



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 08:25 AM EST

PDB ID : 6PE4
EMDB ID : EMD-20322
Title : Yeast Vo motor in complex with 1 VopQ molecule
Authors : Peng, W.; Li, Y.; Tomchick, D.R.; Orth, K.
Deposited on : 2019-06-20
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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

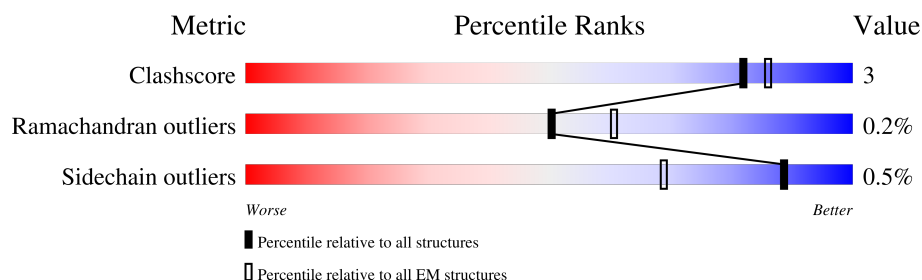
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	1012	<div> <div>17%</div> <div>68%</div> <div>7%</div> <div>25%</div> </div>
2	B	265	<div> <div>19%</div> <div>80%</div> </div>
3	D	345	<div> <div>12%</div> <div>86%</div> <div>14%</div> </div>
4	E	73	<div> <div>12%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
5	F	85	<div> <div>42%</div> <div>81%</div> <div>6%</div> <div>13%</div> </div>
6	G	213	<div> <div>7%</div> <div>82%</div> <div>11%</div> <div>7%</div> </div>
7	H	164	<div> <div>88%</div> <div>7%</div> </div>
8	I	160	<div> <div>95%</div> </div>

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Mol	Chain	Length	Quality of chain
8	J	160	<div><div></div><div>98%</div><div></div></div>
8	K	160	<div><div></div><div>92%</div><div>6%</div></div>
8	L	160	<div><div></div><div>94%</div><div>6%</div></div>
8	M	160	<div><div></div><div>97%</div><div></div></div>
8	N	160	<div><div>5%</div><div>91%</div><div>9%</div></div>
8	O	160	<div><div></div><div>97%</div><div></div></div>
8	P	160	<div><div></div><div>89%</div><div>9%</div></div>
9	Q	513	<div><div>37%</div><div>67%</div><div>5%</div><div>28%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24914 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 V-type proton ATPase subunit a, vacuolar isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	758	Total	C	N	O	S	0	0
			6142	4008	999	1100	35		

There are 172 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	841	SER	-	expression tag	UNP P32563
A	842	MET	-	expression tag	UNP P32563
A	843	GLU	-	expression tag	UNP P32563
A	844	LYS	-	expression tag	UNP P32563
A	845	ARG	-	expression tag	UNP P32563
A	846	ARG	-	expression tag	UNP P32563
A	847	TRP	-	expression tag	UNP P32563
A	848	LYS	-	expression tag	UNP P32563
A	849	LYS	-	expression tag	UNP P32563
A	850	ASN	-	expression tag	UNP P32563
A	851	PHE	-	expression tag	UNP P32563
A	852	ILE	-	expression tag	UNP P32563
A	853	ALA	-	expression tag	UNP P32563
A	854	VAL	-	expression tag	UNP P32563
A	855	SER	-	expression tag	UNP P32563
A	856	ALA	-	expression tag	UNP P32563
A	857	ALA	-	expression tag	UNP P32563
A	858	ASN	-	expression tag	UNP P32563
A	859	ARG	-	expression tag	UNP P32563
A	860	PHE	-	expression tag	UNP P32563
A	861	LYS	-	expression tag	UNP P32563
A	862	LYS	-	expression tag	UNP P32563
A	863	ILE	-	expression tag	UNP P32563
A	864	SER	-	expression tag	UNP P32563
A	865	SER	-	expression tag	UNP P32563
A	866	SER	-	expression tag	UNP P32563
A	867	GLY	-	expression tag	UNP P32563
A	868	ALA	-	expression tag	UNP P32563

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Chain	Residue	Modelled	Actual	Comment	Reference
A	869	LEU	-	expression tag	UNP P32563
A	870	ASP	-	expression tag	UNP P32563
A	871	TYR	-	expression tag	UNP P32563
A	872	ASP	-	expression tag	UNP P32563
A	873	ILE	-	expression tag	UNP P32563
A	874	PRO	-	expression tag	UNP P32563
A	875	THR	-	expression tag	UNP P32563
A	876	THR	-	expression tag	UNP P32563
A	877	ALA	-	expression tag	UNP P32563
A	878	SER	-	expression tag	UNP P32563
A	879	GLU	-	expression tag	UNP P32563
A	880	ASN	-	expression tag	UNP P32563
A	881	LEU	-	expression tag	UNP P32563
A	882	TYR	-	expression tag	UNP P32563
A	883	PHE	-	expression tag	UNP P32563
A	884	GLN	-	expression tag	UNP P32563
A	885	GLY	-	expression tag	UNP P32563
A	886	GLU	-	expression tag	UNP P32563
A	887	LEU	-	expression tag	UNP P32563
A	888	LYS	-	expression tag	UNP P32563
A	889	THR	-	expression tag	UNP P32563
A	890	ALA	-	expression tag	UNP P32563
A	891	ALA	-	expression tag	UNP P32563
A	892	LEU	-	expression tag	UNP P32563
A	893	ALA	-	expression tag	UNP P32563
A	894	GLN	-	expression tag	UNP P32563
A	895	HIS	-	expression tag	UNP P32563
A	896	ASP	-	expression tag	UNP P32563
A	897	GLU	-	expression tag	UNP P32563
A	898	ALA	-	expression tag	UNP P32563
A	899	VAL	-	expression tag	UNP P32563
A	900	ASP	-	expression tag	UNP P32563
A	901	ASN	-	expression tag	UNP P32563
A	902	PHE	-	expression tag	UNP P32563
A	903	ASN	-	expression tag	UNP P32563
A	904	LYS	-	expression tag	UNP P32563
A	905	GLU	-	expression tag	UNP P32563
A	906	GLN	-	expression tag	UNP P32563
A	907	GLN	-	expression tag	UNP P32563
A	908	ASN	-	expression tag	UNP P32563
A	909	ALA	-	expression tag	UNP P32563
A	910	PHE	-	expression tag	UNP P32563

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Chain	Residue	Modelled	Actual	Comment	Reference
A	911	TYR	-	expression tag	UNP P32563
A	912	GLU	-	expression tag	UNP P32563
A	913	ILE	-	expression tag	UNP P32563
A	914	LEU	-	expression tag	UNP P32563
A	915	HIS	-	expression tag	UNP P32563
A	916	LEU	-	expression tag	UNP P32563
A	917	PRO	-	expression tag	UNP P32563
A	918	ASN	-	expression tag	UNP P32563
A	919	LEU	-	expression tag	UNP P32563
A	920	ASN	-	expression tag	UNP P32563
A	921	GLU	-	expression tag	UNP P32563
A	922	GLU	-	expression tag	UNP P32563
A	923	GLN	-	expression tag	UNP P32563
A	924	ARG	-	expression tag	UNP P32563
A	925	ASN	-	expression tag	UNP P32563
A	926	ALA	-	expression tag	UNP P32563
A	927	PHE	-	expression tag	UNP P32563
A	928	ILE	-	expression tag	UNP P32563
A	929	GLN	-	expression tag	UNP P32563
A	930	SER	-	expression tag	UNP P32563
A	931	LEU	-	expression tag	UNP P32563
A	932	LYS	-	expression tag	UNP P32563
A	933	ASP	-	expression tag	UNP P32563
A	934	ASP	-	expression tag	UNP P32563
A	935	PRO	-	expression tag	UNP P32563
A	936	SER	-	expression tag	UNP P32563
A	937	GLN	-	expression tag	UNP P32563
A	938	SER	-	expression tag	UNP P32563
A	939	ALA	-	expression tag	UNP P32563
A	940	ASN	-	expression tag	UNP P32563
A	941	LEU	-	expression tag	UNP P32563
A	942	LEU	-	expression tag	UNP P32563
A	943	ALA	-	expression tag	UNP P32563
A	944	GLU	-	expression tag	UNP P32563
A	945	ALA	-	expression tag	UNP P32563
A	946	LYS	-	expression tag	UNP P32563
A	947	LYS	-	expression tag	UNP P32563
A	948	LEU	-	expression tag	UNP P32563
A	949	ASN	-	expression tag	UNP P32563
A	950	ASP	-	expression tag	UNP P32563
A	951	ALA	-	expression tag	UNP P32563
A	952	GLN	-	expression tag	UNP P32563

