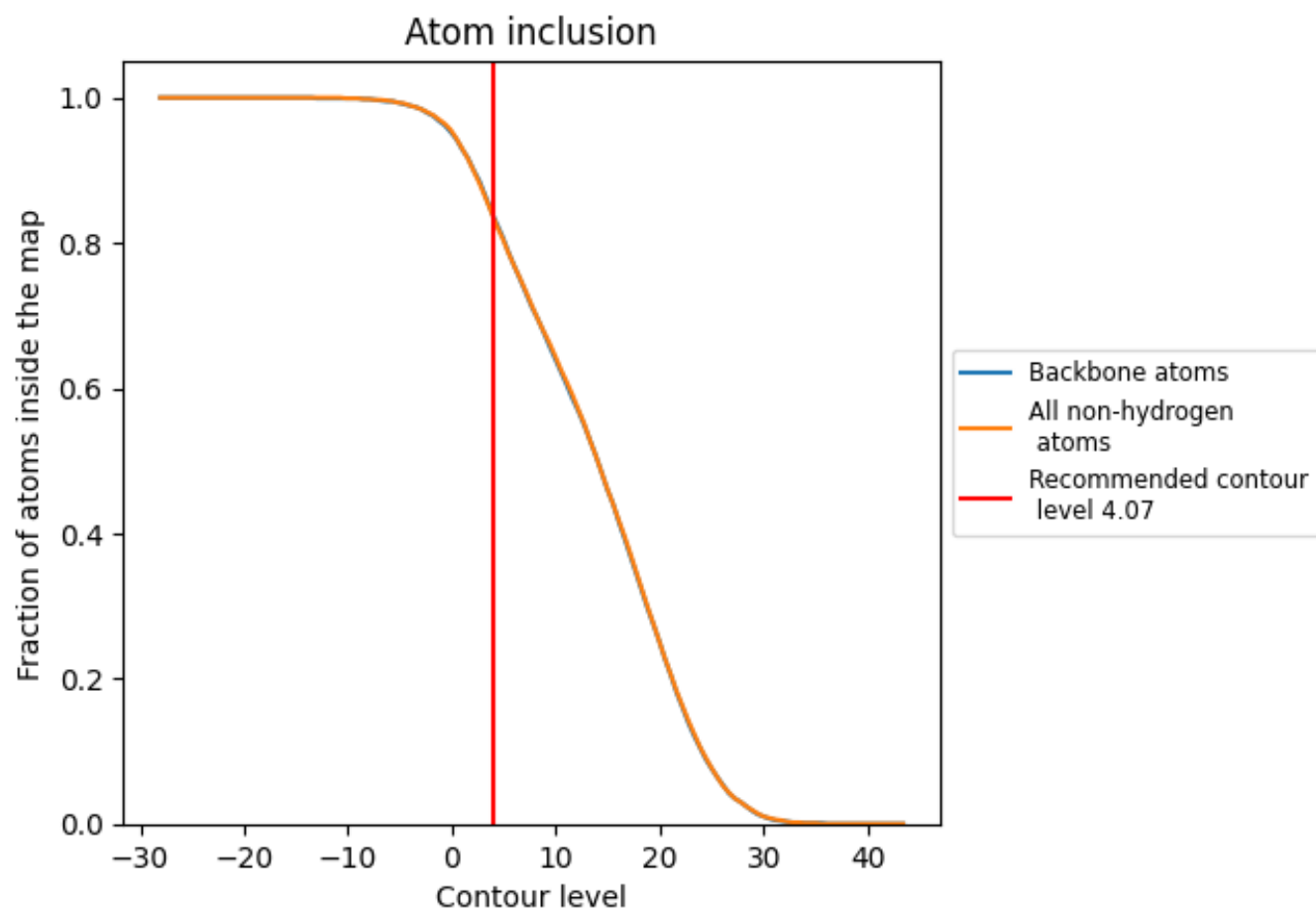
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.8320	 0.5180
A	 0.8360	 0.4900
B	 0.8910	 0.4930
C	 0.8180	 0.4500
D	 0.7820	 0.3780
E	 0.8000	 0.4290
F	 0.6540	 0.4140
H	 0.8540	 0.5640
I	 0.8640	 0.5380
J	 0.8380	 0.4810
K	 0.8210	 0.4790
L	 0.8490	 0.5340
M	 0.8570	 0.5500
N	 0.8280	 0.5390
h	 0.8530	 0.5330
i	 0.8490	 0.5380
j	 0.8660	 0.5650
k	 0.8420	 0.5320
l	 0.8000	 0.4700
m	 0.7890	 0.4490
n	 0.8160	 0.4960

