wwPDB EM Validation Summary Report

Dec 13, 2022 – 12:08 AM EST

PDB ID	:	1MHS
Title	:	Model of Neurospora crassa proton ATPase
Authors	:	Kuhlbrandt, W.
Deposited on	:	2002-08-21
Resolution	:	8.00 Å(reported)
Based on initial model	:	?

This is a wwPDB EM Validation Summary Report for a publicly released PDB/EMDB 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 (i)) were used in the production of this report:

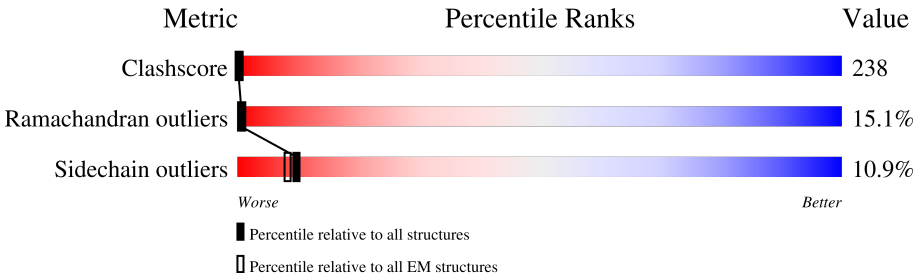
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 8.00 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	920	14% 62% 20% .
1	B	920	14% 62% 20% .

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14082 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 Plasma Membrane ATPase.

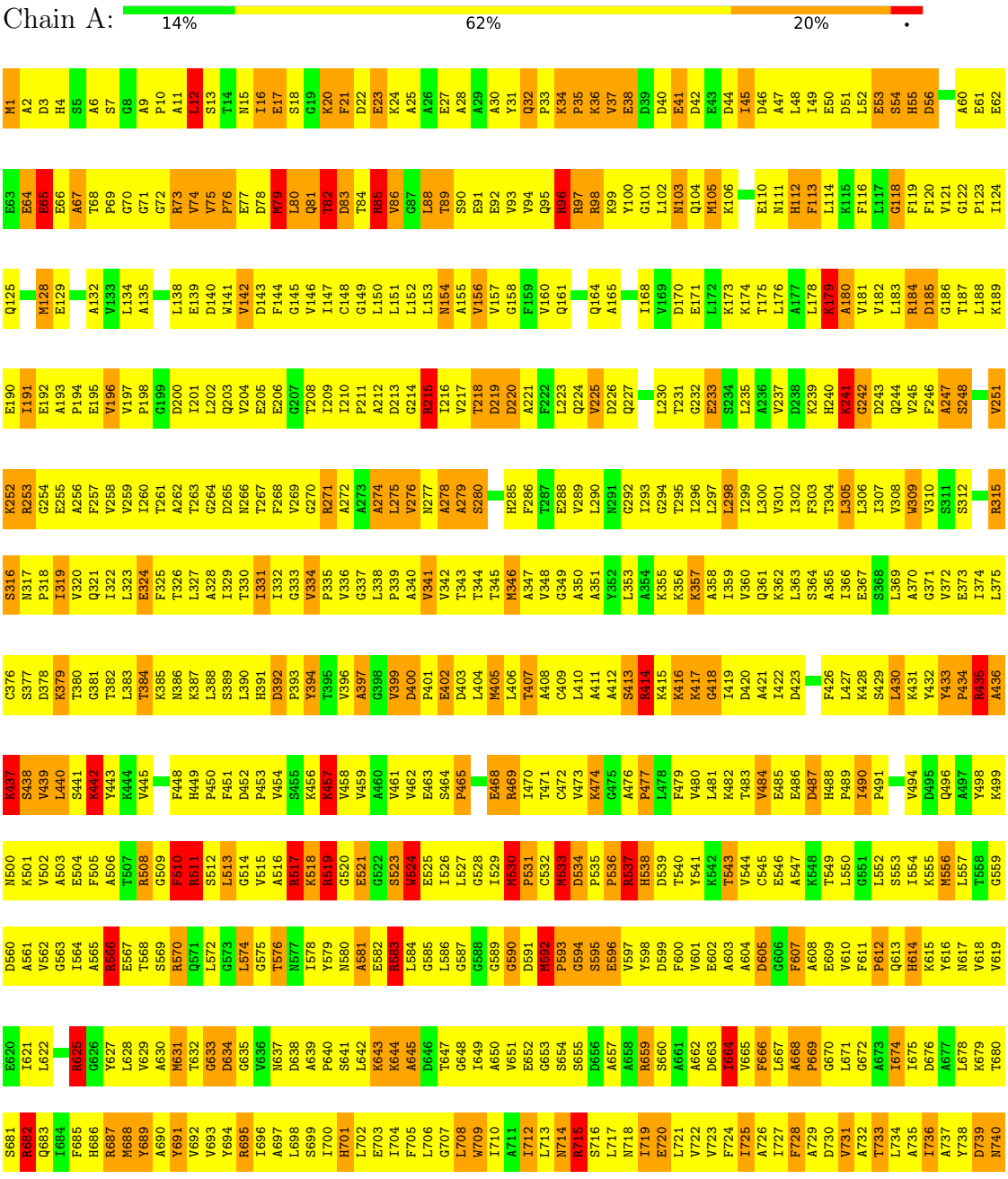
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	920	Total	C	N	O	S	0	0
			7041	4518	1166	1332	25		
1	B	920	Total	C	N	O	S	0	0
			7041	4518	1166	1332	25		