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Chain	Residue	Modelled	Actual	Comment	Reference
A	953	ALA	-	expression tag	UNP P32563
A	954	PRO	-	expression tag	UNP P32563
A	955	LYS	-	expression tag	UNP P32563
A	956	VAL	-	expression tag	UNP P32563
A	957	ASP	-	expression tag	UNP P32563
A	958	ASN	-	expression tag	UNP P32563
A	959	PHE	-	expression tag	UNP P32563
A	960	ASN	-	expression tag	UNP P32563
A	961	LYS	-	expression tag	UNP P32563
A	962	GLU	-	expression tag	UNP P32563
A	963	GLN	-	expression tag	UNP P32563
A	964	GLN	-	expression tag	UNP P32563
A	965	ASN	-	expression tag	UNP P32563
A	966	ALA	-	expression tag	UNP P32563
A	967	PHE	-	expression tag	UNP P32563
A	968	TYR	-	expression tag	UNP P32563
A	969	GLU	-	expression tag	UNP P32563
A	970	ILE	-	expression tag	UNP P32563
A	971	LEU	-	expression tag	UNP P32563
A	972	HIS	-	expression tag	UNP P32563
A	973	LEU	-	expression tag	UNP P32563
A	974	PRO	-	expression tag	UNP P32563
A	975	ASN	-	expression tag	UNP P32563
A	976	LEU	-	expression tag	UNP P32563
A	977	ASN	-	expression tag	UNP P32563
A	978	GLU	-	expression tag	UNP P32563
A	979	GLU	-	expression tag	UNP P32563
A	980	GLN	-	expression tag	UNP P32563
A	981	ARG	-	expression tag	UNP P32563
A	982	ASN	-	expression tag	UNP P32563
A	983	ALA	-	expression tag	UNP P32563
A	984	PHE	-	expression tag	UNP P32563
A	985	ILE	-	expression tag	UNP P32563
A	986	GLN	-	expression tag	UNP P32563
A	987	SER	-	expression tag	UNP P32563
A	988	LEU	-	expression tag	UNP P32563
A	989	LYS	-	expression tag	UNP P32563
A	990	ASP	-	expression tag	UNP P32563
A	991	ASP	-	expression tag	UNP P32563
A	992	PRO	-	expression tag	UNP P32563
A	993	SER	-	expression tag	UNP P32563
A	994	GLN	-	expression tag	UNP P32563

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Chain	Residue	Modelled	Actual	Comment	Reference
A	995	SER	-	expression tag	UNP P32563
A	996	ALA	-	expression tag	UNP P32563
A	997	ASN	-	expression tag	UNP P32563
A	998	LEU	-	expression tag	UNP P32563
A	999	LEU	-	expression tag	UNP P32563
A	1000	ALA	-	expression tag	UNP P32563
A	1001	GLU	-	expression tag	UNP P32563
A	1002	ALA	-	expression tag	UNP P32563
A	1003	LYS	-	expression tag	UNP P32563
A	1004	LYS	-	expression tag	UNP P32563
A	1005	LEU	-	expression tag	UNP P32563
A	1006	ASN	-	expression tag	UNP P32563
A	1007	ASP	-	expression tag	UNP P32563
A	1008	ALA	-	expression tag	UNP P32563
A	1009	GLN	-	expression tag	UNP P32563
A	1010	ALA	-	expression tag	UNP P32563
A	1011	PRO	-	expression tag	UNP P32563
A	1012	LYS	-	expression tag	UNP P32563

- Molecule 2 is a protein called V0 assembly protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	53	Total	C	N	O	S	0	0
			406	268	59	77	2		

- Molecule 3 is a protein called V-type proton ATPase subunit d.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	345	Total	C	N	O	S	0	0
			2802	1779	454	555	14		

- Molecule 4 is a protein called V-type proton ATPase subunit e.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	69	Total	C	N	O	S	0	0
			554	369	91	88	6		

- Molecule 5 is a protein called Uncharacterized protein YPR170W-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	74	Total	C	N	O	S	0	0
			561	374	86	98	3		

- Molecule 6 is a protein called V-type proton ATPase subunit c''.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	199	Total	C	N	O	S	0	0
			1484	989	229	259	7		

- Molecule 7 is a protein called V-type proton ATPase subunit c'.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	158	Total	C	N	O	S	0	0
			1149	758	180	199	12		

- Molecule 8 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	159	Total	C	N	O	S	0	0
			1140	751	182	199	8		
8	J	159	Total	C	N	O	S	0	0
			1140	751	182	199	8		
8	K	159	Total	C	N	O	S	0	0
			1140	751	182	199	8		
8	L	159	Total	C	N	O	S	0	0
			1140	751	182	199	8		
8	M	159	Total	C	N	O	S	0	0
			1140	751	182	199	8		
8	N	159	Total	C	N	O	S	0	0
			1140	751	182	199	8		
8	O	158	Total	C	N	O	S	0	0
			1132	746	181	198	7		
8	P	158	Total	C	N	O	S	0	0
			1132	746	181	198	7		

- Molecule 9 is a protein called Cation transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	369	Total	C	N	O	S	0	0
			2712	1686	469	542	15		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	-20	MET	-	initiating methionine	UNP A0A0L7YPA6
Q	-19	GLY	-	expression tag	UNP A0A0L7YPA6
Q	-18	SER	-	expression tag	UNP A0A0L7YPA6

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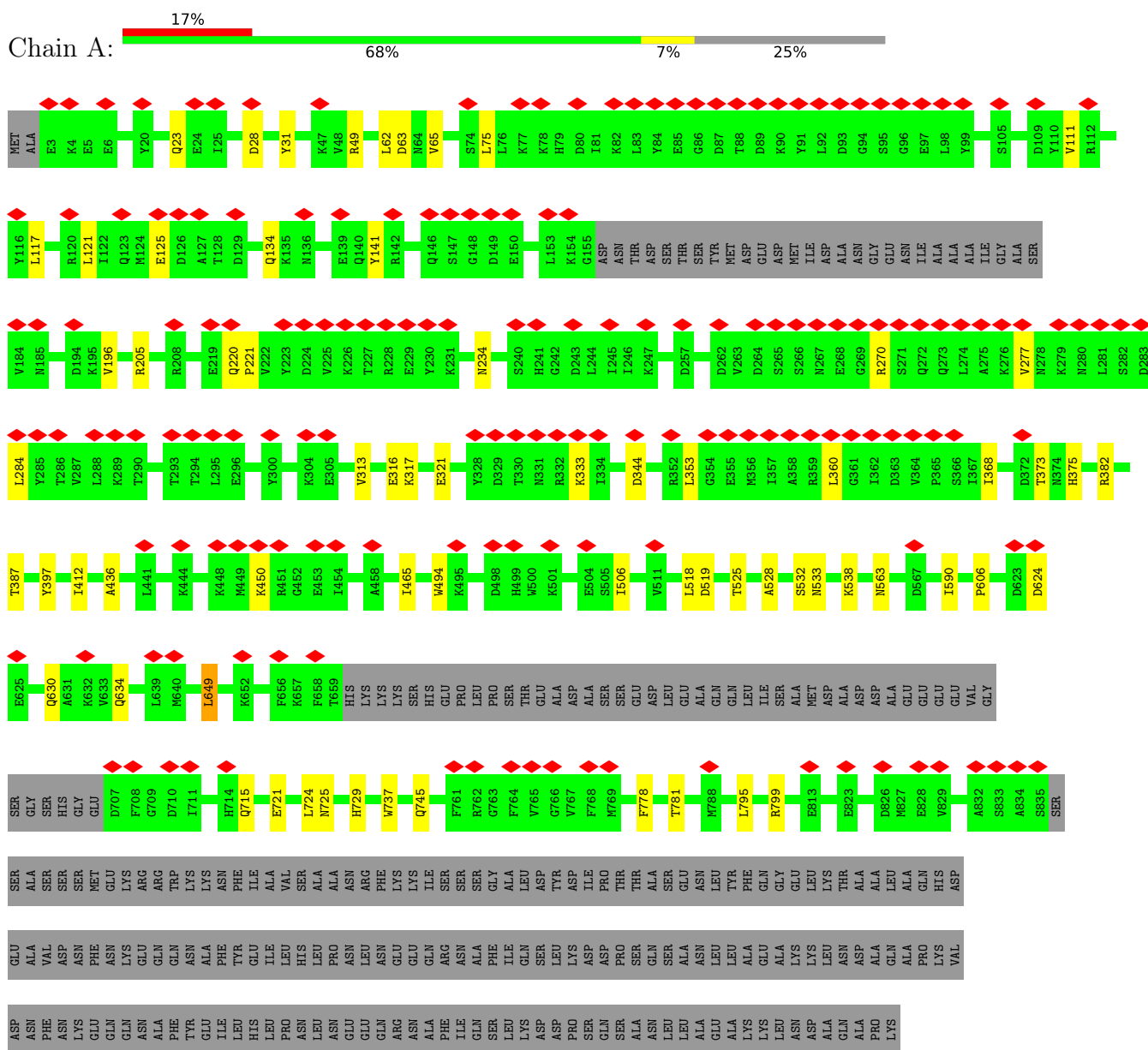
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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-17	SER	-	expression tag	UNP A0A0L7YPA6
Q	-16	HIS	-	expression tag	UNP A0A0L7YPA6
Q	-15	HIS	-	expression tag	UNP A0A0L7YPA6
Q	-14	HIS	-	expression tag	UNP A0A0L7YPA6
Q	-13	HIS	-	expression tag	UNP A0A0L7YPA6
Q	-12	HIS	-	expression tag	UNP A0A0L7YPA6
Q	-11	HIS	-	expression tag	UNP A0A0L7YPA6
Q	-10	SER	-	expression tag	UNP A0A0L7YPA6
Q	-9	GLN	-	expression tag	UNP A0A0L7YPA6
Q	-8	ASP	-	expression tag	UNP A0A0L7YPA6
Q	-7	LEU	-	expression tag	UNP A0A0L7YPA6
Q	-6	ASP	-	expression tag	UNP A0A0L7YPA6
Q	-5	GLU	-	expression tag	UNP A0A0L7YPA6
Q	-4	VAL	-	expression tag	UNP A0A0L7YPA6
Q	-3	ASP	-	expression tag	UNP A0A0L7YPA6
Q	-2	ALA	-	expression tag	UNP A0A0L7YPA6
Q	-1	GLY	-	expression tag	UNP A0A0L7YPA6
Q	0	SER	-	expression tag	UNP A0A0L7YPA6
Q	283	THR	ALA	conflict	UNP A0A0L7YPA6

