



Full wwPDB EM Validation Report ⓘ

Apr 8, 2024 – 10:16 AM EDT

PDB ID : 8TSW
EMDB ID : EMD-41601
Title : S. thermodepolymerans KpsMT-KpsE Apo 1
Authors : Kuklewicz, J.; Zimmer, J.
Deposited on : 2023-08-12
Resolution : 3.10 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

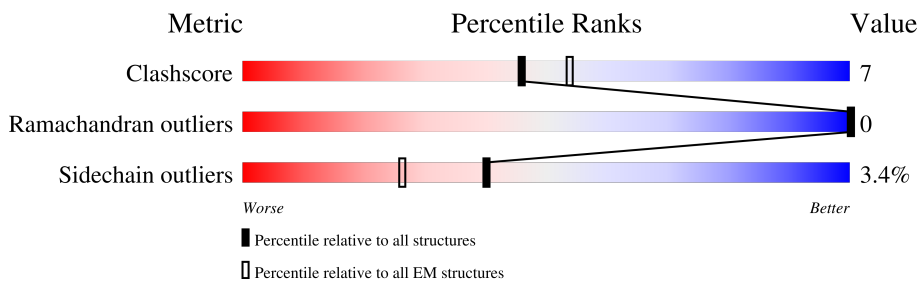
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



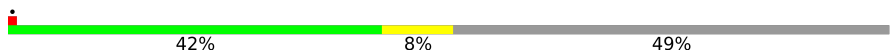
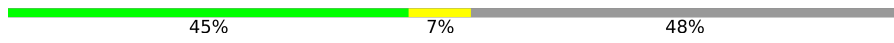


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	234	
1	B	234	
2	C	274	
2	D	274	
3	E	390	
3	F	390	
3	G	390	
3	H	390	

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Mol	Chain	Length	Quality of chain
3	I	390	 42% 8% 49%
3	J	390	 45% 7% 48%
3	K	390	 50% 9% 46%
3	L	390	 35% 9% 55%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 20326 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ABC transporter ATP-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	214	1687	1068	292	316	11	0	0
1	B	214	1687	1068	292	316	11	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	ASP	-	expression tag	UNP A0A2S5T4B3
A	228	TYR	-	expression tag	UNP A0A2S5T4B3
A	229	LYS	-	expression tag	UNP A0A2S5T4B3
A	230	ASP	-	expression tag	UNP A0A2S5T4B3
A	231	ASP	-	expression tag	UNP A0A2S5T4B3
A	232	ASP	-	expression tag	UNP A0A2S5T4B3
A	233	ASP	-	expression tag	UNP A0A2S5T4B3
A	234	LYS	-	expression tag	UNP A0A2S5T4B3
B	227	ASP	-	expression tag	UNP A0A2S5T4B3
B	228	TYR	-	expression tag	UNP A0A2S5T4B3
B	229	LYS	-	expression tag	UNP A0A2S5T4B3
B	230	ASP	-	expression tag	UNP A0A2S5T4B3
B	231	ASP	-	expression tag	UNP A0A2S5T4B3
B	232	ASP	-	expression tag	UNP A0A2S5T4B3
B	233	ASP	-	expression tag	UNP A0A2S5T4B3
B	234	LYS	-	expression tag	UNP A0A2S5T4B3

- Molecule 2 is a protein called Transport permease protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	255	2033	1364	342	320	7	0	0
2	D	255	2033	1364	342	320	7	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	MET	-	initiating methionine	UNP A0A2S5T447
C	-1	GLY	-	expression tag	UNP A0A2S5T447
C	0	LYS	-	expression tag	UNP A0A2S5T447
C	1	ILE	-	expression tag	UNP A0A2S5T447
C	2	HIS	-	expression tag	UNP A0A2S5T447
C	3	LEU	-	expression tag	UNP A0A2S5T447
D	-2	MET	-	initiating methionine	UNP A0A2S5T447
D	-1	GLY	-	expression tag	UNP A0A2S5T447
D	0	LYS	-	expression tag	UNP A0A2S5T447
D	1	ILE	-	expression tag	UNP A0A2S5T447
D	2	HIS	-	expression tag	UNP A0A2S5T447
D	3	LEU	-	expression tag	UNP A0A2S5T447

- Molecule 3 is a protein called Capsular biosynthesis protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	198	Total 1624	C 1051	N 277	O 288	S 8	0	0
3	F	204	Total 1672	C 1081	N 285	O 297	S 9	0	0
3	G	209	Total 1713	C 1103	N 297	O 305	S 8	0	0
3	H	174	Total 1434	C 925	N 244	O 259	S 6	0	0
3	I	198	Total 1624	C 1051	N 277	O 288	S 8	0	0
3	J	204	Total 1672	C 1081	N 285	O 297	S 9	0	0
3	K	209	Total 1713	C 1103	N 297	O 305	S 8	0	0
3	L	174	Total 1434	C 925	N 244	O 259	S 6	0	0

