



# wwPDB EM Validation Summary Report ⓘ

May 25, 2025 – 01:02 PM EDT

PDB ID : 8TSH / pdb\_00008tsh  
EMDB ID : EMD-41592  
Title : S. thermodepolymerans KpsMT(E151Q)-KpsE in complex with ATP  
Authors : Kuklewicz, J.; Zimmer, J.  
Deposited on : 2023-08-11  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

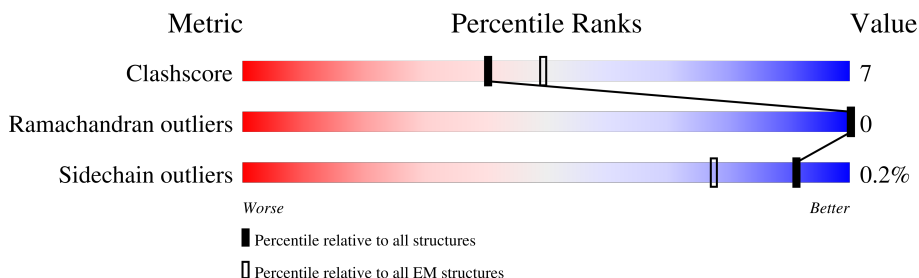
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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.





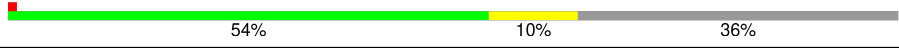

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	73% 20% 7%
1	B	234	74% 19% 7%
2	C	274	75% 19% 5%
2	D	274	76% 18% 7%
3	E	390	52% 14% 35%
3	F	390	55% 13% 32%
3	G	390	56% 11% 33%
3	H	390	57% 8% 35%

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Mol	Chain	Length	Quality of chain
3	I	390	 55% 9% 36%
3	J	390	 56% 11% 33%
3	K	390	 54% 10% 36%
3	L	390	 56% 9% 35%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24254 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
1	A	217	Total	C	N	O	S	0	0
			1708	1081	298	318	11		
1	B	217	Total	C	N	O	S	0	0
			1708	1081	298	318	11		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	GLN	GLU	engineered mutation	UNP A0A2S5T4B3
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	151	GLN	GLU	engineered mutation	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
2	C	259	Total	C	N	O	S	0	0
			2062	1383	347	325	7		

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

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
3	E	255	Total	C	N	O	S	0	0
			2073	1333	358	374	8		
3	F	265	Total	C	N	O	S	0	0
			2158	1385	376	389	8		
3	G	263	Total	C	N	O	S	0	0
			2140	1374	372	386	8		
3	H	254	Total	C	N	O	S	0	0
			2065	1326	359	372	8		
3	I	251	Total	C	N	O	S	0	0
			2032	1307	349	368	8		
3	J	260	Total	C	N	O	S	0	0
			2115	1359	366	382	8		
3	K	251	Total	C	N	O	S	0	0
			2042	1308	354	372	8		
3	L	253	Total	C	N	O	S	0	0
			2054	1320	356	370	8		

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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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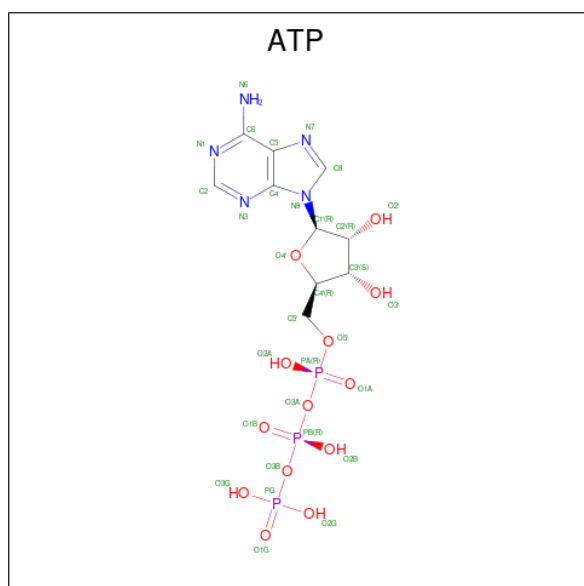
Chain	Residue	Modelled	Actual	Comment	Reference
J	377	SER	-	expression tag	UNP A0A2S5T4A0
J	378	HIS	-	expression tag	UNP A0A2S5T4A0
J	379	HIS	-	expression tag	UNP A0A2S5T4A0
J	380	HIS	-	expression tag	UNP A0A2S5T4A0
J	381	HIS	-	expression tag	UNP A0A2S5T4A0
J	382	HIS	-	expression tag	UNP A0A2S5T4A0
J	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

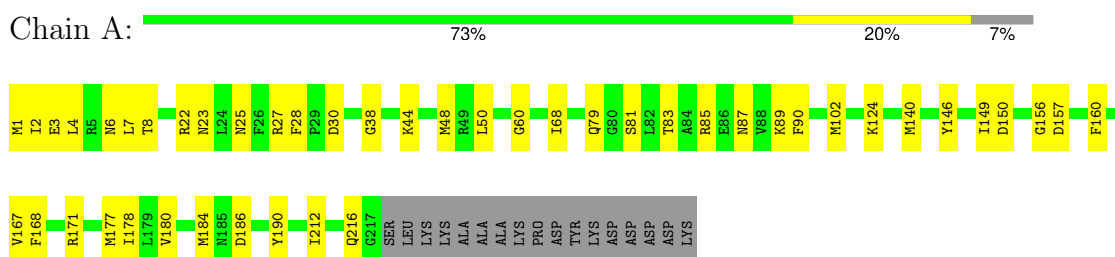
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula:  $Mg$ ) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	Mg 1	0
5	B	1	Total 1	Mg 1	0

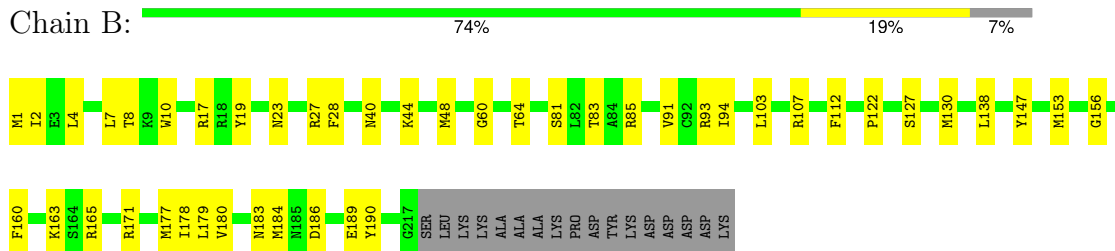
### 3 Residue-property plots

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.

