



## Full wwPDB EM Validation Report ⓘ

Jul 8, 2024 – 05:20 am BST

PDB ID : 7PXA  
EMDB ID : EMD-13695  
Title : Open-gate mycobacterium 20S CP proteasome in complex MPA - global 3D refinement  
Authors : Jomaa, A.; Kavalchuk, M.; Weber-Ban, E.  
Deposited on : 2021-10-08  
Resolution : 2.80 Å(reported)  
Based on initial model : 5KWA

This is a Full wwPDB EM Validation 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.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) : 2.37.1

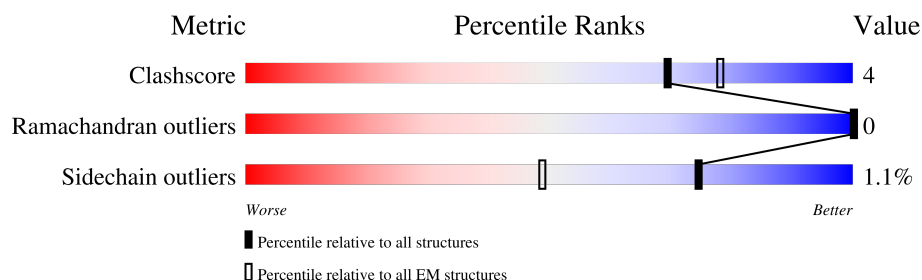
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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  $\geq 3$ , 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	0	248	 6% 74% 12% 13%
1	2	248	 5% 75% 10% 13%
1	4	248	 6% 76% 10% 13%
1	6	248	 7% 75% 11% 13%
1	8	248	 6% 74% 12% 13%
1	I	248	 22% 70% 16% 14%
1	K	248	 20% 75% 13% 12%
1	O	248	 22% 72% 15% 13%

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Mol	Chain	Length	Quality of chain
1	Q	248	
1	T	248	
1	X	248	
1	Z	248	
1	d	248	
1	f	248	
2	1	609	
2	A	609	
2	B	609	
2	C	609	
2	D	609	
2	E	609	
2	F	609	
3	H	291	
3	J	291	
3	L	291	
3	M	291	
3	N	291	
3	P	291	
3	R	291	
3	S	291	
3	U	291	
3	V	291	
3	W	291	
3	Y	291	

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Mol	Chain	Length	Quality of chain
3	a	291	<div><div></div><div>77%</div><div>23%</div></div>
3	b	291	<div><div></div><div>76%</div><div>23%</div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 46614 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	2	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	4	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	6	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	8	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	I	214	Total	C	N	O	S	0	0
			1650	1033	302	312	3		
1	K	217	Total	C	N	O	S	0	0
			1668	1044	305	316	3		
1	O	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	Q	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	T	214	Total	C	N	O	S	0	0
			1650	1033	302	312	3		
1	X	214	Total	C	N	O	S	0	0
			1650	1033	302	312	3		
1	Z	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	d	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	f	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		

- Molecule 2 is a protein called AAA ATPase forming ring-shaped complexes.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	5	Total	C	N	O	0	0
			42	28	6	8		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	5	Total	C	N	O	0	0
			42	28	6	8		
2	B	5	Total	C	N	O	0	0
			42	28	6	8		
2	C	7	Total	C	N	O	0	0
			56	35	9	12		
2	D	5	Total	C	N	O	0	0
			42	28	6	8		
2	E	7	Total	C	N	O	0	0
			56	35	9	12		
2	F	6	Total	C	N	O	0	0
			50	32	8	10		

- Molecule 3 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	J	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		
3	L	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	M	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	N	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	P	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		
3	R	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	S	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	U	234	Total	C	N	O	S	0	0
			1715	1072	295	343	5		
3	V	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		
3	W	234	Total	C	N	O	S	0	0
			1715	1072	295	343	5		
3	Y	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		
3	a	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		

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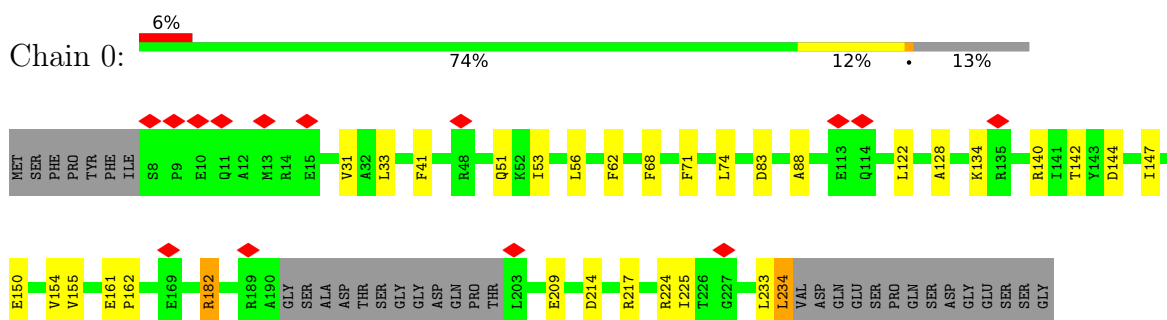
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		

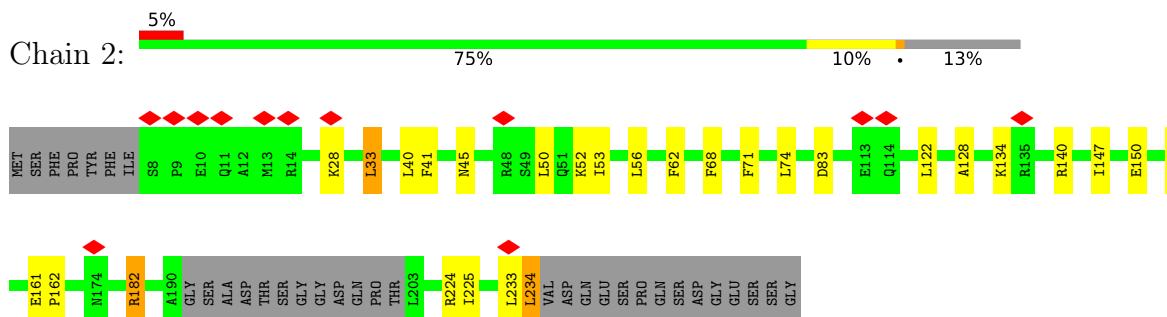
### 3 Residue-property plots [i](#)

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.

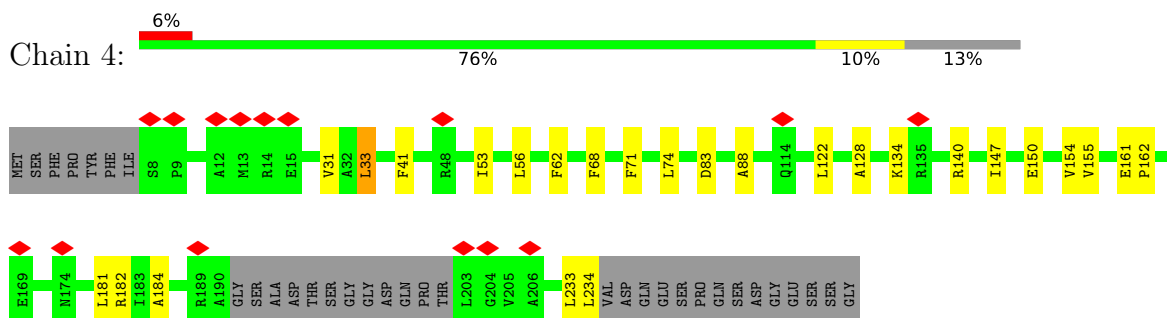
- Molecule 1: Proteasome subunit alpha



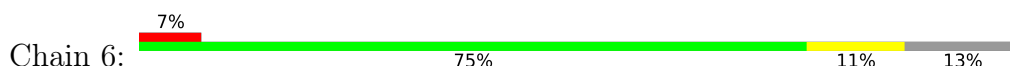
- Molecule 1: Proteasome subunit alpha



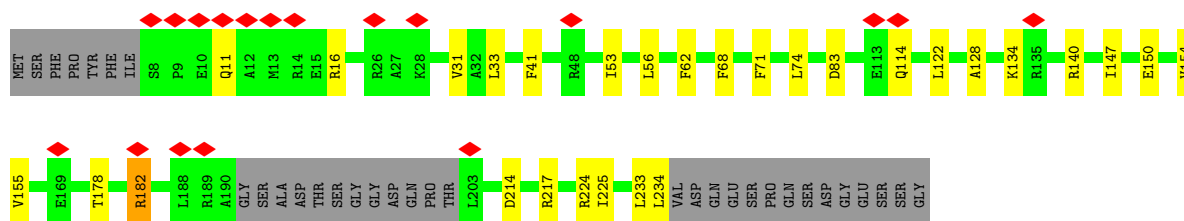
- Molecule 1: Proteasome subunit alpha



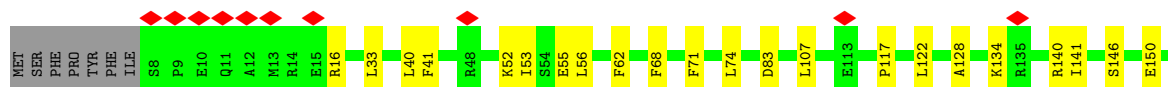
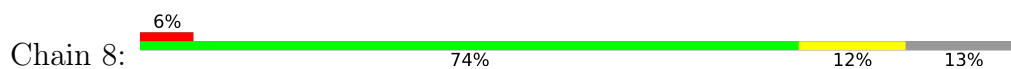
- Molecule 1: Proteasome subunit alpha



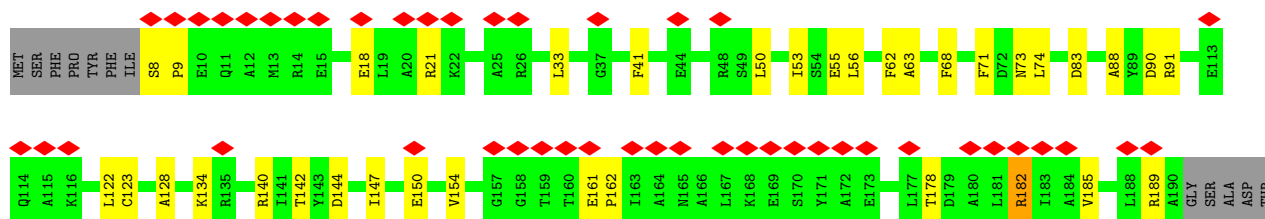




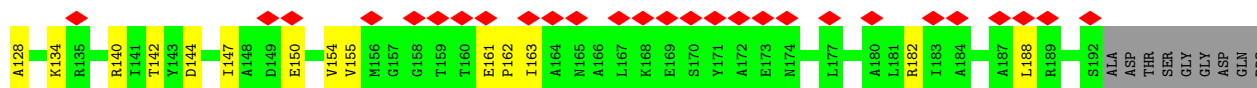
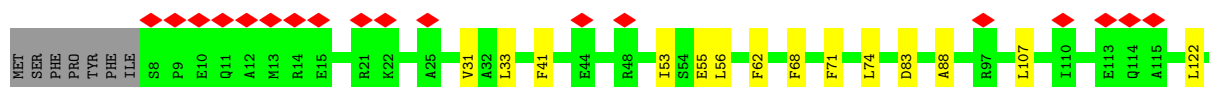
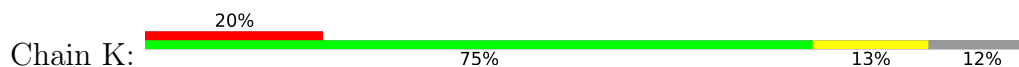
- Molecule 1: Proteasome subunit alpha



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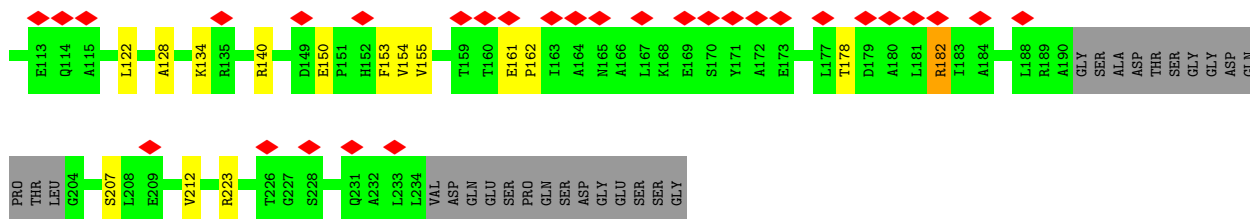