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	MET	-	initiating methionine	UNP A0A2S5T4A0
E	-1	GLY	-	expression tag	UNP A0A2S5T4A0
E	0	LYS	-	expression tag	UNP A0A2S5T4A0
E	1	ILE	-	expression tag	UNP A0A2S5T4A0
E	2	HIS	-	expression tag	UNP A0A2S5T4A0
E	77	CYS	LEU	conflict	UNP A0A2S5T4A0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	138	CYS	SER	conflict	UNP A0A2S5T4A0
E	372	GLY	-	expression tag	UNP A0A2S5T4A0
E	373	SER	-	expression tag	UNP A0A2S5T4A0
E	374	GLY	-	expression tag	UNP A0A2S5T4A0
E	375	SER	-	expression tag	UNP A0A2S5T4A0
E	376	GLY	-	expression tag	UNP A0A2S5T4A0
E	377	SER	-	expression tag	UNP A0A2S5T4A0
E	378	HIS	-	expression tag	UNP A0A2S5T4A0
E	379	HIS	-	expression tag	UNP A0A2S5T4A0
E	380	HIS	-	expression tag	UNP A0A2S5T4A0
E	381	HIS	-	expression tag	UNP A0A2S5T4A0
E	382	HIS	-	expression tag	UNP A0A2S5T4A0
E	383	HIS	-	expression tag	UNP A0A2S5T4A0
E	384	HIS	-	expression tag	UNP A0A2S5T4A0
E	385	HIS	-	expression tag	UNP A0A2S5T4A0
E	386	HIS	-	expression tag	UNP A0A2S5T4A0
E	387	HIS	-	expression tag	UNP A0A2S5T4A0
F	-2	MET	-	initiating methionine	UNP A0A2S5T4A0
F	-1	GLY	-	expression tag	UNP A0A2S5T4A0
F	0	LYS	-	expression tag	UNP A0A2S5T4A0
F	1	ILE	-	expression tag	UNP A0A2S5T4A0
F	2	HIS	-	expression tag	UNP A0A2S5T4A0
F	77	CYS	LEU	conflict	UNP A0A2S5T4A0
F	138	CYS	SER	conflict	UNP A0A2S5T4A0
F	372	GLY	-	expression tag	UNP A0A2S5T4A0
F	373	SER	-	expression tag	UNP A0A2S5T4A0
F	374	GLY	-	expression tag	UNP A0A2S5T4A0
F	375	SER	-	expression tag	UNP A0A2S5T4A0
F	376	GLY	-	expression tag	UNP A0A2S5T4A0
F	377	SER	-	expression tag	UNP A0A2S5T4A0
F	378	HIS	-	expression tag	UNP A0A2S5T4A0
F	379	HIS	-	expression tag	UNP A0A2S5T4A0
F	380	HIS	-	expression tag	UNP A0A2S5T4A0
F	381	HIS	-	expression tag	UNP A0A2S5T4A0
F	382	HIS	-	expression tag	UNP A0A2S5T4A0
F	383	HIS	-	expression tag	UNP A0A2S5T4A0
F	384	HIS	-	expression tag	UNP A0A2S5T4A0
F	385	HIS	-	expression tag	UNP A0A2S5T4A0
F	386	HIS	-	expression tag	UNP A0A2S5T4A0
F	387	HIS	-	expression tag	UNP A0A2S5T4A0
G	-2	MET	-	initiating methionine	UNP A0A2S5T4A0
G	-1	GLY	-	expression tag	UNP A0A2S5T4A0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	LYS	-	expression tag	UNP A0A2S5T4A0
G	1	ILE	-	expression tag	UNP A0A2S5T4A0
G	2	HIS	-	expression tag	UNP A0A2S5T4A0
G	77	CYS	LEU	conflict	UNP A0A2S5T4A0
G	138	CYS	SER	conflict	UNP A0A2S5T4A0
G	372	GLY	-	expression tag	UNP A0A2S5T4A0
G	373	SER	-	expression tag	UNP A0A2S5T4A0
G	374	GLY	-	expression tag	UNP A0A2S5T4A0
G	375	SER	-	expression tag	UNP A0A2S5T4A0
G	376	GLY	-	expression tag	UNP A0A2S5T4A0
G	377	SER	-	expression tag	UNP A0A2S5T4A0
G	378	HIS	-	expression tag	UNP A0A2S5T4A0
G	379	HIS	-	expression tag	UNP A0A2S5T4A0
G	380	HIS	-	expression tag	UNP A0A2S5T4A0
G	381	HIS	-	expression tag	UNP A0A2S5T4A0
G	382	HIS	-	expression tag	UNP A0A2S5T4A0
G	383	HIS	-	expression tag	UNP A0A2S5T4A0
G	384	HIS	-	expression tag	UNP A0A2S5T4A0
G	385	HIS	-	expression tag	UNP A0A2S5T4A0
G	386	HIS	-	expression tag	UNP A0A2S5T4A0
G	387	HIS	-	expression tag	UNP A0A2S5T4A0
H	-2	MET	-	initiating methionine	UNP A0A2S5T4A0
H	-1	GLY	-	expression tag	UNP A0A2S5T4A0
H	0	LYS	-	expression tag	UNP A0A2S5T4A0
H	1	ILE	-	expression tag	UNP A0A2S5T4A0
H	2	HIS	-	expression tag	UNP A0A2S5T4A0
H	77	CYS	LEU	conflict	UNP A0A2S5T4A0
H	138	CYS	SER	conflict	UNP A0A2S5T4A0
H	372	GLY	-	expression tag	UNP A0A2S5T4A0
H	373	SER	-	expression tag	UNP A0A2S5T4A0
H	374	GLY	-	expression tag	UNP A0A2S5T4A0
H	375	SER	-	expression tag	UNP A0A2S5T4A0
H	376	GLY	-	expression tag	UNP A0A2S5T4A0
H	377	SER	-	expression tag	UNP A0A2S5T4A0
H	378	HIS	-	expression tag	UNP A0A2S5T4A0
H	379	HIS	-	expression tag	UNP A0A2S5T4A0
H	380	HIS	-	expression tag	UNP A0A2S5T4A0
H	381	HIS	-	expression tag	UNP A0A2S5T4A0
H	382	HIS	-	expression tag	UNP A0A2S5T4A0
H	383	HIS	-	expression tag	UNP A0A2S5T4A0
H	384	HIS	-	expression tag	UNP A0A2S5T4A0
H	385	HIS	-	expression tag	UNP A0A2S5T4A0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	386	HIS	-	expression tag	UNP A0A2S5T4A0
H	387	HIS	-	expression tag	UNP A0A2S5T4A0
I	-2	MET	-	initiating methionine	UNP A0A2S5T4A0
I	-1	GLY	-	expression tag	UNP A0A2S5T4A0
I	0	LYS	-	expression tag	UNP A0A2S5T4A0
I	1	ILE	-	expression tag	UNP A0A2S5T4A0
I	2	HIS	-	expression tag	UNP A0A2S5T4A0
I	77	CYS	LEU	conflict	UNP A0A2S5T4A0
I	138	CYS	SER	conflict	UNP A0A2S5T4A0
I	372	GLY	-	expression tag	UNP A0A2S5T4A0
I	373	SER	-	expression tag	UNP A0A2S5T4A0
I	374	GLY	-	expression tag	UNP A0A2S5T4A0
I	375	SER	-	expression tag	UNP A0A2S5T4A0
I	376	GLY	-	expression tag	UNP A0A2S5T4A0
I	377	SER	-	expression tag	UNP A0A2S5T4A0
I	378	HIS	-	expression tag	UNP A0A2S5T4A0
I	379	HIS	-	expression tag	UNP A0A2S5T4A0
I	380	HIS	-	expression tag	UNP A0A2S5T4A0
I	381	HIS	-	expression tag	UNP A0A2S5T4A0
I	382	HIS	-	expression tag	UNP A0A2S5T4A0
I	383	HIS	-	expression tag	UNP A0A2S5T4A0
I	384	HIS	-	expression tag	UNP A0A2S5T4A0
I	385	HIS	-	expression tag	UNP A0A2S5T4A0
I	386	HIS	-	expression tag	UNP A0A2S5T4A0
I	387	HIS	-	expression tag	UNP A0A2S5T4A0
J	-2	MET	-	initiating methionine	UNP A0A2S5T4A0
J	-1	GLY	-	expression tag	UNP A0A2S5T4A0
J	0	LYS	-	expression tag	UNP A0A2S5T4A0
J	1	ILE	-	expression tag	UNP A0A2S5T4A0
J	2	HIS	-	expression tag	UNP A0A2S5T4A0
J	77	CYS	LEU	conflict	UNP A0A2S5T4A0
J	138	CYS	SER	conflict	UNP A0A2S5T4A0
J	372	GLY	-	expression tag	UNP A0A2S5T4A0
J	373	SER	-	expression tag	UNP A0A2S5T4A0
J	374	GLY	-	expression tag	UNP A0A2S5T4A0
J	375	SER	-	expression tag	UNP A0A2S5T4A0
J	376	GLY	-	expression tag	UNP A0A2S5T4A0
J	377	SER	-	expression tag	UNP A0A2S5T4A0
J	378	HIS	-	expression tag	UNP A0A2S5T4A0
J	379	HIS	-	expression tag	UNP A0A2S5T4A0
J	380	HIS	-	expression tag	UNP A0A2S5T4A0
J	381	HIS	-	expression tag	UNP A0A2S5T4A0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	382	HIS	-	expression tag	UNP A0A2S5T4A0
J	383	HIS	-	expression tag	UNP A0A2S5T4A0
J	384	HIS	-	expression tag	UNP A0A2S5T4A0
J	385	HIS	-	expression tag	UNP A0A2S5T4A0
J	386	HIS	-	expression tag	UNP A0A2S5T4A0
J	387	HIS	-	expression tag	UNP A0A2S5T4A0
K	-2	MET	-	initiating methionine	UNP A0A2S5T4A0
K	-1	GLY	-	expression tag	UNP A0A2S5T4A0
K	0	LYS	-	expression tag	UNP A0A2S5T4A0
K	1	ILE	-	expression tag	UNP A0A2S5T4A0
K	2	HIS	-	expression tag	UNP A0A2S5T4A0
K	77	CYS	LEU	conflict	UNP A0A2S5T4A0
K	138	CYS	SER	conflict	UNP A0A2S5T4A0
K	372	GLY	-	expression tag	UNP A0A2S5T4A0
K	373	SER	-	expression tag	UNP A0A2S5T4A0
K	374	GLY	-	expression tag	UNP A0A2S5T4A0
K	375	SER	-	expression tag	UNP A0A2S5T4A0
K	376	GLY	-	expression tag	UNP A0A2S5T4A0
K	377	SER	-	expression tag	UNP A0A2S5T4A0
K	378	HIS	-	expression tag	UNP A0A2S5T4A0
K	379	HIS	-	expression tag	UNP A0A2S5T4A0
K	380	HIS	-	expression tag	UNP A0A2S5T4A0
K	381	HIS	-	expression tag	UNP A0A2S5T4A0
K	382	HIS	-	expression tag	UNP A0A2S5T4A0
K	383	HIS	-	expression tag	UNP A0A2S5T4A0
K	384	HIS	-	expression tag	UNP A0A2S5T4A0
K	385	HIS	-	expression tag	UNP A0A2S5T4A0
K	386	HIS	-	expression tag	UNP A0A2S5T4A0
K	387	HIS	-	expression tag	UNP A0A2S5T4A0
L	-2	MET	-	initiating methionine	UNP A0A2S5T4A0
L	-1	GLY	-	expression tag	UNP A0A2S5T4A0
L	0	LYS	-	expression tag	UNP A0A2S5T4A0
L	1	ILE	-	expression tag	UNP A0A2S5T4A0
L	2	HIS	-	expression tag	UNP A0A2S5T4A0
L	77	CYS	LEU	conflict	UNP A0A2S5T4A0
L	138	CYS	SER	conflict	UNP A0A2S5T4A0
L	372	GLY	-	expression tag	UNP A0A2S5T4A0
L	373	SER	-	expression tag	UNP A0A2S5T4A0
L	374	GLY	-	expression tag	UNP A0A2S5T4A0
L	375	SER	-	expression tag	UNP A0A2S5T4A0
L	376	GLY	-	expression tag	UNP A0A2S5T4A0
L	377	SER	-	expression tag	UNP A0A2S5T4A0

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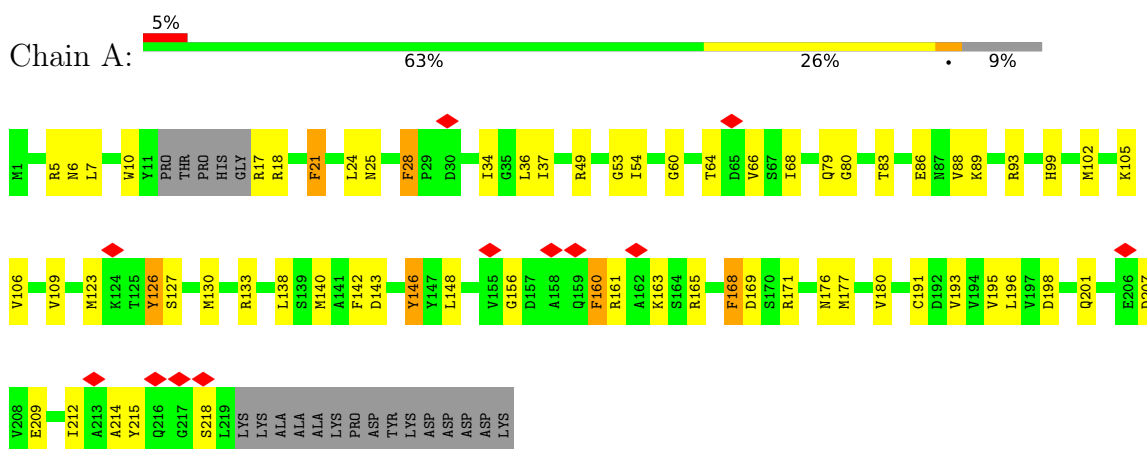
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Chain	Residue	Modelled	Actual	Comment	Reference
L	378	HIS	-	expression tag	UNP A0A2S5T4A0
L	379	HIS	-	expression tag	UNP A0A2S5T4A0
L	380	HIS	-	expression tag	UNP A0A2S5T4A0
L	381	HIS	-	expression tag	UNP A0A2S5T4A0
L	382	HIS	-	expression tag	UNP A0A2S5T4A0
L	383	HIS	-	expression tag	UNP A0A2S5T4A0
L	384	HIS	-	expression tag	UNP A0A2S5T4A0
L	385	HIS	-	expression tag	UNP A0A2S5T4A0
L	386	HIS	-	expression tag	UNP A0A2S5T4A0
L	387	HIS	-	expression tag	UNP A0A2S5T4A0

