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PDB ID	:	7TMS
EMDB ID	:	EMD-26001
Title	:	V-ATPase from Saccharomyces cerevisiae, State 2
Authors	:	Vasanthakumar, T.; Keon, K.A.; Bueler, S.A.; Jaskolka, M.C.; Rubinstein,
		J.L.
Deposited on	:	2022-01-20
Resolution	:	3.80  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 (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
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)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is 3.80 Å.

Ramachandran outliers

Sidechain outliers

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	;	Percentile Ranks	Value
Ramachandran outliers			0.0%
Sidechain outliers			0.3%
	Worse		Better
	Percentile relativ	ve to all structures	
	Percentile relativ	ve to all EM structures	
		<b>XX71</b> , 1, , , , , 1, <b>2</b> , , ,	
Metric		whole archive	EM structures
		(# Entries)	(# Entries)

154571

154315

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 $<=5\%$
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.

4023

3826

Mol	Chain	Length	Quality of chain	
1	А	617	96%	•
1	С	617	96%	·
1	Е	617	96%	·
2	В	517	92%	8%
2	D	517	92%	8%
2	F	517	92%	8%
3	G	233	95%	5%
3	Ι	233	95%	5%
3	K	233	<u>6%</u> 96%	•

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Mol	Chain	Length	Quality of chain	
4	Н	114	98%	
4	J	114	97%	·
4	L	114	21%	
5	М	256	86%	• 13%
6	N	118	33%	
7	0	392		Q%
8	Р	478	91%	970
0	1	\$40	17%	0%
10	a h	040	87%	13%
10	d	200	20% 80%	
11	с	213	92%	7%
12	d	345	98%	••
13	е	73	88%	12%
14	f	85	74%	26%
15	g	160	99%	
15	h	160	99%	
15	i	160	99%	
15	j	160	99%	
15	k	160	99%	
15	1	160	99%	
15	m	160	99%	
15	n	160	99%	
16	0	164	96%	



# 2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 57652 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 H(+)-transporting two-sector ATPase.

Mol	Chain	Residues		At	AltConf	Trace			
1	А	593	Total	С	N	0	S	0	0
			4542	2888	756	878	20		
1	C	593	Total	С	Ν	Ο	$\mathbf{S}$	0	0
1	U		4547	2887	757	883	20	0	0
1	Е	E 502	Total	С	Ν	0	$\mathbf{S}$	0	0
1		E (	090	4578	2904	760	894	20	0

• Molecule 2 is a protein called Vacuolar proton pump subunit B.

Mol	Chain	Residues		At	AltConf	Trace			
2	В	475	Total	С	Ν	0	$\mathbf{S}$	0	0
	D	410	3677	2328	631	706	12	0	0
0	Л	475	Total	С	Ν	0	S	0	0
	D	410	3694	2337	632	713	12	0	0
0	Б	178	Total	С	Ν	0	S	0	0
	T,	410	3731	2358	641	720	12	0	U

• Molecule 3 is a protein called V-ATPase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace			
3	С	221	Total	С	Ν	0	S	0	0			
5	G	221	1325	826	250	248	1	0	0			
2	Т	221	Total	С	Ν	0	S	0	0			
J	1	221	1346	846	256	242	2	0	0			
2	K	224	Total	С	Ν	0	S	0	0			
3	n	n	K	К	224	1263	783	243	236	1	0	

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	Н	112	Total 556	C 332	N 112	O 112	0	0

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Mol	Chain	Residues		Ato	ms	AltConf	Trace	
4	J	111	Total 562	C 338	N 112	O 112	0	0
4	L	111	Total 556	C 332	N 113	0 111	0	0

• Molecule 5 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace	
5	М	223	Total 1463	C 896	N 279	0 283	${ m S}{ m 5}$	0	0

• Molecule 6 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
6	Ν	115	Total 587	C 357	N 115	0 115	0	0

• Molecule 7 is a protein called V-type proton ATPase subunit C.