- Molecule 1: Proteasome subunit alpha

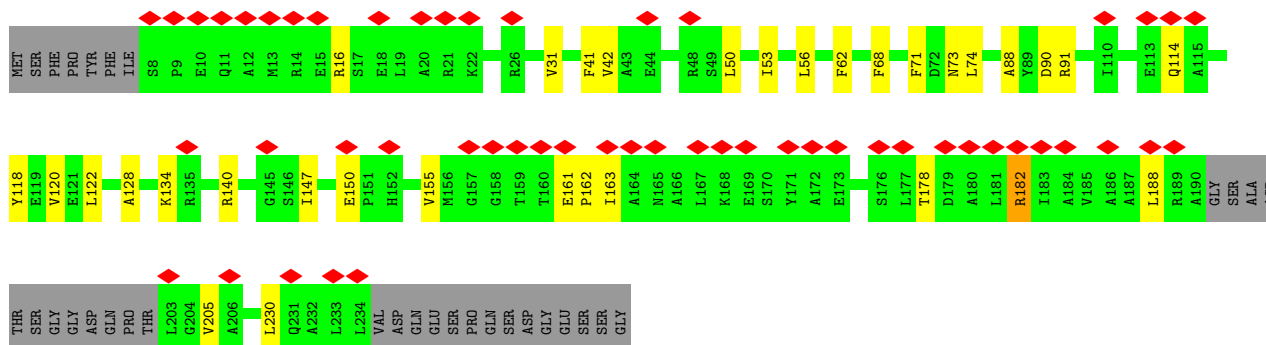
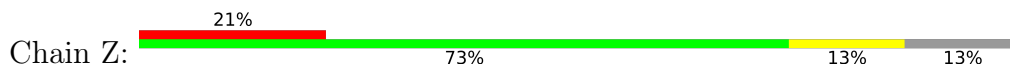


- Molecule 1: Proteasome subunit alpha

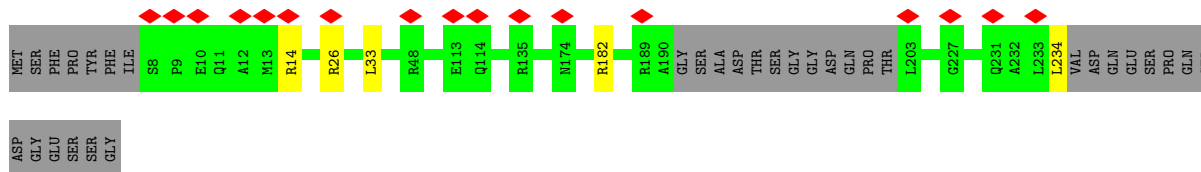
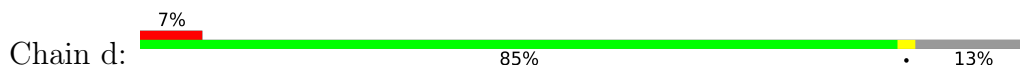




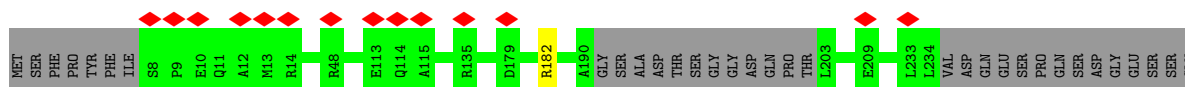
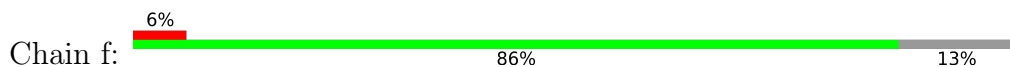
- Molecule 1: Proteasome subunit alpha



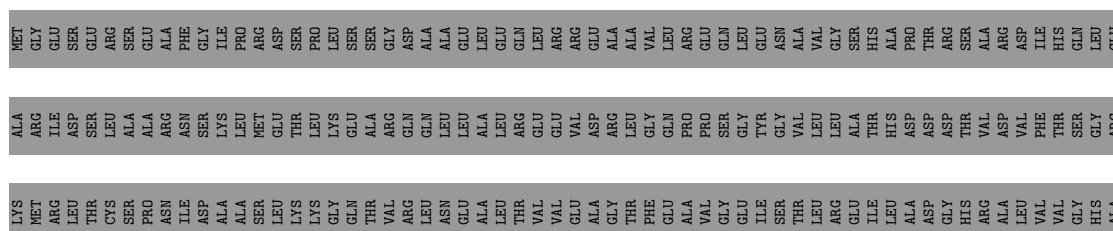
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha



- Molecule 2: AAA ATPase forming ring-shaped complexes



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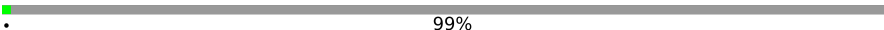
Chain A:  99%

[illegible]



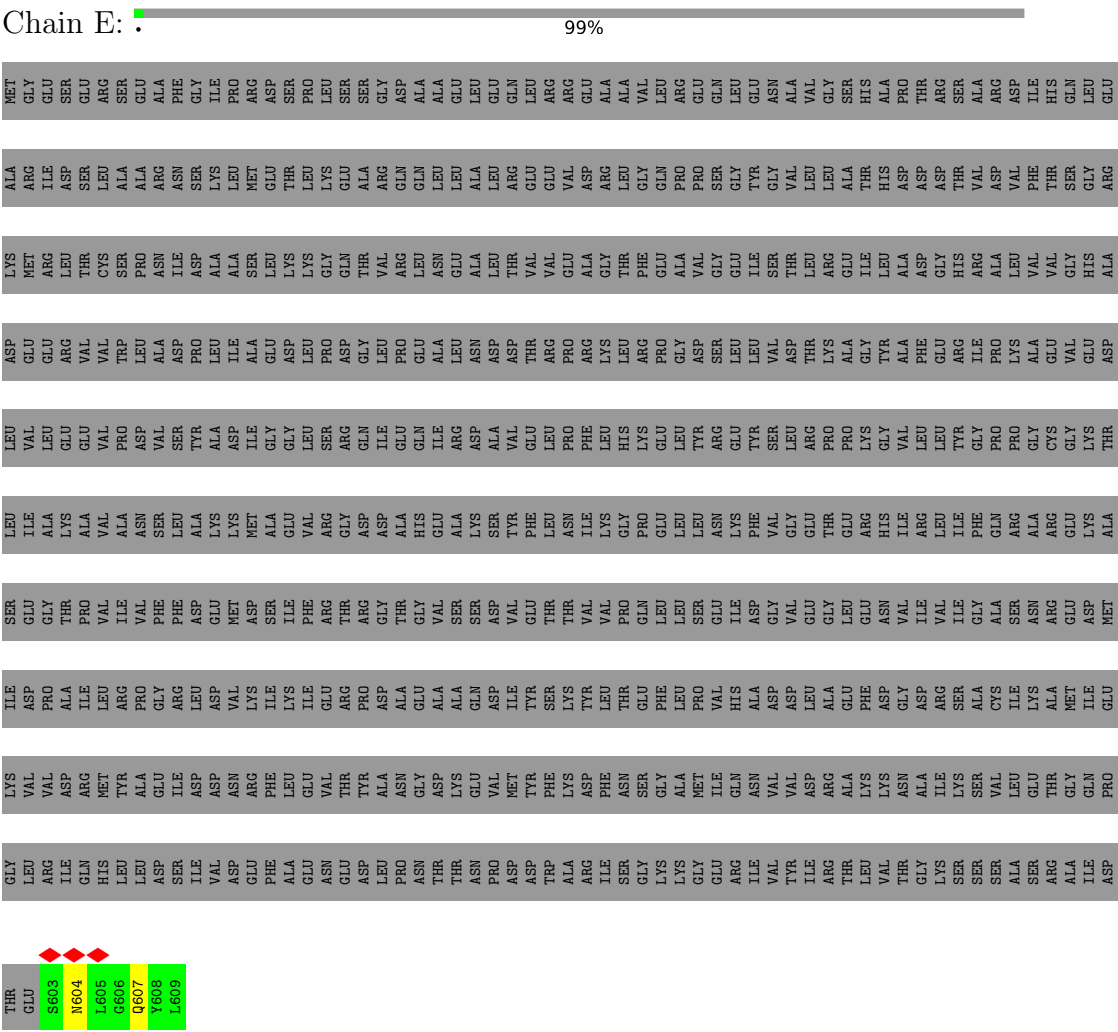
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GLU	ARG	VAL	ASP	GLY	GLU	ALA	LEU	VAL
S603	ARG	VAL	PRO	GLY	THR	LYS	LEU	GLU
N604	ILE	ASP	ALA	THR	PRO	ALA	GLU	GLY
L605	GLN	ARG	ILE	VAL	VAL	VAL	VAL	VAL
L609	HIS	MET	LEU	VAL	ILE	ALA	PRO	VAL
	LEU	TYR	ARG	ILE	ILE	ASN	ASN	ASP
	ASP	GLU	GLY	PHE	PHE	ASP	SER	VAL
	SER	ILE	ARG	ASP	LEU	ALA	ALA	TYR
	ILE	ASP	LEU	GLU	GLU	LYS	ASP	ALA
	VAL	ASN	VAL	ASP	MET	LYS	ASP	ASP
	GLU	ARG	LYS	ASP	GLY	ILE	ILE	GLY
	PHE	PHE	ILE	SER	ALA	ALA	GLY	GLY
	ALA	LEU	LYS	ILE	ILE	VAL	VAL	LEU
	ASN	VAL	GLU	ARG	THR	GLU	ARG	SER
	GLU	THR	THR	THR	GLY	VAL	GLN	GLN
	ASN	GLY	GLU	VAL	GLY	ALA	GLN	ILE
	THR	ASP	ALA	VAL	THR	SER	ALA	ILE
	THR	LYS	GLN	SER	SER	SER	LYS	ARG
	PRO	VAL	ASP	ASP	VAL	VAL	TYR	VAL
	ASP	MET	ILE	VAL	THR	PHE	GLU	VAL
	ASP	TYR	THR	GLU	THR	THR	GLU	LEU
	TRP	PHE	SER	SER	SER	ASN	ASN	LEU
	ALA	LYS	LYS	THR	THR	ILE	ASN	PRO
	ARG	ASP	TYR	VAL	VAL	ILE	TYR	ARG
	ILE	PHE	LEU	VAL	GLY	GLY	ASN	GLY
	SER	ASN	THR	PRO	GLN	HIS	GLY	HIS
	GLY	SER	PHE	GLU	LEU	GLN	LYS	LYS
	LYS	GLY	ALA	LEU	LEU	GLU	GLY	GLU
	LYS	MET	PRO	SER	LEU	LEU	LEU	LEU
	GLY	ILE	VAL	THR	ASN	ASN	THR	TYR
	ARG	GLN	GLY	ILE	GLY	THR	ARG	ARG
	THR	THR	ALA	ASP	GLU	VAL	GLY	PRO
	THR	LYS	PHE	ASN	GLU	ARG	GLY	PRO
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	ILE	ASN	VAL	GLY	VAL	ILE	VAL	GLY
	THR	ASN	ASP	VAL	ASN	VAL	GLY	GLY
	GLY	ALA	ALA	ILE	ILE	ARG	LEU	LEU
	LYS	ILE	ARG	LYS	THR	THR	ILE	TYR
	THR	THR	LYS	ILE	GLY	ARG	PHE	GLY
	VAL	VAL	VAL	ALA	VAL	GLN	GLN	PRO
	THR	ASN	ASP	GLY	ASN	THR	GLN	PRO
	THR	ASN	ILE	THR	VAL	ALA	ALA	PRO
	GLY	LYS	ARG	ALA	VAL	ARG	GLY	GLY
	ASN	GLN	THR	GLY	GLU	GLY	GLY	GLY
	ASP	ILE	GLU	MET	THR	THR	LYS	THR

- Molecule 2: AAA ATPase forming ring-shaped complexes

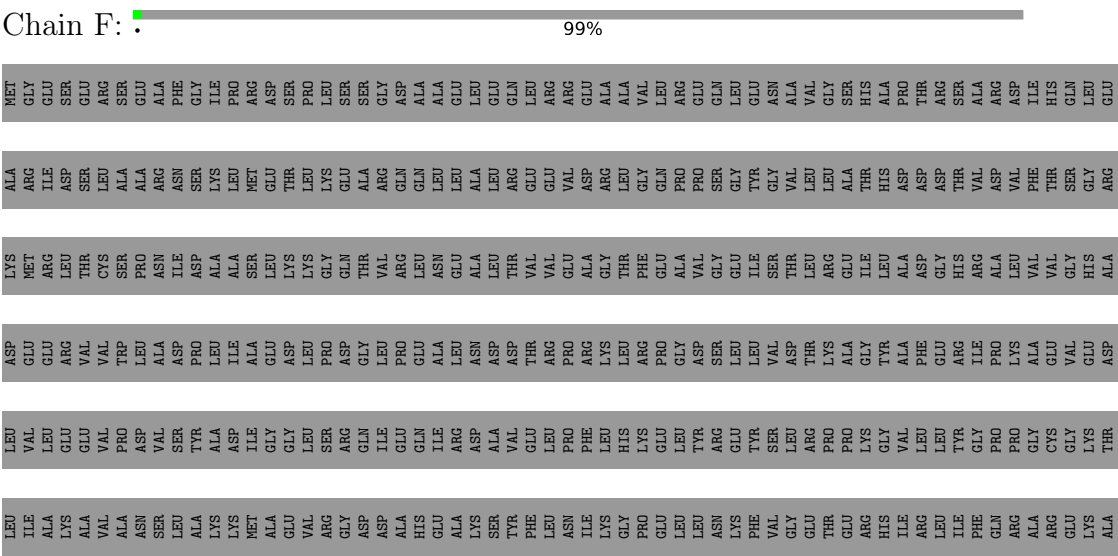
Chain D: 