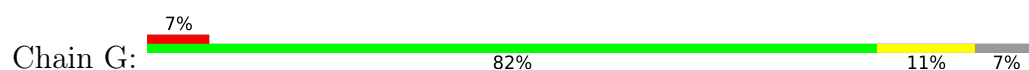
3 Residue-property plots

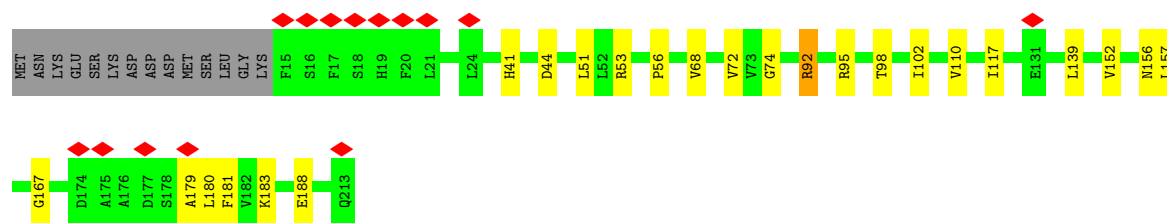
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: V-type proton ATPase subunit a, vacuolar isoform

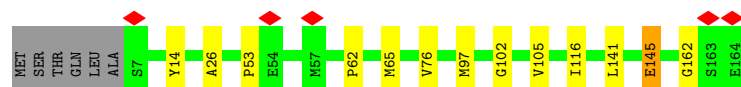
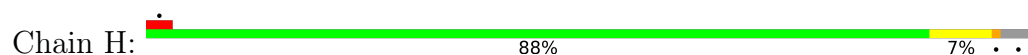


- Molecule 2: V0 assembly protein 1

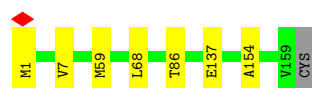
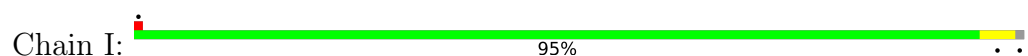




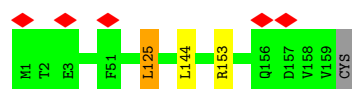
- Molecule 7: V-type proton ATPase subunit c'



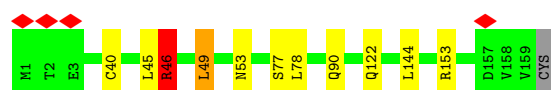
- Molecule 8: V-type proton ATPase subunit c



- Molecule 8: V-type proton ATPase subunit c



- Molecule 8: V-type proton ATPase subunit c

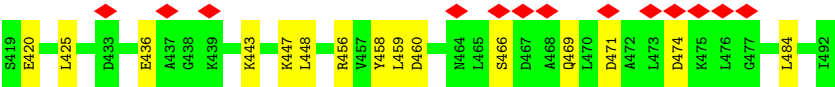


- Molecule 8: V-type proton ATPase subunit c



- Molecule 8: V-type proton ATPase subunit c





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108491	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.158	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.035	Depositor
Map size (\AA)	299.6, 299.6, 299.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/6295	0.61	3/8520 (0.0%)
2	B	0.34	0/412	0.58	0/562
3	D	0.42	0/2861	0.65	2/3880 (0.1%)
4	E	0.34	0/570	0.65	0/778
5	F	0.31	0/578	0.54	0/793
6	G	0.43	0/1515	0.61	0/2057
7	H	0.44	0/1172	0.68	0/1587
8	I	0.41	0/1158	0.64	1/1574 (0.1%)
8	J	0.41	0/1158	0.63	2/1574 (0.1%)
8	K	0.42	0/1158	0.69	2/1574 (0.1%)
8	L	0.40	0/1158	0.62	0/1574
8	M	0.40	0/1158	0.64	1/1574 (0.1%)
8	N	0.42	0/1158	0.69	0/1574
8	O	0.41	0/1150	0.66	0/1564
8	P	0.44	0/1150	0.70	3/1564 (0.2%)
9	Q	0.32	0/2752	0.62	1/3726 (0.0%)
All	All	0.39	0/25403	0.63	15/34475 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	K	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	135	ASP	CB-CG-OD1	10.04	127.34	118.30
1	A	649	LEU	CA-CB-CG	8.41	134.64	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	49	LEU	CA-CB-CG	7.84	133.34	115.30
3	D	248	LEU	CA-CB-CG	6.09	129.31	115.30
8	K	144	LEU	CA-CB-CG	5.91	128.89	115.30
8	P	144	LEU	CA-CB-CG	5.81	128.67	115.30
8	P	141	LEU	CA-CB-CG	5.70	128.41	115.30
1	A	724	LEU	CA-CB-CG	5.62	128.24	115.30
8	I	68	LEU	CA-CB-CG	5.46	127.86	115.30
3	D	76	LEU	CA-CB-CG	5.40	127.72	115.30
8	J	144	LEU	CA-CB-CG	5.37	127.64	115.30
1	A	117	LEU	CA-CB-CG	5.21	127.28	115.30
8	J	125	LEU	CA-CB-CG	5.14	127.13	115.30
8	P	68	LEU	CA-CB-CG	5.12	127.08	115.30
8	M	91	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	K	46	ARG	Sidechain

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	6142	0	6125	35	0
2	B	406	0	426	3	0
3	D	2802	0	2689	30	0
4	E	554	0	575	6	0
5	F	561	0	551	3	0
6	G	1484	0	1549	15	0
7	H	1149	0	1200	8	0
8	I	1140	0	1214	4	0
8	J	1140	0	1214	2	0
8	K	1140	0	1214	8	0
8	L	1140	0	1214	7	0
8	M	1140	0	1214	2	0
8	N	1140	0	1214	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	O	1132	0	1202	2	0
8	P	1132	0	1202	9	0
9	Q	2712	0	2597	19	0
All	All	24914	0	25400	128	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 3.