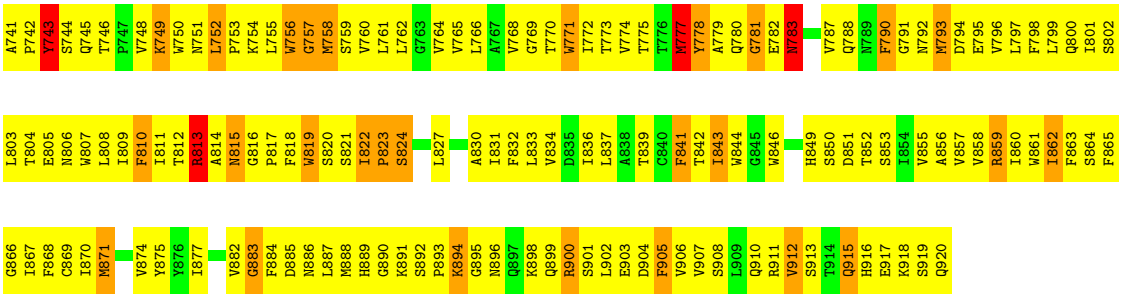
3 Residue-property plots (i)

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. 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. 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: Plasma Membrane ATPase

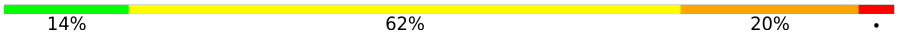
Chain A:

