



wwPDB NMR Structure Validation Summary Report ⓘ

May 19, 2016 – 04:30 PM EDT

PDB ID : 4AQZ
Title : B2 domain of Neisseria meningitidis Pilus assembly protein PilQ
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Deposited on : 2012-04-20

This is a wwPDB NMR 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/NMRValidationReportHelp>

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:

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

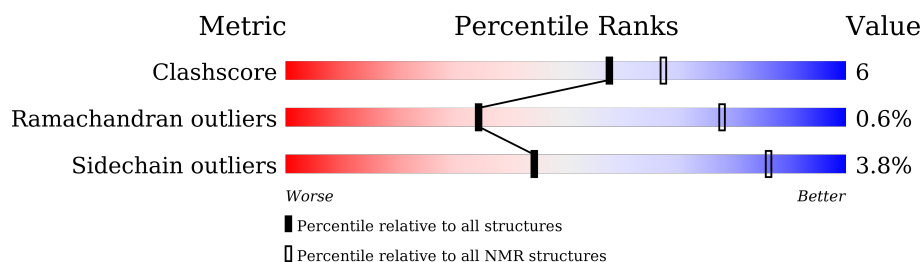
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	138	 66% 9% 25%

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:225-A:327 (103)	0.26	15

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 7, 14, 18, 20
2	8, 9, 15, 17, 19
3	5, 6, 11
4	12, 13
Single-model clusters	10; 16

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2073 atoms, of which 1005 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ.

Mol	Chain	Residues	Atoms						Trace
1	A	138	Total	C	H	N	O	S	0
			2073	666	1005	202	196	4	

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	MET	-	EXPRESSION TAG	UNP Q70M91
A	193	GLY	-	EXPRESSION TAG	UNP Q70M91
A	194	SER	-	EXPRESSION TAG	UNP Q70M91
A	195	SER	-	EXPRESSION TAG	UNP Q70M91
A	196	HIS	-	EXPRESSION TAG	UNP Q70M91
A	197	HIS	-	EXPRESSION TAG	UNP Q70M91
A	198	HIS	-	EXPRESSION TAG	UNP Q70M91
A	199	HIS	-	EXPRESSION TAG	UNP Q70M91
A	200	HIS	-	EXPRESSION TAG	UNP Q70M91
A	201	HIS	-	EXPRESSION TAG	UNP Q70M91
A	202	GLY	-	EXPRESSION TAG	UNP Q70M91
A	203	LEU	-	EXPRESSION TAG	UNP Q70M91
A	204	VAL	-	EXPRESSION TAG	UNP Q70M91
A	205	PRO	-	EXPRESSION TAG	UNP Q70M91
A	206	ARG	-	EXPRESSION TAG	UNP Q70M91
A	207	GLY	-	EXPRESSION TAG	UNP Q70M91
A	208	SER	-	EXPRESSION TAG	UNP Q70M91
A	209	HIS	-	EXPRESSION TAG	UNP Q70M91
A	210	MET	-	EXPRESSION TAG	UNP Q70M91
A	211	ALA	-	EXPRESSION TAG	UNP Q70M91
A	212	SER	-	EXPRESSION TAG	UNP Q70M91
A	213	MET	-	EXPRESSION TAG	UNP Q70M91
A	214	THR	-	EXPRESSION TAG	UNP Q70M91
A	215	GLY	-	EXPRESSION TAG	UNP Q70M91
A	216	GLY	-	EXPRESSION TAG	UNP Q70M91
A	217	GLN	-	EXPRESSION TAG	UNP Q70M91
A	218	GLN	-	EXPRESSION TAG	UNP Q70M91
A	219	MET	-	EXPRESSION TAG	UNP Q70M91
A	220	GLY	-	EXPRESSION TAG	UNP Q70M91
A	221	ARG	-	EXPRESSION TAG	UNP Q70M91

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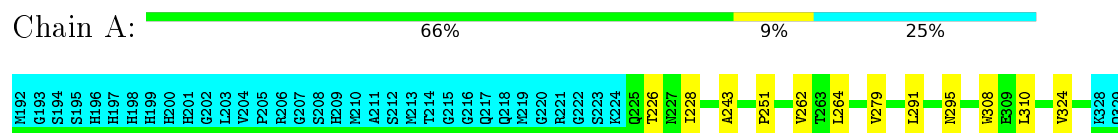
Chain	Residue	Modelled	Actual	Comment	Reference
A	222	GLY	-	EXPRESSION TAG	UNP Q70M91
A	223	SER	-	EXPRESSION TAG	UNP Q70M91