Mol	Chain	Residues		Ator	AltConf	Trace		
7	О	357	Total 1808	C 1093	N 357	O 358	0	0

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

Mol	Chain	Residues		Ator	AltConf	Trace		
8	Р	440	Total 2229	C 1345	N 441	0 443	0	0

• Molecule 9 is a protein called V-type proton ATPase subunit a, vacuolar isoform.

Mol	Chain	Residues		At	AltConf	Trace			
9	a	734	Total 5362	C 3488	N 888	O 956	S 30	0	0

• Molecule 10 is a protein called V0 assembly protein 1.

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
10	b	52	Total 400	C 267	N 59	0 72	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0



• Molecule 11 is a protein called V-type proton ATPase subunit c".

Mol	Chain	Residues		At	oms		AltConf	Trace	
11	с	198	Total 1464	C 974	N 227	O 256	${f S}7$	0	0

• Molecule 12 is a protein called V-type proton ATPase subunit d.

Mol	Chain	Residues		At	AltConf	Trace			
12	d	343	Total 2769	C 1761	N 451	0 544	S 13	0	0

• Molecule 13 is a protein called V-type proton ATPase subunit e.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
13	е	64	Total 510	C 343	N 83	O 79	${ m S}{ m 5}$	0	0

• Molecule 14 is a protein called Yeast V-ATPase subunit f.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
14	f	63	Total	С	Ν	0	$\mathbf{S}$	0	0
11	I	00	467	308	73	83	3	0	0

• Molecule 15 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues		At	oms			AltConf	Trace
15	G	150	Total	С	Ν	0	S	0	0
10	g	109	1128	743	179	199	7	0	0
15	h	150	Total	С	Ν	Ο	S	0	0
10	11	105	1137	749	182	199	7	0	0
15	i	150	Total	С	Ν	Ο	$\mathbf{S}$	0	0
10	1	105	1137	749	182	199	7	0	0
15	;	150	Total	С	Ν	Ο	$\mathbf{S}$	0	0
10	J	109	1137	749	182	199	7	0	0
15	Ŀ	150	Total	С	Ν	Ο	$\mathbf{S}$	0	0
10	K	109	1129	744	180	198	7	0	0
15	1	150	Total	С	Ν	0	$\mathbf{S}$	0	0
10	1	109	1131	746	181	197	7	0	0
15	m	150	Total	С	Ν	0	$\mathbf{S}$	0	0
10	111	109	1137	749	182	199	7	0	0
15	n	150	Total	С	Ν	0	S	0	0
10	11	109	1130	743	182	198	7	U	



• Molecule 16 is a protein called V-type proton ATPase subunit c'.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
16	О	158	Total 1123	С 740	N 178	0 194	S 11	0	0

• Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues			AltConf			
17	Е	1	Total 27	C 10	N 5	O 10	Р 2	0



# 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: H(+)-transporting two-sector ATPase

















Chain e:	88%	12%
MET SER SER 112 HG7 PR0 CLU CLU	ALA GLU	
• Molecule 14: Y	/east V-ATPase subunit f	
Chain f:	74%	26%
MET ARG PRO VAL VAL VAL VAL THR GLY GLY ALA MIL	L16 L57 L57 L50 V03 V73 ARG ARG ARG ARG ARG ARG ARG ARG ARG CUU LEU LUU SER ARG ARG CUU LUU ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG	
• Molecule 15: V	<i>V</i> -type proton ATPase subunit c	
Chain g:	99%	
MI R117 V159 CVS		
• Molecule 15: V	<i>V</i> -type proton ATPase subunit c	
Chain h:	99%	
M1 Y76 V159 CYS		
• Molecule 15: V	V-type proton ATPase subunit c	
Chain i:	99%	
M1 V159 CVS		
• Molecule 15: V	-type proton ATPase subunit c	
Chain j:	99%	<del>.</del> .
M1 Y76 N151 V159 CYS		
• Molecule 15: V	V-type proton ATPase subunit c	
Chain k:	99%	
MI V159 CYS		