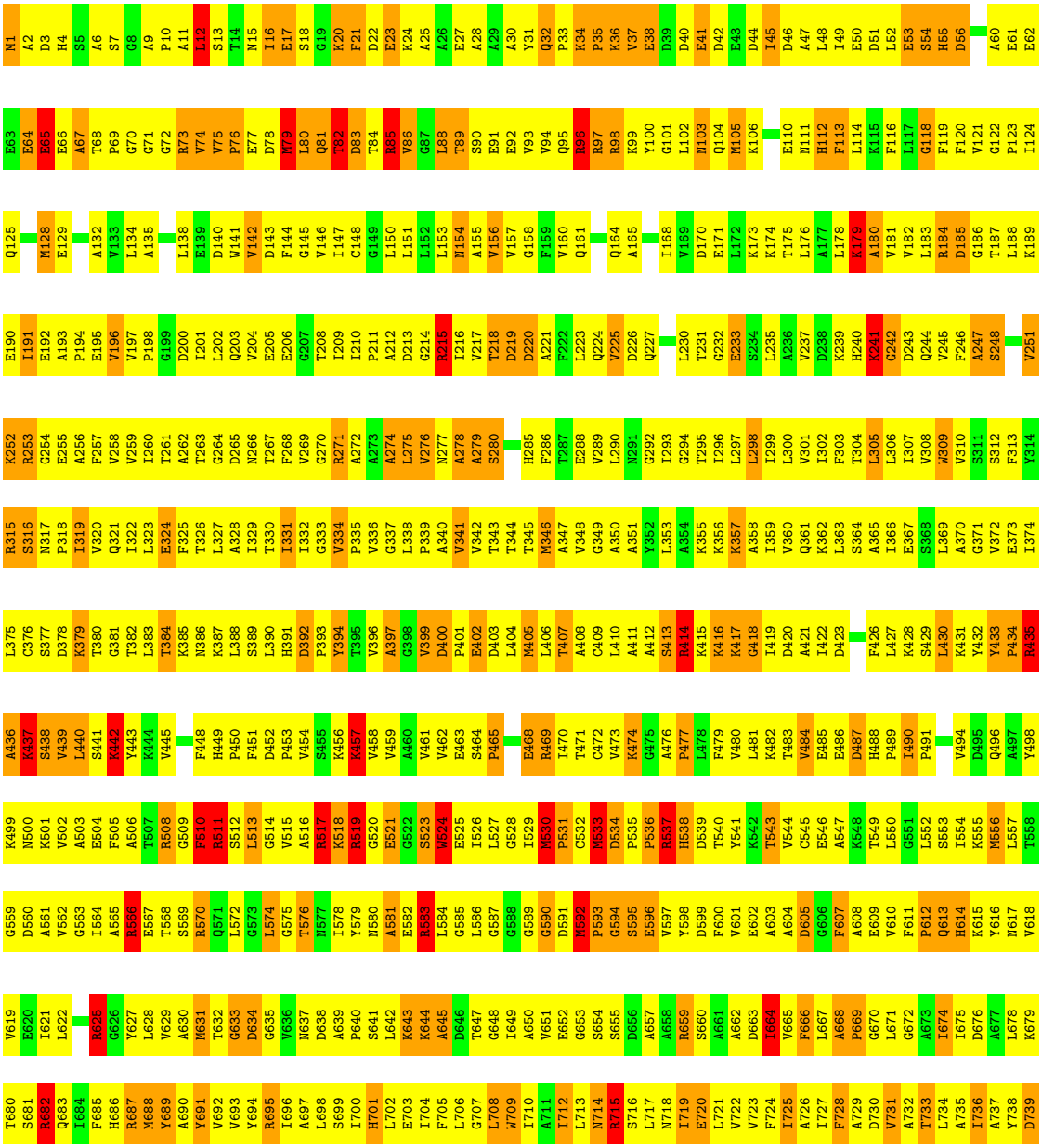


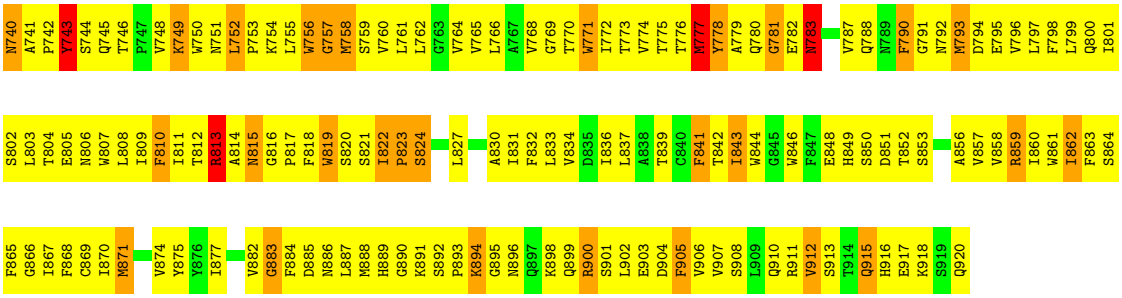


• Molecule 1: Plasma Membrane ATPase

Chain B:






N740 A741 P742 Y743 S744 Q745 T746 P747 V748 K749 W750 N751 L752 P753 K754 L755 W756 G757 M758 S759 V760 L761 L762 G763 V764 V765 L766 A767 V768 G769 T770 W771 I772 T773 V774 T775 T776 M777 Y778 A779 Q780 G781 E782 N783 V787 Q788 N789 F790 G791 N792 M793 D794 E795 V796 L797 F798 L799 Q800 I801
S802 L803 T804 E805 N806 W807 L808 I809 F810 I811 T812 R813 A814 N815 G816 P817 F818 W819 S820 S821 I822 P823 S824 L827 A830 I831 F832 L833 V834 D835 I836 L837 A838 T839 C840 F841 T842 I843 W844 G845 W846 F847 E848 H849 S850 D851 T852 S853 A856 V857 V858 R859 I860 W861 I862 F863 S864
F865 G866 I867 F868 C869 I870 M871 V874 Y875 Y876 I877 V882 G883 F884 D885 N886 L887 M888 H889 G890 K891 S892 P893 K894 G895 N896 Q897 K898 Q899 R900 S901 L902 E903 D904 F905 V906 V907 S908 L909 Q910 R911 V912 S913 T914 Q915 H916 E917 K918 S919 Q920

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	167.00Å 167.00Å 250.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 8.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-8.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14082	wwPDB-VP
Average B, all atoms (Å^2)	4.0	wwPDB-VP

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	0.91	1/7181 (0.0%)	1.25	50/9748 (0.5%)
1	B	0.91	1/7181 (0.0%)	1.25	50/9748 (0.5%)
All	All	0.91	2/14362 (0.0%)	1.25	100/19496 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	524	TRP	NE1-CE2	-5.12	1.30	1.37
1	B	524	TRP	NE1-CE2	-5.10	1.30	1.37

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	695	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	B	695	ARG	NE-CZ-NH2	7.72	124.16	120.30
1	A	813	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	B	570	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	B	813	ARG	NE-CZ-NH2	7.58	124.09	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7041	0	7087	3372	43

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7041	0	7087	3392	45
All	All	14082	0	14174	6713	61

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 238.

The worst 5 of 6713 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:A:859:ARG:HG2	1:B:309:TRP:CZ2	1.28	1.69
1:A:510:PHE:CZ	1:A:512:SER:HB3	1.28	1.66
1:B:810:PHE:CE2	1:B:823:PRO:HD2	1.22	1.64
1:A:510:PHE:CD1	1:A:531:PRO:HB3	1.17	1.64
1:A:74:VAL:CG2	1:A:76:PRO:HD2	1.26	1.63

The worst 5 of 61 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:C	1:A:139:GLU:OE1[4_555]	0.66	1.54
1:B:848:GLU:CD	1:B:849:HIS:CB[5_675]	0.74	1.46
1:B:848:GLU:CA	1:B:848:GLU:O[5_675]	0.91	1.29
1:A:138:LEU:CA	1:A:139:GLU:OE1[4_555]	1.02	1.18
1:B:848:GLU:CD	1:B:849:HIS:CG[5_675]	1.03	1.17

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	A	918/920 (100%)	655 (71%)	124 (14%)	139 (15%)	0 3
1	B	918/920 (100%)	655 (71%)	124 (14%)	139 (15%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1836/1840 (100%)	1310 (71%)	248 (14%)	278 (15%)	0 3

5 of 278 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	A	16	ILE
1	A	17	GLU
1	A	23	GLU
1	A	30	ALA

5.3.2 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 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	751/751 (100%)	669 (89%)	82 (11%)	6 23
1	B	751/751 (100%)	669 (89%)	82 (11%)	6 23
All	All	1502/1502 (100%)	1338 (89%)	164 (11%)	10 23

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	435	ARG
1	B	674	ILE
1	B	452	ASP
1	B	533	MET
1	B	725	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	449	HIS
1	B	718	ASN
1	B	488	HIS

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Mol	Chain	Res	Type
1	B	624	GLN
1	B	896	ASN

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.