wwPDB X-ray Structure Validation Summary Report (i)

Oct 1, 2023 – 10:43 PM EDT

PDB ID	:	6N1G
Title	:	Crystal structure of Aquaglyceroporin AQP7
Authors	:	Vahedi-Faridi, A.; Lodowski, D.; Kowatz, T.
Deposited on	:	2018-11-08
Resolution	:	4.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15472 atoms, of which 7776 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-7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	249	Total	C	H	N	O	S	0	0	0
			3826	1266	1920	308	319	13			
1	C	249	Total	C	H	N	O	S	0	0	0
			3826	1266	1920	308	319	13			
1	B	249	Total	C	H	N	O	S	0	0	0
			3826	1266	1920	308	319	13			
1	D	249	Total	C	H	N	O	S	0	0	0
			3826	1266	1920	308	319	13			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	343	GLY	-	expression tag	UNP O14520
A	344	GLY	-	expression tag	UNP O14520
A	345	SER	-	expression tag	UNP O14520
A	346	LEU	-	expression tag	UNP O14520
A	347	GLU	-	expression tag	UNP O14520
A	348	VAL	-	expression tag	UNP O14520
A	349	LEU	-	expression tag	UNP O14520
A	350	PHE	-	expression tag	UNP O14520
A	351	GLN	-	expression tag	UNP O14520
A	352	GLY	-	expression tag	UNP O14520
A	353	PRO	-	expression tag	UNP O14520
A	354	ALA	-	expression tag	UNP O14520
A	355	ALA	-	expression tag	UNP O14520
A	356	TYR	-	expression tag	UNP O14520
A	357	PRO	-	expression tag	UNP O14520
A	358	TYR	-	expression tag	UNP O14520
A	359	ASP	-	expression tag	UNP O14520
A	360	VAL	-	expression tag	UNP O14520
A	361	PRO	-	expression tag	UNP O14520
A	362	ASP	-	expression tag	UNP O14520
A	363	TYR	-	expression tag	UNP O14520

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Chain	Residue	Modelled	Actual	Comment	Reference
A	364	ALA	-	expression tag	UNP O14520
A	365	ALA	-	expression tag	UNP O14520
A	366	ALA	-	expression tag	UNP O14520
A	367	HIS	-	expression tag	UNP O14520
A	368	HIS	-	expression tag	UNP O14520
A	369	HIS	-	expression tag	UNP O14520
A	370	HIS	-	expression tag	UNP O14520
A	371	HIS	-	expression tag	UNP O14520
A	372	HIS	-	expression tag	UNP O14520
A	373	HIS	-	expression tag	UNP O14520
A	374	HIS	-	expression tag	UNP O14520
A	375	HIS	-	expression tag	UNP O14520
A	376	HIS	-	expression tag	UNP O14520
C	343	GLY	-	expression tag	UNP O14520
C	344	GLY	-	expression tag	UNP O14520
C	345	SER	-	expression tag	UNP O14520
C	346	LEU	-	expression tag	UNP O14520
C	347	GLU	-	expression tag	UNP O14520
C	348	VAL	-	expression tag	UNP O14520
C	349	LEU	-	expression tag	UNP O14520
C	350	PHE	-	expression tag	UNP O14520
C	351	GLN	-	expression tag	UNP O14520
C	352	GLY	-	expression tag	UNP O14520
C	353	PRO	-	expression tag	UNP O14520
C	354	ALA	-	expression tag	UNP O14520
C	355	ALA	-	expression tag	UNP O14520
C	356	TYR	-	expression tag	UNP O14520
C	357	PRO	-	expression tag	UNP O14520
C	358	TYR	-	expression tag	UNP O14520
C	359	ASP	-	expression tag	UNP O14520
C	360	VAL	-	expression tag	UNP O14520
C	361	PRO	-	expression tag	UNP O14520
C	362	ASP	-	expression tag	UNP O14520
C	363	TYR	-	expression tag	UNP O14520
C	364	ALA	-	expression tag	UNP O14520
C	365	ALA	-	expression tag	UNP O14520
C	366	ALA	-	expression tag	UNP O14520
C	367	HIS	-	expression tag	UNP O14520
C	368	HIS	-	expression tag	UNP O14520
C	369	HIS	-	expression tag	UNP O14520
C	370	HIS	-	expression tag	UNP O14520
C	371	HIS	-	expression tag	UNP O14520

