



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2017 – 04:24 pm GMT

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29102

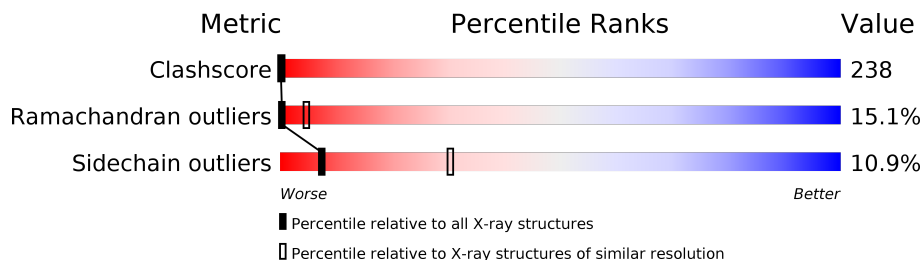
1 Overall quality at a glance

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1036 (11.50-3.80)
Ramachandran outliers	110173	1004 (11.50-3.76)
Sidechain outliers	110143	1099 (11.50-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	920	
1	B	920	

2 Entry composition

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 ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

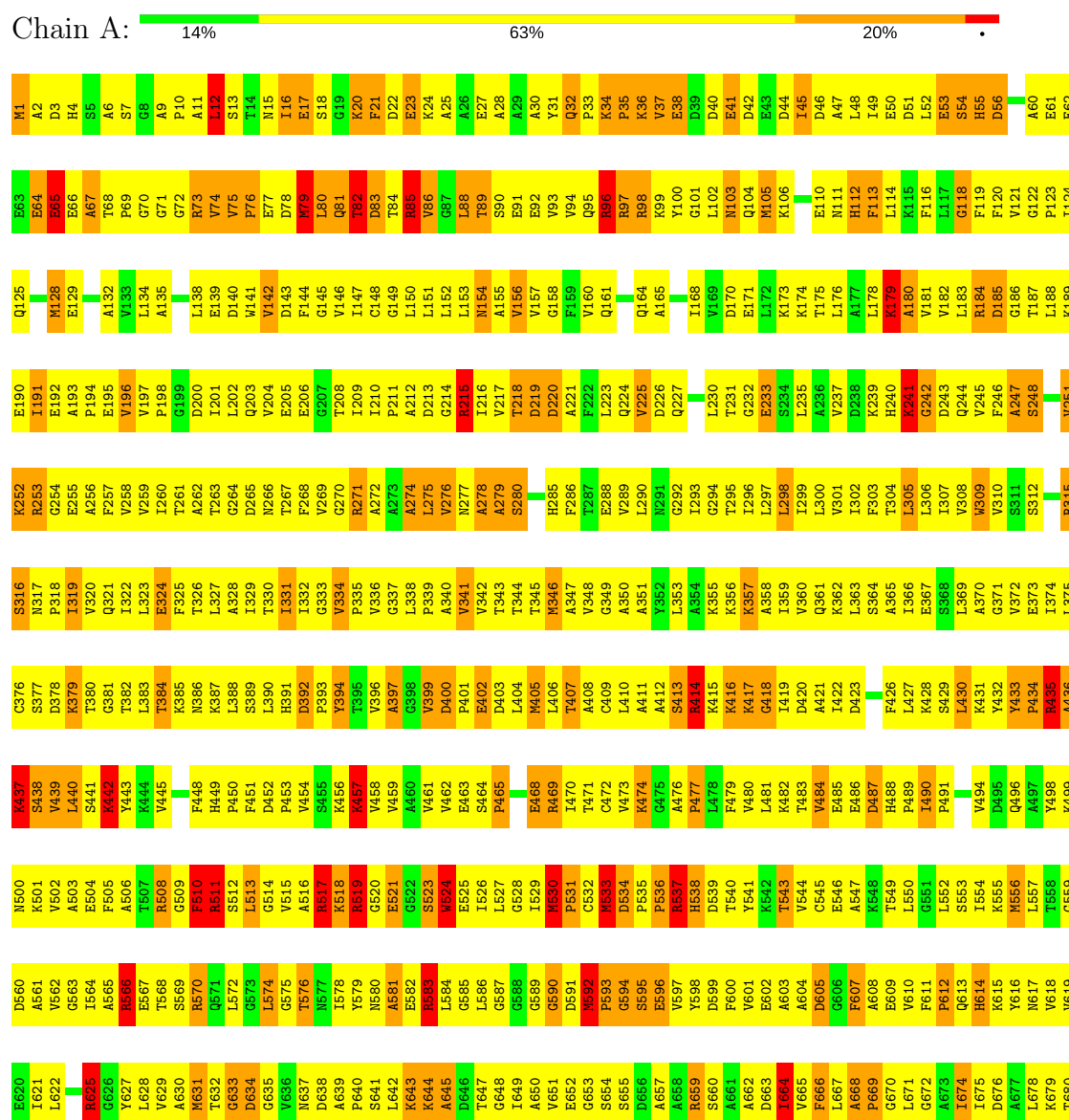
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	920	Total	C	N	O	S	0	0	0
			7041	4518	1166	1332	25			
1	B	920	Total	C	N	O	S	0	0	0
			7041	4518	1166	1332	25			

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

Note EDS was not executed.

• Molecule 1: Plasma Membrane ATPase





F866	G866	I867	F868	C869	I870	N871		V874	Y875	N876	I877		V882	G883	F884	D885	N886	L887	H888	H889	G890	K891	S892	P893	K894	G895	N896	N897	K898	Q899	R900	S901	L902	E903	D904	F905	V906	V907	S908	L909	Q910	R911	V912	S913	T914	Q915	H916	E917	K918	S919	Q920								
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
N740	A741	P742	N743	S744	Q745	T746	F747	V748	K749	W750	N751	L752	P753	K754	L755	W756	G757	W758	S759	V760	L761	L762	G763	V764	V765	L766	N767	V768	G769	T770	W771	L772	T773	V774	T775	T776	N777	Y778	A779	Q780	G781	E782	N783		V787	Q788	N789	F790	G791	N792	N793	D794	E795	V796	L797	F798	L799	Q800	I801

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - 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(°)	Ideal(°)
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

Continued on next page...

Continued from previous page...

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 [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 X-ray entries followed by that with respect to entries of similar resolution.

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 5
1	B	918/920 (100%)	655 (71%)	124 (14%)	139 (15%)	0 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1836/1840 (100%)	1310 (71%)	248 (14%)	278 (15%)	0 5

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 ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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%)	7 30
1	B	751/751 (100%)	669 (89%)	82 (11%)	7 30
All	All	1502/1502 (100%)	1338 (89%)	164 (11%)	7 30

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

Mol	Chain	Res	Type
1	A	777	MET
1	B	82	THR
1	B	728	PHE
1	A	783	ASN
1	B	18	SER

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

Mol	Chain	Res	Type
1	A	896	ASN
1	B	161	GLN
1	B	780	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	4	HIS
1	B	125	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 carbohydrates 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 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.