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

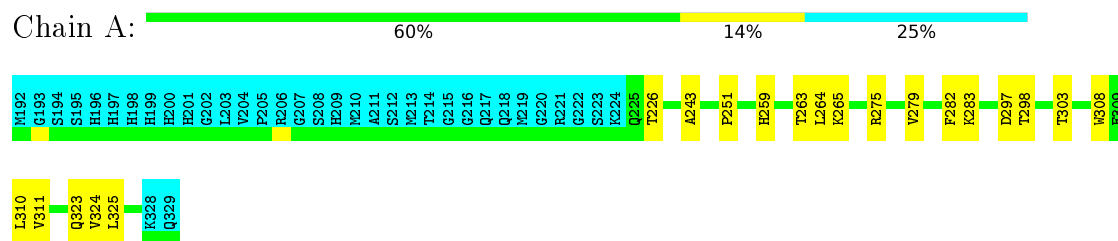
- Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 15. Colouring as in section 4.1 above.

- Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ



5 Refinement protocol and experimental data overview

The models were refined using the following method: *CYANA2.1 AND CNS1.2 WATER REFINEMENT*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA2.1	refinement	
TOPSPIN2.1	structure solution	
CCPN ANALYSIS	structure solution	
CYANA2.1	structure solution	
CNS1.2	structure solution	
TALOSPLUS	structure solution	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	4aqz_cs.cif
Number of chemical shift lists	1
Total number of shifts	1484
Number of shifts mapped to atoms	1484
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 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 (average) 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	0.89±0.03	0±0/822 (0.0±0.0%)	0.71±0.03	0±0/1119 (0.0±0.0%)
All	All	0.89	0/16440 (0.0%)	0.71	1/22380 (0.0%)

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	Planarity
1	A	0.0±0.0	0.1±0.4
All	All	0	3

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	231	ARG	NE-CZ-NH2	-5.09	117.75	120.30	10	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	231	ARG	Sidechain	2
1	A	293	ARG	Sidechain	1

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	806	755	822	10±2
All	All	16120	15100	16440	197

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 6.

5 of 62 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:251:PRO:HB3	1:A:264:LEU:HD13	0.65	1.68	3	12
1:A:308:TRP:CZ3	1:A:310:LEU:HB2	0.64	2.28	15	11
1:A:279:VAL:HA	1:A:282:PHE:CD2	0.61	2.30	14	3
1:A:225:GLN:O	1:A:245:LEU:HD23	0.60	1.96	10	1
1:A:226:THR:HA	1:A:243:ALA:O	0.60	1.97	18	17

6.3 Torsion angles [i](#)

6.3.1 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 NMR 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	103/138 (75%)	99±2 (96±2%)	4±2 (4±2%)	1±1 (1±1%)	34	78
All	All	2060/2760 (75%)	1971 (96%)	77 (4%)	12 (1%)	34	78

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	295	ASN	6
1	A	279	VAL	5
1	A	225	GLN	1

6.3.2 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 NMR 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	89/116 (77%)	86±2 (96±2%)	3±2 (4±2%)	44	86
All	All	1780/2320 (77%)	1712 (96%)	68 (4%)	44	86

5 of 24 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	291	LEU	7
1	A	262	VAL	6
1	A	283	LYS	6
1	A	324	VAL	5
1	A	296	ASN	5

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: 4aqz_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1484
Number of shifts mapped to atoms	1484
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	123	-0.05 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	113	0.08 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	123	-1.79 ± 0.25	Should be applied
^{15}N	116	-0.83 ± 0.52	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 1131 atoms were assigned a chemical shift out of a possible 1274. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	505/505 (100%)	201/201 (100%)	206/206 (100%)	98/98 (100%)
Sidechain	563/680 (83%)	344/394 (87%)	214/254 (84%)	5/32 (16%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	63/89 (71%)	32/47 (68%)	30/35 (86%)	1/7 (14%)
Overall	1131/1274 (89%)	577/642 (90%)	450/495 (91%)	104/137 (76%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	304	THR	HG23	-0.22	2.29 – -0.01	-5.9
1	A	304	THR	HG22	-0.22	2.29 – -0.01	-5.9
1	A	304	THR	HG21	-0.22	2.29 – -0.01	-5.9
1	A	279	VAL	HG11	-0.58	2.13 – -0.47	-5.4
1	A	279	VAL	HG12	-0.58	2.13 – -0.47	-5.4
1	A	279	VAL	HG13	-0.58	2.13 – -0.47	-5.4

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