All (128) 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:D:163:LYS:HZ1	9:Q:456:ARG:HD2	1.51	0.76
3:D:163:LYS:HZ1	9:Q:456:ARG:CD	2.01	0.74
3:D:163:LYS:NZ	9:Q:456:ARG:CD	2.54	0.70
3:D:163:LYS:NZ	9:Q:456:ARG:HD3	2.08	0.69
9:Q:388:VAL:HG11	9:Q:401:ASP:HB2	1.77	0.66
7:H:76:VAL:HG21	7:H:105:VAL:HG21	1.78	0.66
8:N:70:VAL:HG21	8:N:97:VAL:HG21	1.78	0.65
8:K:122:GLN:NE2	9:Q:420:GLU:O	2.29	0.65
7:H:65:MET:O	7:H:145:GLU:OE1	2.16	0.63
8:L:45:LEU:HD21	9:Q:448:LEU:HB2	1.83	0.61
1:A:518:LEU:HA	4:E:55:GLN:HE22	1.67	0.59
3:D:50:ASP:OD2	6:G:92:ARG:NH2	2.35	0.59
3:D:149:TYR:HA	3:D:153:LEU:HB2	1.83	0.58
8:K:122:GLN:OE1	8:L:47:PRO:HB3	2.04	0.58
8:P:2:THR:HG22	8:P:4:LEU:H	1.70	0.57
1:A:387:THR:HG23	1:A:412:ILE:HD11	1.87	0.56
3:D:163:LYS:HZ2	9:Q:456:ARG:HD3	1.71	0.56
9:Q:436:GLU:OE1	9:Q:443:LYS:NZ	2.38	0.56
3:D:106:ASN:ND2	3:D:131:GLY:O	2.39	0.56
8:J:153:ARG:NH1	8:K:78:LEU:O	2.39	0.55
8:N:77:SER:OG	8:N:90:GLN:NE2	2.39	0.55
2:B:244:ILE:HD13	8:P:30:TYR:HD2	1.72	0.54
3:D:186:LYS:NZ	3:D:242:LEU:O	2.37	0.54
8:I:137:GLU:O	8:I:137:GLU:HG3	2.08	0.54
3:D:18:ARG:NH2	3:D:302:GLN:O	2.41	0.53
5:F:39:VAL:HA	5:F:44:ASP:OD2	2.09	0.53
8:P:10:PRO:HA	8:P:82:GLN:HE21	1.74	0.53
8:M:122:GLN:NE2	8:N:44:VAL:O	2.42	0.53
8:K:45:LEU:O	8:K:46:ARG:HG2	2.07	0.53
5:F:34:ASN:HD22	5:F:39:VAL:HG11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:178:GLU:OE1	3:D:181:ARG:NH2	2.42	0.52
7:H:62:PRO:HG3	7:H:141:LEU:HD21	1.91	0.52
8:K:153:ARG:NH2	8:L:75:CYS:O	2.43	0.52
6:G:74:GLY:HA3	6:G:157:LEU:HA	1.92	0.51
3:D:249:TYR:O	3:D:253:THR:OG1	2.24	0.51
4:E:64:ARG:HG3	4:E:67:LEU:HB2	1.90	0.51
7:H:116:ILE:HD11	7:H:145:GLU:HG2	1.92	0.51
6:G:102:ILE:HD11	6:G:181:PHE:HZ	1.75	0.51
1:A:317:LYS:NZ	1:A:321:GLU:OE2	2.40	0.51
1:A:649:LEU:HA	1:A:715:GLN:HG3	1.92	0.50
8:L:63:ILE:HD11	8:L:108:ILE:HD12	1.93	0.50
1:A:75:LEU:HD11	1:A:125:GLU:HG3	1.94	0.50
1:A:533:ASN:HB2	1:A:737:TRP:HE1	1.77	0.49
1:A:62:LEU:HD12	1:A:313:VAL:HG13	1.94	0.49
1:A:31:TYR:OH	1:A:316:GLU:OE1	2.31	0.49
3:D:86:GLN:OE1	8:P:117:ARG:NH1	2.43	0.49
8:K:49:LEU:O	8:K:53:ASN:ND2	2.45	0.49
1:A:721:GLU:O	1:A:725:ASN:ND2	2.46	0.49
6:G:110:VAL:HG13	6:G:156:ASN:HB3	1.95	0.48
1:A:506:ILE:HD11	4:E:67:LEU:HD23	1.96	0.48
1:A:141:TYR:HE2	1:A:277:VAL:HG21	1.77	0.48
9:Q:466:SER:H	9:Q:469:GLN:HE21	1.59	0.48
1:A:28:ASP:OD2	1:A:360:LEU:HD21	2.14	0.48
1:A:353:LEU:HD22	1:A:368:ILE:HD11	1.96	0.48
7:H:26:ALA:HB2	7:H:102:GLY:HA2	1.95	0.48
1:A:134:GLN:HG3	1:A:284:LEU:HD11	1.96	0.47
3:D:200:ILE:HD12	3:D:306:ILE:HD11	1.94	0.47
8:O:56:PRO:HB3	8:O:133:LEU:HD21	1.94	0.47
8:M:146:VAL:HG11	8:N:21:ILE:HG21	1.95	0.47
8:N:34:LYS:HE3	8:N:113:ASP:OD2	2.15	0.47
3:D:59:SER:HB3	3:D:62:SER:H	1.80	0.47
3:D:164:ASN:OD1	9:Q:456:ARG:NH2	2.34	0.47
8:I:1:MET:HB3	8:I:7:VAL:HG23	1.97	0.47
9:Q:418:LEU:HD21	9:Q:425:LEU:HD22	1.97	0.47
2:B:250:THR:HG22	3:D:88:SER:HB3	1.96	0.46
3:D:152:VAL:HG23	3:D:153:LEU:HD22	1.96	0.46
9:Q:146:SER:OG	9:Q:343:ALA:O	2.33	0.46
4:E:63:ARG:HH22	8:P:156:GLN:HB2	1.81	0.46
8:L:34:LYS:HE3	8:L:113:ASP:OD2	2.16	0.46
8:L:45:LEU:HD13	9:Q:459:LEU:HB2	1.96	0.46
1:A:606:PRO:HB3	1:A:624:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLN:HB3	1:A:333:LYS:HE2	1.97	0.46
1:A:49:ARG:HH22	3:D:35:GLN:HG3	1.81	0.46
8:L:77:SER:OG	8:L:90:GLN:NE2	2.50	0.45
8:N:153:ARG:O	8:N:155:THR:N	2.38	0.45
8:J:125:LEU:HD11	8:K:40:CYS:HA	1.98	0.45
1:A:494:TRP:HD1	1:A:519:ASP:OD2	2.00	0.45
1:A:745:GLN:HG2	8:P:148:LEU:HD21	1.99	0.45
9:Q:212:LEU:HD11	9:Q:484:LEU:HB3	1.98	0.45
6:G:179:ALA:O	6:G:183:LYS:NZ	2.49	0.45
3:D:118:ARG:HB2	3:D:122:GLU:OE2	2.17	0.45
8:K:77:SER:OG	8:K:90:GLN:NE2	2.50	0.45
6:G:41:HIS:HB3	6:G:44:ASP:OD2	2.16	0.45
1:A:196:VAL:HG21	1:A:234:ASN:HD21	1.82	0.45
9:Q:447:LYS:HG2	9:Q:460:ASP:HB3	1.98	0.45
1:A:436:ALA:HB2	1:A:465:ILE:HG22	1.99	0.44
1:A:795:LEU:HD22	8:P:134:ILE:HG13	2.00	0.44
2:B:214:ILE:HA	6:G:53:ARG:HH22	1.82	0.44
6:G:117:ILE:HG21	6:G:152:VAL:HG11	1.99	0.44
9:Q:212:LEU:HD12	9:Q:215:ILE:HD12	1.99	0.44
3:D:33:LEU:HD22	3:D:42:LEU:HD12	2.00	0.43
1:A:373:THR:HG1	1:A:375:HIS:HD1	1.65	0.43
4:E:22:TRP:O	4:E:34:ARG:NH2	2.51	0.43
8:I:86:THR:HG23	8:I:154:ALA:HB1	2.01	0.43
1:A:778:PHE:HA	1:A:781:THR:HG22	2.01	0.43
4:E:68:ARG:HA	4:E:69:PRO:HD3	1.86	0.43
6:G:51:LEU:HD23	7:H:14:TYR:HB2	2.00	0.43
1:A:397:TYR:HA	6:G:98:THR:HG21	2.00	0.43
1:A:725:ASN:O	1:A:729:HIS:HB2	2.18	0.43
3:D:281:THR:OG1	3:D:282:GLY:N	2.51	0.43
1:A:205:ARG:NH2	3:D:155:ASP:OD2	2.40	0.43
8:N:84:LEU:HD12	8:O:7:VAL:HG12	2.01	0.43
6:G:68:VAL:HG21	8:P:146:VAL:HG21	2.00	0.43
1:A:121:LEU:O	1:A:125:GLU:HB2	2.18	0.42
9:Q:471:ASP:O	9:Q:474:ASP:HB2	2.19	0.42
1:A:65:VAL:HG21	1:A:111:VAL:HG22	2.01	0.42
5:F:4:VAL:HG13	5:F:6:SER:H	1.85	0.42
3:D:84:ARG:HG2	3:D:92:ARG:HH11	1.83	0.41
3:D:248:LEU:HB2	3:D:252:ALA:HB3	2.01	0.41
1:A:63:ASP:HB3	1:A:317:LYS:HE3	2.02	0.41
7:H:97:MET:HG3	7:H:162:GLY:HA3	2.02	0.41
9:Q:456:ARG:NH1	9:Q:458:TYR:OH	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:LYS:HD3	1:A:590:ILE:HG23	2.02	0.41
6:G:167:GLY:HA2	6:G:188:GLU:OE2	2.20	0.41
1:A:528:ALA:O	1:A:532:SER:HB3	2.21	0.41
3:D:173:ASP:OD1	3:D:176:ASN:ND2	2.54	0.41
1:A:220:GLN:HA	1:A:221:PRO:HD3	1.96	0.41
3:D:36:CYS:O	3:D:335:ARG:NH1	2.53	0.41
1:A:344:ASP:OD2	1:A:382:ARG:NH2	2.54	0.41
3:D:211:LEU:HD13	3:D:310:TRP:CD1	2.55	0.41
6:G:180:LEU:HD21	7:H:53:PRO:HB3	2.01	0.41
3:D:146:GLU:OE2	3:D:169:ALA:HA	2.21	0.41
8:I:59:MET:O	8:I:137:GLU:OE2	2.39	0.41
8:N:56:PRO:HG3	8:N:133:LEU:HD21	2.03	0.41
3:D:234:ASP:HB3	3:D:237:LEU:HD23	2.03	0.40
1:A:630:GLN:O	1:A:634:GLN:HG2	2.22	0.40
6:G:72:VAL:HG13	8:P:139:LEU:HB3	2.02	0.40
6:G:56:PRO:HG3	6:G:139:LEU:HD23	2.04	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	752/1012 (74%)	692 (92%)	59 (8%)	1 (0%)	51	83
2	B	51/265 (19%)	46 (90%)	5 (10%)	0	100	100
3	D	343/345 (99%)	317 (92%)	24 (7%)	2 (1%)	25	59
4	E	67/73 (92%)	58 (87%)	9 (13%)	0	100	100
5	F	72/85 (85%)	68 (94%)	4 (6%)	0	100	100
6	G	197/213 (92%)	194 (98%)	3 (2%)	0	100	100
7	H	156/164 (95%)	152 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
8	J	157/160 (98%)	156 (99%)	1 (1%)	0	100	100
8	K	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
8	L	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
8	M	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
8	N	157/160 (98%)	151 (96%)	5 (3%)	1 (1%)	25	59
8	O	156/160 (98%)	152 (97%)	4 (3%)	0	100	100
8	P	156/160 (98%)	150 (96%)	6 (4%)	0	100	100
9	Q	363/513 (71%)	323 (89%)	39 (11%)	1 (0%)	41	73
All	All	3255/3950 (82%)	3066 (94%)	184 (6%)	5 (0%)	50	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	N	154	ALA
9	Q	85	PRO
3	D	134	ASP
3	D	133	PHE
1	A	525	THR