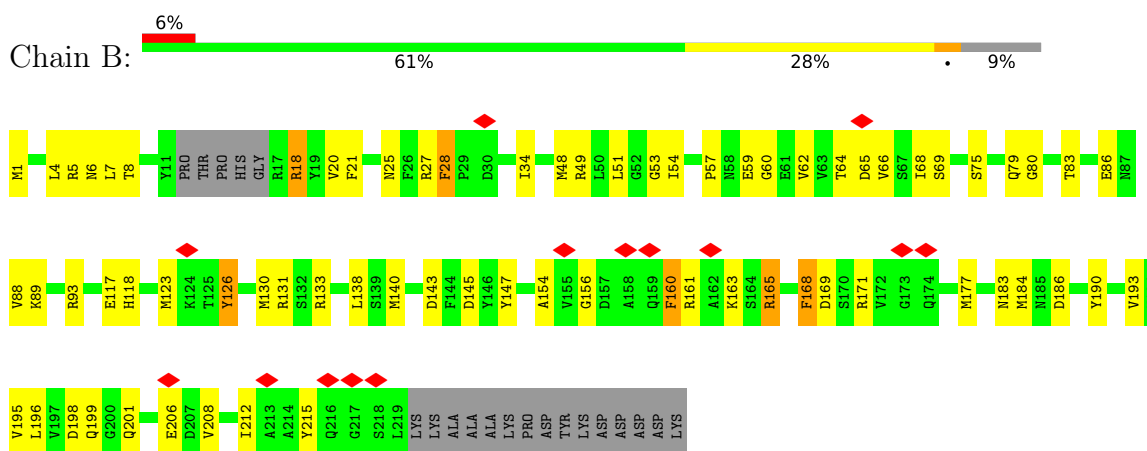
3 Residue-property plots

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.

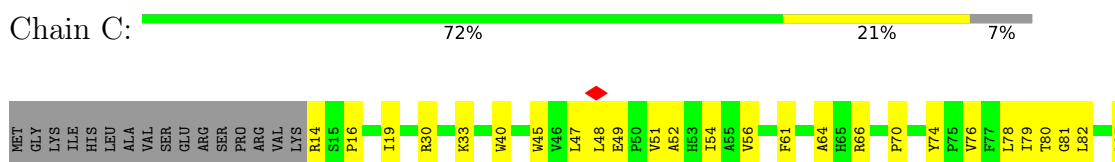
- Molecule 1: ABC transporter ATP-binding protein



- Molecule 1: ABC transporter ATP-binding protein



- Molecule 2: Transport permease protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43811	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	39.371	Depositor
Minimum map value	-18.574	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.889	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/1718	0.55	0/2313
1	B	0.26	0/1718	0.56	0/2313
2	C	0.27	0/2089	0.53	0/2848
2	D	0.27	0/2089	0.53	0/2848
3	E	0.27	0/1658	0.52	0/2250
3	F	0.25	0/1707	0.52	0/2317
3	G	0.25	0/1748	0.49	0/2371
3	H	0.25	0/1465	0.51	0/1986
3	I	0.25	0/1658	0.52	0/2250
3	J	0.25	0/1707	0.50	0/2317
3	K	0.25	0/1748	0.49	0/2371
3	L	0.25	0/1465	0.52	0/1986
All	All	0.26	0/20770	0.52	0/28170

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1687	0	1652	38	0
1	B	1687	0	1652	41	0
2	C	2033	0	2151	38	0
2	D	2033	0	2151	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1624	0	1650	21	0
3	F	1672	0	1697	17	0
3	G	1713	0	1736	12	0
3	H	1434	0	1436	20	0
3	I	1624	0	1650	17	0
3	J	1672	0	1697	17	0
3	K	1713	0	1736	9	0
3	L	1434	0	1436	20	0
All	All	20326	0	20644	271	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 7.