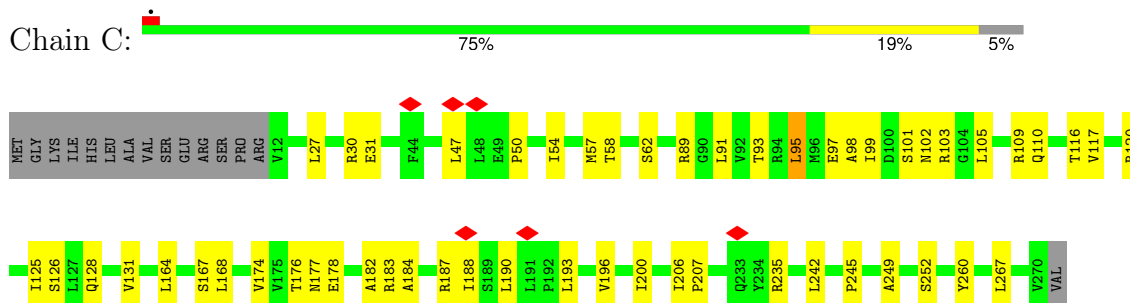
- Molecule 1: ABC transporter ATP-binding protein



- Molecule 1: ABC transporter ATP-binding protein



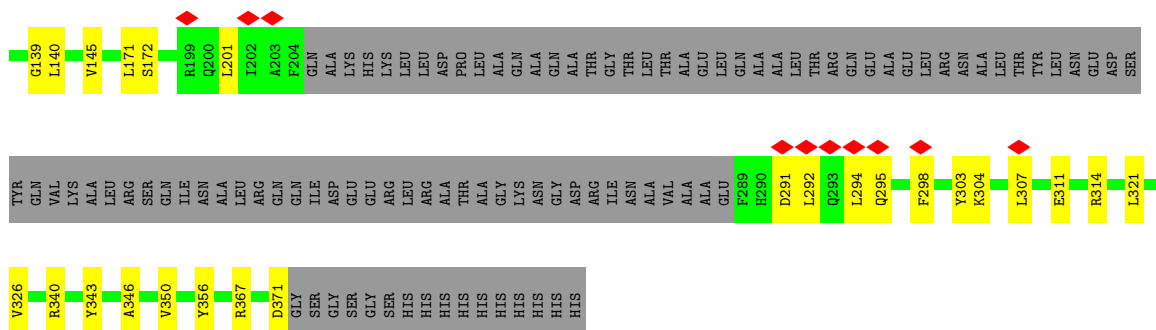
- Molecule 2: Transport permease protein



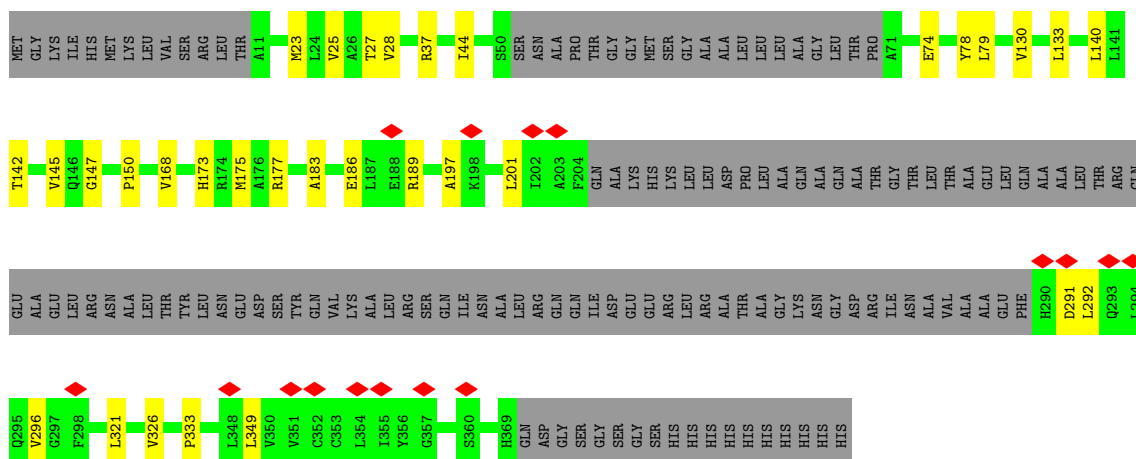
- Molecule 2: Transport permease protein



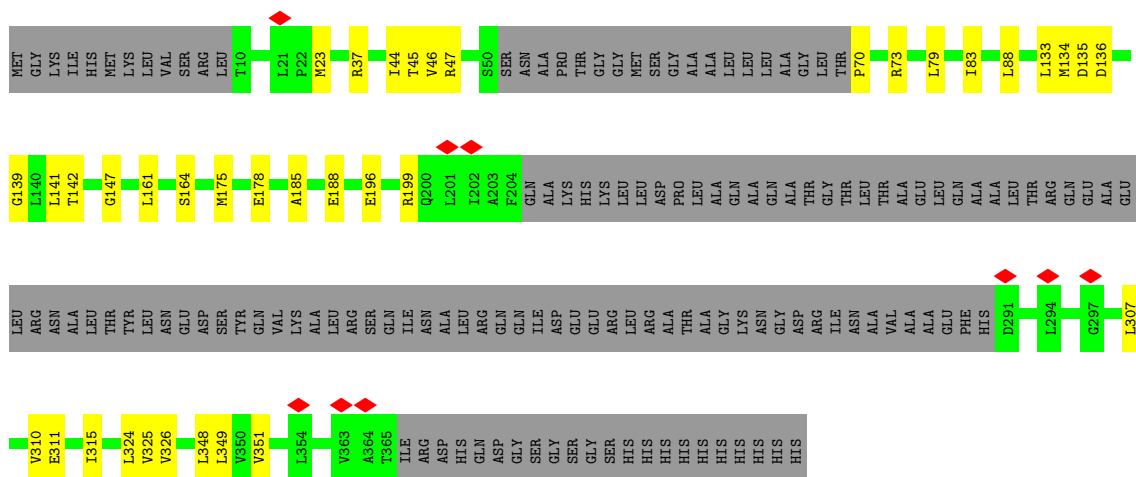




- Molecule 3: Capsular biosynthesis protein



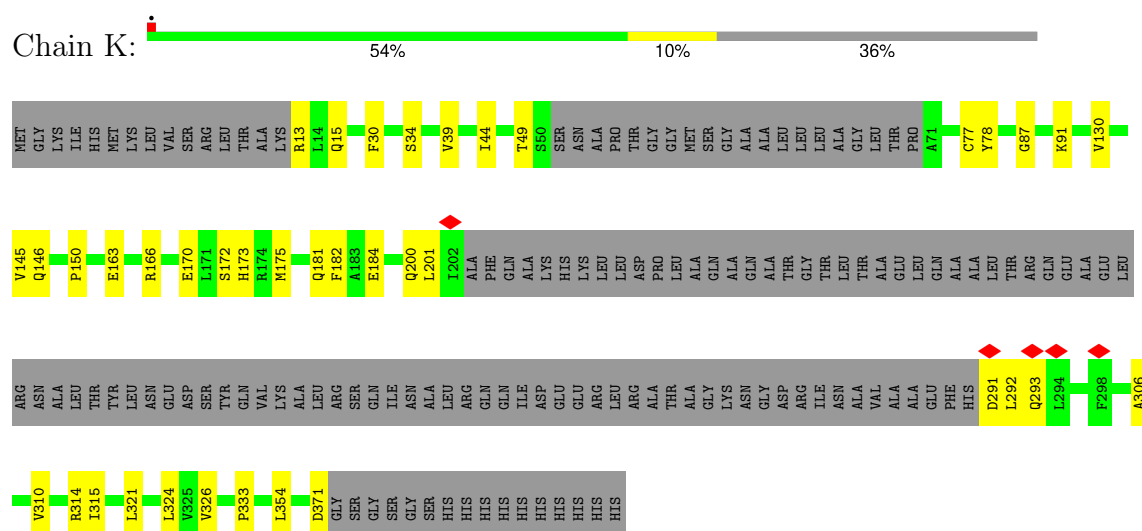
- Molecule 3: Capsular biosynthesis protein