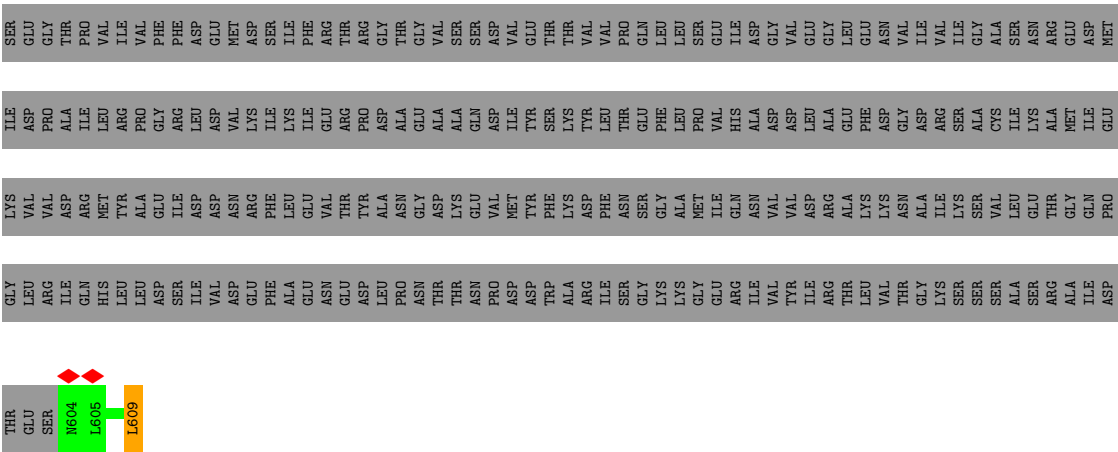
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SER	ARG	VAL	PRO	GLY	ALA	LEU	LEU	GLU	ARG	ILE	SER
ASN	ILE	ASP	ALA	THR	LYS	GLU	GLU	ARG	THR	ASP	GLU
L605	GLN	ARG	ILE	PRO	VAL	VAL	VAL	VAL	CYS	LEU	ARG
L609	HIS	MET	LEU	VAL	VAL	PRO	VAL	VAL	VAL	ALA	SER
	LEU	TYR	ARG	ILE	ASN	ASP	TRP	LEU	SER	ALA	GLU
	ASP	ALA	GLY	PHE	SER	VAL	ALA	ALA	ASN	ARG	ALA
	SER	ILE	ARG	PHE	LEU	SER	LEU	ASP	ILE	ASN	PHE
	ILE	ASP	LEU	ASP	ALA	TYR	TYR	PRO	ASP	SER	GLY
	VAL	ASP	ASP	GLU	LYS	ALA	LEU	LEU	ALA	LYS	ILE
	ASP	ASN	VAL	MET	LYS	ASP	ILE	ALA	ALA	LEU	PRO
	GLU	ARG	LYS	ASP	MET	ILE	ALA	ALA	SER	MET	ARG
	PHE	PHE	ILE	SER	ALA	GLY	GLU	GLU	LEU	ASP	ASP
	ALA	LEU	LYS	ILE	VAL	GLY	GLY	ASP	LYS	THR	SER
	GLU	GLU	ILE	PHE	VAL	ARG	LEU	LEU	GLY	LEU	PRO
	ASN	VAL	GLU	ARG	GLY	SER	SER	PRO	GLY	LYS	LEU
	GLU	THR	ARG	THR	GLY	GLN	GLN	GLU	GLN	LEU	LEU
	ASP	TYR	PRO	GLY	ASP	ARG	ARG	ASP	GLN	GLU	SER
	LEU	ALA	ASP	GLY	ALA	ILE	ILE	LEU	VAL	ALA	GLY
	PRO	ASN	ALA	THR	ALA	GLU	GLU	PRO	ARG	GLN	ALA
	ASN	GLY	ALA	GLY	HIS	GLN	LYS	LEU	ASN	LEU	ALA
	THR	ASP	ALA	VAL	GLU	ILE	GLU	ALA	ASN	LEU	ALA
	LYS	LYS	ALA	SER	GLA	ARG	LEU	LEU	GLU	LEU	GLU
	ASN	GLU	GLN	SER	LYS	ASP	ASP	ASN	ALA	ALA	GLU
	PRO	VAL	ASP	ASP	SER	ALA	ASP	ASP	LEU	LEU	GLU
	ASP	MET	ILE	VAL	TYR	VAL	VAL	ASP	LEU	LEU	GLN
	ASP	TYR	THR	GLU	PHE	GLU	GLU	THR	VAL	GLU	LEU
	ALA	LYS	LYS	THR	LEU	LEU	LEU	ARG	VAL	GLU	ARG
	ARG	ASP	TYR	VAL	ILE	PHE	PHE	PRO	GLU	VAL	THR
	ILE	PHE	LEU	VAL	LYS	LEU	GLY	LYS	GLY	GLY	ALA
	SER	ASN	THR	PRO	GLY	HIS	HIS	LEU	THR	LEU	SER
	GLY	SER	GLU	GLN	LEU	GLU	LYS	ARG	PHE	ALA	ALA
	LYS	GLY	PHE	LEU	LEU	GLU	LYS	PRO	GLU	VAL	ARG
	LYS	ALA	LEU	VAL	VAL	ARG	LEU	LYS	ALA	VAL	THR
	GLY	MET	PRO	SER	LEU	TYR	ASP	VAL	VAL	VAL	ILE
	GLU	ILE	VAL	GLU	ASN	GLU	SER	ASP	GLY	ASP	THR
	ARG	GLN	HIS	ILE	LYS	TYR	LEU	LEU	HIS	THR	ALA
	ILE	ASN	ALA	ASP	PHE	VAL	LEU	VAL	THR	ALA	SER
	VAL	VAL	ASP	GLY	VAL	SER	GLY	VAL	ALA	ASP	ARG
	TYR	VAL	ASP	VAL	GLY	LEU	ARG	THR	THR	THR	THR
	ILE	ASP	LEU	GLU	ILE	ARG	THR	ASP	ALA	ASP	THR
	ARG	ALA	ALA	GLY	THR	ARG	LYS	GLY	ARG	ASP	THR
	THR	ALA	GLU	LEU	ARG	PRO	GLY	HIS	THR	VAL	ALA
	LEU	LYS	PHE	GLU	HIS	LYS	GLY	TYR	LEU	ASP	ARG
	VAL	LYS	ASP	ASN	ASP	TYR	LEU	VAL	ALA	ALA	THR
	THR	ASN	GLY	VAL	VAL	SER	SER	THR	ALA	ALA	ALA
	GLY	SER	GLU	GLN	LEU	GLU	GLU	GLU	LEU	THR	GLN
	LYS	GLY	ILE	ILE	VAL	GLY	LYS	VAL	GLY	GLY	GLY
	THR	ASN	THR	MET	ALA	THR	THR	ASP	HIS	ALA	THR
	GLY	ILE	GLU	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	ARG	PRO	THR	ALA	ALA	THR	THR	ASP	ALA	ASP	GLY

● Molecule 2: AAA ATPase forming ring-shaped complexes

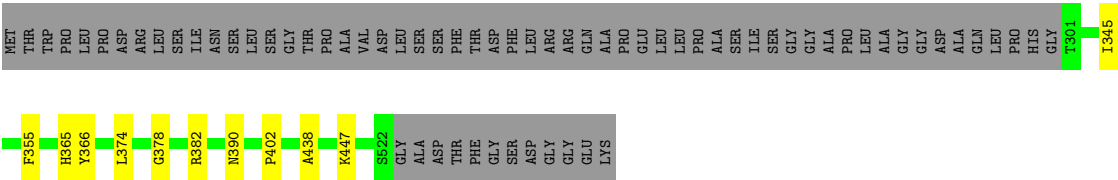


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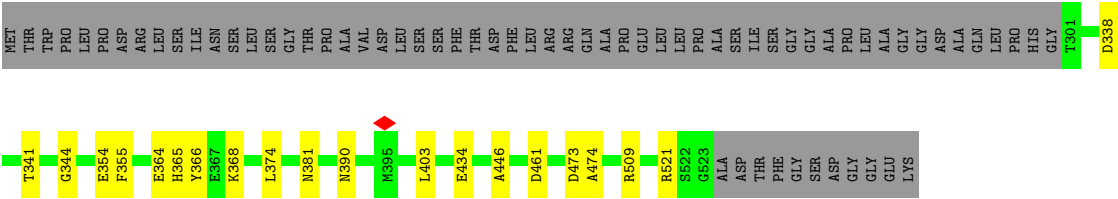




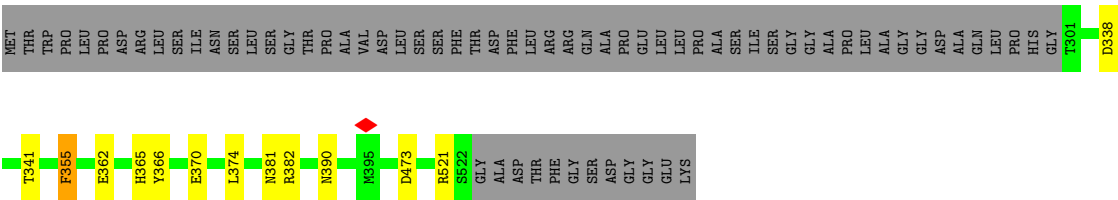
• Molecule 3: Proteasome subunit beta



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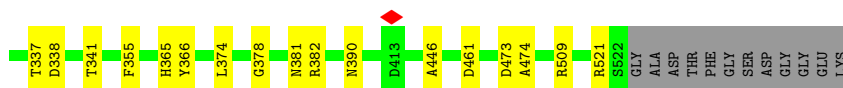
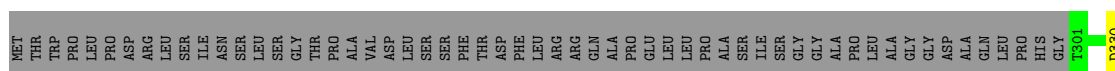
• Molecule 3: Proteasome subunit beta



• Molecule 3: Proteasome subunit beta

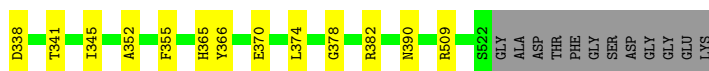
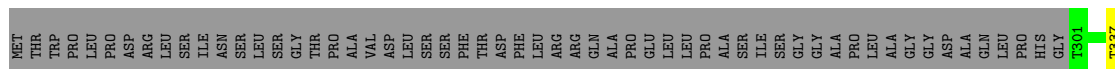






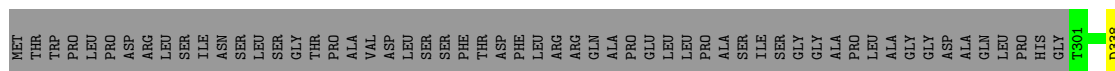
- Molecule 3: Proteasome subunit beta

Chain N: 71% 5% 24%



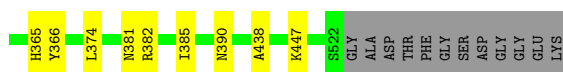
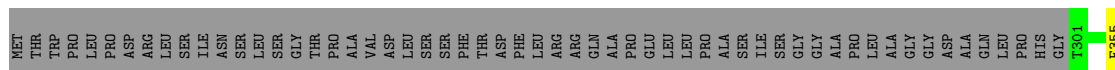
- Molecule 3: Proteasome subunit beta

Chain P: 74% 23%



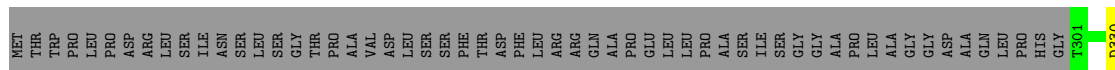
- Molecule 3: Proteasome subunit beta

Chain R: 73% 24%



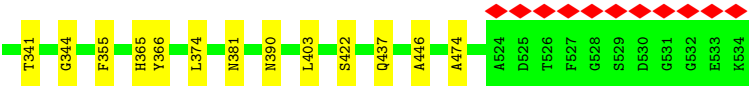
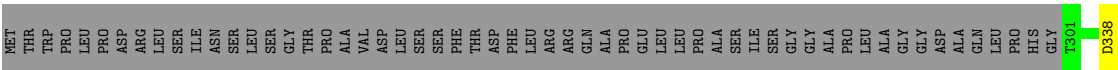
- Molecule 3: Proteasome subunit beta

Chain S: 71% 5% 24%



- Molecule 3: Proteasome subunit beta

Chain U: 76% 5% 20%



• Molecule 3: Proteasome subunit beta



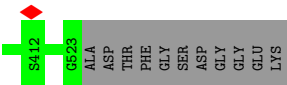
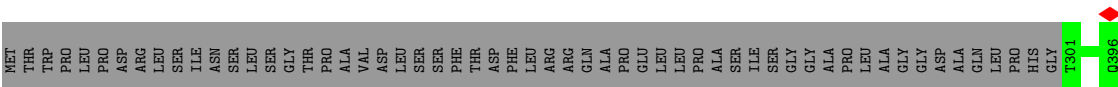
• Molecule 3: Proteasome subunit beta