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	664/875 (76%)	660 (99%)	4 (1%)	86	94
2	B	47/244 (19%)	47 (100%)	0	100	100
3	D	309/309 (100%)	305 (99%)	4 (1%)	69	87
4	E	62/65 (95%)	62 (100%)	0	100	100
5	F	61/72 (85%)	61 (100%)	0	100	100
6	G	155/168 (92%)	153 (99%)	2 (1%)	69	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	120/125 (96%)	119 (99%)	1 (1%)	81	92
8	I	118/119 (99%)	118 (100%)	0	100	100
8	J	118/119 (99%)	118 (100%)	0	100	100
8	K	118/119 (99%)	117 (99%)	1 (1%)	81	92
8	L	118/119 (99%)	118 (100%)	0	100	100
8	M	118/119 (99%)	117 (99%)	1 (1%)	81	92
8	N	118/119 (99%)	118 (100%)	0	100	100
8	O	117/119 (98%)	117 (100%)	0	100	100
8	P	117/119 (98%)	116 (99%)	1 (1%)	78	91
9	Q	275/418 (66%)	275 (100%)	0	100	100
All	All	2635/3228 (82%)	2621 (100%)	14 (0%)	89	94

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	ARG
1	A	450	LYS
1	A	563	ASN
1	A	799	ARG
3	D	21	ARG
3	D	163	LYS
3	D	303	GLN
3	D	337	ARG
6	G	92	ARG
6	G	95	ARG
7	H	145	GLU
8	K	46	ARG
8	M	1	MET
8	P	138	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	311	GLN
1	A	563	ASN
3	D	7	ASN
3	D	176	ASN

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Mol	Chain	Res	Type
4	E	55	GLN
5	F	34	ASN
6	G	100	ASN
8	K	90	GLN
8	L	90	GLN
8	N	90	GLN
9	Q	202	ASN
9	Q	366	GLN
9	Q	469	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.

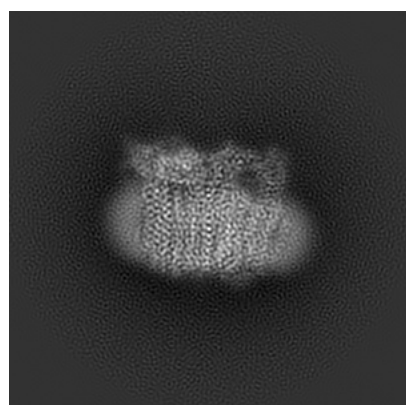
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20322. These allow visual inspection of the internal detail of the map and identification of artifacts.

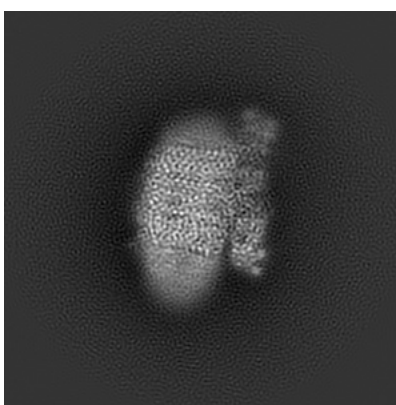
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

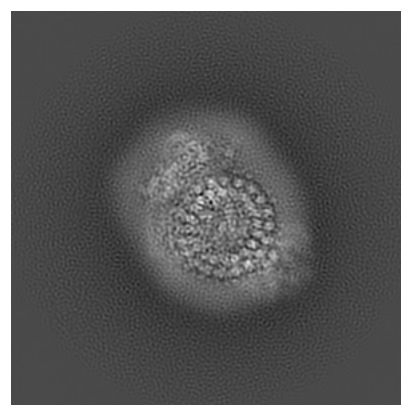
6.1.1 Primary map



X



Y

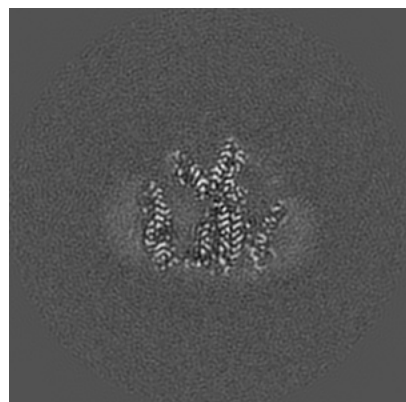


Z

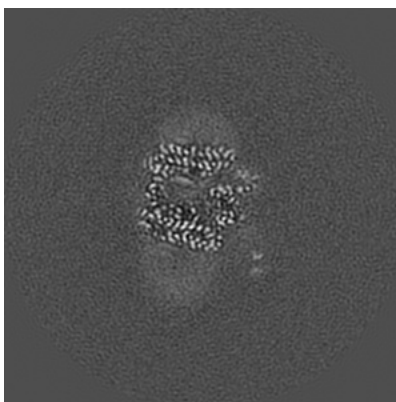
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