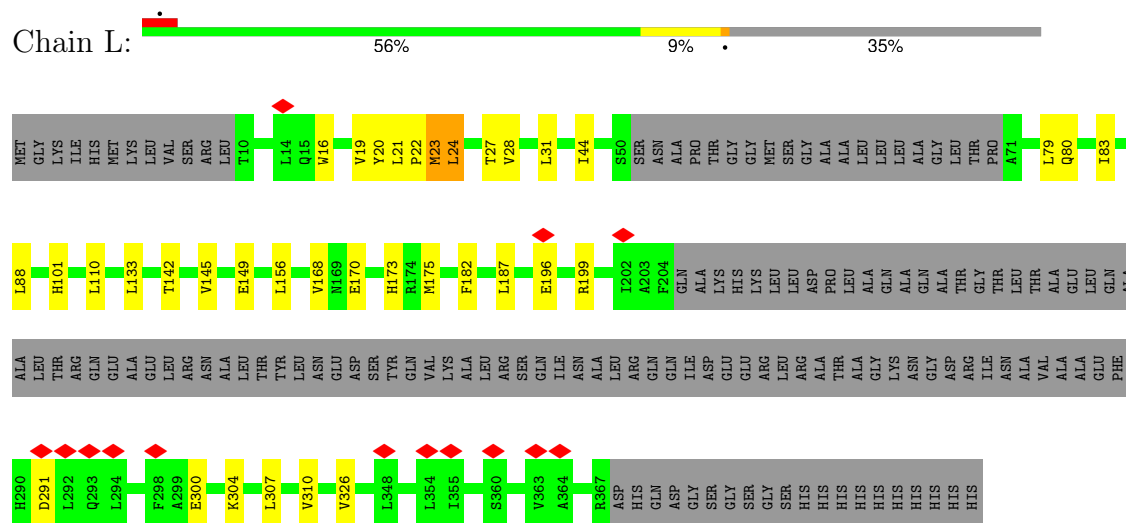
- Molecule 3: Capsular biosynthesis protein



- Molecule 3: Capsular biosynthesis protein



- Molecule 3: Capsular biosynthesis protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36731	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	36.066	Depositor
Minimum map value	-16.932	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.862	Depositor
Recommended contour level	4	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

### 5.1 Standard geometry

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

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	0.10	0/1743	0.27	0/2351
1	B	0.10	0/1743	0.29	0/2351
2	C	0.13	0/2118	0.33	0/2887
2	D	0.12	0/2089	0.30	0/2848
3	E	0.12	0/2113	0.28	0/2863
3	F	0.21	0/2199	0.31	0/2978
3	G	0.13	0/2181	0.29	0/2955
3	H	0.12	0/2105	0.29	0/2852
3	I	0.13	0/2071	0.30	0/2807
3	J	0.13	0/2157	0.31	0/2923
3	K	0.13	0/2080	0.30	0/2819
3	L	0.24	0/2093	0.39	0/2836
All	All	0.15	0/24692	0.31	0/33470

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1708	0	1670	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1708	0	1669	28	0
2	C	2062	0	2187	39	0
2	D	2033	0	2151	37	0
3	E	2073	0	2090	34	0
3	F	2158	0	2180	31	0
3	G	2140	0	2159	31	0
3	H	2065	0	2081	20	0
3	I	2032	0	2054	22	0
3	J	2115	0	2129	31	0
3	K	2042	0	2055	26	0
3	L	2054	0	2077	24	0
4	A	31	0	12	0	0
4	B	31	0	12	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	24254	0	24526	331	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.

The worst 5 of 331 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:C:95:LEU:HD13	2:C:117:VAL:HB	1.70	0.73
3:K:200:GLN:HE22	3:K:292:LEU:HD22	1.54	0.72
3:E:187:LEU:HD11	3:E:307:LEU:HD22	1.72	0.70
3:F:28:VAL:O	3:F:32:VAL:HB	1.92	0.70
1:B:8:THR:HG22	1:B:23:ASN:H	1.57	0.69

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	215/234 (92%)	207 (96%)	8 (4%)	0	100	100
1	B	215/234 (92%)	205 (95%)	10 (5%)	0	100	100
2	C	257/274 (94%)	248 (96%)	9 (4%)	0	100	100
2	D	253/274 (92%)	247 (98%)	6 (2%)	0	100	100
3	E	249/390 (64%)	244 (98%)	5 (2%)	0	100	100
3	F	259/390 (66%)	251 (97%)	8 (3%)	0	100	100
3	G	257/390 (66%)	251 (98%)	6 (2%)	0	100	100
3	H	248/390 (64%)	244 (98%)	4 (2%)	0	100	100
3	I	245/390 (63%)	242 (99%)	3 (1%)	0	100	100
3	J	254/390 (65%)	249 (98%)	5 (2%)	0	100	100
3	K	245/390 (63%)	243 (99%)	2 (1%)	0	100	100
3	L	247/390 (63%)	242 (98%)	5 (2%)	0	100	100
All	All	2944/4136 (71%)	2873 (98%)	71 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	180/194 (93%)	180 (100%)	0	100	100
1	B	180/194 (93%)	180 (100%)	0	100	100
2	C	219/232 (94%)	218 (100%)	1 (0%)	86	92
2	D	215/232 (93%)	215 (100%)	0	100	100
3	E	221/325 (68%)	221 (100%)	0	100	100
3	F	231/325 (71%)	231 (100%)	0	100	100
3	G	229/325 (70%)	229 (100%)	0	100	100
3	H	220/325 (68%)	220 (100%)	0	100	100
3	I	217/325 (67%)	217 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	226/325 (70%)	225 (100%)	1 (0%)	89	94
3	K	219/325 (67%)	219 (100%)	0	100	100
3	L	219/325 (67%)	216 (99%)	3 (1%)	62	81
All	All	2576/3452 (75%)	2571 (100%)	5 (0%)	91	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	95	LEU
3	J	296	VAL
3	L	23	MET
3	L	24	LEU
3	L	110	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	157	ASN
3	L	119	GLN
3	F	48	GLN
3	K	200	GLN
3	E	200	GLN

### 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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ATP	A	301	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
4	ATP	B	301	5	28,33,33	0.65	0	34,52,52	0.60	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	301	-	-	7/18/38/38	0/3/3/3
4	ATP	B	301	5	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	ATP	C5-C6-N6	2.31	123.83	120.31
4	B	301	ATP	C5-C6-N6	2.30	123.82	120.31

