



wwPDB EM Validation Summary Report ⓘ

Feb 20, 2025 – 08:44 AM EST

PDB ID : 8VXX
Title : Human Aquaporin 2 from 2D electron diffraction data
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for Membrane Protein Structure (TEMIMPS)
Deposited on : 2024-01-31
Resolution : 2.60 Å(reported)

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 ⓘ 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:

MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

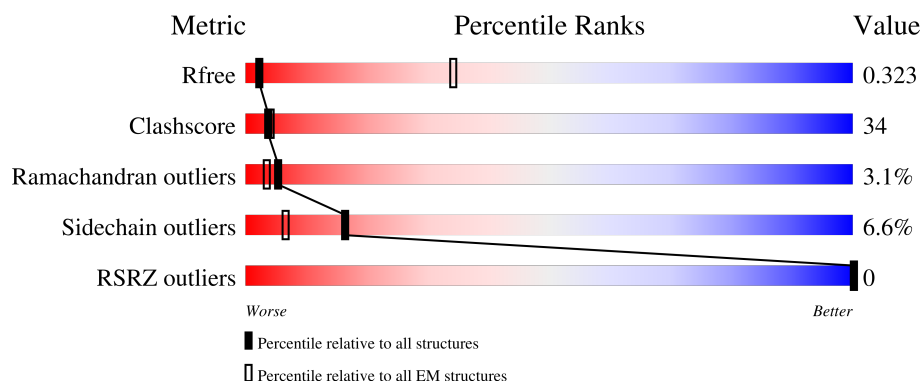
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 2.60 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)
R_{free}	164678	53
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RSRZ outliers	164674	54

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	252	50% (green), 44% (yellow), 5% (orange)
1	B	252	58% (green), 37% (yellow), 5% (orange)
1	X	252	45% (green), 47% (yellow), 7% (orange), . (red)
1	Y	252	52% (green), 42% (yellow), . (orange), . (red)

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7512 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.

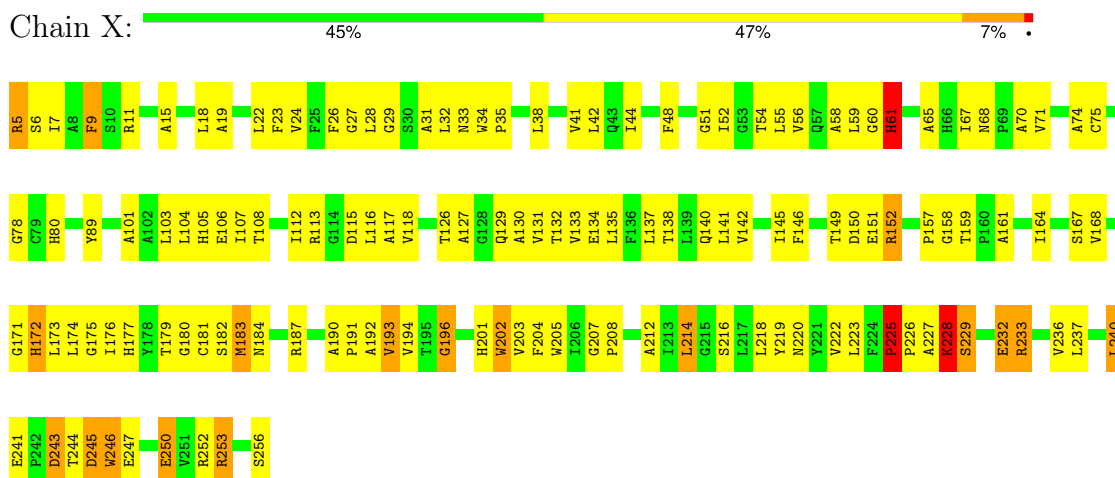
- Molecule 1 is a protein called Aquaporin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	252	Total	C	N	O	S	0	0
			1878	1218	320	334	6		
1	Y	252	Total	C	N	O	S	0	0
			1878	1218	320	334	6		
1	A	252	Total	C	N	O	S	0	0
			1878	1218	320	334	6		
1	B	252	Total	C	N	O	S	0	0
			1878	1218	320	334	6		

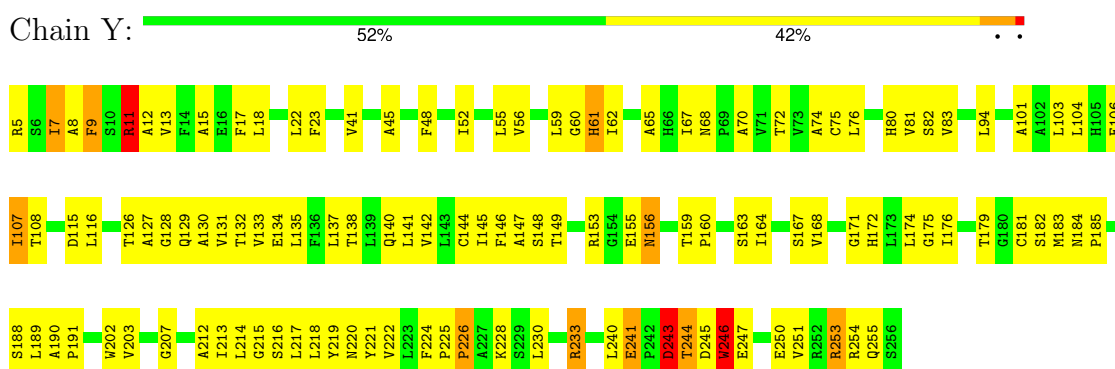
3 Residue-property plots

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. 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.