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Chain	Residue	Modelled	Actual	Comment	Reference
C	372	HIS	-	expression tag	UNP O14520
C	373	HIS	-	expression tag	UNP O14520
C	374	HIS	-	expression tag	UNP O14520
C	375	HIS	-	expression tag	UNP O14520
C	376	HIS	-	expression tag	UNP O14520
B	343	GLY	-	expression tag	UNP O14520
B	344	GLY	-	expression tag	UNP O14520
B	345	SER	-	expression tag	UNP O14520
B	346	LEU	-	expression tag	UNP O14520
B	347	GLU	-	expression tag	UNP O14520
B	348	VAL	-	expression tag	UNP O14520
B	349	LEU	-	expression tag	UNP O14520
B	350	PHE	-	expression tag	UNP O14520
B	351	GLN	-	expression tag	UNP O14520
B	352	GLY	-	expression tag	UNP O14520
B	353	PRO	-	expression tag	UNP O14520
B	354	ALA	-	expression tag	UNP O14520
B	355	ALA	-	expression tag	UNP O14520
B	356	TYR	-	expression tag	UNP O14520
B	357	PRO	-	expression tag	UNP O14520
B	358	TYR	-	expression tag	UNP O14520
B	359	ASP	-	expression tag	UNP O14520
B	360	VAL	-	expression tag	UNP O14520
B	361	PRO	-	expression tag	UNP O14520
B	362	ASP	-	expression tag	UNP O14520
B	363	TYR	-	expression tag	UNP O14520
B	364	ALA	-	expression tag	UNP O14520
B	365	ALA	-	expression tag	UNP O14520
B	366	ALA	-	expression tag	UNP O14520
B	367	HIS	-	expression tag	UNP O14520
B	368	HIS	-	expression tag	UNP O14520
B	369	HIS	-	expression tag	UNP O14520
B	370	HIS	-	expression tag	UNP O14520
B	371	HIS	-	expression tag	UNP O14520
B	372	HIS	-	expression tag	UNP O14520
B	373	HIS	-	expression tag	UNP O14520
B	374	HIS	-	expression tag	UNP O14520
B	375	HIS	-	expression tag	UNP O14520
B	376	HIS	-	expression tag	UNP O14520
D	343	GLY	-	expression tag	UNP O14520
D	344	GLY	-	expression tag	UNP O14520
D	345	SER	-	expression tag	UNP O14520

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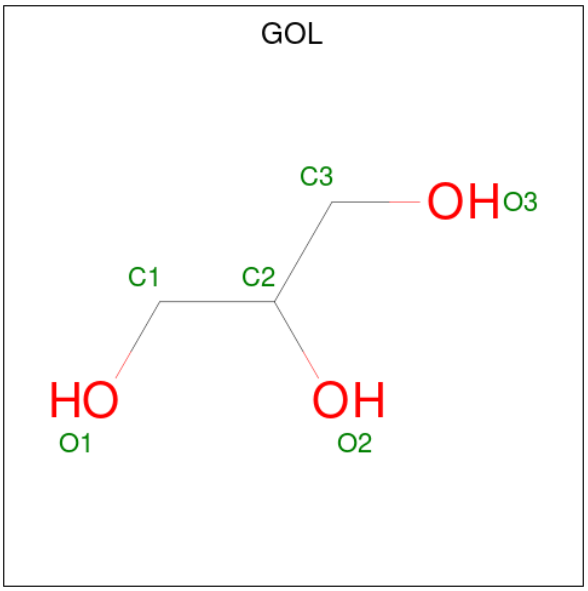
Chain	Residue	Modelled	Actual	Comment	Reference
D	346	LEU	-	expression tag	UNP O14520
D	347	GLU	-	expression tag	UNP O14520
D	348	VAL	-	expression tag	UNP O14520
D	349	LEU	-	expression tag	UNP O14520
D	350	PHE	-	expression tag	UNP O14520
D	351	GLN	-	expression tag	UNP O14520
D	352	GLY	-	expression tag	UNP O14520
D	353	PRO	-	expression tag	UNP O14520
D	354	ALA	-	expression tag	UNP O14520
D	355	ALA	-	expression tag	UNP O14520
D	356	TYR	-	expression tag	UNP O14520
D	357	PRO	-	expression tag	UNP O14520
D	358	TYR	-	expression tag	UNP O14520
D	359	ASP	-	expression tag	UNP O14520
D	360	VAL	-	expression tag	UNP O14520
D	361	PRO	-	expression tag	UNP O14520
D	362	ASP	-	expression tag	UNP O14520
D	363	TYR	-	expression tag	UNP O14520
D	364	ALA	-	expression tag	UNP O14520
D	365	ALA	-	expression tag	UNP O14520
D	366	ALA	-	expression tag	UNP O14520
D	367	HIS	-	expression tag	UNP O14520
D	368	HIS	-	expression tag	UNP O14520
D	369	HIS	-	expression tag	UNP O14520
D	370	HIS	-	expression tag	UNP O14520
D	371	HIS	-	expression tag	UNP O14520
D	372	HIS	-	expression tag	UNP O14520
D	373	HIS	-	expression tag	UNP O14520
D	374	HIS	-	expression tag	UNP O14520
D	375	HIS	-	expression tag	UNP O14520
D	376	HIS	-	expression tag	UNP O14520