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

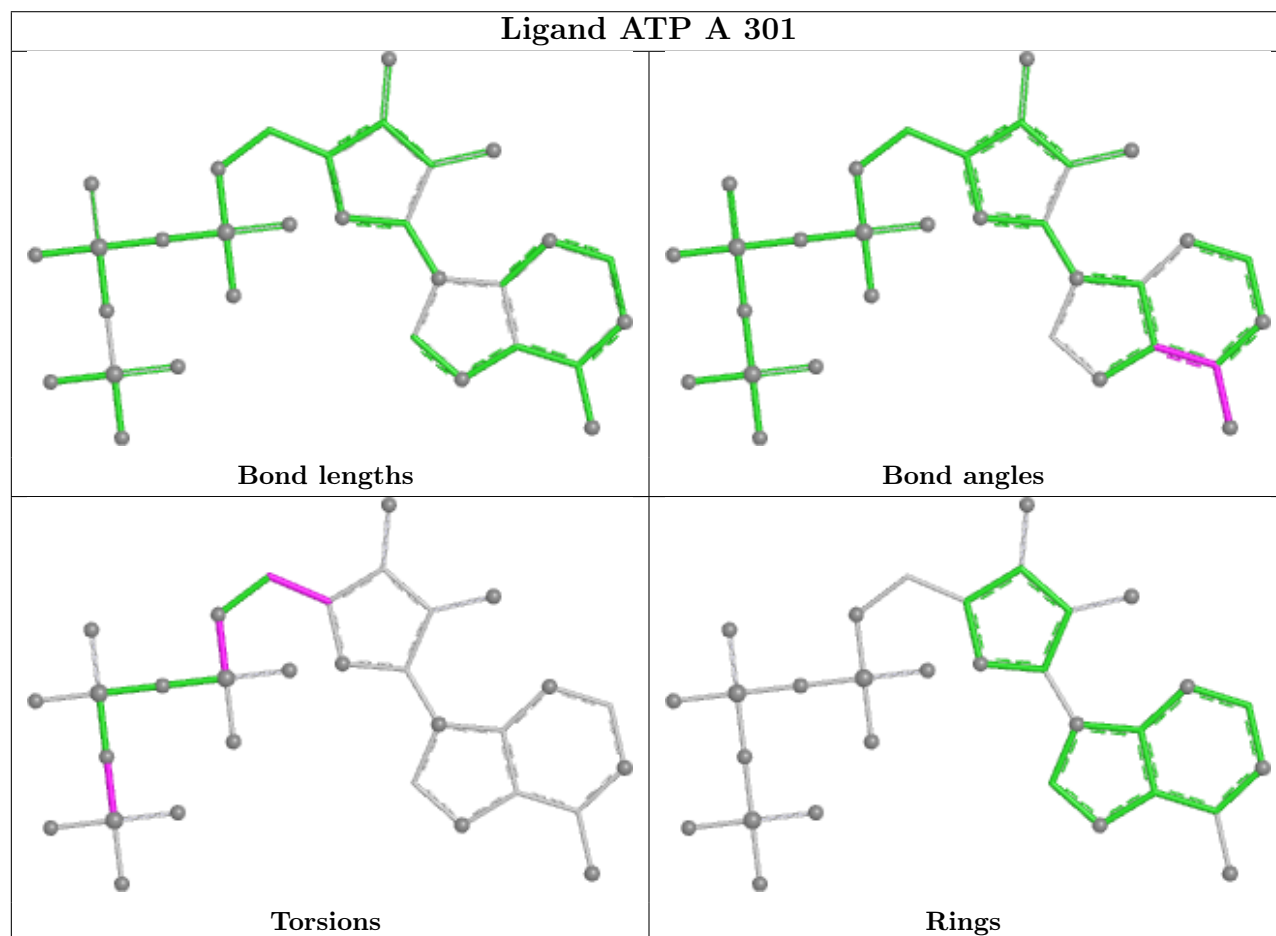
Mol	Chain	Res	Type	Atoms
4	A	301	ATP	PB-O3B-PG-O2G
4	A	301	ATP	C5'-O5'-PA-O3A
4	B	301	ATP	C5'-O5'-PA-O3A
4	A	301	ATP	O4'-C4'-C5'-O5'
4	B	301	ATP	O4'-C4'-C5'-O5'

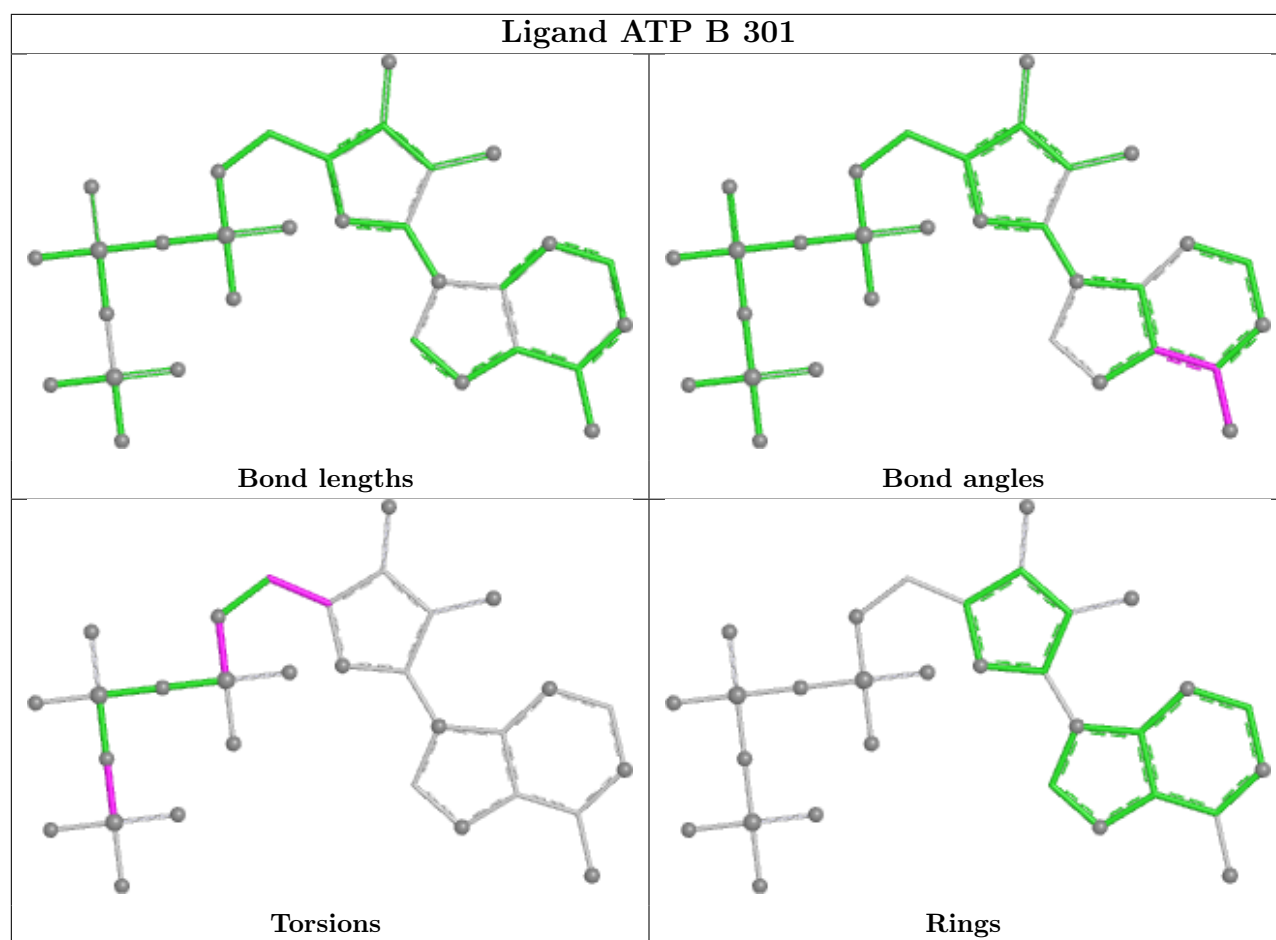
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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.