• Molecul	e 15: V-type proton ATPase subunit c	
Chain l:	99%	<mark></mark>
MI K81 V159 CYS		
• Molecul	e 15: V-type proton ATPase subunit c	
Chain m:	99%	
M1 V159 CYS		
• Molecul	e 15: V-type proton ATPase subunit c	
Chain n:	99%	
M1 Y76		
• Molecul	e 16: V-type proton ATPase subunit c'	
Chain o:	96%	





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56915	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	43	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	52.654	Depositor
Minimum map value	-4.139	Depositor
Average map value	0.078	Depositor
Map value standard deviation	1.456	Depositor
Recommended contour level	5.0	Depositor
Map size (Å)	360.49997, 360.49997, 360.49997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^{\circ}$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2016666, 1.2016666, 1.2016666	Depositor



# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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		
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.29	0/4641	0.50	0/6296	
1	С	0.29	0/4646	0.48	0/6300	
1	Е	0.29	0/4677	0.49	0/6339	
2	В	0.30	0/3747	0.54	0/5084	
2	D	0.30	0/3764	0.52	0/5105	
2	F	0.29	0/3801	0.51	0/5151	
3	G	0.25	0/1333	0.47	0/1834	
3	Ι	0.26	0/1355	0.45	0/1855	
3	Κ	0.24	0/1273	0.45	0/1762	
4	Н	0.21	0/556	0.33	0/774	
4	J	0.23	0/563	0.33	0/782	
4	L	0.23	0/557	0.33	0/775	
5	М	0.25	0/1472	0.51	0/1992	
6	Ν	0.23	0/592	0.40	0/828	
7	0	0.24	0/1822	0.42	0/2553	
8	Р	0.23	0/2239	0.36	0/3128	
9	а	0.28	0/5490	0.52	0/7497	
10	b	0.26	0/406	0.49	0/553	
11	с	0.30	0/1494	0.51	0/2031	
12	d	0.30	0/2828	0.54	0/3837	
13	е	0.27	0/525	0.53	0/718	
14	f	0.29	0/481	0.43	0/661	
15	g	0.30	0/1146	0.52	0/1560	
15	h	0.30	0/1155	0.54	0/1571	
15	i	0.29	0/1155	0.54	0/1571	
15	j	0.29	0/1155	0.53	0/1571	
15	k	0.29	0/1147	0.54	0/1562	
15	1	0.29	0/1149	0.54	0/1563	
15	m	0.31	0/1155	0.55	0/1571	
15	n	0.30	0/1148	0.56	0/1562	
16	0	0.31	0/1145	0.54	0/1554	
All	All	0.28	0/58617	0.50	0/79940	