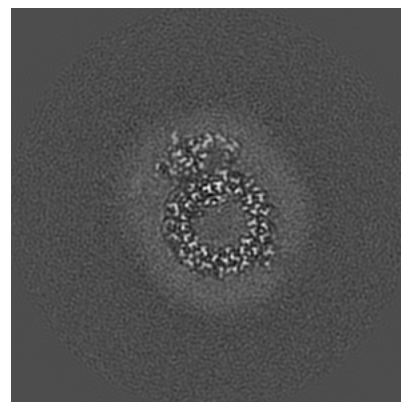
6.2.1 Primary map



X Index: 140



Y Index: 140

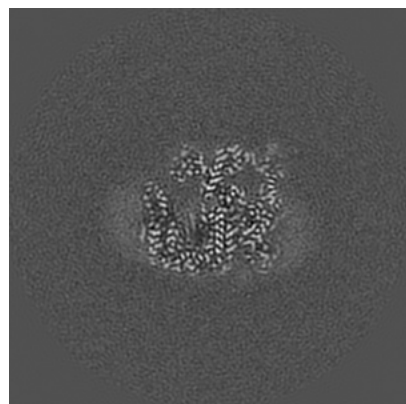


Z Index: 140

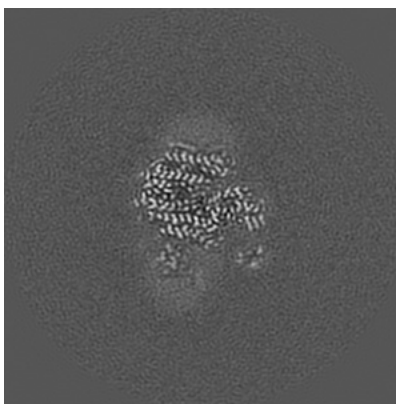
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

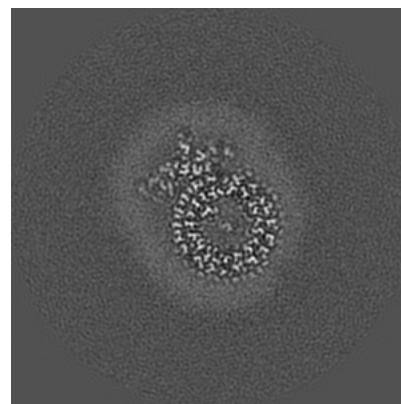
6.3.1 Primary map



X Index: 132



Y Index: 148

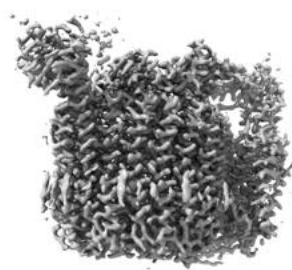


Z Index: 123

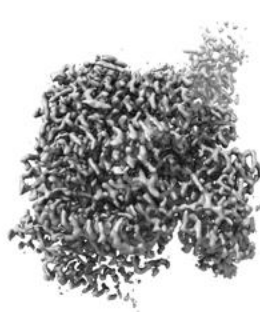
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

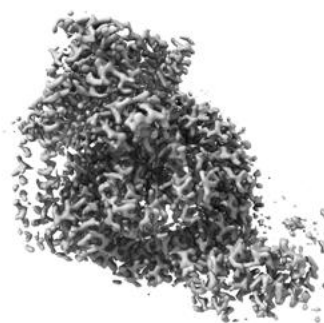
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

