



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 26, 2017 – 05:40 PM EDT

PDB ID : 3LLQ
Title : Aquaporin structure from plant pathogen Agrobacterium Tumerfaciens
Authors : Liu, Q.; Hillerich, B.; Love, J.; New York Consortium on Membrane Protein Structure (NYCOMPS)
Deposited on : unknown
Resolution : 2.01 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)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

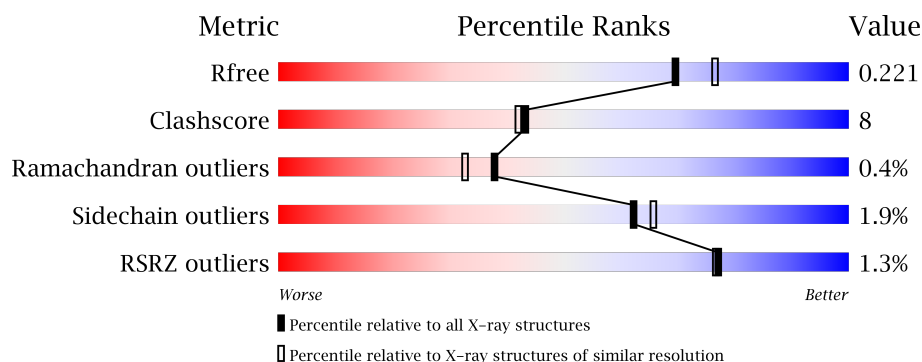
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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))
R_{free}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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.

Mol	Chain	Length	Quality of chain
1	A	256	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 17%, yellow 17%, yellow 70%, green 70%, green 97%, grey 97%, grey 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%; text-align: center;"> </div> </div> </div>
1	B	256	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 18%, yellow 18%, yellow 71%, green 71%, green 98%, grey 98%, grey 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%; text-align: center;"> </div> </div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3395 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 Aquaporin Z 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1642	1094	265	280	3			
1	B	233	Total	C	N	O	S	0	0	0
			1691	1130	271	287	3			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	expression tag	UNP Q8UJW4
A	-26	ASP	-	expression tag	UNP Q8UJW4
A	-25	TYR	-	expression tag	UNP Q8UJW4
A	-24	LYS	-	expression tag	UNP Q8UJW4
A	-23	ASP	-	expression tag	UNP Q8UJW4
A	-22	ASP	-	expression tag	UNP Q8UJW4
A	-21	ASP	-	expression tag	UNP Q8UJW4
A	-20	ASP	-	expression tag	UNP Q8UJW4
A	-19	LYS	-	expression tag	UNP Q8UJW4
A	-18	HIS	-	expression tag	UNP Q8UJW4
A	-17	HIS	-	expression tag	UNP Q8UJW4
A	-16	HIS	-	expression tag	UNP Q8UJW4
A	-15	HIS	-	expression tag	UNP Q8UJW4
A	-14	HIS	-	expression tag	UNP Q8UJW4
A	-13	HIS	-	expression tag	UNP Q8UJW4
A	-12	HIS	-	expression tag	UNP Q8UJW4
A	-11	HIS	-	expression tag	UNP Q8UJW4
A	-10	HIS	-	expression tag	UNP Q8UJW4
A	-9	HIS	-	expression tag	UNP Q8UJW4
A	-8	GLU	-	expression tag	UNP Q8UJW4
A	-7	ASN	-	expression tag	UNP Q8UJW4
A	-6	LEU	-	expression tag	UNP Q8UJW4
A	-5	TYR	-	expression tag	UNP Q8UJW4
A	-4	PHE	-	expression tag	UNP Q8UJW4
A	-3	GLN	-	expression tag	UNP Q8UJW4