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	C	1	Total C H O 14 3 8 3	0	0
2	C	1	Total C H O 14 3 8 3	0	0
2	C	1	Total C H O 14 3 8 3	0	0
2	B	1	Total C H O 14 3 8 3	0	0
2	B	1	Total C H O 14 3 8 3	0	0
2	B	1	Total C H O 14 3 8 3	14	0
2	D	1	Total C H O 14 3 8 3	0	0
2	D	1	Total C H O 14 3 8 3	0	0
2	D	1	Total C H O 14 3 8 3	0	0
2	D	1	Total C H O 14 3 8 3	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	385.66Å 385.66Å 385.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.71 – 4.00	Depositor
% Data completeness (in resolution range)	87.9 (32.71-4.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	50.00 (at 4.00Å)	Xtriage
Refinement program	PHENIX (1.14_3235: ???)	Depositor
R, R_{free}	0.232 , 0.277	Depositor
Wilson B-factor (Å^2)	132.5	Xtriage
Anisotropy	0.000	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15472	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 88.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7106e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	D	402	-	5,5,5	0.86	0	5,5,5	1.01	0
2	GOL	C	403	-	5,5,5	0.97	0	5,5,5	0.80	0
2	GOL	A	402	-	5,5,5	0.83	0	5,5,5	0.93	0
2	GOL	C	402	-	5,5,5	0.86	0	5,5,5	0.99	0
2	GOL	B	403	-	5,5,5	0.96	0	5,5,5	1.00	0
2	GOL	D	401	-	5,5,5	1.25	1 (20%)	5,5,5	1.07	0
2	GOL	D	403	-	5,5,5	0.87	0	5,5,5	1.02	0
2	GOL	D	404	-	5,5,5	0.84	0	5,5,5	0.96	0
2	GOL	A	401	-	5,5,5	1.11	0	5,5,5	0.97	0
2	GOL	B	402	-	5,5,5	0.86	0	5,5,5	0.94	0
2	GOL	C	401	-	5,5,5	1.29	1 (20%)	5,5,5	0.84	0
2	GOL	B	401	-	5,5,5	1.33	2 (40%)	5,5,5	0.79	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	402	-	-	0/4/4/4	-
2	GOL	C	403	-	-	2/4/4/4	-
2	GOL	A	402	-	-	0/4/4/4	-
2	GOL	C	402	-	-	2/4/4/4	-
2	GOL	B	403	-	-	0/4/4/4	-
2	GOL	D	401	-	-	0/4/4/4	-
2	GOL	D	403	-	-	0/4/4/4	-
2	GOL	D	404	-	-	2/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	B	402	-	-	0/4/4/4	-
2	GOL	C	401	-	-	2/4/4/4	-
2	GOL	B	401	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	GOL	C1-C2	2.27	1.61	1.51
2	D	401	GOL	C1-C2	2.09	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	GOL	C1-C2	2.09	1.60	1.51
2	B	401	GOL	C3-C2	2.04	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	402	GOL	O1-C1-C2-C3
2	C	403	GOL	O1-C1-C2-O2
2	C	403	GOL	O1-C1-C2-C3
2	A	401	GOL	O2-C2-C3-O3
2	D	404	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.