All (271) 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)
3:F:3:MET:HG2	3:F:4:LYS:H	1.46	0.79
2:D:66:ARG:HH12	2:D:70:PRO:HA	1.55	0.72
2:C:66:ARG:HH12	2:C:70:PRO:HA	1.56	0.69
3:H:90:GLN:O	3:H:94:GLN:NE2	2.25	0.69
2:D:31:GLU:HG3	2:D:123:LEU:HD13	1.75	0.68
1:A:53:GLY:HA3	2:C:109:ARG:HG3	1.76	0.67
1:A:68:ILE:O	2:C:109:ARG:NH2	2.31	0.64
1:A:80:GLY:HA2	1:A:123:MET:HB2	1.79	0.64
2:C:102:ASN:HB3	2:C:105:LEU:HD12	1.80	0.62
1:B:49:ARG:HG2	1:B:54:ILE:HD12	1.82	0.62
1:B:34:ILE:HD11	1:B:195:VAL:HG23	1.81	0.62
3:K:135:ASP:O	3:K:139:GLY:N	2.33	0.61
2:D:178:GLU:N	2:D:178:GLU:OE1	2.34	0.61
3:I:339:PRO:O	3:I:344:ASN:ND2	2.34	0.61
1:B:68:ILE:O	2:D:109:ARG:NH2	2.35	0.60
2:D:102:ASN:HB3	2:D:105:LEU:HD12	1.81	0.60
1:B:143:ASP:OD1	1:B:171:ARG:NH2	2.32	0.60
1:A:88:VAL:HG23	1:A:138:LEU:HD13	1.84	0.59
3:G:135:ASP:O	3:G:139:GLY:N	2.35	0.59
1:A:209:GLU:HA	1:A:212:ILE:HD12	1.84	0.59
3:H:28:VAL:O	3:H:32:VAL:HB	2.02	0.59
1:B:53:GLY:HA3	2:D:109:ARG:HG3	1.83	0.59
1:B:147:TYR:HB2	1:B:177:MET:HG2	1.85	0.58
1:B:160:PHE:HA	1:B:163:LYS:HZ2	1.68	0.58
3:G:50:SER:OG	3:G:319:ARG:NH2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:N	1:B:65:ASP:OD1	2.36	0.58
2:C:95:LEU:HD12	2:C:117:VAL:HG13	1.85	0.58
3:E:339:PRO:O	3:E:344:ASN:ND2	2.36	0.58
3:F:136:ASP:OD1	3:F:136:ASP:N	2.36	0.58
1:B:198:ASP:OD2	1:B:199:GLN:NE2	2.36	0.57
2:C:101:SER:OG	2:C:102:ASN:OD1	2.23	0.57
1:B:186:ASP:O	1:B:190:TYR:HB2	2.04	0.57
2:D:101:SER:OG	2:D:102:ASN:OD1	2.22	0.57
3:I:23:MET:HE1	3:I:349:LEU:HB2	1.86	0.57
3:K:49:THR:O	3:L:179:GLN:NE2	2.38	0.56
2:D:96:MET:HE1	2:D:186:VAL:HG21	1.87	0.56
3:J:130:VAL:HG22	3:J:145:VAL:HG22	1.87	0.56
1:B:140:MET:O	1:B:171:ARG:NH1	2.36	0.56
1:B:130:MET:HA	1:B:133:ARG:HD2	1.87	0.56
2:C:178:GLU:N	2:C:178:GLU:OE2	2.39	0.56
2:D:95:LEU:HD12	2:D:117:VAL:HG13	1.86	0.56
3:E:175:MET:HG2	3:L:49:THR:HG22	1.88	0.56
1:B:4:LEU:HG	1:B:62:VAL:HG12	1.87	0.56
1:A:156:GLY:O	1:A:161:ARG:NH2	2.36	0.56
1:A:83:THR:N	1:A:86:GLU:OE1	2.37	0.55
3:J:39:VAL:HG21	3:J:338:TYR:HD2	1.71	0.55
3:K:130:VAL:HG22	3:K:145:VAL:HG22	1.88	0.55
1:B:196:LEU:HD13	1:B:215:TYR:HE1	1.71	0.55
3:F:130:VAL:HG22	3:F:145:VAL:HG22	1.88	0.55
3:F:39:VAL:HG21	3:F:338:TYR:HD2	1.72	0.55
3:L:320:LYS:NZ	3:L:323:SER:OG	2.39	0.55
1:B:75:SER:HB2	1:B:131:ARG:HD3	1.88	0.55
3:L:135:ASP:O	3:L:139:GLY:N	2.40	0.55
1:A:130:MET:HA	1:A:133:ARG:HD2	1.89	0.54
1:B:88:VAL:HG23	1:B:138:LEU:HD13	1.88	0.54
3:E:174:ARG:HG3	3:E:177:ARG:HH21	1.72	0.54
1:A:37:ILE:HG12	1:A:215:TYR:OH	2.08	0.54
1:B:80:GLY:HA2	1:B:123:MET:HB2	1.88	0.54
2:C:96:MET:HE1	2:C:186:VAL:HG21	1.89	0.54
2:C:81:GLY:HA3	2:C:227:ARG:HH21	1.73	0.54
3:I:8:ARG:HH21	3:I:13:ARG:HD3	1.72	0.54
2:C:79:ILE:HD11	2:C:135:ALA:HB1	1.90	0.54
3:F:137:ILE:H	3:F:137:ILE:HD12	1.72	0.54
3:G:130:VAL:HG22	3:G:145:VAL:HG22	1.88	0.54
1:B:79:GLN:HG3	2:D:30:ARG:HD2	1.90	0.53
3:E:136:ASP:OD1	3:E:136:ASP:N	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLN:HG3	2:C:30:ARG:HD2	1.90	0.53
2:C:54:ILE:HD12	2:C:78:LEU:HD23	1.89	0.53
2:D:54:ILE:HD12	2:D:78:LEU:HD23	1.89	0.53
3:L:163:GLU:OE2	3:L:166:ARG:NH2	2.41	0.53
3:F:28:VAL:O	3:F:32:VAL:HB	2.09	0.53
3:J:133:LEU:HB2	3:J:142:THR:HG23	1.90	0.53
2:C:45:TRP:O	2:C:49:GLU:HG2	2.08	0.53
3:J:28:VAL:O	3:J:32:VAL:HB	2.09	0.53
2:D:45:TRP:O	2:D:49:GLU:HG2	2.09	0.52
2:D:81:GLY:HA3	2:D:227:ARG:HH21	1.73	0.52
3:G:158:ARG:HG2	3:G:330:PRO:HG2	1.90	0.52
3:H:163:GLU:OE2	3:H:166:ARG:NH2	2.39	0.52
2:C:130:ILE:O	2:C:134:ILE:HG22	2.10	0.52
1:A:49:ARG:HG2	1:A:54:ILE:HD12	1.90	0.52
2:D:78:LEU:O	2:D:82:LEU:HB2	2.09	0.52
3:F:39:VAL:HG22	3:F:146:GLN:HG2	1.91	0.52
3:I:136:ASP:OD1	3:I:136:ASP:N	2.34	0.52
3:K:169:ASN:ND2	3:K:322:LYS:O	2.38	0.52
1:A:143:ASP:OD1	1:A:171:ARG:NH2	2.35	0.52
1:B:7:LEU:HA	1:B:60:GLY:HA3	1.92	0.52
3:J:10:THR:OG1	3:J:11:ALA:N	2.42	0.51
3:G:48:GLN:HA	3:G:322:LYS:HD2	1.91	0.51
1:B:156:GLY:O	1:B:161:ARG:NH2	2.36	0.51
3:E:25:VAL:HA	3:E:28:VAL:HG22	1.92	0.51
3:F:46:VAL:HG11	3:F:75:ASP:HB3	1.92	0.51
3:I:46:VAL:HG12	3:I:322:LYS:HE2	1.93	0.51
3:J:39:VAL:HG22	3:J:146:GLN:HG2	1.91	0.51
3:L:92:LEU:HB3	3:L:98:LEU:HD11	1.93	0.51
3:H:92:LEU:HB3	3:H:98:LEU:HD11	1.93	0.51
3:E:37:ARG:HA	3:E:147:GLY:O	2.11	0.51
3:J:136:ASP:OD1	3:J:136:ASP:N	2.36	0.51
3:G:371:ASP:N	3:G:371:ASP:OD1	2.40	0.51
2:C:61:PHE:HB3	2:C:64:ALA:HB3	1.93	0.50
3:K:158:ARG:HG2	3:K:330:PRO:HG2	1.93	0.50
1:B:28:PHE:HE1	1:B:195:VAL:HG21	1.77	0.50
1:B:5:ARG:O	1:B:60:GLY:HA2	2.10	0.50
1:A:146:TYR:HD1	1:A:176:ASN:HD22	1.58	0.50
3:I:23:MET:O	3:I:27:THR:OG1	2.21	0.50
3:I:37:ARG:HA	3:I:147:GLY:O	2.10	0.50
1:A:34:ILE:HD11	1:A:195:VAL:HG23	1.93	0.50
2:D:76:VAL:O	2:D:80:THR:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:48:GLN:NE2	3:F:321:LEU:O	2.42	0.50
3:H:73:ARG:NH2	3:H:136:ASP:O	2.40	0.49
1:A:214:ALA:O	1:A:218:SER:OG	2.30	0.49
2:C:182:ALA:O	2:C:186:VAL:HG13	2.12	0.49
2:D:193:LEU:HA	2:D:196:VAL:HG22	1.94	0.49
1:A:28:PHE:HE1	1:A:195:VAL:HG21	1.77	0.49
2:C:76:VAL:O	2:C:80:THR:HG23	2.13	0.49
3:H:158:ARG:HG2	3:H:330:PRO:HG2	1.95	0.49
3:H:135:ASP:O	3:H:139:GLY:N	2.46	0.49
1:B:83:THR:N	1:B:86:GLU:OE2	2.45	0.49
2:C:66:ARG:HH22	2:C:70:PRO:HB3	1.78	0.49
3:E:347:THR:O	3:E:351:VAL:HG12	2.13	0.49
2:D:182:ALA:O	2:D:186:VAL:HG13	2.12	0.48
3:H:174:ARG:HA	3:H:177:ARG:NH1	2.28	0.48
2:D:76:VAL:HA	2:D:79:ILE:HG22	1.94	0.48
2:C:52:ALA:O	2:C:56:VAL:HG12	2.13	0.48
1:B:1:MET:SD	1:B:27:ARG:NH2	2.86	0.48
1:B:86:GLU:HA	1:B:89:LYS:HG2	1.94	0.48
1:A:5:ARG:O	1:A:60:GLY:HA3	2.14	0.48
2:D:52:ALA:O	2:D:56:VAL:HG12	2.14	0.48
2:C:76:VAL:HA	2:C:79:ILE:HG22	1.96	0.48
2:C:99:ILE:HD13	2:C:113:PRO:HB3	1.96	0.48
2:C:193:LEU:HA	2:C:196:VAL:HG22	1.95	0.48
3:E:49:THR:OG1	3:E:321:LEU:O	2.31	0.47
3:L:73:ARG:NH2	3:L:136:ASP:O	2.34	0.47
1:B:160:PHE:HA	1:B:163:LYS:NZ	2.28	0.47
3:G:73:ARG:NH1	3:G:136:ASP:O	2.47	0.47
2:D:16:PRO:HB3	3:K:370:GLN:HA	1.97	0.47
2:D:257:LEU:HB3	3:K:361:LEU:HD13	1.97	0.47
1:B:123:MET:HA	1:B:126:TYR:HB2	1.97	0.47
3:L:79:LEU:O	3:L:83:ILE:HG12	2.15	0.47
1:A:68:ILE:HG22	2:C:109:ARG:HH22	1.79	0.47
3:H:320:LYS:NZ	3:H:323:SER:OG	2.47	0.47
3:L:48:GLN:OE1	3:L:49:THR:N	2.47	0.47
1:B:4:LEU:HD23	1:B:7:LEU:HD12	1.97	0.47
2:C:78:LEU:O	2:C:82:LEU:HB2	2.15	0.47
3:J:29:TYR:HE1	3:J:109:PRO:HD2	1.80	0.47
3:E:83:ILE:HA	3:E:88:LEU:HD23	1.95	0.47
3:F:29:TYR:HE1	3:F:109:PRO:HD2	1.80	0.47
3:L:158:ARG:HG2	3:L:330:PRO:HG2	1.97	0.47
3:L:173:HIS:HB3	3:L:177:ARG:HH21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:24:LEU:O	3:I:28:VAL:HG13	2.16	0.46
3:I:83:ILE:HA	3:I:88:LEU:HD23	1.97	0.46
3:I:75:ASP:OD1	3:I:75:ASP:N	2.49	0.46
3:I:130:VAL:HG22	3:I:145:VAL:HG22	1.96	0.46
1:A:168:PHE:HE1	1:A:177:MET:HG3	1.79	0.46
3:E:25:VAL:O	3:E:28:VAL:HG22	2.16	0.46
3:F:363:VAL:HA	3:F:366:ILE:HG22	1.96	0.46
3:G:72:SER:O	3:G:76:THR:HG23	2.16	0.46
3:G:136:ASP:OD1	3:G:136:ASP:N	2.47	0.46
2:D:99:ILE:HD13	2:D:113:PRO:HB3	1.97	0.46
1:A:123:MET:HA	1:A:126:TYR:HB2	1.97	0.46
1:B:208:VAL:O	1:B:212:ILE:HG12	2.16	0.46
3:H:41:GLU:OE1	3:H:144:ARG:NE	2.45	0.46
1:A:86:GLU:HA	1:A:89:LYS:HG2	1.98	0.45
3:K:73:ARG:NH1	3:K:136:ASP:O	2.46	0.45
1:B:168:PHE:HE1	1:B:177:MET:HG3	1.80	0.45
3:K:136:ASP:N	3:K:136:ASP:OD1	2.46	0.45
1:A:34:ILE:HD13	1:A:193:VAL:HG23	1.98	0.45
3:I:92:LEU:HD13	3:I:156:LEU:HD11	1.96	0.45
3:H:79:LEU:O	3:H:83:ILE:HG12	2.15	0.45
3:L:174:ARG:HA	3:L:177:ARG:NH1	2.31	0.45
2:C:96:MET:HA	2:C:173:ALA:HB2	1.98	0.45
3:E:75:ASP:OD1	3:E:75:ASP:N	2.50	0.45
1:A:64:THR:HG22	1:A:66:VAL:H	1.81	0.45
2:D:149:VAL:HG11	2:D:232:PRO:HB3	1.98	0.45
3:E:46:VAL:HG12	3:E:322:LYS:HE2	1.99	0.45
1:B:117:GLU:OE2	1:B:118:HIS:NE2	2.50	0.45
2:C:149:VAL:HG11	2:C:232:PRO:HB3	1.99	0.45
2:D:61:PHE:HB3	2:D:64:ALA:HB3	1.98	0.45
3:E:15:GLN:HB3	3:E:20:TYR:CE2	2.51	0.44
3:G:319:ARG:HH12	3:H:179:GLN:HB3	1.82	0.44
1:B:123:MET:O	1:B:131:ARG:NH2	2.50	0.44
2:C:16:PRO:HB3	3:G:370:GLN:HA	1.99	0.44
3:L:41:GLU:OE1	3:L:144:ARG:NE	2.48	0.44
3:E:130:VAL:HG22	3:E:145:VAL:HG22	1.98	0.44
1:A:5:ARG:NH1	1:A:25:ASN:OD1	2.51	0.44
1:A:123:MET:N	1:A:123:MET:SD	2.91	0.44
3:L:23:MET:O	3:L:27:THR:OG1	2.32	0.44
2:D:97:GLU:HB2	2:D:120:ARG:NH2	2.33	0.44
1:B:5:ARG:NH2	1:B:6:ASN:HD22	2.16	0.44
2:C:45:TRP:HA	2:C:48:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:VAL:O	2:C:54:ILE:HG22	2.18	0.44
2:D:96:MET:HA	2:D:173:ALA:HB2	1.99	0.44
1:A:207:ASP:OD1	1:A:207:ASP:N	2.47	0.43
2:C:121:ALA:O	2:C:125:ILE:HG12	2.18	0.43
2:D:51:VAL:O	2:D:54:ILE:HG22	2.18	0.43
3:F:37:ARG:HA	3:F:147:GLY:O	2.19	0.43
2:D:45:TRP:HA	2:D:48:LEU:HG	2.00	0.43
1:B:48:MET:HA	1:B:51:LEU:HD12	2.00	0.43
1:A:196:LEU:HD13	1:A:215:TYR:HE1	1.83	0.43
1:A:5:ARG:O	1:A:60:GLY:CA	2.67	0.43
1:A:93:ARG:NH1	3:F:368:ASP:OD1	2.51	0.43
2:C:47:LEU:HD23	2:C:47:LEU:HA	1.89	0.43
3:E:14:LEU:HG	3:E:356:TYR:HE1	1.84	0.43
3:H:38:TYR:N	3:H:147:GLY:O	2.50	0.43
3:H:173:HIS:HB3	3:H:177:ARG:HH21	1.83	0.43
3:L:159:ALA:HA	3:L:162:GLU:HG2	2.01	0.43
1:B:64:THR:HG22	1:B:66:VAL:H	1.82	0.43
2:D:66:ARG:HH22	2:D:70:PRO:HB3	1.83	0.43
3:H:44:ILE:HD13	3:H:161:LEU:HD22	2.00	0.43
3:L:92:LEU:HD23	3:L:156:LEU:HD11	2.00	0.43
3:J:361:LEU:HD23	3:J:361:LEU:HA	1.83	0.43
1:A:99:HIS:HA	1:A:102:MET:HE2	2.01	0.43
2:D:121:ALA:O	2:D:125:ILE:HG12	2.19	0.43
3:J:363:VAL:HA	3:J:366:ILE:HG22	2.01	0.43
3:J:79:LEU:HD23	3:J:79:LEU:HA	1.88	0.42
3:E:44:ILE:HG22	3:E:326:VAL:HA	2.01	0.42
3:L:44:ILE:HG22	3:L:326:VAL:HG12	2.01	0.42
3:L:174:ARG:HE	3:L:174:ARG:HB3	1.70	0.42
3:F:361:LEU:HD23	3:F:361:LEU:HA	1.83	0.42
2:D:79:ILE:HD11	2:D:135:ALA:HB1	2.00	0.42
1:B:93:ARG:NH1	3:J:368:ASP:OD1	2.52	0.42
1:B:8:THR:HB	1:B:59:GLU:HB2	2.00	0.42
3:F:11:ALA:HA	3:F:14:LEU:HB3	2.01	0.42
3:I:44:ILE:HG22	3:I:326:VAL:HA	2.00	0.42
3:L:167:PHE:CE1	3:L:171:LEU:HD13	2.54	0.42
3:E:15:GLN:HG3	3:E:356:TYR:CZ	2.54	0.42
3:E:29:TYR:O	3:E:34:SER:N	2.48	0.42
3:I:151:GLU:OE1	3:I:151:GLU:N	2.41	0.42
3:J:72:SER:OG	3:J:73:ARG:N	2.50	0.42
3:I:18:LEU:HD23	3:I:356:TYR:HD1	1.85	0.42
1:A:160:PHE:HA	1:A:163:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:VAL:HG12	1:B:206:GLU:HA	2.02	0.42
3:H:159:ALA:HA	3:H:162:GLU:HG2	2.01	0.42
3:H:174:ARG:HE	3:H:174:ARG:HB3	1.63	0.42
3:J:322:LYS:HE3	3:J:322:LYS:HB3	1.93	0.42
2:D:180:PRO:HA	2:D:183:ARG:HG3	2.02	0.41
3:I:39:VAL:HG22	3:I:146:GLN:HG2	2.02	0.41
3:J:37:ARG:HA	3:J:147:GLY:O	2.19	0.41
2:C:102:ASN:OD1	2:C:102:ASN:N	2.53	0.41
2:D:181:GLN:O	2:D:185:ILE:HG22	2.20	0.41
3:E:92:LEU:HD13	3:E:156:LEU:HD11	2.01	0.41
1:A:36:LEU:HB3	1:A:180:VAL:HG22	2.02	0.41
3:J:75:ASP:N	3:J:75:ASP:OD1	2.54	0.41
1:A:7:LEU:HB2	1:A:21:PHE:CZ	2.55	0.41
1:B:154:ALA:HB3	1:B:161:ARG:HG3	2.02	0.41
2:C:33:LYS:HD2	2:C:33:LYS:HA	1.94	0.41
3:F:322:LYS:HE3	3:F:322:LYS:HB3	1.94	0.41
3:H:44:ILE:HG22	3:H:326:VAL:HG12	2.03	0.41
2:C:181:GLN:O	2:C:185:ILE:HG22	2.21	0.41
1:A:105:LYS:HZ3	1:A:142:PHE:HA	1.85	0.41
1:B:18:ARG:HH21	1:B:20:VAL:HG13	1.86	0.41
3:I:163:GLU:OE2	3:I:166:ARG:NH1	2.54	0.41
2:C:152:LEU:HD23	2:C:152:LEU:HA	1.89	0.41
2:C:180:PRO:HA	2:C:183:ARG:HG3	2.02	0.41
3:E:163:GLU:OE2	3:E:166:ARG:NH1	2.53	0.41
3:G:75:ASP:OD2	3:G:322:LYS:NZ	2.49	0.41
3:H:150:PRO:HB3	3:H:333:PRO:HG2	2.03	0.41
2:D:33:LYS:HD2	2:D:33:LYS:HA	1.91	0.41
3:H:23:MET:O	3:H:27:THR:OG1	2.27	0.41
2:D:60:LEU:HB3	2:D:61:PHE:CD1	2.56	0.40
2:D:208:PRO:O	2:D:211:LEU:HB2	2.20	0.40
1:A:6:ASN:HA	1:A:24:LEU:O	2.22	0.40
1:B:161:ARG:O	1:B:165:ARG:HD3	2.21	0.40
1:A:148:LEU:HD13	1:A:148:LEU:HA	1.96	0.40
2:C:14:ARG:HB3	2:C:19:ILE:HD11	2.04	0.40
3:E:86:MET:HE2	3:E:123:LEU:HD22	2.03	0.40
3:J:39:VAL:HG21	3:J:338:TYR:CD2	2.53	0.40
1:A:106:VAL:HA	1:A:109:VAL:HG12	2.03	0.40
1:A:140:MET:O	1:A:171:ARG:NH1	2.41	0.40
2:C:74:TYR:CE1	2:C:78:LEU:HD13	2.57	0.40
3:F:3:MET:HG2	3:F:4:LYS:N	2.23	0.40
3:L:38:TYR:N	3:L:147:GLY:O	2.51	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	210/234 (90%)	200 (95%)	10 (5%)	0	100	100
1	B	210/234 (90%)	203 (97%)	7 (3%)	0	100	100
2	C	253/274 (92%)	244 (96%)	9 (4%)	0	100	100
2	D	253/274 (92%)	241 (95%)	12 (5%)	0	100	100
3	E	192/390 (49%)	188 (98%)	4 (2%)	0	100	100
3	F	198/390 (51%)	189 (96%)	9 (4%)	0	100	100
3	G	203/390 (52%)	198 (98%)	5 (2%)	0	100	100
3	H	168/390 (43%)	164 (98%)	4 (2%)	0	100	100
3	I	192/390 (49%)	188 (98%)	4 (2%)	0	100	100
3	J	198/390 (51%)	190 (96%)	8 (4%)	0	100	100
3	K	203/390 (52%)	199 (98%)	4 (2%)	0	100	100
3	L	168/390 (43%)	164 (98%)	4 (2%)	0	100	100
All	All	2448/4136 (59%)	2368 (97%)	80 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/194 (92%)	163 (92%)	15 (8%)	11	38
1	B	178/194 (92%)	163 (92%)	15 (8%)	11	38
2	C	215/232 (93%)	208 (97%)	7 (3%)	38	69
2	D	215/232 (93%)	209 (97%)	6 (3%)	43	73
3	E	180/325 (55%)	176 (98%)	4 (2%)	52	78
3	F	186/325 (57%)	179 (96%)	7 (4%)	33	66
3	G	189/325 (58%)	187 (99%)	2 (1%)	73	89
3	H	158/325 (49%)	155 (98%)	3 (2%)	57	81
3	I	180/325 (55%)	176 (98%)	4 (2%)	52	78
3	J	186/325 (57%)	180 (97%)	6 (3%)	39	69
3	K	189/325 (58%)	187 (99%)	2 (1%)	73	89
3	L	158/325 (49%)	153 (97%)	5 (3%)	39	69
All	All	2212/3452 (64%)	2136 (97%)	76 (3%)	40	69