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)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	Perce	ntiles
1	А	591/617~(96%)	565~(96%)	26~(4%)	0	100	100
1	С	591/617~(96%)	570 (96%)	21~(4%)	0	100	100
1	Е	591/617~(96%)	574 (97%)	17 (3%)	0	100	100
2	В	473/517~(92%)	454 (96%)	19~(4%)	0	100	100
2	D	473/517~(92%)	467 (99%)	6 (1%)	0	100	100
2	F	476/517~(92%)	466 (98%)	10 (2%)	0	100	100
3	G	219/233~(94%)	212 (97%)	7 (3%)	0	100	100
3	Ι	219/233~(94%)	216 (99%)	3~(1%)	0	100	100
3	K	222/233~(95%)	220 (99%)	2(1%)	0	100	100
4	Н	110/114 (96%)	109 (99%)	1 (1%)	0	100	100
4	J	109/114~(96%)	108 (99%)	1 (1%)	0	100	100
4	L	109/114~(96%)	109 (100%)	0	0	100	100
5	М	221/256~(86%)	212 (96%)	9~(4%)	0	100	100
6	Ν	113/118~(96%)	105 (93%)	8 (7%)	0	100	100
7	Ο	353/392~(90%)	332 (94%)	21 (6%)	0	100	100
8	Р	434/478 (91%)	421 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
9	a	728/840~(87%)	686 (94%)	41 (6%)	1 (0%)	51	83
10	b	50/265~(19%)	48 (96%)	2 (4%)	0	100	100
11	с	196/213~(92%)	187 (95%)	9(5%)	0	100	100
12	d	341/345~(99%)	326 (96%)	15 (4%)	0	100	100
13	е	62/73~(85%)	59~(95%)	3(5%)	0	100	100
14	f	61/85~(72%)	57 (93%)	4 (7%)	0	100	100
15	g	157/160~(98%)	155 (99%)	2 (1%)	0	100	100
15	h	157/160~(98%)	154 (98%)	3 (2%)	0	100	100
15	i	157/160~(98%)	154 (98%)	3 (2%)	0	100	100
15	j	157/160~(98%)	151 (96%)	6 (4%)	0	100	100
15	k	157/160~(98%)	153 (98%)	4 (2%)	0	100	100
15	1	157/160~(98%)	153 (98%)	4 (2%)	0	100	100
15	m	157/160~(98%)	154 (98%)	3 (2%)	0	100	100
15	n	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
16	О	156/164~(95%)	151 (97%)	4 (3%)	1 (1%)	25	62
All	All	8154/8952 (91%)	7880 (97%)	272 (3%)	2(0%)	100	100

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All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	0	54	GLU
9	а	334	ILE

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Percei	ntiles
1	А	485/516~(94%)	484 (100%)	1 (0%)	93	97
1	С	484/516~(94%)	484 (100%)	0	100	100
1	Ε	497/516~(96%)	497 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
2	В	391/444~(88%)	391~(100%)	0	100	100
2	D	395/444~(89%)	395~(100%)	0	100	100
2	F	401/444~(90%)	400 (100%)	1 (0%)	93	97
3	G	65/208~(31%)	65~(100%)	0	100	100
3	Ι	70/208~(34%)	70 (100%)	0	100	100
3	К	40/208~(19%)	39~(98%)	1 (2%)	47	70
4	Н	1/94~(1%)	1 (100%)	0	100	100
4	J	3/94~(3%)	3~(100%)	0	100	100
4	L	2/94~(2%)	2(100%)	0	100	100
5	М	100/221~(45%)	98~(98%)	2(2%)	55	75
6	Ν	6/104~(6%)	6 (100%)	0	100	100
7	Ο	16/348~(5%)	16 (100%)	0	100	100
8	Р	12/439~(3%)	12 (100%)	0	100	100
9	a	488/728~(67%)	487 (100%)	1 (0%)	93	97
10	b	46/244~(19%)	46 (100%)	0	100	100
11	с	150/168~(89%)	149 (99%)	1 (1%)	84	91
12	d	302/309~(98%)	298~(99%)	4(1%)	69	82
13	е	55/65~(85%)	55~(100%)	0	100	100
14	f	48/72~(67%)	48 (100%)	0	100	100
15	g	115/119~(97%)	114 (99%)	1 (1%)	78	88
15	h	117/119~(98%)	117 (100%)	0	100	100
15	i	117/119~(98%)	117 (100%)	0	100	100
15	j	117/119~(98%)	116 (99%)	1 (1%)	78	88
15	k	115/119~(97%)	115 (100%)	0	100	100
15	1	115/119 (97%)	114 (99%)	1 (1%)	78	88
15	m	117/119~(98%)	117 (100%)	0	100	100
15	n	114/119~(96%)	114 (100%)	0	100	100
16	0	$\overline{112/125}~(90\%)$	112 (100%)	0	100	100
All	All	$5096/75\overline{61}\ (67\%)$	5082 (100%)	14 (0%)	92	96

