

Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2K88
Title	:	Association of subunit d (Vma6p) and E (Vma4p) with G (Vma10p) and the
		NMR solution structure of subunit G (G1-59) of the Saccharomyces cerevisiae
		V1VO ATPase
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Deposited on	:	2008-09-04

This is a Full wwPDB NMR Structure 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/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

Ramachandran outliers

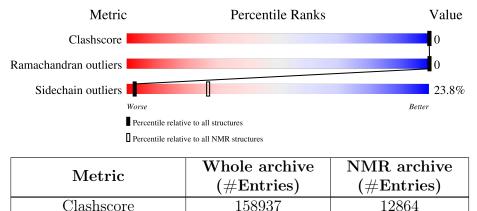
Sidechain outliers

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $SOLUTION\ NMR$

The overall completeness of chemical shifts assignment was not calculated.

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.



154571

154315

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

11451

11428

Mol	Chain	Length	Quality of chain		
1	А	60	30%	•	68%



2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues					
Well-defined core Residue range (total) Backbone RMSD (Å) Medoid model					
1	A:36-A:54 (19)	0.07	1		

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models		
1	1, 3, 4, 5, 6, 8		
2	7, 9, 10		
Single-model clusters	2		



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 993 atoms, of which 507 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Vacuolar proton pump subunit G.

Mol	Chain	Residues	Atoms				Trace		
1	٨	60	Total	С	Η	Ν	0	S	0
	A	60	993	303	507	86	95	2	U

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MET	-	expression tag	UNP P48836
А	2	VAL	-	expression tag	UNP P48836
А	60	CYS	-	expression tag	UNP P48836



4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Vacuolar proton pump subunit G

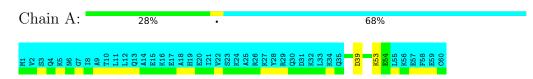
Chain A:	30%	·	68%	
M1 V2 K5 K5 K5 K5 G7 C7 A9 A9 A9 A9 A9 A9 A9 A9 A9 A10 A10 A10 A10 A10 A10 A10 A10 A10 A10	L11 L12 Q13 A14 E15 E15 E17 A18 H19	E20 121 V22 V22 V22 K24 K24 K24 K26 R26 R26 R26 R26 R26 R27 C32 D31 D31	L33 K34 Q35 F55 F58 F58 F58 F58 F58 C60	

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

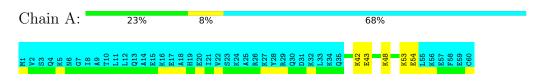
4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Vacuolar proton pump subunit G



4.2.2 Score per residue for model 2

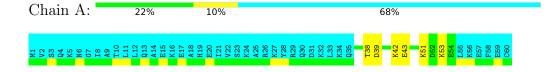
• Molecule 1: Vacuolar proton pump subunit G





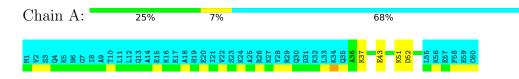
4.2.3 Score per residue for model 3

• Molecule 1: Vacuolar proton pump subunit G



4.2.4 Score per residue for model 4

• Molecule 1: Vacuolar proton pump subunit G



4.2.5 Score per residue for model 5

• Molecule 1: Vacuolar proton pump subunit G

Chain A:	28%	·	68%
М1 5 V 2 6 4 4 1 6 6 7 7 9 8 9 7 9 8 9 7 9 8 1 7 9 8 1 7 9 8 1 7 9 8 1 7 1 8	710 111 712 712 713 713 713 713 713 713 713 713 713 713	H19 E20 121 X22 A25 A25 A25 K27 K27	728 0331 0331 0331 0331 0332 0335 0335 0335 0335 0335 0335 0335

4.2.6 Score per residue for model 6

• Molecule 1: Vacuolar proton pump subunit G

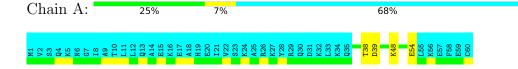
Chain A:	30%	•	68%
M1 V2 Q4 N6 G7 B1 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7	A 9 1110 1111 11110 1110 11110	121 V22 S23 A25 A25 K27 Y28 R29 Q30 D31	K32 K34 K51 K55 F55 F55 F55 F55 F55 F55 F55 F55 K50

4.2.7 Score per residue for model 7



4.2.8 Score per residue for model 8

• Molecule 1: Vacuolar proton pump subunit G



4.2.9 Score per residue for model 9

• Molecule 1: Vacuolar proton pump subunit G

Chain A:	25%	7%	68%
M1 V2 K5 G4 G7 G7 A9 A9	111 111 111 111 111 111 111 111 111 11	E20 E20 V22 S23 K24 R26 R26	V22 V22 V23 V23 V23 V23 V23 V23 V23 V23

4.2.10 Score per residue for model 10

• Molecule 1: Vacuolar proton pump subunit G

Chain A:	27%	5%	68%
M1 V2 V2 V2 V2 V2 V2 V2 V2 V2 V2 V2 V2 V2	Q13 A14 E15 K16 E17 A18 H19 E20	121 V22 S23 A25 A25 R24 R26 R23 R32 R33 R33 R33 R33 R37 R37 R37 R37 R37 R37	E43 K51 F55 E57 C60 C60



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: torsion angle dynamics.

Of the 10 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	refinement	3.0

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	А	152	155	155	0 ± 0
All	All	1520	1550	1550	-

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 -.

There are no clashes.

6.3 Torsion angles (i)

6.3.1 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 NMR 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	19/60~(32%)	19±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	190/600~(32%)	190 (100%)	0 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.



6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR 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	А	16/52~(31%)	$12\pm2~(76\pm11\%)$	$4\pm2~(24\pm11\%)$	2 27
All	All	160/520~(31%)	122 (76%)	38 (24%)	2 27

All 11 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	51	LYS	6
1	А	43	GLU	5
1	А	48	LYS	5
1	А	37	LYS	5
1	А	53	LYS	4
1	А	38	THR	4
1	А	39	ASP	3
1	А	42	LYS	2
1	А	54	GLU	2
1	А	52	ASP	1
1	А	50	GLN	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.



6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



7 Chemical shift validation (i)

No chemical shift data were provided