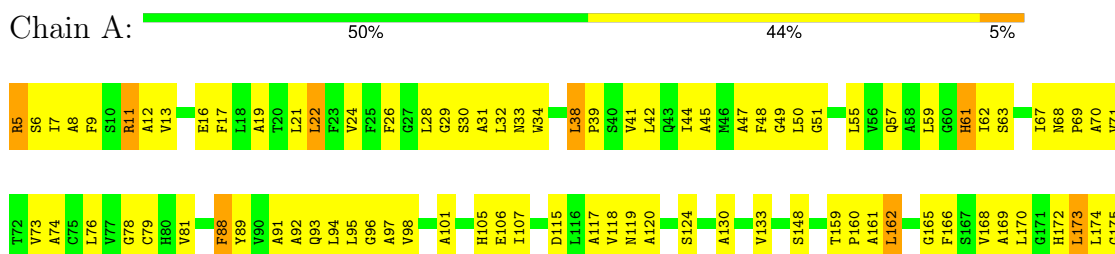
• Molecule 1: Aquaporin-2



• Molecule 1: Aquaporin-2

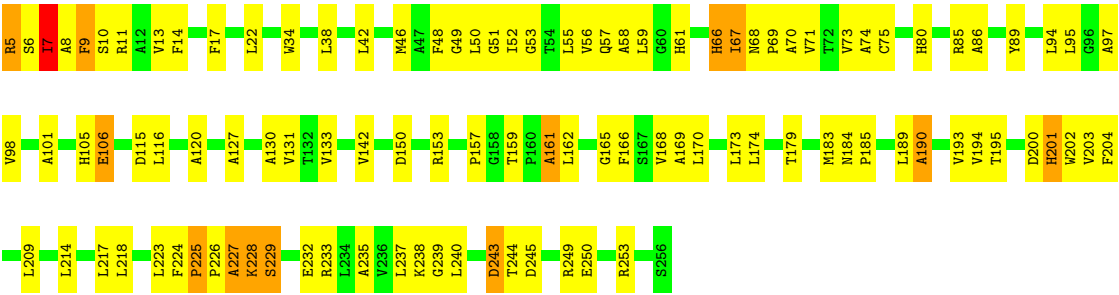


• Molecule 1: Aquaporin-2





• Molecule 1: Aquaporin-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.70Å 94.70Å 250.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.96 – 2.60 66.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	71.0 (66.96-2.60) 71.0 (66.96-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.42Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.293 , 0.296 0.327 , 0.323	Depositor DCC
R_{free} test set	47875 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.11 , 13.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.169 for k,h,-l	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	7512	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.61	1/1922 (0.1%)	1.01	8/2626 (0.3%)
1	B	0.58	0/1922	0.92	4/2626 (0.2%)
1	X	0.64	0/1922	0.93	3/2626 (0.1%)
1	Y	0.59	0/1922	0.91	3/2626 (0.1%)
All	All	0.61	1/7688 (0.0%)	0.94	18/10504 (0.2%)

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
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	TRP	CB-CG	5.42	1.59	1.50

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	PRO	C-N-CD	-7.67	103.72	120.60
1	A	162	LEU	CB-CG-CD1	-7.20	98.77	111.00
1	X	246	TRP	N-CA-C	6.90	129.62	111.00
1	Y	11	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	Y	225	PRO	C-N-CD	-6.30	106.74	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	7	ILE	Peptide

5.2 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 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	1878	0	1903	146	0
1	B	1878	0	1903	107	0
1	X	1878	0	1903	182	0
1	Y	1878	0	1903	118	0
All	All	7512	0	7612	513	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 34.

The worst 5 of 513 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:11:ARG:NH2	1:B:224:PHE:O	1.89	1.06
1:B:68:ASN:ND2	1:B:183:MET:O	1.94	1.00
1:A:67:ILE:O	1:A:184:ASN:ND2	1.98	0.95
1:A:68:ASN:ND2	1:A:183:MET:O	1.99	0.95
1:X:11:ARG:NH2	1:Y:224:PHE:O	2.11	0.83

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	250/252 (99%)	210 (84%)	35 (14%)	5 (2%)	6	12
1	B	250/252 (99%)	210 (84%)	28 (11%)	12 (5%)	2	2
1	X	250/252 (99%)	208 (83%)	33 (13%)	9 (4%)	3	4
1	Y	250/252 (99%)	217 (87%)	28 (11%)	5 (2%)	6	12
All	All	1000/1008 (99%)	845 (84%)	124 (12%)	31 (3%)	5	5

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	225	PRO
1	X	228	LYS
1	Y	241	GLU
1	Y	243	ASP
1	A	225	PRO

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	194/195 (100%)	181 (93%)	13 (7%)	13	29
1	B	194/195 (100%)	186 (96%)	8 (4%)	26	51
1	X	194/195 (100%)	178 (92%)	16 (8%)	9	20
1	Y	194/195 (100%)	180 (93%)	14 (7%)	12	26
All	All	776/780 (100%)	725 (93%)	51 (7%)	16	30

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	253	ARG
1	A	106	GLU
1	B	237	LEU
1	Y	255	GLN
1	A	38	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	105	HIS
1	X	201	HIS
1	X	220	ASN
1	A	172	HIS
1	A	201	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 oligosaccharides 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.