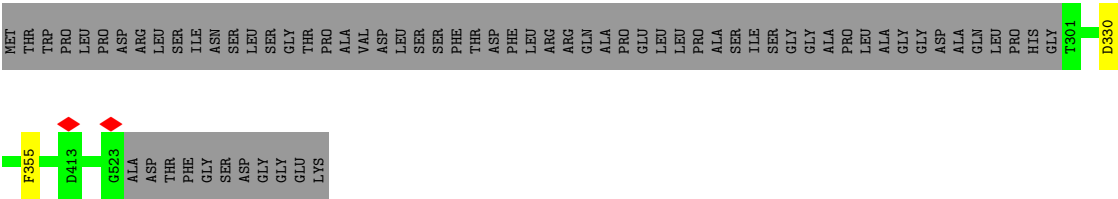
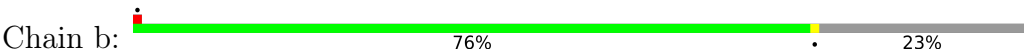
• Molecule 3: Proteasome subunit beta



• Molecule 3: Proteasome subunit beta



• Molecule 3: Proteasome subunit beta



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	222719	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0236	Depositor
Map size ( $\text{\AA}$ )	430.144, 430.144, 430.144	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.222, 1.222, 1.222	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	0	0.24	0/1683	0.41	0/2274
1	2	0.24	0/1683	0.41	0/2274
1	4	0.24	0/1683	0.41	0/2274
1	6	0.24	0/1683	0.40	0/2274
1	8	0.24	0/1683	0.40	0/2274
1	I	0.24	0/1675	0.40	0/2263
1	K	0.24	0/1693	0.40	0/2287
1	O	0.24	0/1683	0.40	0/2274
1	Q	0.24	0/1683	0.40	0/2274
1	T	0.24	0/1675	0.40	0/2263
1	X	0.24	0/1675	0.40	0/2263
1	Z	0.24	0/1683	0.40	0/2274
1	d	0.24	0/1683	0.41	0/2274
1	f	0.24	0/1683	0.41	0/2274
2	1	0.23	0/42	0.43	0/54
2	A	0.23	0/42	0.43	0/54
2	B	0.26	0/42	0.43	0/54
2	C	0.25	0/56	0.51	0/73
2	D	0.23	0/42	0.43	0/54
2	E	0.24	0/56	0.43	0/73
2	F	0.26	0/50	0.41	0/65
3	H	0.24	0/1660	0.42	0/2251
3	J	0.24	0/1664	0.42	0/2256
3	L	0.24	0/1660	0.42	0/2251
3	M	0.24	0/1660	0.42	0/2251
3	N	0.24	0/1660	0.42	0/2251
3	P	0.24	0/1664	0.42	0/2256
3	R	0.24	0/1660	0.42	0/2251
3	S	0.24	0/1660	0.42	0/2251
3	U	0.24	0/1740	0.42	0/2357
3	V	0.24	0/1664	0.42	0/2256
3	W	0.24	0/1740	0.43	0/2357
3	Y	0.24	0/1664	0.42	0/2256
3	a	0.24	0/1664	0.42	0/2256

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	b	0.24	0/1664	0.43	0/2256
All	All	0.24	0/47302	0.41	0/63999