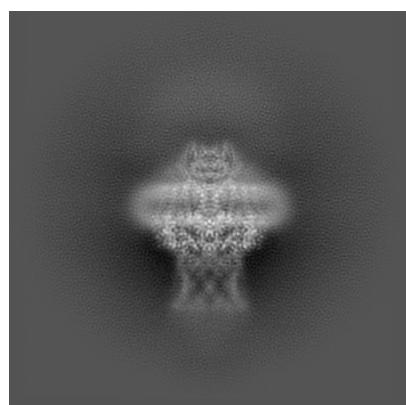
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41592. These allow visual inspection of the internal detail of the map and identification of artifacts.

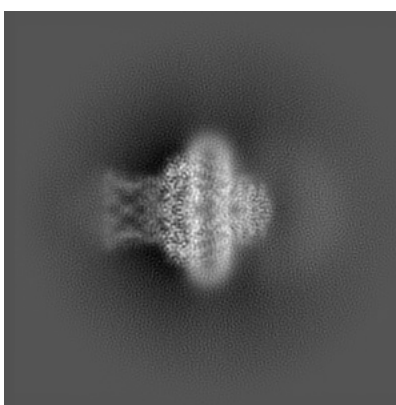
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

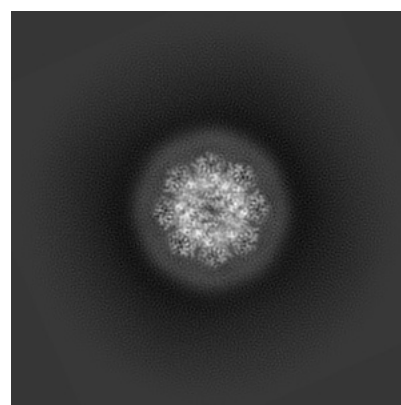
#### 6.1.1 Primary map



X



Y

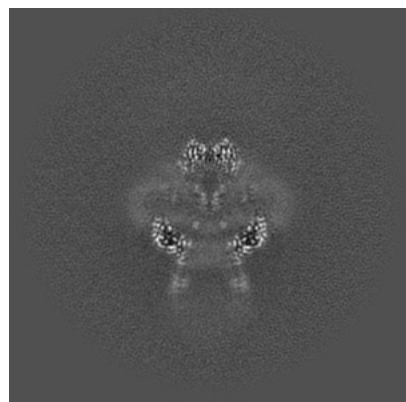


Z

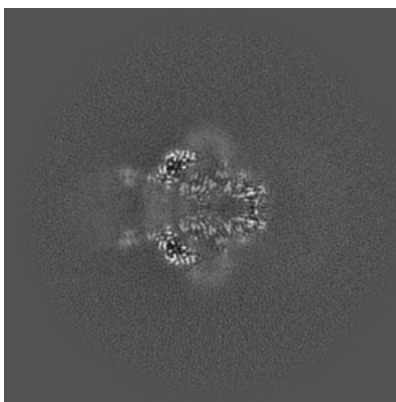
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

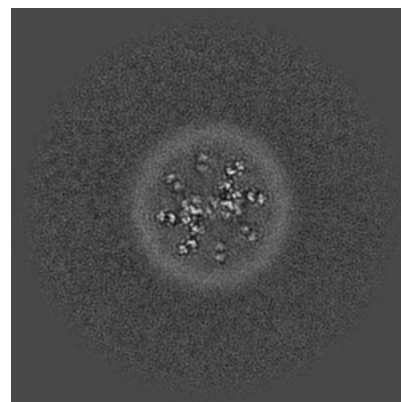
#### 6.2.1 Primary map



X Index: 180



Y Index: 180



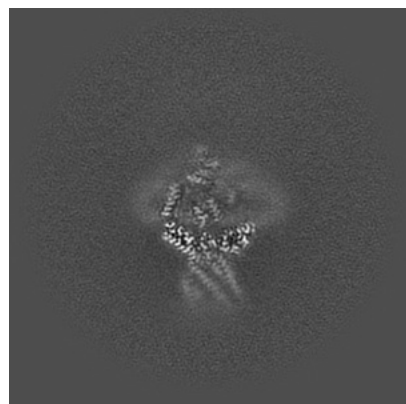
Z Index: 180



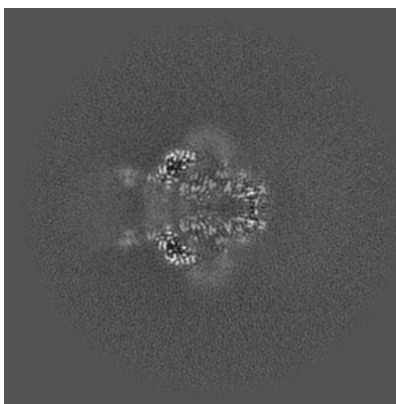
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

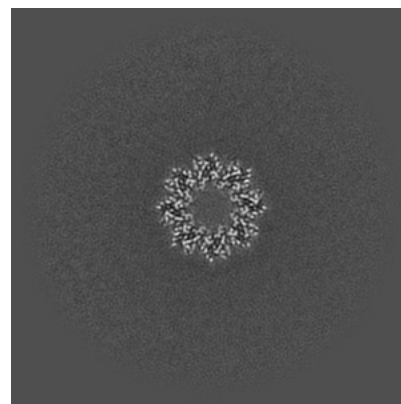
### 6.3.1 Primary map



X Index: 156



Y Index: 180

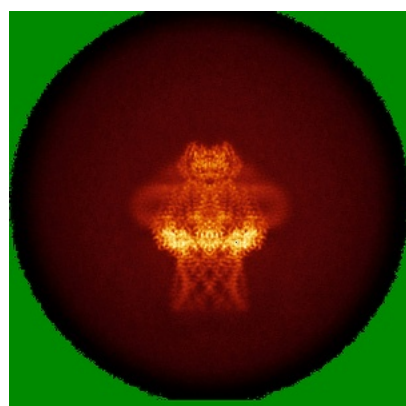


Z Index: 151

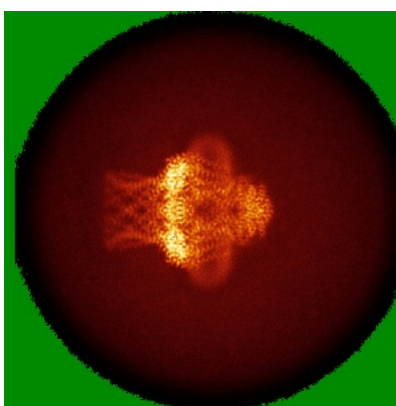
The images above show the largest variance slices of the map in three orthogonal directions.

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

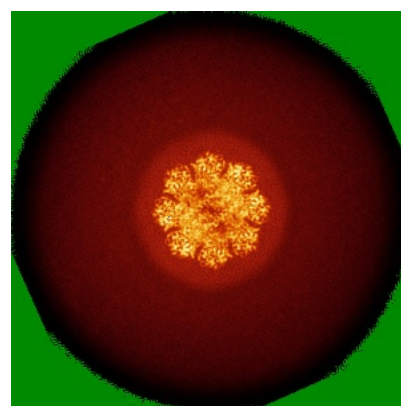
### 6.4.1 Primary map



X



Y



Z

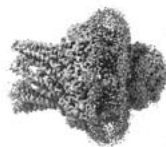
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 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.