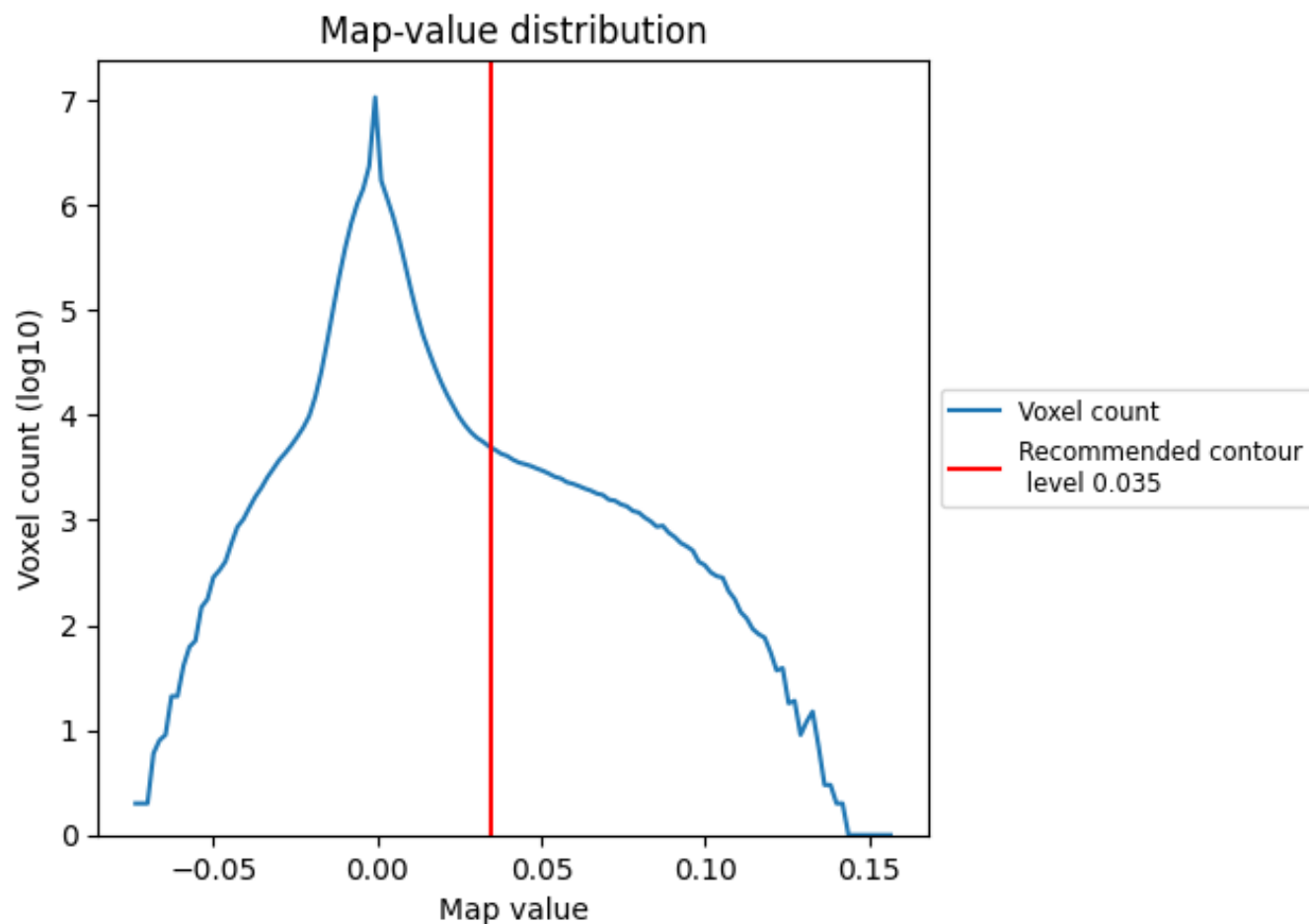
6.5 Mask visualisation

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

7 Map analysis [i](#)

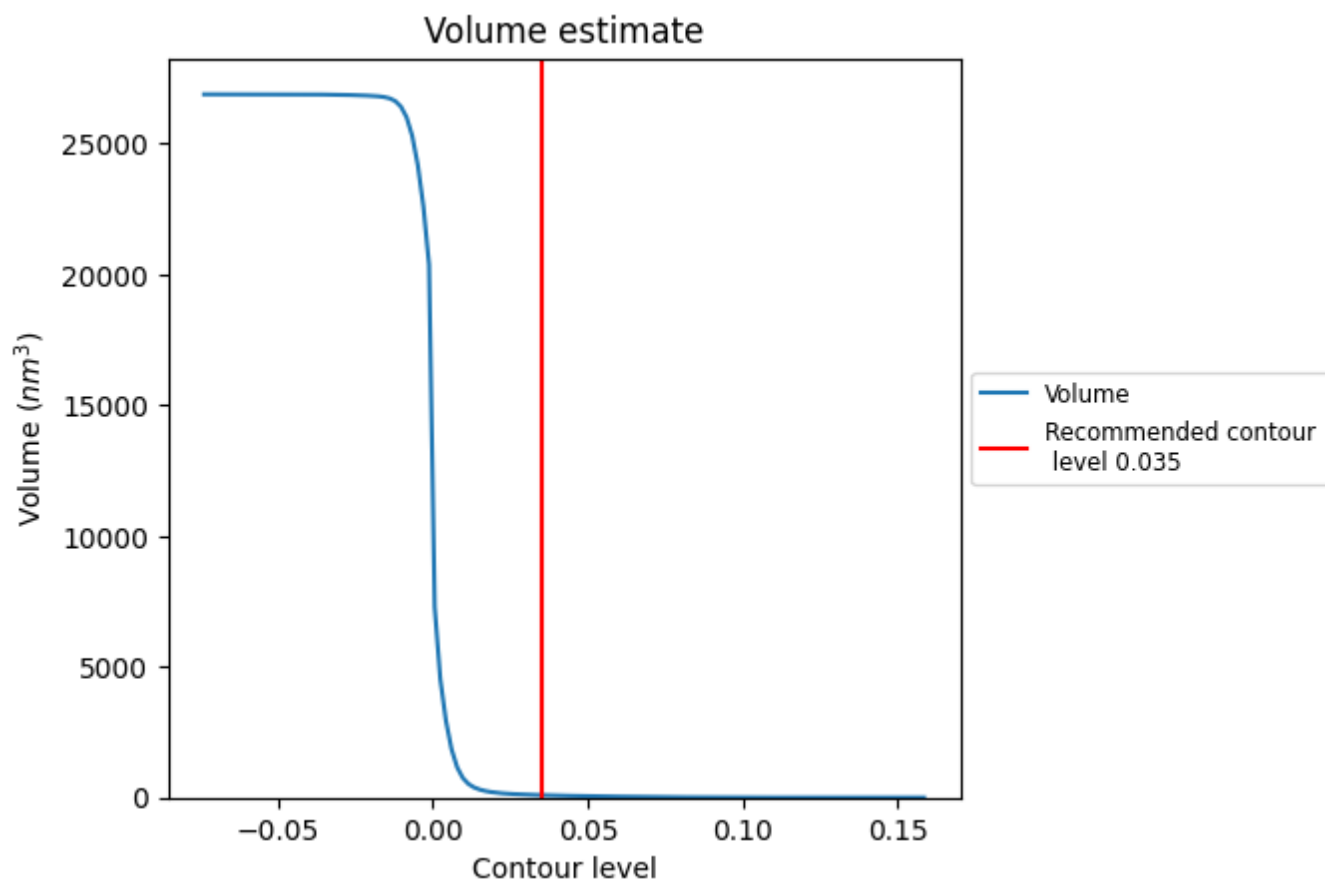
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

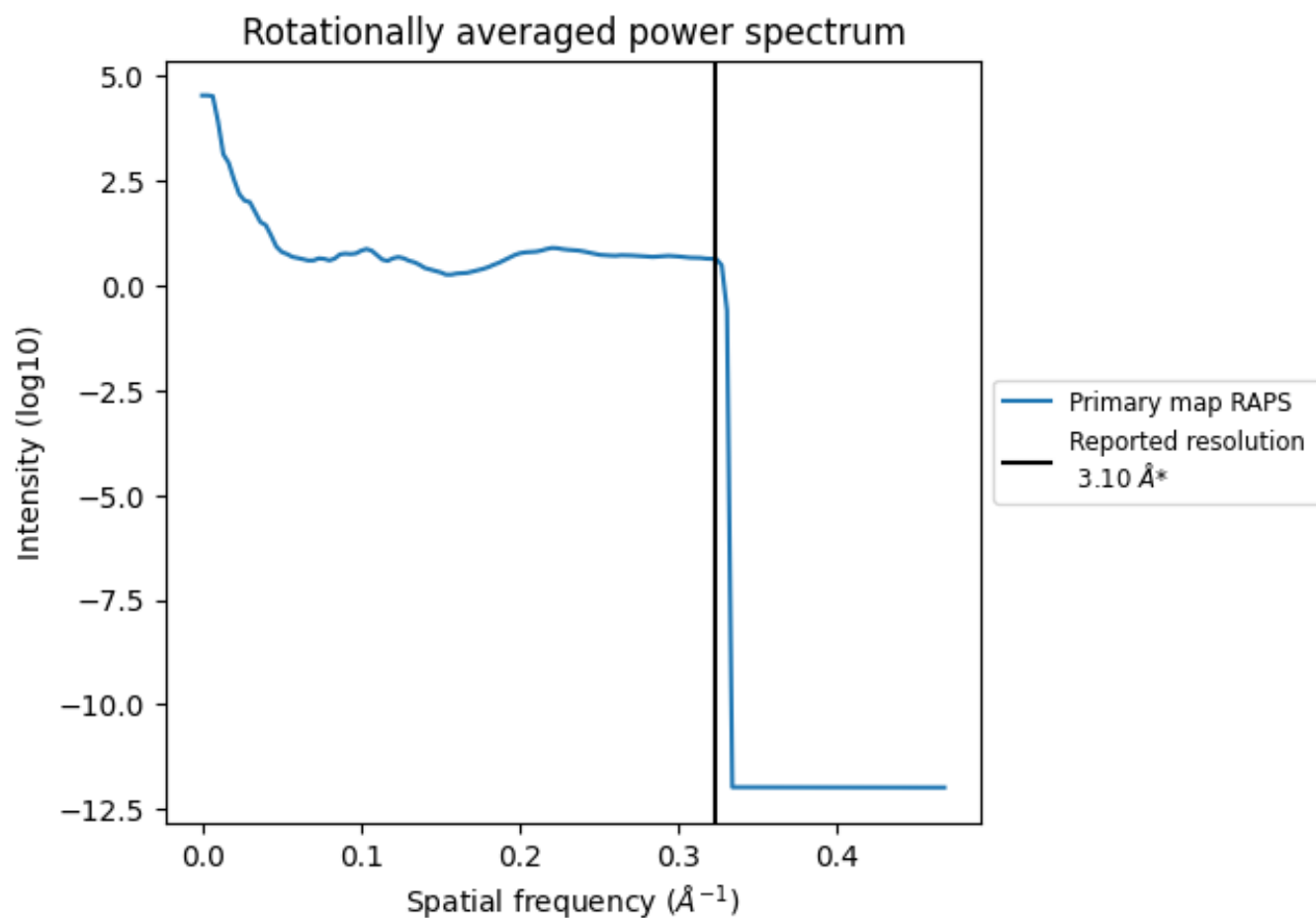
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm³; this corresponds to an approximate mass of 84 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 0.323 \AA^{-1}

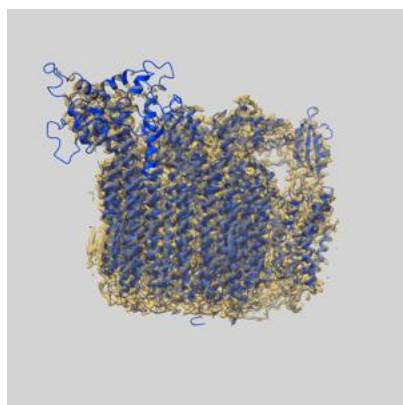
8 Fourier-Shell correlation ⓘ

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

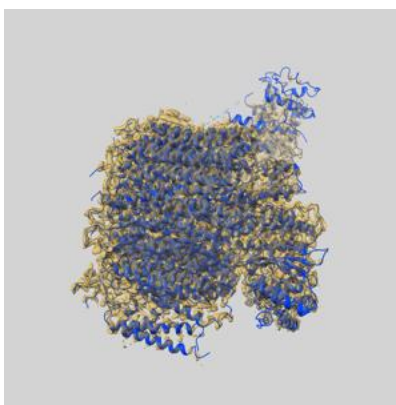
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20322 and PDB model 6PE4. Per-residue inclusion information can be found in section [3](#) on page [11](#).