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	0	1658	0	1659	18	0
1	2	1658	0	1659	16	0
1	4	1658	0	1659	13	0
1	6	1658	0	1659	14	0
1	8	1658	0	1659	17	0
1	I	1650	0	1648	25	0
1	K	1668	0	1667	18	0
1	O	1658	0	1659	22	0
1	Q	1658	0	1659	21	0
1	T	1650	0	1648	19	0
1	X	1650	0	1648	19	0
1	Z	1658	0	1659	18	0
1	d	1658	0	1659	0	0
1	f	1658	0	1659	0	0
2	1	42	0	41	1	0
2	A	42	0	41	0	0
2	B	42	0	41	0	0
2	C	56	0	52	0	0
2	D	42	0	41	0	0
2	E	56	0	52	2	0
2	F	50	0	47	1	0
3	H	1636	0	1625	7	0
3	J	1640	0	1628	10	0
3	L	1636	0	1625	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	1636	0	1625	10	0
3	N	1636	0	1625	8	0
3	P	1640	0	1628	5	0
3	R	1636	0	1625	6	0
3	S	1636	0	1625	9	0
3	U	1715	0	1690	8	0
3	V	1640	0	1628	8	0
3	W	1715	0	1690	7	0
3	Y	1640	0	1628	10	0
3	a	1640	0	1628	0	0
3	b	1640	0	1628	0	0
All	All	46614	0	46414	291	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 (291) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:74:LEU:HD23	1:6:122:LEU:HD11	1.73	0.70
1:Z:74:LEU:HD23	1:Z:122:LEU:HD11	1.73	0.70
1:0:74:LEU:HD23	1:0:122:LEU:HD11	1.72	0.70
1:8:74:LEU:HD23	1:8:122:LEU:HD11	1.74	0.69
1:2:74:LEU:HD23	1:2:122:LEU:HD11	1.74	0.68
1:K:74:LEU:HD23	1:K:122:LEU:HD11	1.76	0.68
1:X:74:LEU:HD23	1:X:122:LEU:HD11	1.76	0.67
1:4:74:LEU:HD23	1:4:122:LEU:HD11	1.76	0.66
3:J:338:ASP:OD1	3:J:341:THR:OG1	2.15	0.65
1:O:186:ALA:HA	1:O:189:ARG:HD2	1.79	0.64
1:I:217:ARG:HG3	1:I:218:PRO:HD2	1.79	0.64
1:O:74:LEU:HD23	1:O:122:LEU:HD11	1.80	0.63
1:I:74:LEU:HD23	1:I:122:LEU:HD11	1.81	0.63
1:T:41:PHE:HB3	1:T:53:ILE:HD13	1.80	0.63
1:T:74:LEU:HD23	1:T:122:LEU:HD11	1.81	0.63
1:6:140:ARG:HH11	1:6:154:VAL:HG13	1.65	0.62
1:X:83:ASP:OD2	3:Y:365:HIS:ND1	2.31	0.62
1:8:52:LYS:HD2	2:F:609:LEU:HD22	1.81	0.62
1:K:140:ARG:HH11	1:K:154:VAL:HG13	1.65	0.61
1:K:205:VAL:HG13	1:K:230:LEU:HD23	1.83	0.60
1:Q:74:LEU:HD23	1:Q:122:LEU:HD11	1.82	0.60
1:X:140:ARG:HH11	1:X:154:VAL:HG13	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:53:ILE:O	1:T:224:ARG:NH2	2.33	0.60
1:6:83:ASP:OD2	3:N:365:HIS:ND1	2.32	0.60
1:8:83:ASP:OD2	3:V:365:HIS:ND1	2.32	0.59
3:M:338:ASP:OD1	3:M:341:THR:OG1	2.20	0.59
1:O:11:GLN:OE1	1:O:14:ARG:NH2	2.36	0.59
1:O:140:ARG:NH2	1:O:150:GLU:OE2	2.36	0.59
1:X:41:PHE:HB3	1:X:53:ILE:HD13	1.85	0.59
3:Y:432:GLU:OE2	3:Y:437:GLN:NE2	2.35	0.59
1:O:83:ASP:OD2	3:P:365:HIS:ND1	2.34	0.59
1:O:178:THR:HG22	1:O:182:ARG:HE	1.69	0.58
3:Y:381:ASN:ND2	1:Z:88:ALA:O	2.38	0.57
1:T:83:ASP:OD2	3:U:365:HIS:ND1	2.33	0.57
1:K:83:ASP:OD2	3:L:365:HIS:ND1	2.34	0.57
1:2:56:LEU:HG	1:2:62:PHE:HB2	1.87	0.57
1:T:182:ARG:NH1	1:T:234:LEU:O	2.37	0.56
1:2:41:PHE:HB3	1:2:53:ILE:HD13	1.86	0.56
1:8:16:ARG:HB3	1:8:117:PRO:HG3	1.87	0.56
1:8:140:ARG:HH11	1:8:154:VAL:HG13	1.69	0.56
1:Q:74:LEU:HD21	1:Q:107:LEU:HD21	1.88	0.56
1:K:53:ILE:O	1:K:224:ARG:NH2	2.38	0.56
3:M:473:ASP:OD1	3:M:521:ARG:NH1	2.36	0.56
1:2:128:ALA:HB2	1:2:134:LYS:HB3	1.88	0.56
1:O:140:ARG:HH11	1:O:154:VAL:HG13	1.70	0.56
1:I:53:ILE:O	1:I:224:ARG:NH2	2.35	0.56
1:I:83:ASP:OD2	3:J:365:HIS:ND1	2.33	0.56
1:I:41:PHE:HB3	1:I:53:ILE:HD13	1.88	0.55
1:8:41:PHE:HB3	1:8:53:ILE:HD13	1.87	0.55
1:8:140:ARG:NH2	1:8:150:GLU:OE2	2.39	0.55
1:Z:140:ARG:NH2	1:Z:150:GLU:OE2	2.36	0.55
1:4:56:LEU:HG	1:4:62:PHE:HB2	1.88	0.55
1:4:140:ARG:HH11	1:4:154:VAL:HG13	1.72	0.55
1:K:128:ALA:HB2	1:K:134:LYS:HB3	1.89	0.55
1:4:128:ALA:HB2	1:4:134:LYS:HB3	1.89	0.55
3:P:381:ASN:ND2	1:Q:88:ALA:O	2.40	0.54
3:L:381:ASN:ND2	1:X:88:ALA:O	2.41	0.54
1:6:41:PHE:HB3	1:6:53:ILE:HD13	1.88	0.54
1:6:53:ILE:O	1:6:224:ARG:NH2	2.35	0.54
1:T:178:THR:HG22	1:T:182:ARG:HE	1.73	0.54
3:J:461:ASP:OD1	3:J:509:ARG:NH2	2.41	0.54
1:8:128:ALA:HB2	1:8:134:LYS:HB3	1.91	0.53
1:O:68:PHE:HA	1:O:71:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:128:ALA:HB2	1:T:134:LYS:HB3	1.90	0.53
1:6:140:ARG:NH2	1:6:150:GLU:OE2	2.42	0.53
1:8:56:LEU:HG	1:8:62:PHE:HB2	1.89	0.53
1:X:31:VAL:HG12	1:X:155:VAL:HG22	1.91	0.53
1:2:140:ARG:NH2	1:2:150:GLU:OE2	2.42	0.52
1:6:225:ILE:HG21	1:6:233:LEU:HD22	1.91	0.52
1:0:56:LEU:HG	1:0:62:PHE:HB2	1.90	0.52
3:L:355:PHE:HZ	3:L:390:ASN:HB2	1.73	0.52
3:S:355:PHE:HZ	3:S:390:ASN:HB2	1.75	0.52
1:I:128:ALA:HB2	1:I:134:LYS:HB3	1.92	0.52
1:0:41:PHE:HB3	1:0:53:ILE:HD13	1.92	0.51
1:8:68:PHE:HA	1:8:71:PHE:CE2	2.45	0.51
1:Z:163:ILE:HD13	1:Z:188:LEU:HD12	1.92	0.51
1:I:88:ALA:O	3:U:381:ASN:ND2	2.44	0.51
3:R:382:ARG:HH21	3:R:385:ILE:HD12	1.76	0.51
1:I:56:LEU:HG	1:I:62:PHE:HB2	1.92	0.51
1:O:128:ALA:HB2	1:O:134:LYS:HB3	1.93	0.51
3:L:338:ASP:OD1	3:L:341:THR:OG1	2.19	0.51
3:Y:355:PHE:HZ	3:Y:390:ASN:HB2	1.76	0.51
1:0:53:ILE:O	1:0:224:ARG:NH2	2.37	0.51
1:I:185:VAL:HG21	1:I:234:LEU:HD11	1.93	0.51
3:P:338:ASP:OD1	3:P:341:THR:OG1	2.19	0.51
1:Q:53:ILE:O	1:Q:224:ARG:NH2	2.38	0.51
1:X:56:LEU:HG	1:X:62:PHE:HB2	1.94	0.51
1:K:140:ARG:NH2	1:K:150:GLU:OE2	2.44	0.50
1:K:68:PHE:HA	1:K:71:PHE:CE2	2.46	0.50
1:I:140:ARG:HH11	1:I:154:VAL:HG13	1.76	0.50
1:Q:68:PHE:HA	1:Q:71:PHE:CE2	2.47	0.50
1:T:68:PHE:HA	1:T:71:PHE:CE2	2.46	0.50
1:K:56:LEU:HG	1:K:62:PHE:HB2	1.92	0.50
1:X:128:ALA:HB2	1:X:134:LYS:HB3	1.94	0.50
3:R:355:PHE:HZ	3:R:390:ASN:HB2	1.75	0.50
3:M:337:THR:HG1	3:M:341:THR:HG1	1.58	0.49
1:T:14:ARG:NH1	1:T:18:GLU:OE2	2.45	0.49
1:I:68:PHE:HA	1:I:71:PHE:CE2	2.47	0.49
1:0:209:GLU:OE2	1:0:224:ARG:NH1	2.45	0.49
1:2:225:ILE:HG21	1:2:233:LEU:HD22	1.95	0.49
3:J:381:ASN:ND2	1:O:88:ALA:O	2.45	0.49
1:Z:31:VAL:HG12	1:Z:155:VAL:HG22	1.93	0.49
1:4:68:PHE:HA	1:4:71:PHE:CE2	2.47	0.49
1:Q:128:ALA:HB2	1:Q:134:LYS:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:604:ASN:OD1	2:E:604:ASN:N	2.46	0.49
1:K:88:ALA:O	3:R:381:ASN:ND2	2.45	0.49
1:Q:56:LEU:HG	1:Q:62:PHE:HB2	1.95	0.48
1:2:53:ILE:O	1:2:224:ARG:NH2	2.46	0.48
1:6:16:ARG:NH2	1:6:114:GLN:O	2.42	0.48
1:6:68:PHE:HA	1:6:71:PHE:CE2	2.48	0.48
3:N:337:THR:OG1	3:N:341:THR:OG1	2.30	0.48
3:W:338:ASP:OD1	3:W:341:THR:OG1	2.20	0.48
3:M:355:PHE:HZ	3:M:390:ASN:HB2	1.77	0.48
1:6:56:LEU:HG	1:6:62:PHE:HB2	1.94	0.48
1:X:68:PHE:HA	1:X:71:PHE:CE2	2.49	0.48
1:Q:83:ASP:OD2	3:R:365:HIS:ND1	2.43	0.48
3:V:473:ASP:OD1	3:V:521:ARG:NH1	2.37	0.48
3:W:364:GLU:HG2	3:W:368:LYS:HE2	1.96	0.48
1:Z:68:PHE:HA	1:Z:71:PHE:CE2	2.49	0.48
1:2:68:PHE:HA	1:2:71:PHE:CE2	2.49	0.48
1:T:56:LEU:HG	1:T:62:PHE:HB2	1.96	0.48
3:U:355:PHE:HZ	3:U:390:ASN:HB2	1.79	0.48
1:K:41:PHE:HB3	1:K:53:ILE:HD13	1.96	0.47
1:Q:41:PHE:HB3	1:Q:53:ILE:HD13	1.95	0.47
1:T:31:VAL:HG12	1:T:155:VAL:HG22	1.95	0.47
3:W:345:ILE:HB	3:W:352:ALA:HB1	1.95	0.47
1:2:28:LYS:HB2	1:2:52:LYS:HZ2	1.80	0.47
1:2:182:ARG:NH1	1:2:234:LEU:O	2.48	0.47
1:I:140:ARG:NH2	1:I:150:GLU:OE2	2.47	0.47
3:M:461:ASP:OD1	3:M:509:ARG:NH2	2.47	0.47
1:O:50:LEU:HD11	1:Q:147:ILE:HG23	1.97	0.47
1:O:140:ARG:NH2	1:O:150:GLU:OE2	2.48	0.47
1:0:128:ALA:HB2	1:0:134:LYS:HB3	1.97	0.47
3:H:355:PHE:HZ	3:H:390:ASN:HB2	1.81	0.46
3:J:355:PHE:HZ	3:J:390:ASN:HB2	1.81	0.46
1:X:178:THR:HG22	1:X:182:ARG:HE	1.80	0.46
3:Y:338:ASP:OD1	3:Y:341:THR:OG1	2.20	0.46
1:0:83:ASP:OD2	3:S:365:HIS:ND1	2.32	0.46
1:I:185:VAL:O	1:I:189:ARG:HG3	2.16	0.46
1:X:212:VAL:HG21	1:X:223:ARG:HH21	1.80	0.46
1:6:128:ALA:HB2	1:6:134:LYS:HB3	1.96	0.46
1:Q:140:ARG:HH11	1:Q:154:VAL:HG13	1.80	0.46
1:I:73:ASN:ND2	1:O:105:GLN:OE1	2.49	0.46
3:V:338:ASP:OD1	3:V:341:THR:OG1	2.21	0.46
1:K:147:ILE:HG23	1:Q:50:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:56:LEU:HG	1:O:62:PHE:HB2	1.97	0.45
1:Z:56:LEU:HG	1:Z:62:PHE:HB2	1.97	0.45
3:R:438:ALA:HB3	3:R:447:LYS:HG3	1.98	0.45
1:K:31:VAL:HG12	1:K:155:VAL:HG22	1.97	0.45
1:Q:31:VAL:HG12	1:Q:155:VAL:HG22	1.99	0.45
3:L:473:ASP:OD1	3:L:521:ARG:NH1	2.41	0.45
1:4:33:LEU:HD21	1:4:184:ALA:HB2	1.98	0.45
1:I:147:ILE:HG23	1:T:50:LEU:HD11	1.97	0.45
1:I:178:THR:HG22	1:I:182:ARG:HE	1.81	0.45
3:P:355:PHE:HZ	3:P:390:ASN:HB2	1.81	0.45
1:T:140:ARG:HH11	1:T:154:VAL:HG13	1.82	0.45
1:T:147:ILE:HG23	1:Z:50:LEU:HD11	1.99	0.45
1:O:140:ARG:HH11	1:O:154:VAL:HG13	1.82	0.45
1:O:182:ARG:NH1	1:O:234:LEU:O	2.50	0.44
1:Z:178:THR:HG22	1:Z:182:ARG:HE	1.81	0.44
1:Q:142:THR:OG1	1:Q:144:ASP:OD1	2.32	0.44
3:V:382:ARG:HH21	3:V:385:ILE:HD12	1.81	0.44
1:I:161:GLU:HB2	1:I:162:PRO:HD3	2.00	0.44
3:V:345:ILE:HB	3:V:352:ALA:HB1	1.99	0.44
1:8:146:SER:HA	2:E:607:GLN:HB2	1.98	0.44
3:H:438:ALA:HB3	3:H:447:LYS:HG3	2.00	0.44
1:X:46:PRO:HA	1:X:207:SER:HA	1.99	0.44
1:2:140:ARG:HH11	1:2:154:VAL:HG13	1.83	0.44
1:8:33:LEU:HD11	1:8:40:LEU:HD23	1.99	0.44
3:N:338:ASP:OD1	3:N:341:THR:OG1	2.20	0.44
1:Z:41:PHE:HB3	1:Z:53:ILE:HD13	1.99	0.44
1:I:50:LEU:HD11	1:O:147:ILE:HG23	1.99	0.44
1:O:16:ARG:HH11	1:O:117:PRO:HD3	1.83	0.44
3:S:473:ASP:OD1	3:S:521:ARG:NH1	2.39	0.44
3:Y:344:GLY:O	3:Y:403:LEU:N	2.51	0.44
1:X:161:GLU:HB2	1:X:162:PRO:HD3	2.00	0.44
1:Z:161:GLU:HB2	1:Z:162:PRO:HD3	1.99	0.44
1:O:68:PHE:HA	1:O:71:PHE:CE2	2.53	0.43
3:N:366:TYR:CD1	3:N:374:LEU:HG	2.53	0.43
1:T:107:LEU:HD12	1:T:141:ILE:HG22	2.01	0.43
1:I:63:ALA:HB3	1:I:123:CYS:HB3	2.01	0.43
3:J:364:GLU:HG2	3:J:368:LYS:HE2	2.00	0.43
3:J:473:ASP:OD1	3:J:521:ARG:NH1	2.45	0.43
1:O:90:ASP:OD1	1:O:91:ARG:N	2.52	0.43
1:4:41:PHE:HB3	1:4:53:ILE:HD13	2.00	0.43
3:J:344:GLY:O	3:J:403:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:225:ILE:HG21	1:O:233:LEU:HD22	2.01	0.43
3:N:355:PHE:HZ	3:N:390:ASN:HB2	1.82	0.43
1:T:63:ALA:HB3	1:T:123:CYS:HB3	2.01	0.43
1:X:72:ASP:O	1:X:76:ARG:HG3	2.19	0.43
3:P:344:GLY:O	3:P:403:LEU:N	2.51	0.43
3:L:362:GLU:OE2	3:L:382:ARG:NE	2.48	0.43
3:H:345:ILE:HA	3:H:402:PRO:HA	2.01	0.43
1:O:33:LEU:HD21	1:O:184:ALA:HB2	2.00	0.43
1:Q:33:LEU:HD21	1:Q:184:ALA:HB2	2.01	0.43
1:2:83:ASP:OD2	3:M:365:HIS:ND1	2.31	0.43
1:4:140:ARG:NH2	1:4:150:GLU:OE2	2.50	0.43
3:N:345:ILE:HB	3:N:352:ALA:HB1	2.01	0.43
3:S:337:THR:OG1	3:S:341:THR:OG1	2.37	0.43
3:U:338:ASP:OD1	3:U:341:THR:OG1	2.17	0.43
1:O:31:VAL:HG12	1:O:155:VAL:HG22	1.99	0.43
1:4:161:GLU:HB2	1:4:162:PRO:HD3	2.00	0.43
1:2:161:GLU:HB2	1:2:162:PRO:HD3	2.01	0.42
1:Q:161:GLU:HB2	1:Q:162:PRO:HD3	2.01	0.42
1:O:88:ALA:O	3:W:381:ASN:ND2	2.52	0.42
3:H:366:TYR:CD1	3:H:374:LEU:HG	2.54	0.42
1:I:142:THR:OG1	1:I:144:ASP:OD1	2.31	0.42
1:K:161:GLU:HB2	1:K:162:PRO:HD3	2.01	0.42
3:N:366:TYR:CZ	3:N:370:GLU:HG3	2.54	0.42
3:N:378:GLY:O	3:N:382:ARG:HG2	2.20	0.42
1:O:163:ILE:HD13	1:O:188:LEU:HD12	2.01	0.42
3:W:366:TYR:CD1	3:W:374:LEU:HG	2.55	0.42
1:Z:118:TYR:HB3	1:Z:120:VAL:HG22	2.02	0.42
1:Z:205:VAL:HG12	1:Z:230:LEU:HG	2.02	0.42
1:O:45:ASN:ND2	1:O:50:LEU:O	2.40	0.42
3:U:422:SER:HB3	3:U:437:GLN:HG2	2.02	0.42
3:Y:318:ARG:HD3	3:Y:493:THR:HG23	2.02	0.42
3:Y:416:SER:O	3:Y:419:ARG:NH1	2.44	0.42
1:O:161:GLU:HB2	1:O:162:PRO:HD3	2.02	0.42
1:8:55:GLU:HB2	1:8:222:PHE:CG	2.55	0.42
1:I:55:GLU:HB2	1:I:222:PHE:CG	2.54	0.42
1:K:142:THR:OG1	1:K:144:ASP:OD1	2.25	0.42
1:Q:44:GLU:HB2	1:Q:188:LEU:HD21	2.02	0.42
1:O:142:THR:OG1	1:O:144:ASP:OD1	2.27	0.42
1:2:45:ASN:ND2	1:2:50:LEU:O	2.38	0.42
1:4:181:LEU:HD23	1:4:233:LEU:HB3	2.00	0.42
1:O:63:ALA:HB3	1:O:123:CYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:338:ASP:OD1	3:S:341:THR:OG1	2.20	0.42
3:U:366:TYR:CD1	3:U:374:LEU:HG	2.55	0.42
3:Y:366:TYR:CD1	3:Y:374:LEU:HG	2.54	0.42
1:O:161:GLU:HB2	1:O:162:PRO:HD3	2.02	0.42
3:S:366:TYR:CD1	3:S:374:LEU:HG	2.55	0.42
3:U:446:ALA:HB2	3:U:474:ALA:HB2	2.01	0.42
3:V:366:TYR:CD1	3:V:374:LEU:HG	2.54	0.42
3:R:366:TYR:CD1	3:R:374:LEU:HG	2.54	0.42
1:Z:31:VAL:HG23	1:Z:42:VAL:HB	2.01	0.42
1:X:33:LEU:HB3	1:X:153:PHE:HB3	2.02	0.41
1:4:88:ALA:O	3:M:381:ASN:ND2	2.53	0.41
3:S:422:SER:HB3	3:S:437:GLN:HG2	2.01	0.41
1:Z:90:ASP:OD1	1:Z:91:ARG:N	2.53	0.41
1:O:214:ASP:HB3	1:O:217:ARG:HG2	2.02	0.41
1:X:107:LEU:HD23	1:X:107:LEU:HA	1.88	0.41
1:Z:16:ARG:NH1	1:Z:114:GLN:O	2.51	0.41
3:H:378:GLY:O	3:H:382:ARG:HG2	2.21	0.41
1:O:165:ASN:O	1:O:169:GLU:HG2	2.20	0.41
1:Q:140:ARG:NH2	1:Q:150:GLU:OE2	2.53	0.41
1:T:161:GLU:HB2	1:T:162:PRO:HD3	2.02	0.41
1:4:83:ASP:OD2	3:H:365:HIS:ND1	2.31	0.41
3:M:366:TYR:CD1	3:M:374:LEU:HG	2.56	0.41
3:J:446:ALA:HB2	3:J:474:ALA:HB2	2.03	0.41
1:Q:225:ILE:HG21	1:Q:233:LEU:HD22	2.03	0.41
1:8:225:ILE:HG21	1:8:233:LEU:HD22	2.01	0.41
3:L:366:TYR:CD1	3:L:374:LEU:HG	2.56	0.41
3:L:366:TYR:CZ	3:L:370:GLU:HG3	2.55	0.41
3:M:446:ALA:HB2	3:M:474:ALA:HB2	2.01	0.41
1:2:33:LEU:HD11	1:2:40:LEU:HD23	2.03	0.41
1:6:178:THR:HG22	1:6:182:ARG:HE	1.86	0.41
1:8:107:LEU:HD12	1:8:141:ILE:HG22	2.02	0.41
3:H:345:ILE:HG12	3:H:402:PRO:HB3	2.03	0.41
3:J:366:TYR:CD1	3:J:374:LEU:HG	2.56	0.41
1:K:107:LEU:HD23	1:K:107:LEU:HA	1.88	0.41
1:Q:118:TYR:HB3	1:Q:120:VAL:HG22	2.03	0.41
1:T:205:VAL:HG13	1:T:230:LEU:HD23	2.02	0.41
1:T:214:ASP:HB3	1:T:217:ARG:HG2	2.02	0.41
3:W:378:GLY:O	3:W:382:ARG:HG2	2.20	0.41
1:O:51:GLN:OE1	1:O:224:ARG:NH2	2.53	0.41
1:6:214:ASP:HB3	1:6:217:ARG:HG2	2.03	0.41
1:X:140:ARG:NH2	1:X:150:GLU:OE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:609:LEU:HD11	1:2:50:LEU:HD13	2.03	0.40
1:I:90:ASP:OD1	1:I:91:ARG:N	2.54	0.40
3:V:422:SER:HB3	3:V:437:GLN:HG2	2.03	0.40
1:Z:128:ALA:HB2	1:Z:134:LYS:HB3	2.03	0.40
1:8:161:GLU:HB2	1:8:162:PRO:HD3	2.02	0.40
1:8:178:THR:O	1:8:182:ARG:HD3	2.22	0.40
1:K:163:ILE:HD13	1:K:188:LEU:HD12	2.03	0.40
3:S:366:TYR:CZ	3:S:370:GLU:HG3	2.56	0.40
3:U:344:GLY:O	3:U:403:LEU:N	2.53	0.40
3:V:369:LEU:HD23	3:V:369:LEU:HA	1.95	0.40
1:X:50:LEU:HD11	1:Z:147:ILE:HG23	2.04	0.40
3:Y:422:SER:HB3	3:Y:437:GLN:HG2	2.02	0.40
1:I:8:SER:HB3	1:I:9:PRO:HD3	2.02	0.40
1:I:150:GLU:HG3	1:I:154:VAL:HG22	2.04	0.40
3:M:378:GLY:O	3:M:382:ARG:HG2	2.21	0.40
3:W:422:SER:HB3	3:W:437:GLN:HG2	2.03	0.40
1:Q:11:GLN:HG2	1:Q:14:ARG:HH22	1.86	0.40
3:S:378:GLY:O	3:S:382:ARG:HG2	2.21	0.40
1:X:90:ASP:OD1	1:X:91:ARG:N	2.55	0.40
1:4:31:VAL:HG12	1:4:155:VAL:HG22	2.02	0.40
1:6:31:VAL:HG12	1:6:155:VAL:HG22	2.03	0.40
1:I:18:GLU:OE1	1:I:21:ARG:NH2	2.39	0.40
1:K:55:GLU:HB2	1:K:222:PHE:CG	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	0	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	2	211/248 (85%)	207 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4	211/248 (85%)	208 (99%)	3 (1%)	0	100	100
1	6	211/248 (85%)	206 (98%)	5 (2%)	0	100	100
1	8	211/248 (85%)	206 (98%)	5 (2%)	0	100	100
1	I	210/248 (85%)	205 (98%)	5 (2%)	0	100	100
1	K	213/248 (86%)	209 (98%)	4 (2%)	0	100	100
1	O	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	Q	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	T	210/248 (85%)	206 (98%)	4 (2%)	0	100	100
1	X	210/248 (85%)	206 (98%)	4 (2%)	0	100	100
1	Z	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	d	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	f	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
2	1	3/609 (0%)	2 (67%)	1 (33%)	0	100	100
2	A	3/609 (0%)	2 (67%)	1 (33%)	0	100	100
2	B	3/609 (0%)	3 (100%)	0	0	100	100
2	C	5/609 (1%)	5 (100%)	0	0	100	100
2	D	3/609 (0%)	2 (67%)	1 (33%)	0	100	100
2	E	5/609 (1%)	4 (80%)	1 (20%)	0	100	100
2	F	4/609 (1%)	4 (100%)	0	0	100	100
3	H	220/291 (76%)	218 (99%)	2 (1%)	0	100	100
3	J	221/291 (76%)	219 (99%)	2 (1%)	0	100	100
3	L	220/291 (76%)	218 (99%)	2 (1%)	0	100	100
3	M	220/291 (76%)	218 (99%)	2 (1%)	0	100	100
3	N	220/291 (76%)	218 (99%)	2 (1%)	0	100	100
3	P	221/291 (76%)	220 (100%)	1 (0%)	0	100	100
3	R	220/291 (76%)	218 (99%)	2 (1%)	0	100	100
3	S	220/291 (76%)	218 (99%)	2 (1%)	0	100	100
3	U	232/291 (80%)	229 (99%)	3 (1%)	0	100	100
3	V	221/291 (76%)	219 (99%)	2 (1%)	0	100	100
3	W	232/291 (80%)	230 (99%)	2 (1%)	0	100	100
3	Y	221/291 (76%)	219 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	a	221/291 (76%)	219 (99%)	2 (1%)	0	100	100
3	b	221/291 (76%)	218 (99%)	3 (1%)	0	100	100
All	All	6089/11809 (52%)	5996 (98%)	93 (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	0	165/192 (86%)	161 (98%)	4 (2%)	49	81
1	2	165/192 (86%)	161 (98%)	4 (2%)	49	81
1	4	165/192 (86%)	161 (98%)	4 (2%)	49	81
1	6	165/192 (86%)	160 (97%)	5 (3%)	41	75
1	8	165/192 (86%)	163 (99%)	2 (1%)	71	92
1	I	164/192 (85%)	161 (98%)	3 (2%)	59	86
1	K	166/192 (86%)	164 (99%)	2 (1%)	71	92
1	O	165/192 (86%)	164 (99%)	1 (1%)	86	96
1	Q	165/192 (86%)	163 (99%)	2 (1%)	71	92
1	T	164/192 (85%)	163 (99%)	1 (1%)	86	96
1	X	164/192 (85%)	163 (99%)	1 (1%)	86	96
1	Z	165/192 (86%)	163 (99%)	2 (1%)	71	92
1	d	165/192 (86%)	160 (97%)	5 (3%)	41	75
1	f	165/192 (86%)	164 (99%)	1 (1%)	86	96
2	1	4/511 (1%)	4 (100%)	0	100	100
2	A	4/511 (1%)	4 (100%)	0	100	100
2	B	4/511 (1%)	4 (100%)	0	100	100
2	C	6/511 (1%)	6 (100%)	0	100	100
2	D	4/511 (1%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	6/511 (1%)	6 (100%)	0	100	100
2	F	5/511 (1%)	4 (80%)	1 (20%)	1	4
3	H	164/217 (76%)	164 (100%)	0	100	100
3	J	164/217 (76%)	162 (99%)	2 (1%)	71	92
3	L	164/217 (76%)	163 (99%)	1 (1%)	86	96
3	M	164/217 (76%)	163 (99%)	1 (1%)	86	96
3	N	164/217 (76%)	163 (99%)	1 (1%)	86	96
3	P	164/217 (76%)	163 (99%)	1 (1%)	86	96
3	R	164/217 (76%)	164 (100%)	0	100	100
3	S	164/217 (76%)	163 (99%)	1 (1%)	86	96
3	U	171/217 (79%)	171 (100%)	0	100	100
3	V	164/217 (76%)	162 (99%)	2 (1%)	71	92
3	W	171/217 (79%)	170 (99%)	1 (1%)	86	96
3	Y	164/217 (76%)	163 (99%)	1 (1%)	86	96
3	a	164/217 (76%)	164 (100%)	0	100	100
3	b	164/217 (76%)	162 (99%)	2 (1%)	71	92
All	All	4651/9303 (50%)	4600 (99%)	51 (1%)	74	92