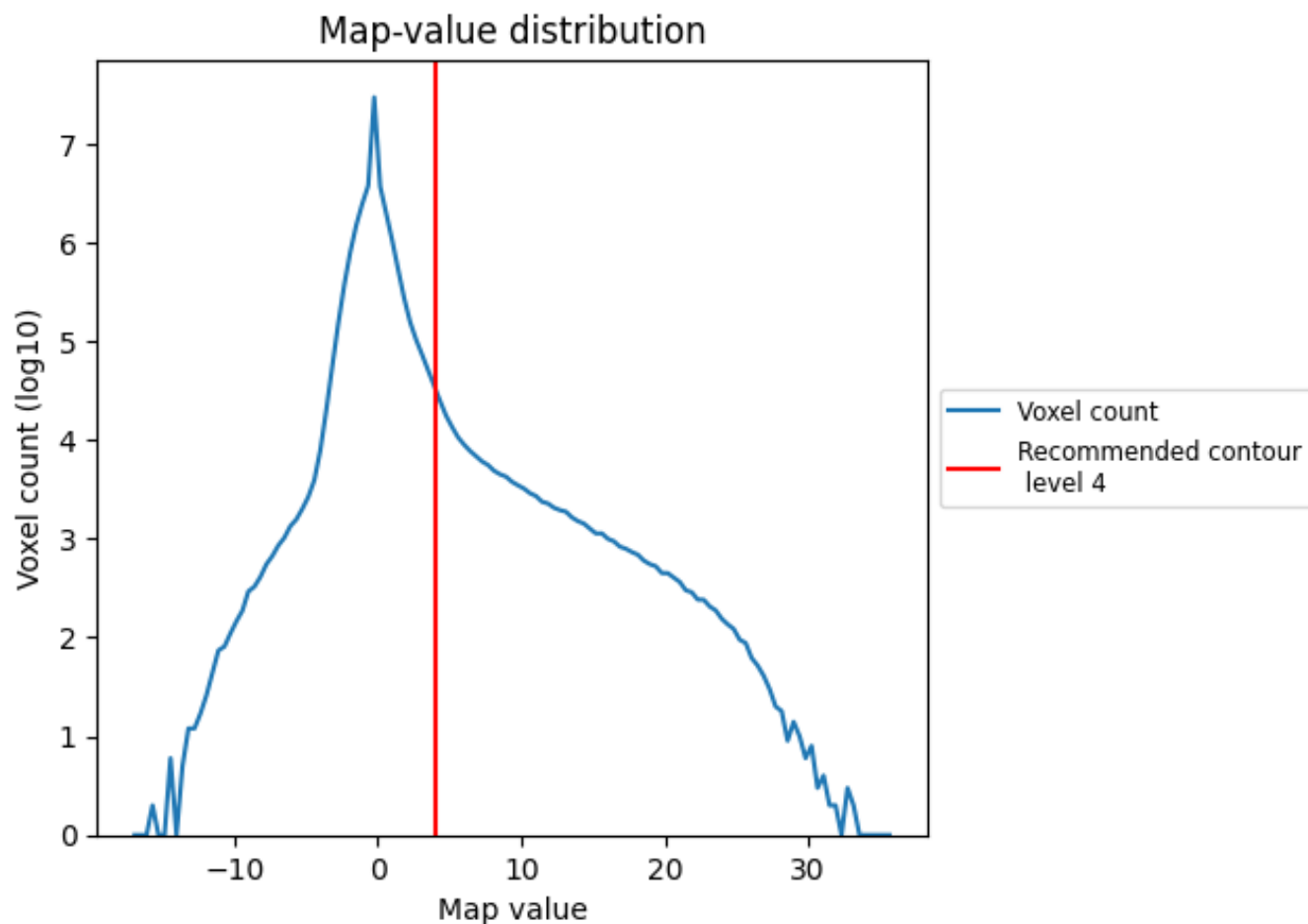
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

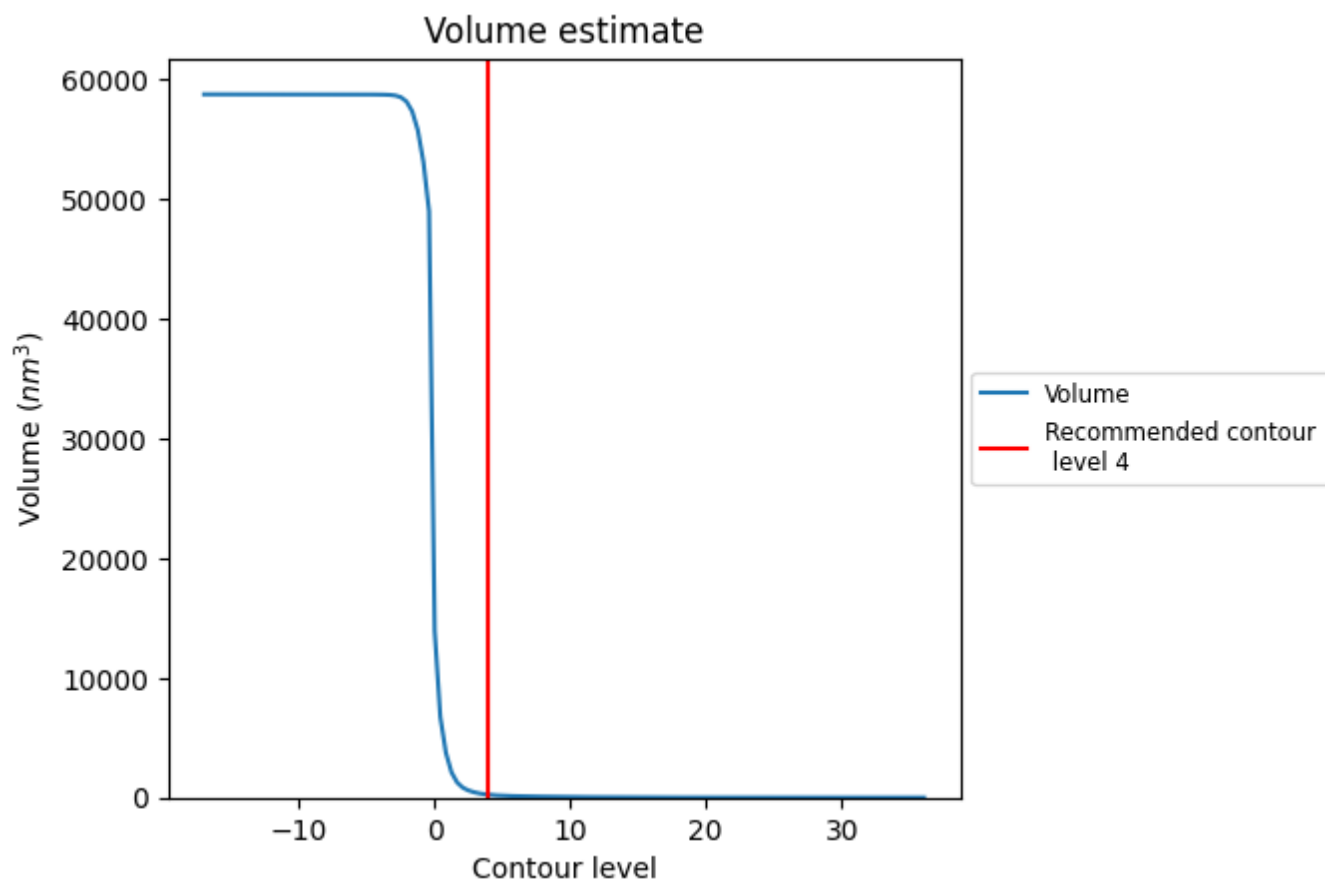
This section contains the results of statistical analysis of the map.