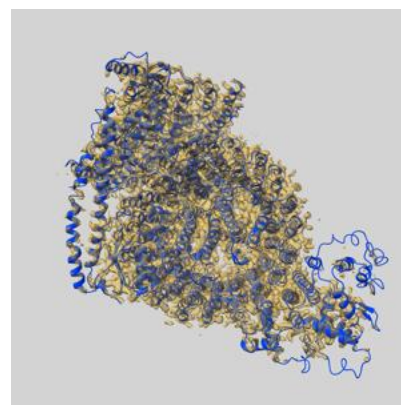
9.1 Map-model overlay [i](#)



X



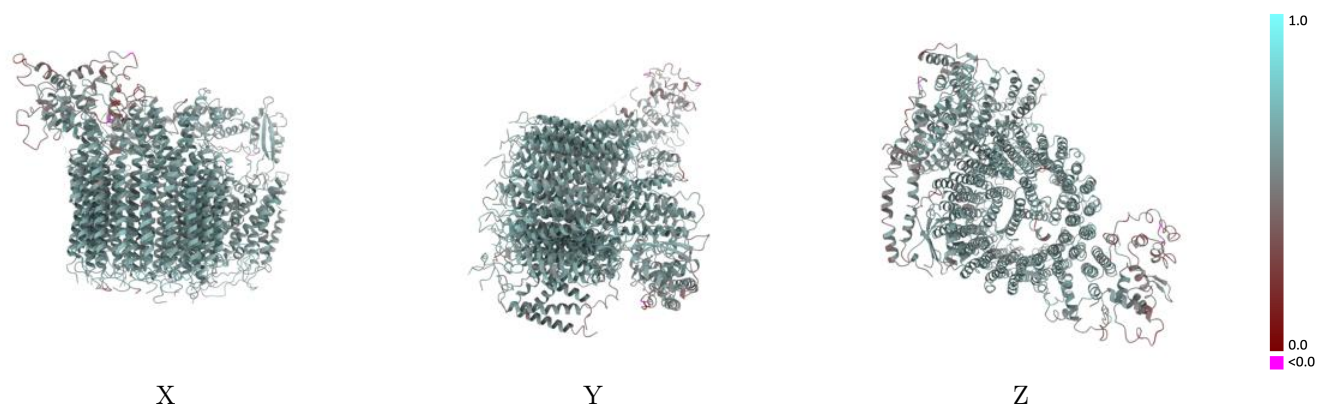
Y



Z

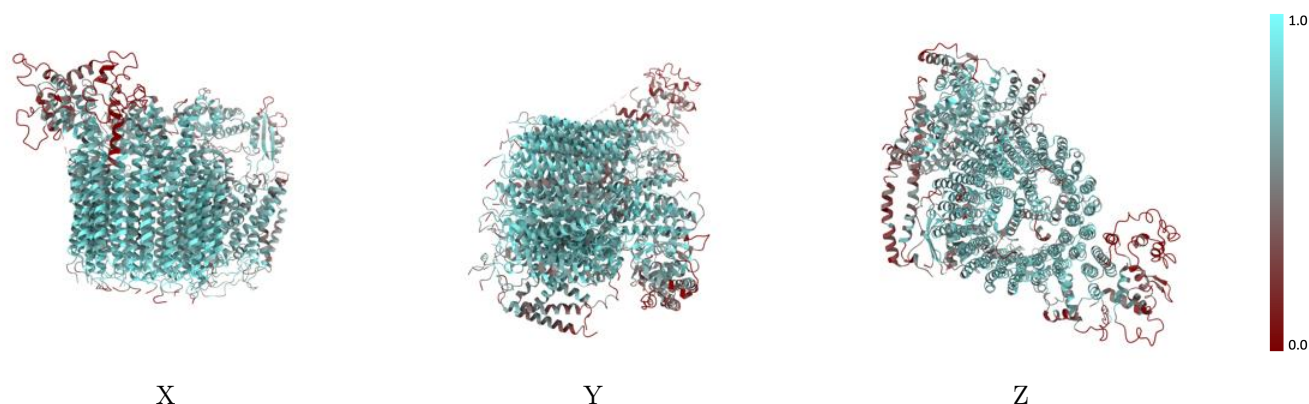
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



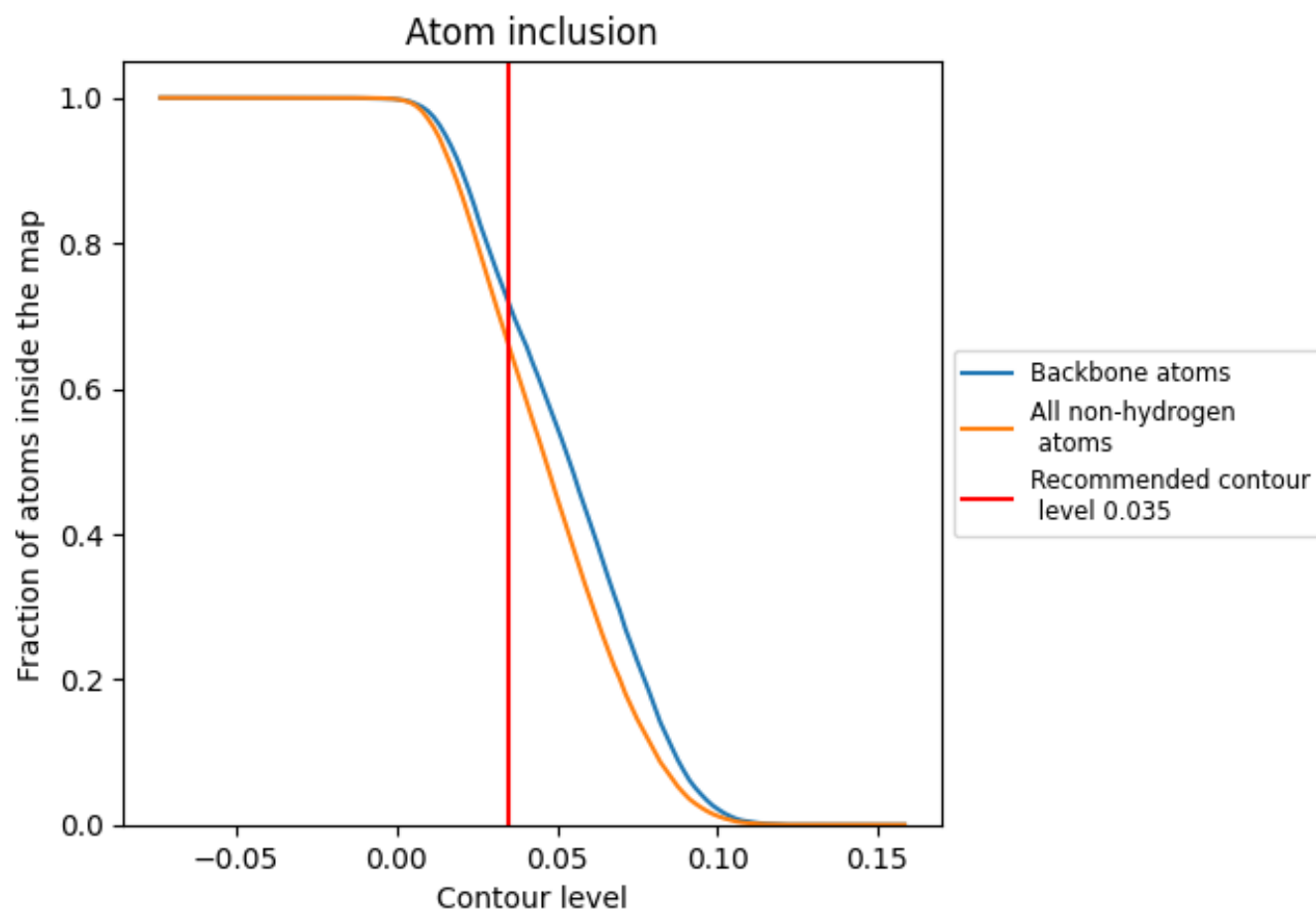
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 66% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6583	 0.5720
A	 0.5848	 0.5560
B	 0.6501	 0.5770
D	 0.6877	 0.5760
E	 0.6476	 0.5630
F	 0.3788	 0.5080
G	 0.7483	 0.5980
H	 0.7641	 0.6040
I	 0.7584	 0.6020
J	 0.7762	 0.6020
K	 0.7762	 0.5900
L	 0.7664	 0.6030
M	 0.7584	 0.5990
N	 0.7575	 0.5960
O	 0.7809	 0.6100
P	 0.7603	 0.6000
Q	 0.3969	 0.4990