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	33	LEU
1	0	147	ILE
1	0	182	ARG
1	0	234	LEU
1	2	33	LEU
1	2	147	ILE
1	2	182	ARG
1	2	234	LEU
1	4	33	LEU
1	4	147	ILE
1	4	182	ARG
1	4	234	LEU
1	6	11	GLN
1	6	33	LEU
1	6	147	ILE

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Mol	Chain	Res	Type
1	6	182	ARG
1	6	234	LEU
1	8	182	ARG
1	8	234	LEU
2	F	609	LEU
1	I	33	LEU
1	I	182	ARG
1	I	217	ARG
3	J	354	GLU
3	J	434	GLU
1	K	33	LEU
1	K	182	ARG
3	L	355	PHE
3	M	330	ASP
3	N	509	ARG
1	O	182	ARG
3	P	432	GLU
1	Q	182	ARG
1	Q	234	LEU
3	S	330	ASP
1	T	182	ARG
3	V	355	PHE
3	V	509	ARG
3	W	330	ASP
1	X	182	ARG
3	Y	330	ASP
1	Z	73	ASN
1	Z	182	ARG
3	b	330	ASP
3	b	355	PHE
1	d	14	ARG
1	d	26	ARG
1	d	33	LEU
1	d	182	ARG
1	d	234	LEU
1	f	182	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	607	GLN
1	I	114	GLN

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Mol	Chain	Res	Type
1	K	114	GLN
1	O	114	GLN
1	Q	114	GLN
1	X	114	GLN

### 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.

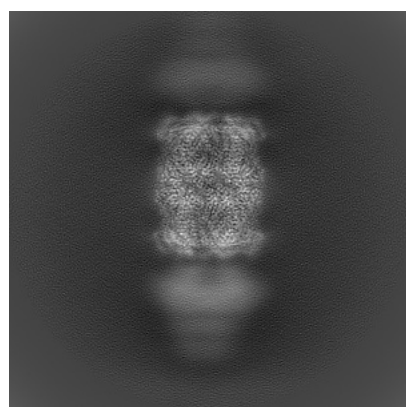
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13695. These allow visual inspection of the internal detail of the map and identification of artifacts.

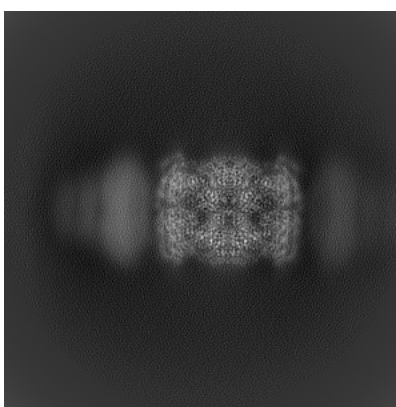
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

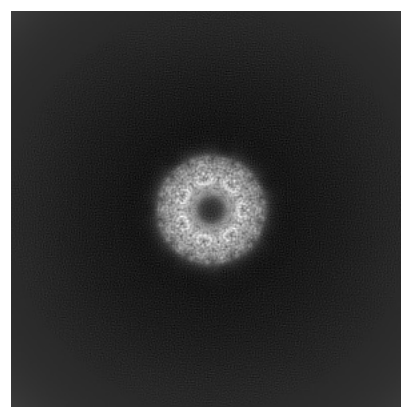
#### 6.1.1 Primary map



X



Y

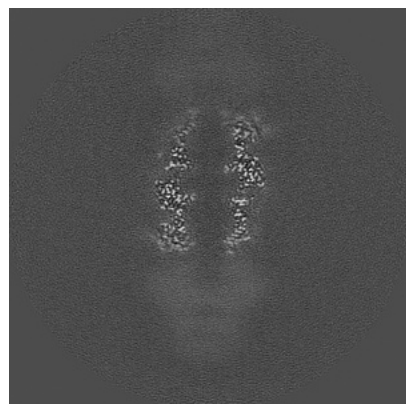


Z

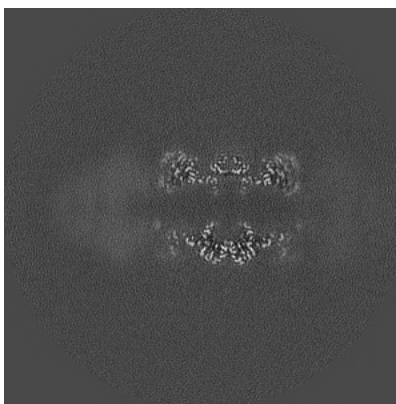
The images above show the map projected in three orthogonal directions.