### 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.

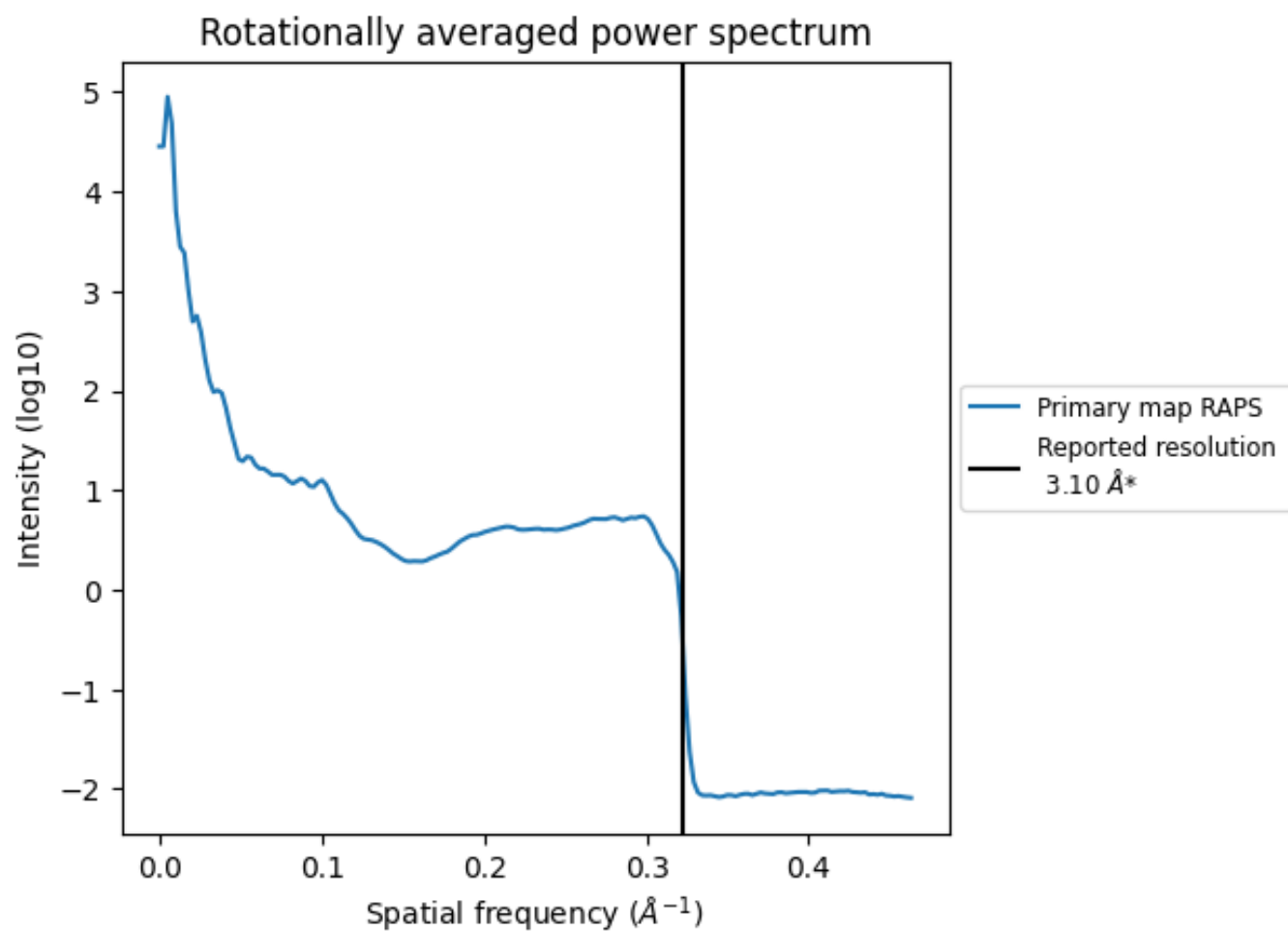
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 241  $\text{nm}^3$ ; this corresponds to an approximate mass of 218 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  $\text{\AA}^{-1}$

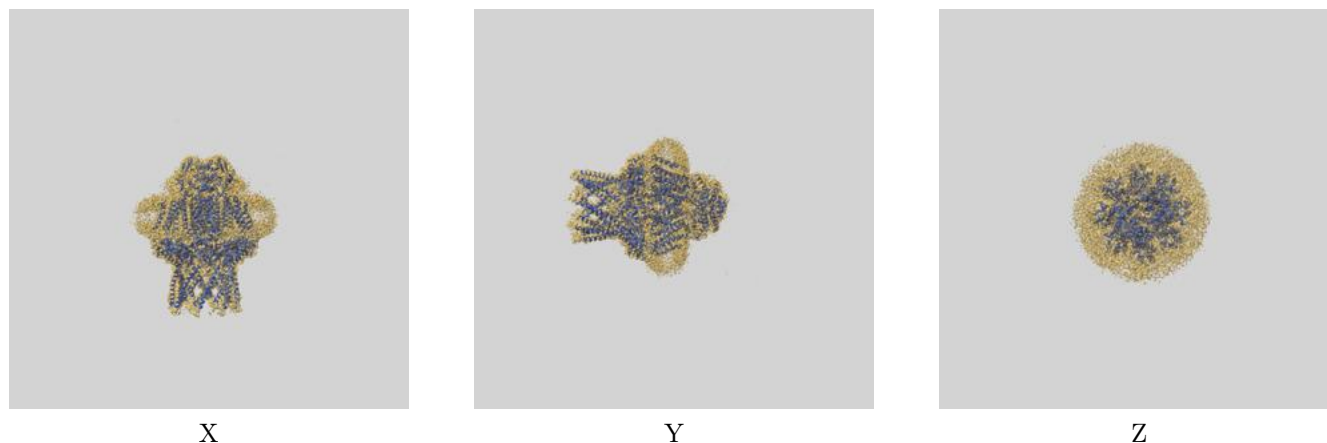
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

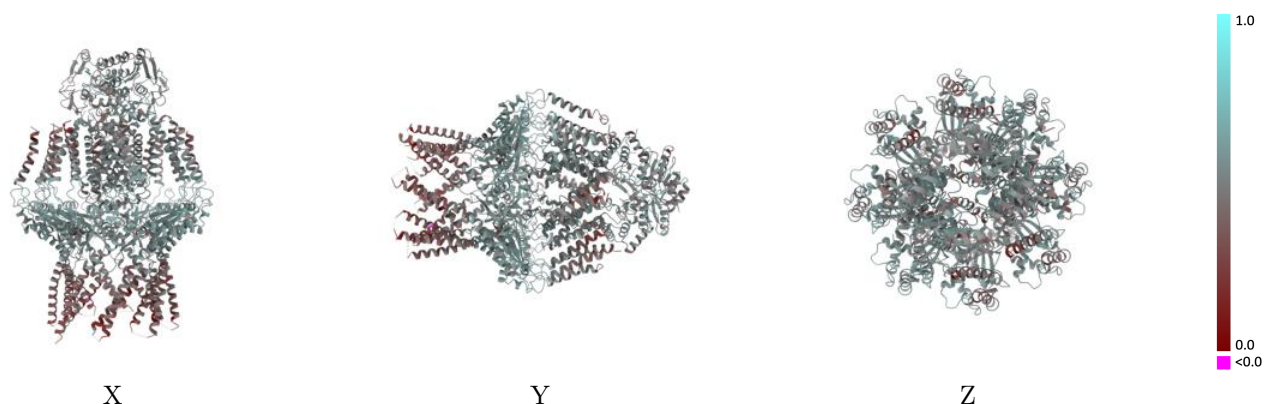
This section contains information regarding the fit between EMDB map EMD-41592 and PDB model 8TSH. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