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	TRP
1	A	17	ARG
1	A	18	ARG
1	A	21	PHE
1	A	28	PHE
1	A	126	TYR
1	A	127	SER
1	A	146	TYR
1	A	160	PHE
1	A	165	ARG
1	A	168	PHE
1	A	169	ASP
1	A	191	CYS
1	A	198	ASP
1	A	201	GLN
1	B	18	ARG
1	B	21	PHE
1	B	25	ASN
1	B	28	PHE
1	B	57	PRO
1	B	69	SER
1	B	126	TYR

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Mol	Chain	Res	Type
1	B	145	ASP
1	B	160	PHE
1	B	165	ARG
1	B	168	PHE
1	B	169	ASP
1	B	183	ASN
1	B	184	MET
1	B	201	GLN
2	C	40	TRP
2	C	97	GLU
2	C	102	ASN
2	C	132	TYR
2	C	204	HIS
2	C	224	GLU
2	C	235	ARG
2	D	40	TRP
2	D	74	TYR
2	D	97	GLU
2	D	102	ASN
2	D	132	TYR
2	D	224	GLU
3	E	20	TYR
3	E	75	ASP
3	E	112	ARG
3	E	135	ASP
3	F	20	TYR
3	F	73	ARG
3	F	75	ASP
3	F	166	ARG
3	F	175	MET
3	F	321	LEU
3	F	338	TYR
3	G	128	SER
3	G	352	CYS
3	H	48	GLN
3	H	77	CYS
3	H	177	ARG
3	I	47	ARG
3	I	75	ASP
3	I	112	ARG
3	I	135	ASP
3	J	20	TYR

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Mol	Chain	Res	Type
3	J	134	MET
3	J	166	ARG
3	J	175	MET
3	J	321	LEU
3	J	338	TYR
3	K	128	SER
3	K	338	TYR
3	L	24	LEU
3	L	30	PHE
3	L	75	ASP
3	L	77	CYS
3	L	177	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	6	ASN
3	E	344	ASN
3	H	94	GLN
3	I	344	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.