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

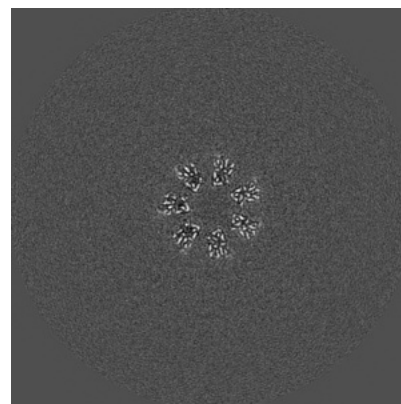
#### 6.2.1 Primary map



X Index: 176



Y Index: 176

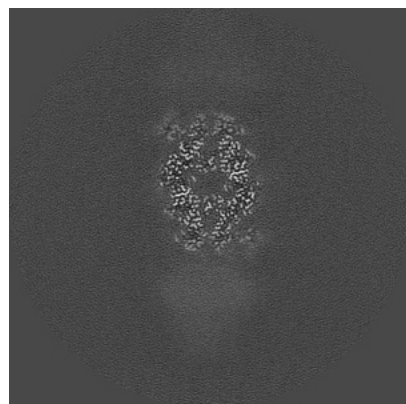


Z Index: 176

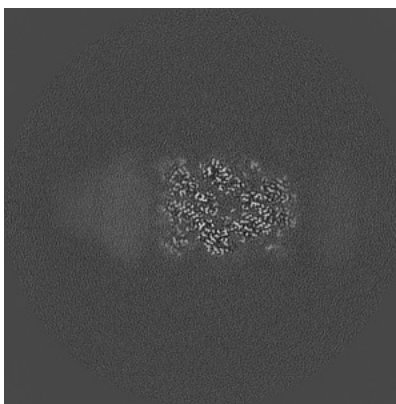
The images above show central slices of the map in three orthogonal directions.

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

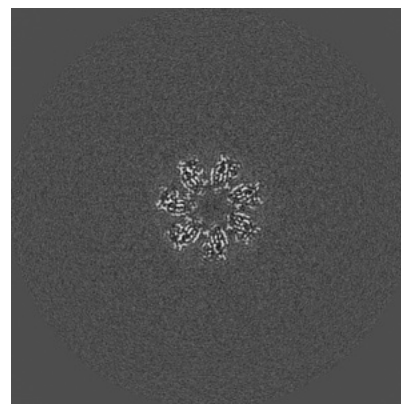
### 6.3.1 Primary map



X Index: 155



Y Index: 152

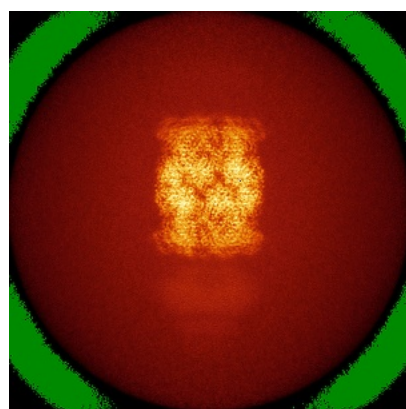


Z Index: 182

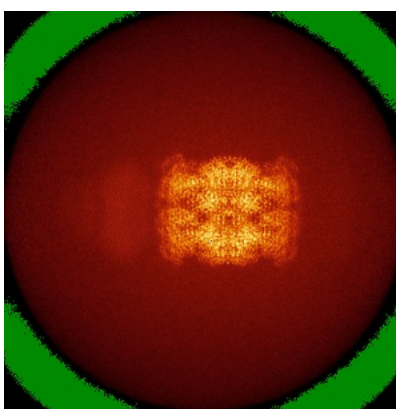
The images above show the largest variance slices of the map in three orthogonal directions.

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

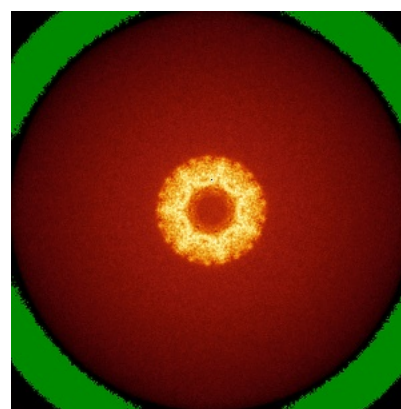
### 6.4.1 Primary map



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 0.0236. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

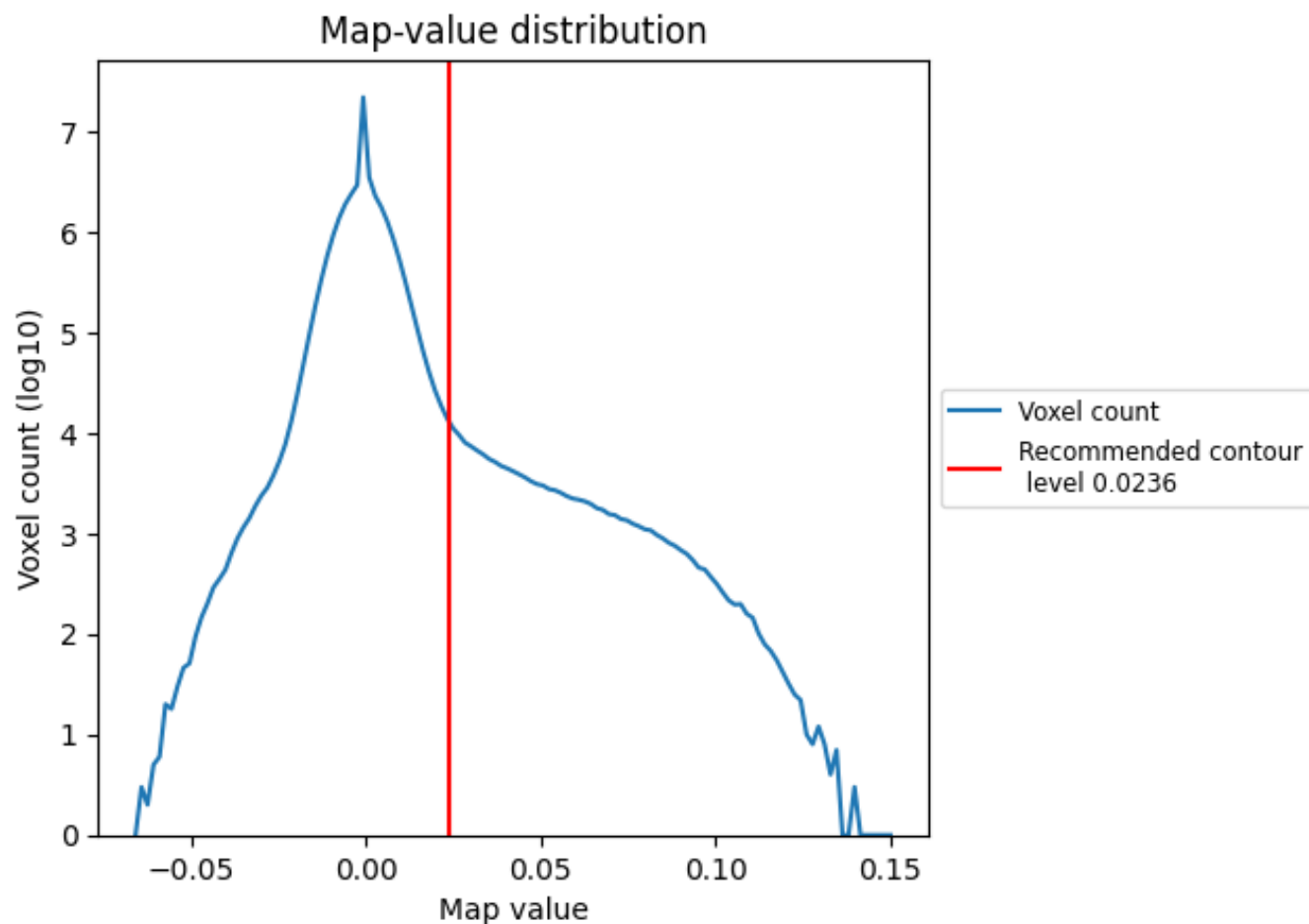
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

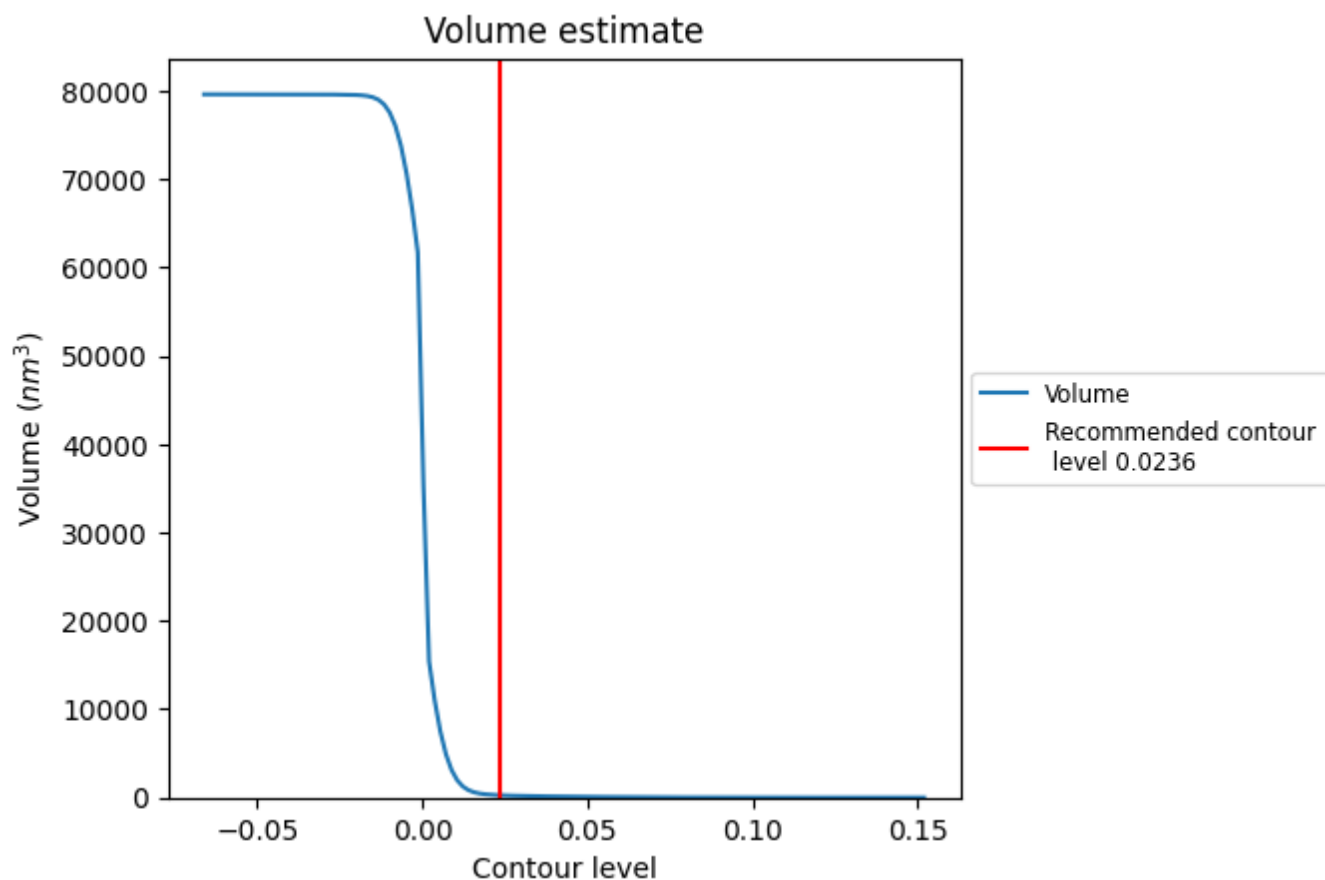
This section contains the results of statistical analysis of the map.