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



Mol	Chain	Res	Type
1	А	504	LYS
2	F	391	MET
3	Κ	166	ARG
5	М	27	GLN
5	М	183	ASN
9	a	241	HIS
11	с	100	ASN
12	d	21	ARG
12	d	78	HIS
12	d	163	LYS
12	d	297	ARG
15	g	117	ARG
15	j	151	ASN
15	1	81	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such side chains are listed below:

Mol	Chain	Res	Type
2	В	331	GLN
2	В	344	HIS
2	В	402	GLN
2	D	402	GLN
1	Е	346	GLN
1	Е	527	GLN
5	М	183	ASN
9	a	311	GLN
9	a	428	HIS
9	a	547	HIS
9	a	729	HIS
11	с	100	ASN
12	d	29	GLN
12	d	78	HIS
12	d	128	HIS
12	d	258	GLN
12	d	303	GLN
12	d	318	GLN
15	g	90	GLN
15	g	121	GLN
15	g	122	GLN
15	g	151	ASN
15	j	53	ASN
15	k	82	GLN
15	m	90	GLN

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Mol	Chain	Res	Type
15	m	151	ASN
15	n	122	GLN
16	0	129	HIS

### 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)

1 ligand is modelled in this entry.

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

Mal	Type	Chain	Dog	Link	Bo	ond leng	ths	B	ond ang	les
	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	ADP	Е	701	-	24,29,29	0.92	1 (4%)	29,45,45	1.39	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ADP	Е	701	-	-	1/12/32/32	0/3/3/3



A11 (	(1)	bond	length	outliers	are	listed	below:	
1111	(+)	bond	longin	outificits	arc	nsucu	DCIOW.	

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
17	Е	701	ADP	C5-C4	2.34	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
17	Е	701	ADP	PA-O3A-PB	-3.24	121.71	132.83
17	Е	701	ADP	N3-C2-N1	-2.89	124.16	128.68
17	Е	701	ADP	C4-C5-N7	-2.61	106.68	109.40
17	Е	701	ADP	C3'-C2'-C1'	2.60	104.89	100.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	Ε	701	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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





## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-26001. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

## 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



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

## 6.2 Central slices (i)

#### 6.2.1 Primary map



X Index: 150

Y Index: 150



Z Index: 150

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: 145

Y Index: 128

Z Index: 90

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



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



## 6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation (i)

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



## 7 Map analysis (i)

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

## 7.1 Map-value distribution (i)



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



## 7.2 Volume estimate (i)



The volume at the recommended contour level is  $451 \text{ nm}^3$ ; this corresponds to an approximate mass of 407 kDa.

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



## 7.3 Rotationally averaged power spectrum (i)



\*Reported resolution corresponds to spatial frequency of 0.263  $\text{\AA}^{-1}$ 



# 8 Fourier-Shell correlation (i)

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-26001 and PDB model 7TMS. 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 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



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



The images above show the model with each residue coloured according 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 (5.0).



## 9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (5.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8210	0.4310
А	0.8330	0.5130
В	0.8460	0.5180
С	0.8730	0.5350
D	0.8610	0.5340
E	0.8880	0.5400
F	0.8690	0.5340
G	0.8190	0.4430
Н	0.6760	0.2540
Ι	0.8830	0.4680
J	0.7950	0.3840
K	0.8820	0.4390
L	0.7430	0.3060
М	0.6520	0.4080
N	0.5740	0.3470
0	0.9410	0.3530
Р	0.9770	0.3850
a	0.6540	0.3070
b	0.7380	0.3410
С	0.8240	0.3610
d	0.7970	0.3600
е	0.7780	0.3490
f	0.7690	0.2900
g	0.8240	0.3590
h	0.8260	0.3680
i	0.8200	0.3680
j	0.8070	0.3410
k	0.8010	0.3320
1	0.7850	0.3350
m	0.7730	0.3380
n	0.7710	0.3340
0	0.8110	0.3490