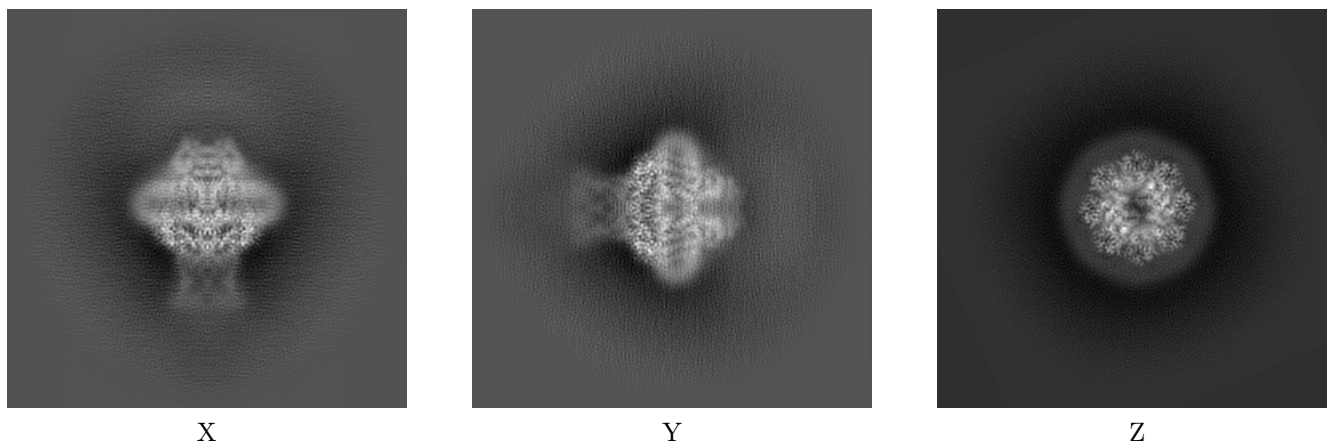
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41601. 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](#)

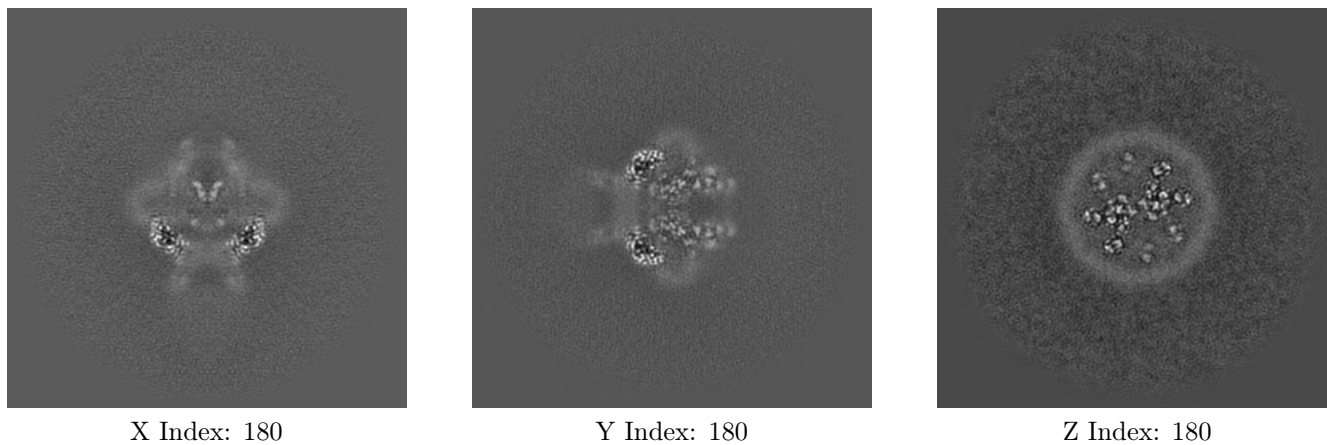
6.1.1 Primary map



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

6.2 Central slices [i](#)

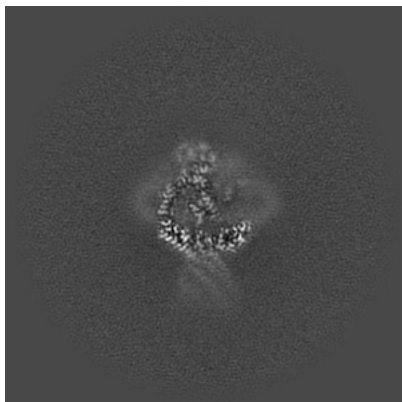
6.2.1 Primary map



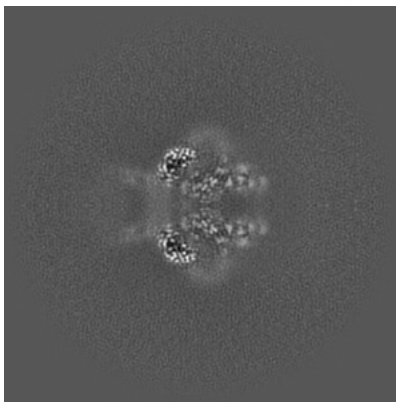
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

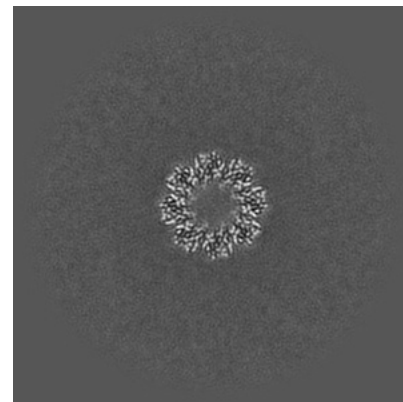
6.3.1 Primary map



X Index: 156



Y Index: 180

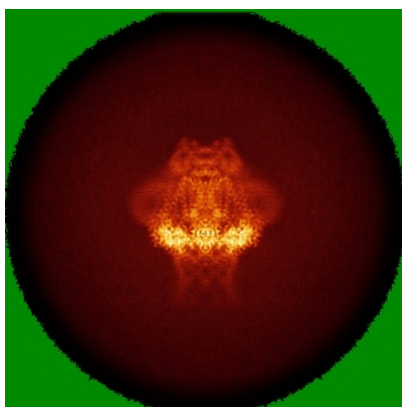


Z Index: 152

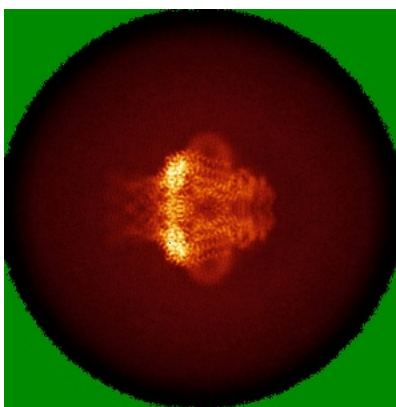
The images above show the largest variance slices of the map in three orthogonal directions.

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

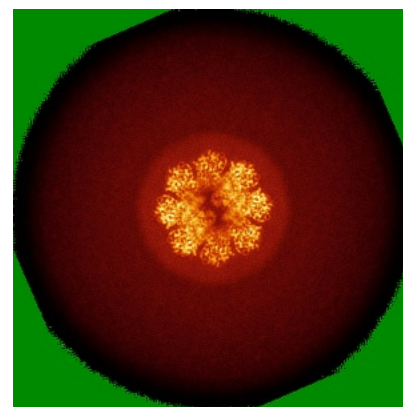
6.4.1 Primary map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