### 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](#)

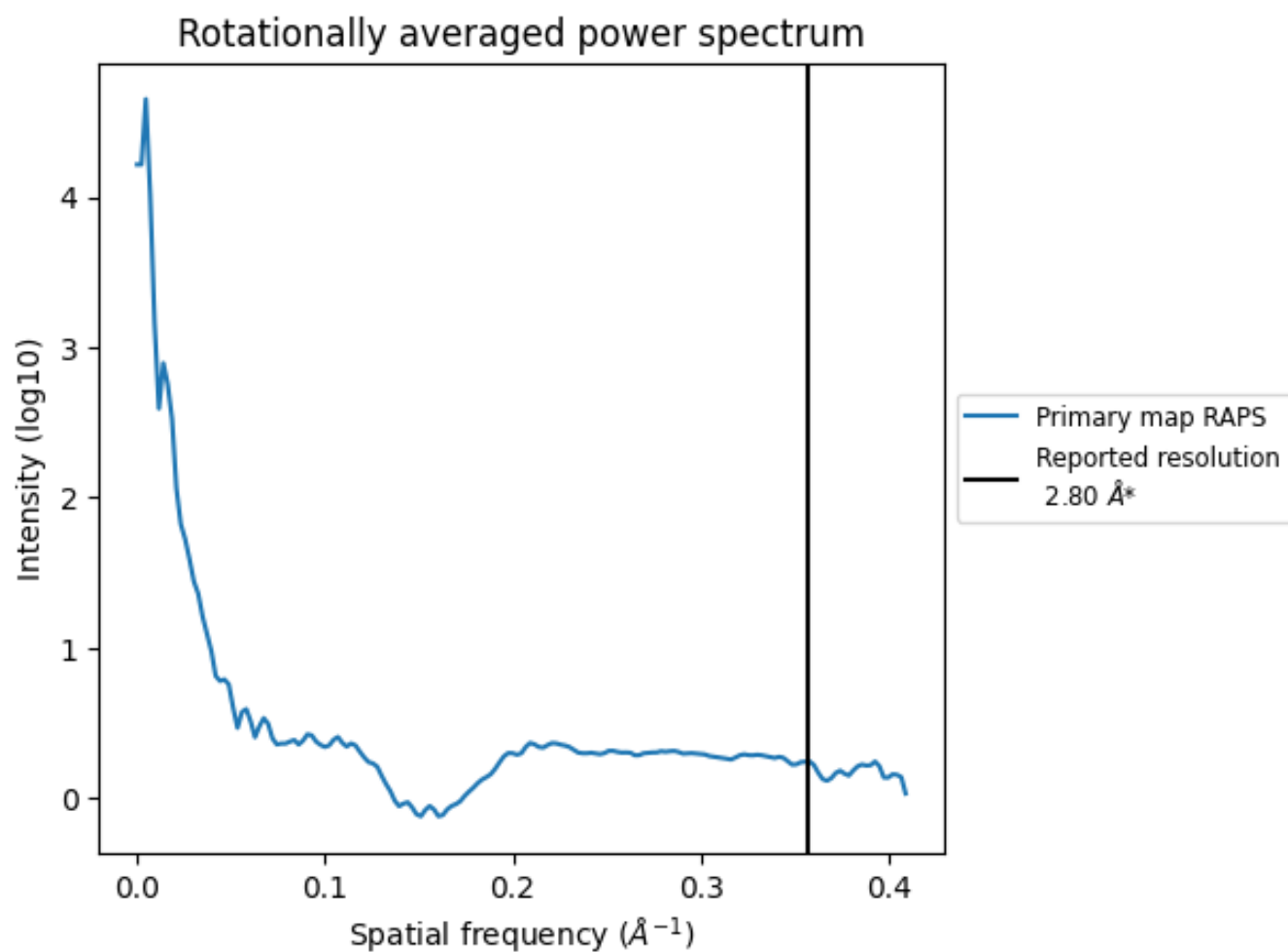


The volume at the recommended contour level is 258 nm<sup>3</sup>; this corresponds to an approximate mass of 233 kDa.

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 0.357 Å<sup>-1</sup>

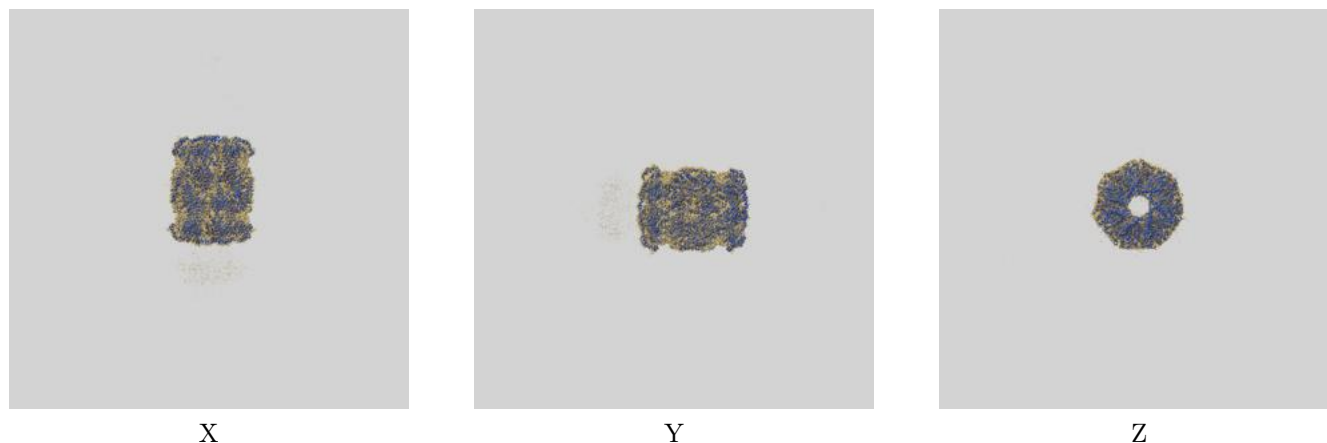
## 8 Fourier-Shell correlation ⓘ

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

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

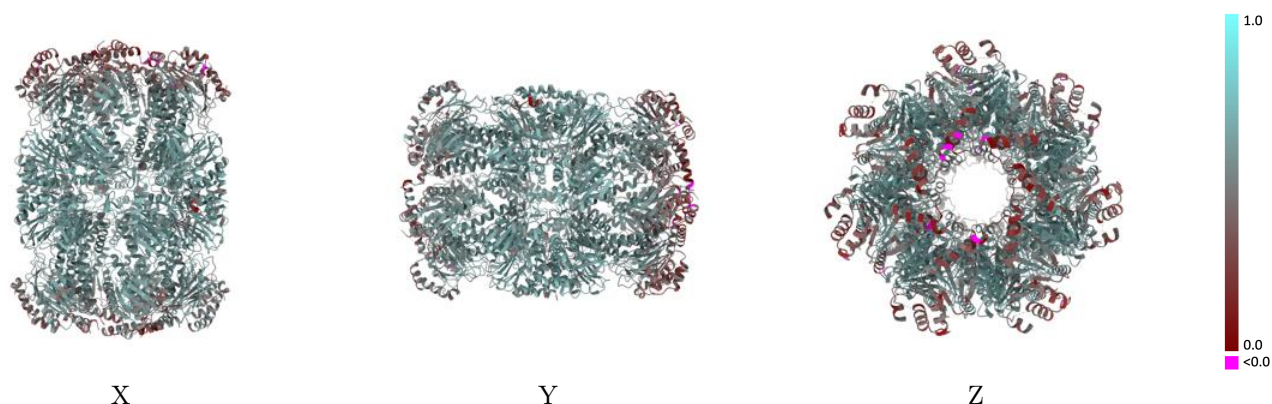
This section contains information regarding the fit between EMDB map EMD-13695 and PDB model 7PXA. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

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



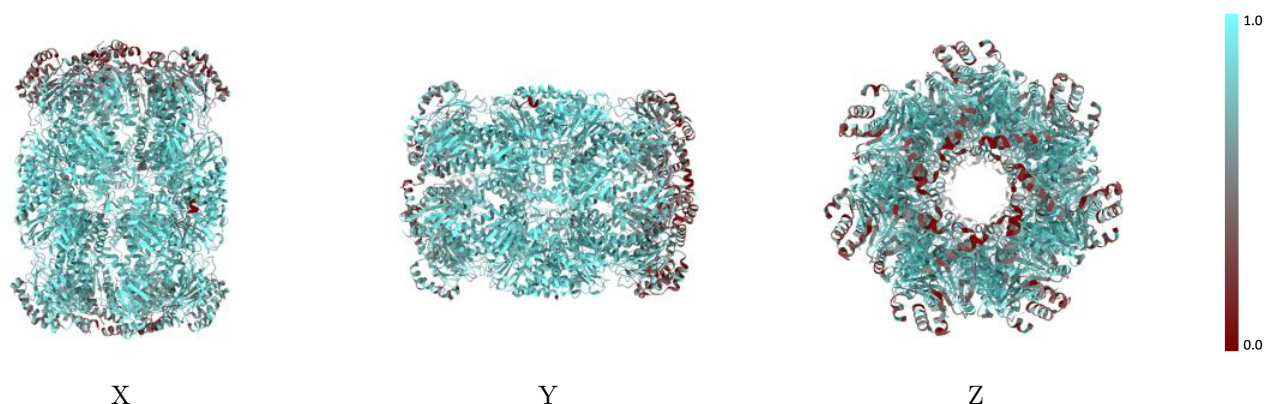
The images above show the 3D surface view of the map at the recommended contour level 0.0236 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



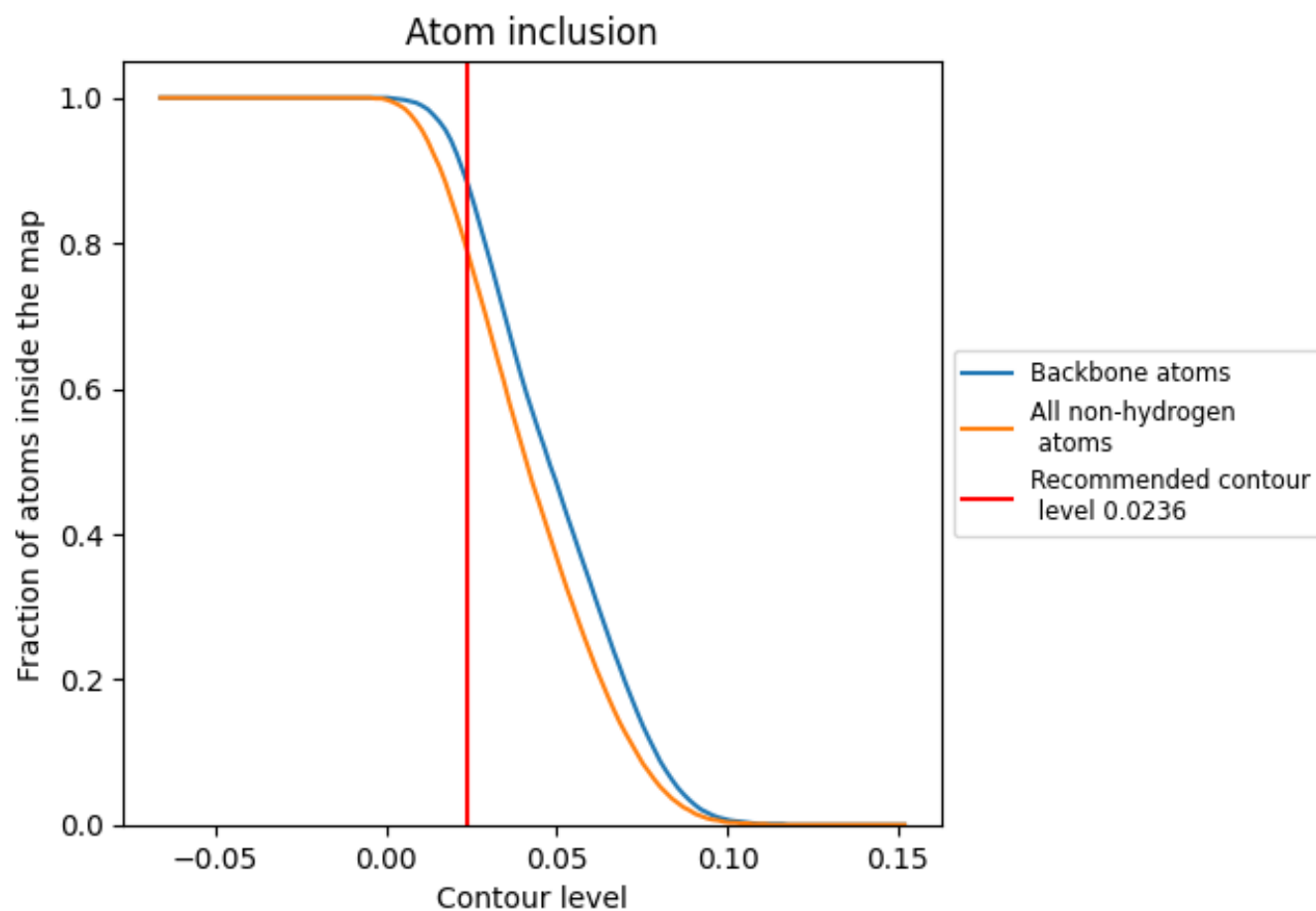
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0236).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0236) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7930	 0.5550
0	 0.7730	 0.5280
1	 0.3900	 0.4280
2	 0.7700	 0.5370
4	 0.7660	 0.5350
6	 0.7630	 0.5270
8	 0.7590	 0.5350
A	 0.5850	 0.4720
B	 0.4880	 0.4510
C	 0.5090	 0.4700
D	 0.5370	 0.4220
E	 0.4550	 0.4440
F	 0.5100	 0.4970
H	 0.9110	 0.6250
I	 0.6100	 0.4580
J	 0.9050	 0.6190
K	 0.6160	 0.4500
L	 0.9080	 0.6240
M	 0.9080	 0.6210
N	 0.9060	 0.6220
O	 0.6120	 0.4580
P	 0.9000	 0.6260
Q	 0.6110	 0.4590
R	 0.9040	 0.6200
S	 0.9040	 0.6210
T	 0.6180	 0.4540
U	 0.8560	 0.5930
V	 0.9060	 0.6210
W	 0.8710	 0.6010
X	 0.6160	 0.4570
Y	 0.9040	 0.6180
Z	 0.6200	 0.4540
a	 0.9010	 0.6210
b	 0.9060	 0.6200
d	 0.7580	 0.5250
f	 0.7710	 0.5370