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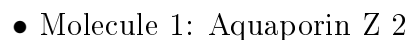
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8UJW4
A	-1	TYR	-	expression tag	UNP Q8UJW4
A	0	VAL	-	expression tag	UNP Q8UJW4
B	-27	MET	-	expression tag	UNP Q8UJW4
B	-26	ASP	-	expression tag	UNP Q8UJW4
B	-25	TYR	-	expression tag	UNP Q8UJW4
B	-24	LYS	-	expression tag	UNP Q8UJW4
B	-23	ASP	-	expression tag	UNP Q8UJW4
B	-22	ASP	-	expression tag	UNP Q8UJW4
B	-21	ASP	-	expression tag	UNP Q8UJW4
B	-20	ASP	-	expression tag	UNP Q8UJW4
B	-19	LYS	-	expression tag	UNP Q8UJW4
B	-18	HIS	-	expression tag	UNP Q8UJW4
B	-17	HIS	-	expression tag	UNP Q8UJW4
B	-16	HIS	-	expression tag	UNP Q8UJW4
B	-15	HIS	-	expression tag	UNP Q8UJW4
B	-14	HIS	-	expression tag	UNP Q8UJW4
B	-13	HIS	-	expression tag	UNP Q8UJW4
B	-12	HIS	-	expression tag	UNP Q8UJW4
B	-11	HIS	-	expression tag	UNP Q8UJW4
B	-10	HIS	-	expression tag	UNP Q8UJW4
B	-9	HIS	-	expression tag	UNP Q8UJW4
B	-8	GLU	-	expression tag	UNP Q8UJW4
B	-7	ASN	-	expression tag	UNP Q8UJW4
B	-6	LEU	-	expression tag	UNP Q8UJW4
B	-5	TYR	-	expression tag	UNP Q8UJW4
B	-4	PHE	-	expression tag	UNP Q8UJW4
B	-3	GLN	-	expression tag	UNP Q8UJW4
B	-2	SER	-	expression tag	UNP Q8UJW4
B	-1	TYR	-	expression tag	UNP Q8UJW4
B	0	VAL	-	expression tag	UNP Q8UJW4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	24	Total O 24 24	0	0
2	B	38	Total O 38 38	0	0

- Molecule 1: Aquaporin Z 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	90.50Å 102.23Å 148.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.18 – 2.01 28.73 – 2.01	Depositor EDS
% Data completeness (in resolution range)	93.1 (31.18-2.01) 93.1 (28.73-2.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.188 , 0.219 0.191 , 0.221	Depositor DCC
R_{free} test set	2197 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.907	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3395	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% 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 [i](#)

5.1 Standard geometry [i](#)

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	1.44	11/1687 (0.7%)	0.99	4/2305 (0.2%)
1	B	1.36	14/1739 (0.8%)	0.91	2/2376 (0.1%)
All	All	1.40	25/3426 (0.7%)	0.95	6/4681 (0.1%)

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	PHE	CG-CD2	7.21	1.49	1.38
1	A	45	LEU	CB-CG	6.94	1.72	1.52
1	B	143	PHE	CD2-CE2	6.82	1.52	1.39
1	A	28	ALA	CA-CB	6.69	1.66	1.52
1	A	149	GLY	N-CA	6.67	1.56	1.46

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	LEU	CA-CB-CG	-7.20	98.73	115.30
1	A	144	LEU	CB-CG-CD1	6.54	122.11	111.00
1	A	144	LEU	CA-CB-CG	-6.52	100.31	115.30
1	A	148	LEU	CB-CG-CD2	-5.56	101.55	111.00
1	A	45	LEU	CB-CG-CD1	-5.52	101.61	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1642	0	1682	27	0
1	B	1691	0	1727	28	0
2	A	24	0	0	0	0
2	B	38	0	0	0	0
All	All	3395	0	3409	52	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 8.

The worst 5 of 52 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:B:144:LEU:HD13	1:B:214:GLY:HA2	1.65	0.77
1:A:144:LEU:HD13	1:A:214:GLY:HA2	1.69	0.73
1:B:147:ILE:HA	1:B:164:ILE:HD11	1.81	0.63
1:B:61:HIS:HD2	1:B:67:SER:OG	1.81	0.63
1:A:144:LEU:HD13	1:A:214:GLY:CA	2.31	0.59

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 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	226/256 (88%)	217 (96%)	8 (4%)	1 (0%)	38	33
1	B	231/256 (90%)	224 (97%)	6 (3%)	1 (0%)	38	33
All	All	457/512 (89%)	441 (96%)	14 (3%)	2 (0%)	38	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183	VAL

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Mol	Chain	Res	Type
1	A	183	VAL

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	158/186 (85%)	155 (98%)	3 (2%)	62	66
1	B	163/186 (88%)	160 (98%)	3 (2%)	64	68
All	All	321/372 (86%)	315 (98%)	6 (2%)	62	66

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	ARG
1	B	187	ARG
1	B	61	HIS
1	A	144	LEU
1	B	144	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	HIS
1	A	191	GLN
1	B	61	HIS
1	B	180	ASN

5.3.3 RNA ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	228/256 (89%)	-0.46	3 (1%) 77 77	19, 31, 43, 59	0
1	B	233/256 (91%)	-0.41	3 (1%) 77 77	21, 30, 43, 55	0
All	All	461/512 (90%)	-0.44	6 (1%) 77 77	19, 30, 43, 59	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	GLY	3.0
1	B	-4	PHE	2.8
1	B	227	LYS	2.5
1	B	223	LEU	2.5
1	A	107	ALA	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.