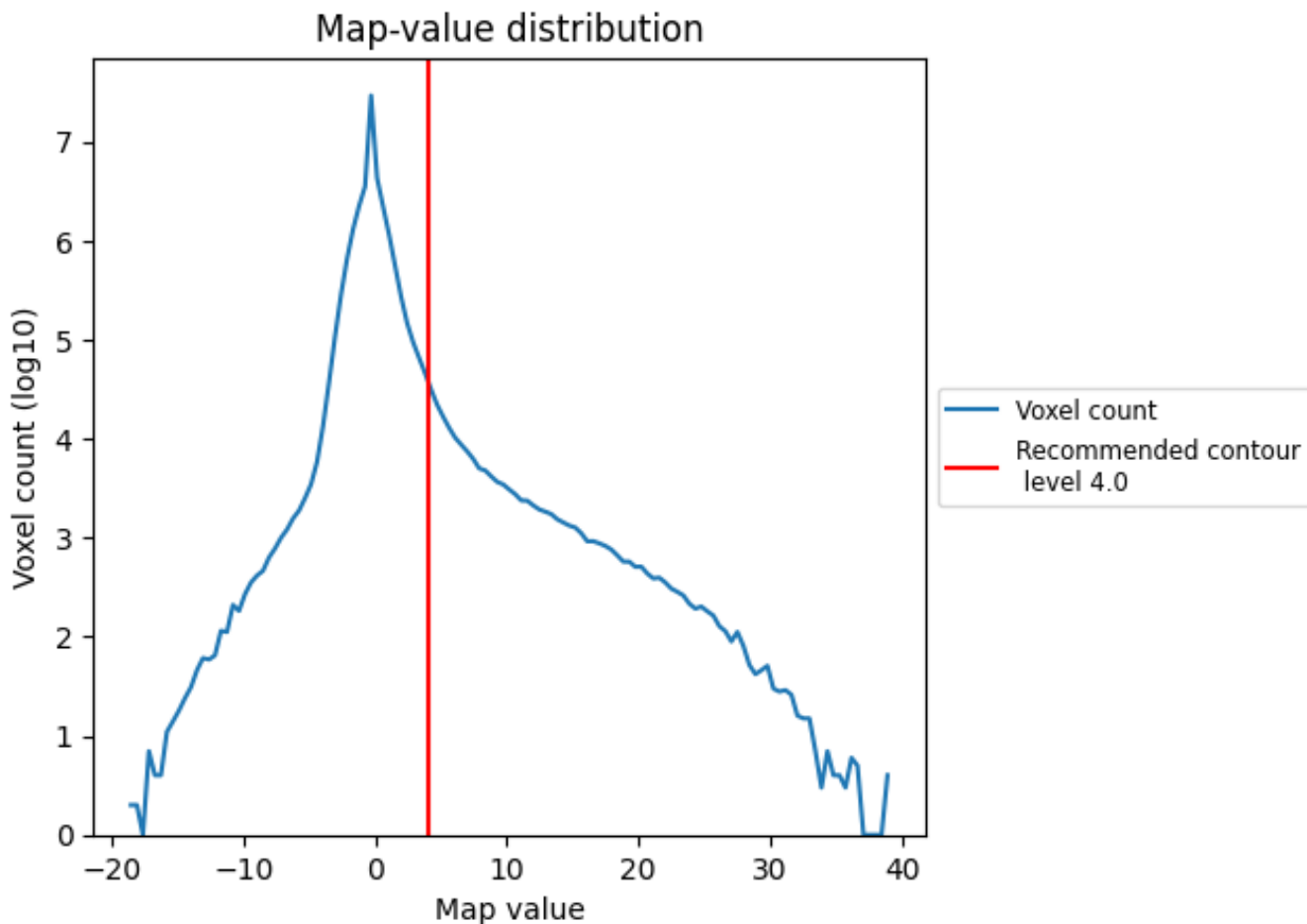
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

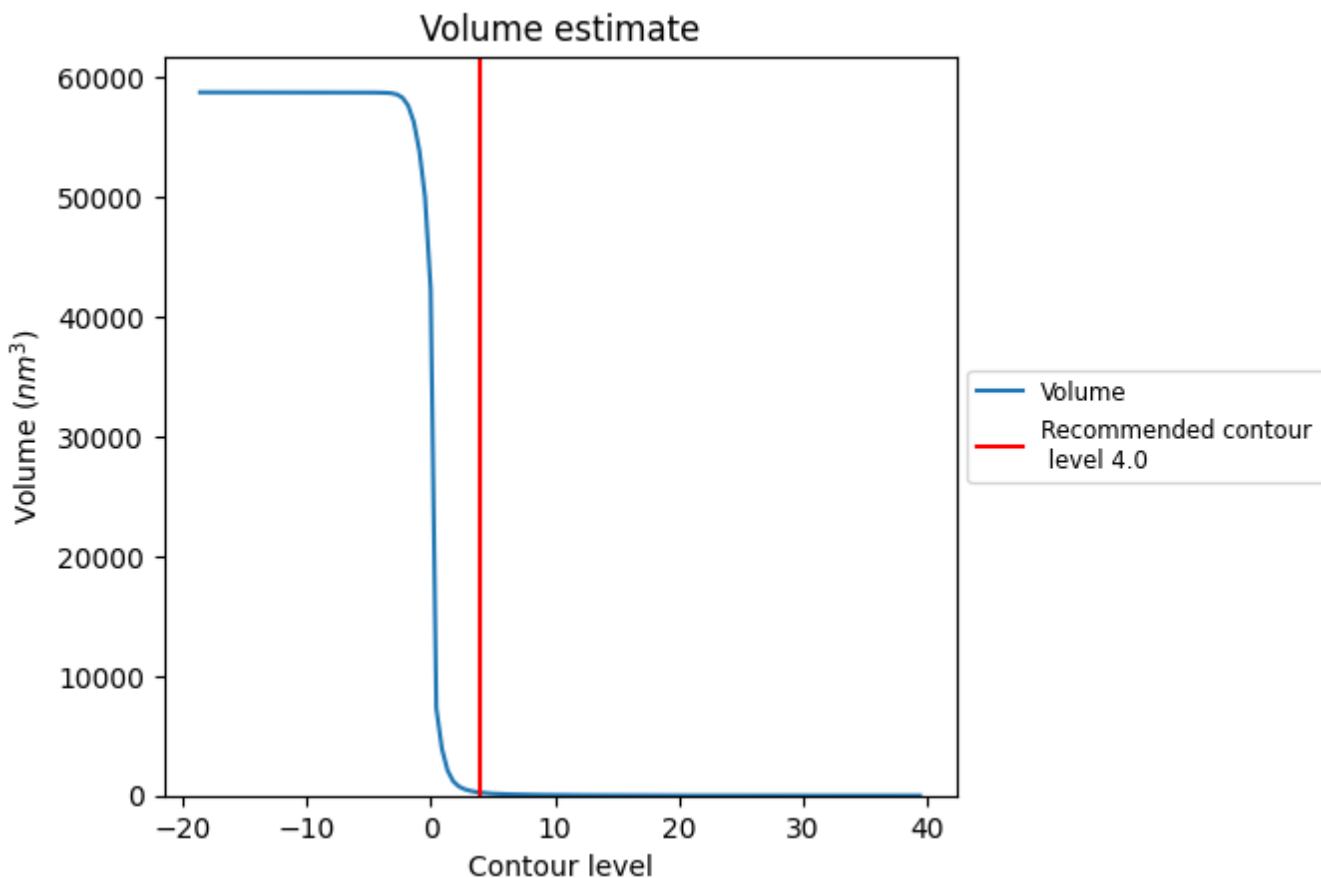
This section contains the results of statistical analysis of the map.

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.

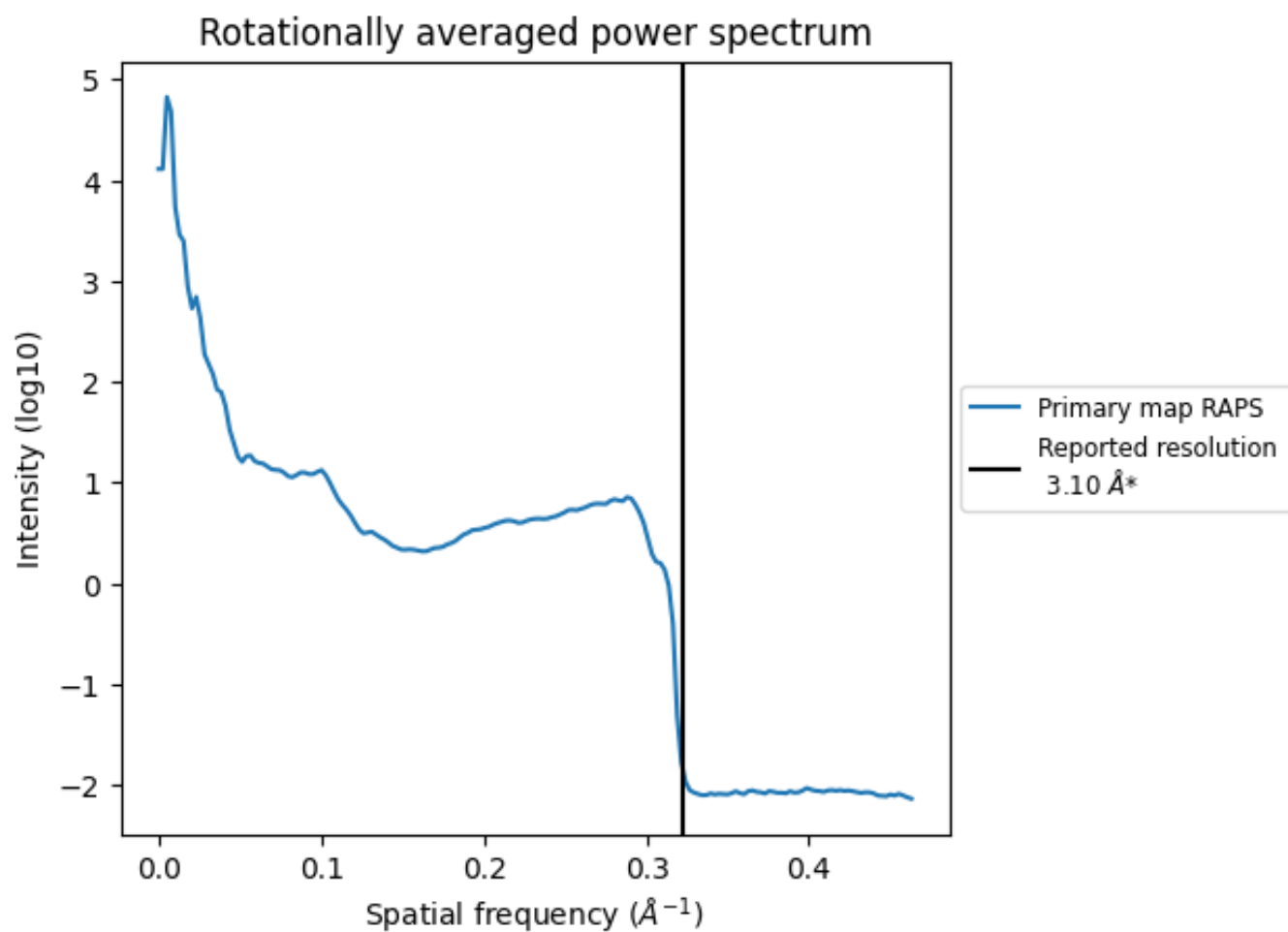
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247 nm³; this corresponds to an approximate mass of 224 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