### 9.1 Map-model overlay [i](#)



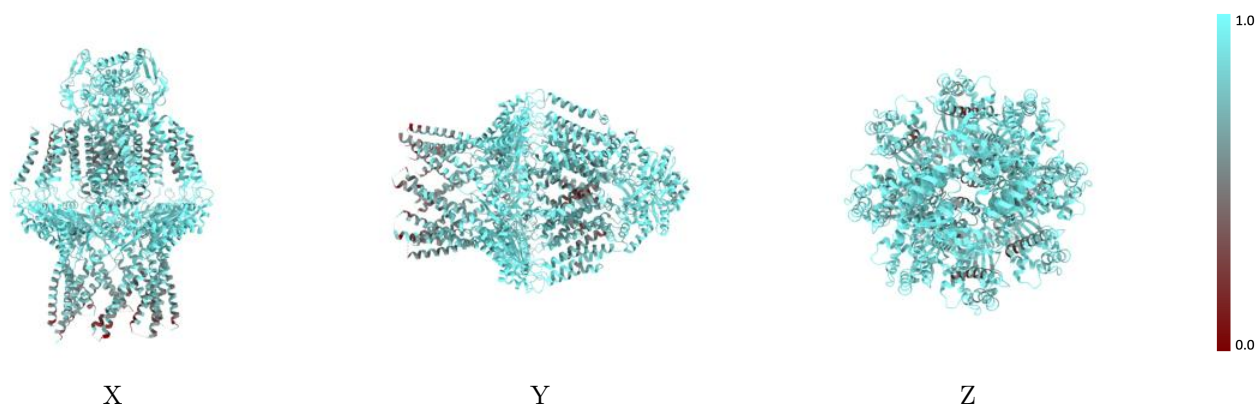
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

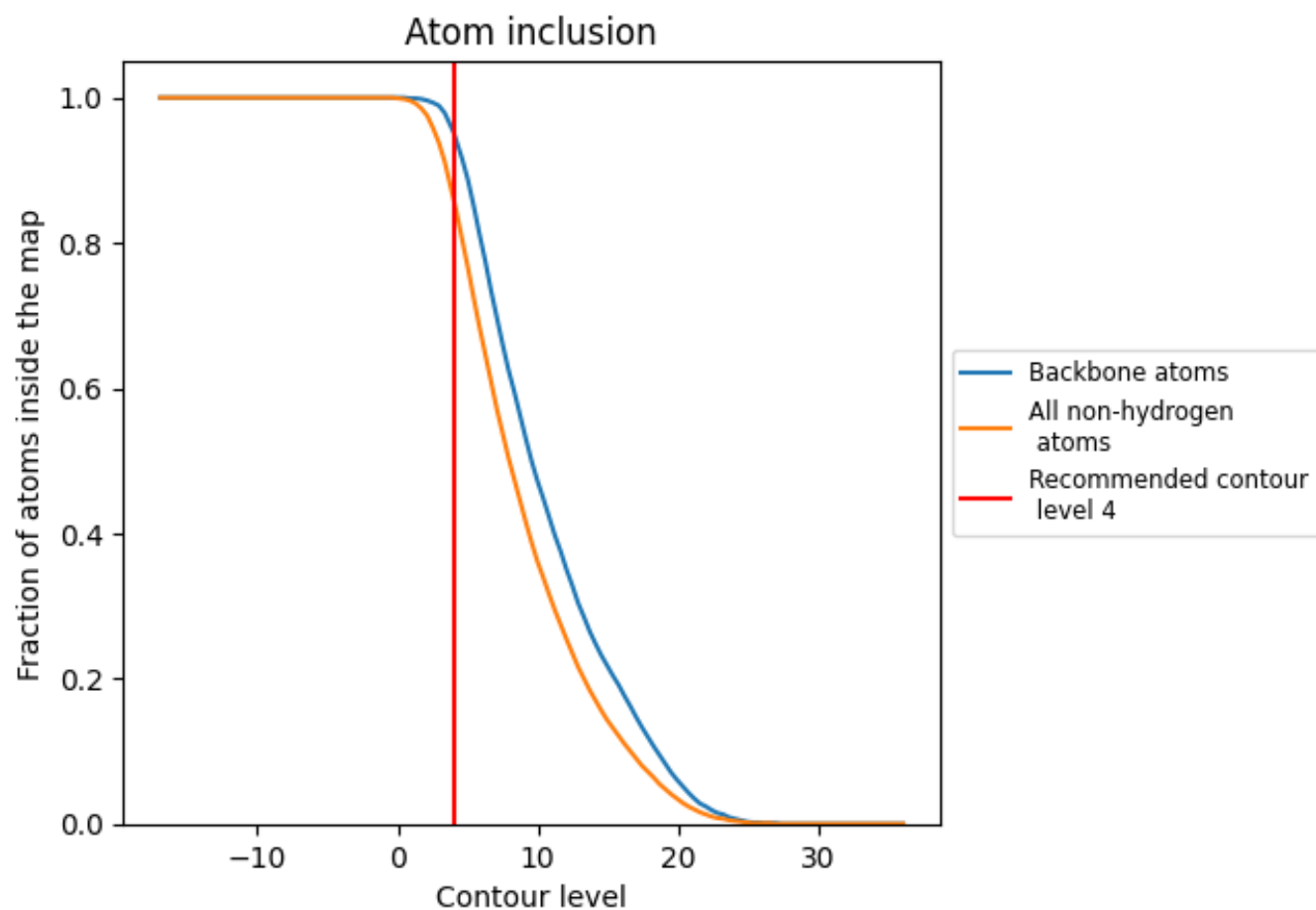
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 86% 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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8600</div>	<div><div></div>0.4990</div>
A	<div><div></div>0.9300</div>	<div><div></div>0.5020</div>
B	<div><div></div>0.9250</div>	<div><div></div>0.5090</div>
C	<div><div></div>0.8420</div>	<div><div></div>0.5120</div>
D	<div><div></div>0.8500</div>	<div><div></div>0.5190</div>
E	<div><div></div>0.8360</div>	<div><div></div>0.4830</div>
F	<div><div></div>0.8560</div>	<div><div></div>0.4960</div>
G	<div><div></div>0.8680</div>	<div><div></div>0.5060</div>
H	<div><div></div>0.8200</div>	<div><div></div>0.4840</div>
I	<div><div></div>0.8470</div>	<div><div></div>0.4920</div>
J	<div><div></div>0.8640</div>	<div><div></div>0.4970</div>
K	<div><div></div>0.8790</div>	<div><div></div>0.5140</div>
L	<div><div></div>0.8310</div>	<div><div></div>0.4800</div>

1.0

0.0

<0.0