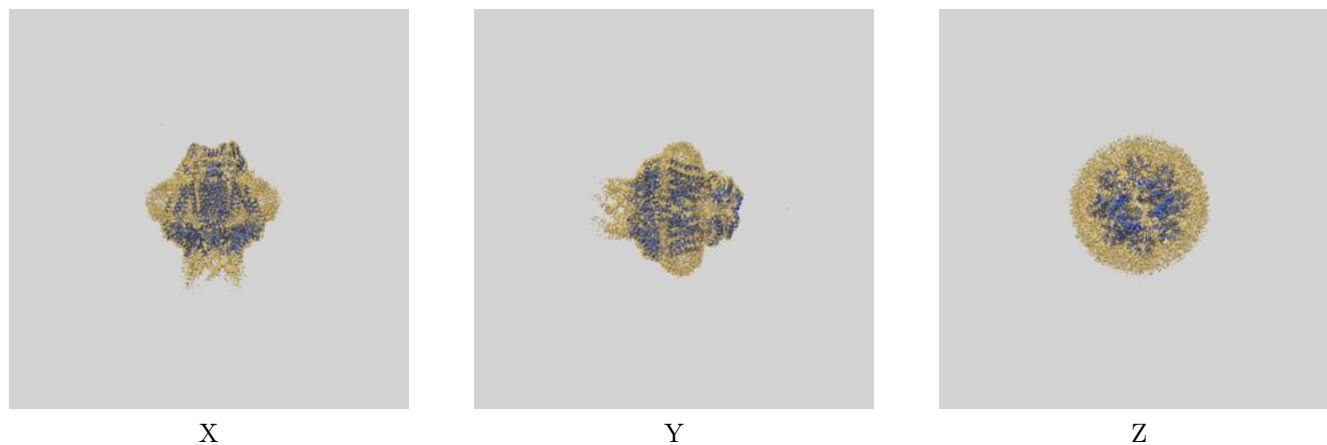
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

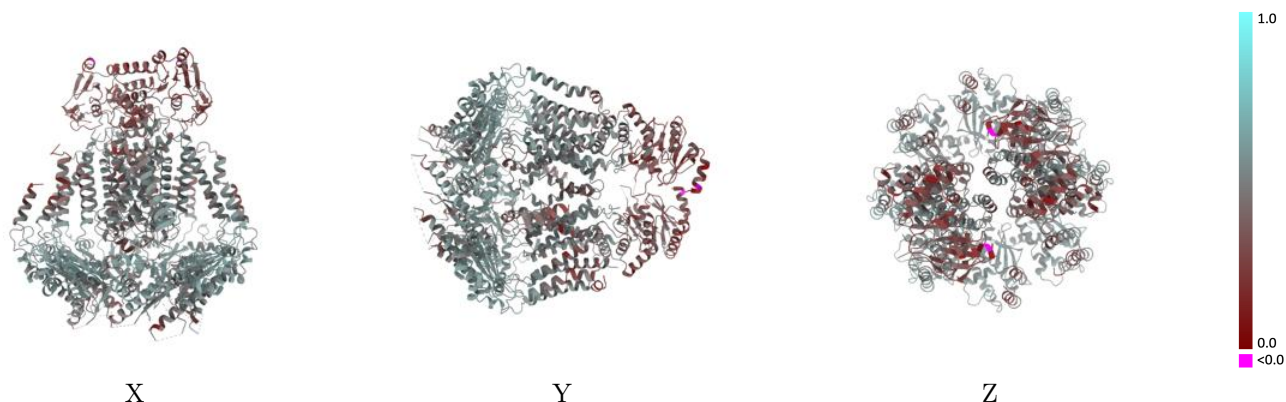
This section contains information regarding the fit between EMDB map EMD-41601 and PDB model 8TSW. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



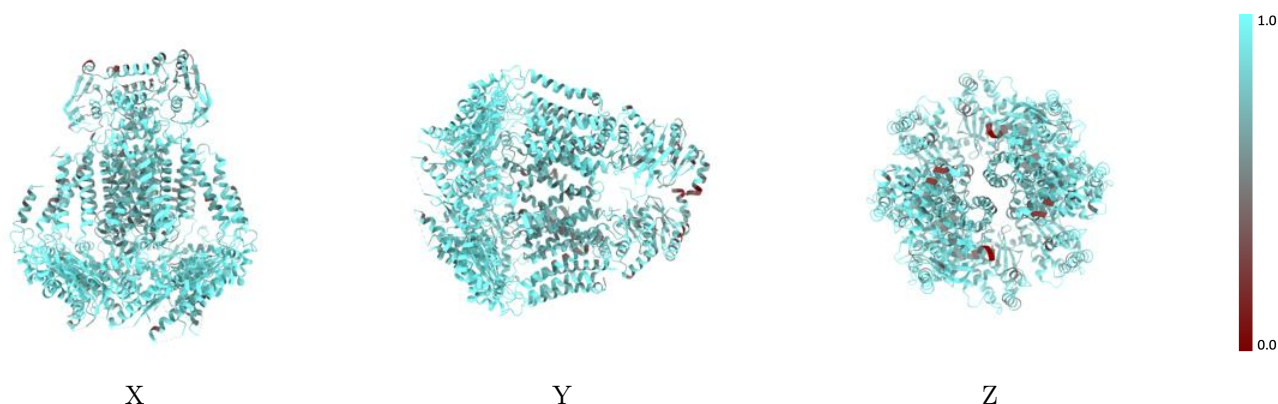
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



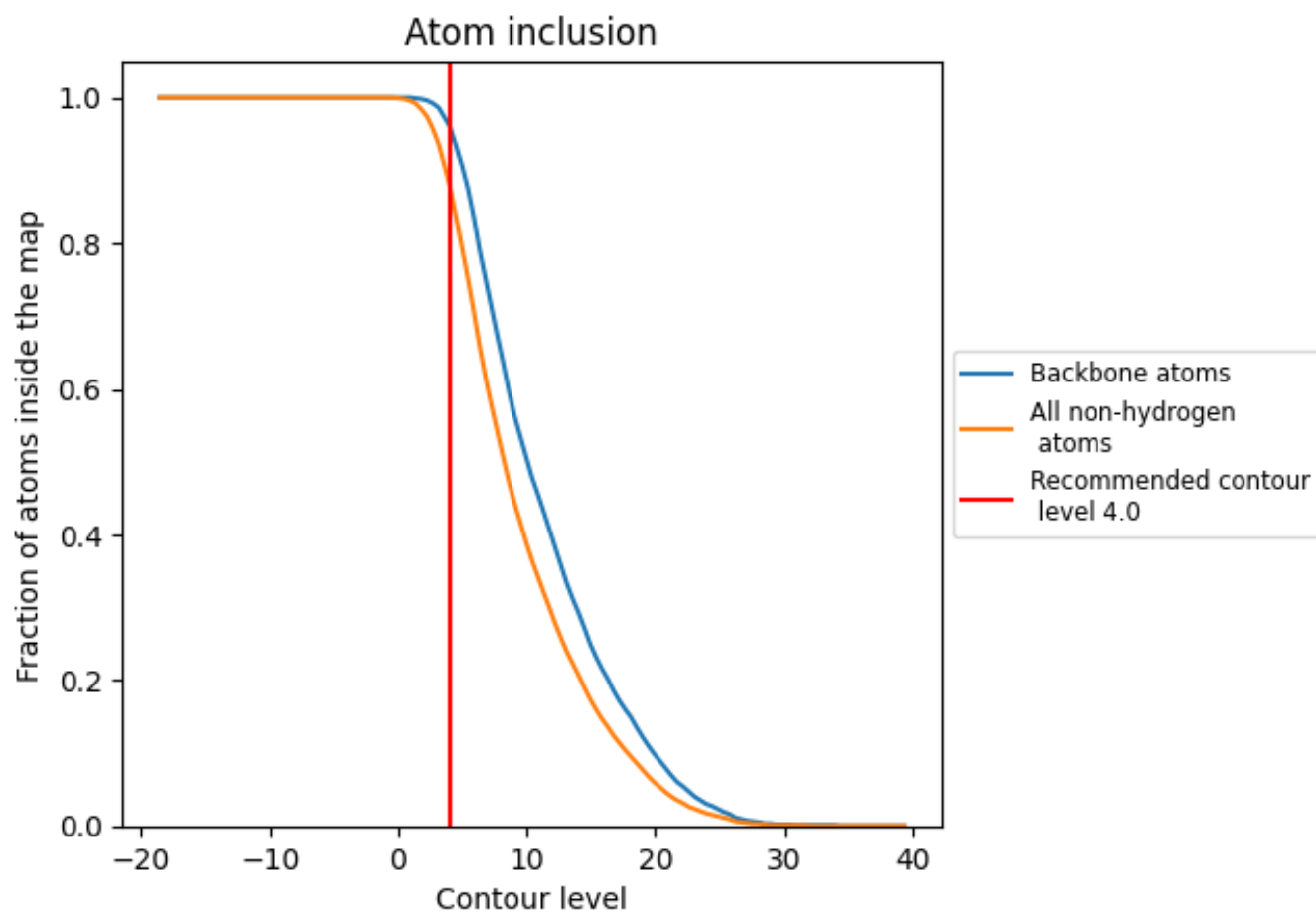
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.0).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 88% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8800	 0.4760
A	 0.8020	 0.3150
B	 0.7970	 0.3190
C	 0.8400	 0.4830
D	 0.8390	 0.4860
E	 0.9040	 0.5060
F	 0.9250	 0.5160
G	 0.9260	 0.5240
H	 0.8930	 0.5110
I	 0.9070	 0.5080
J	 0.9220	 0.5160
K	 0.9270	 0.5230
L	 0.8960	 0.5100

