



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 4AR0 / pdb_00004ar0
BMRB ID : 18459
Title : N0 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.

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<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

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 : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

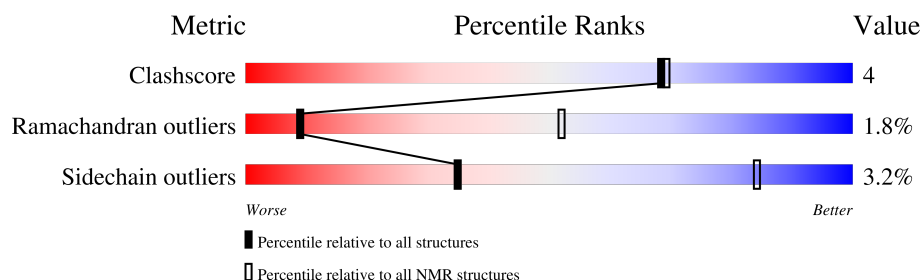
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	128	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:345-A:421 (77)	0.84	1

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 5 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2026 atoms, of which 1011 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	128	Total	C	H	N	O	S	0
			2026	637	1011	177	194	7	

There are 29 discrepancies between the modelled and reference sequences:

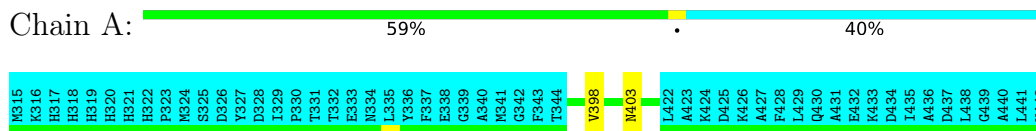
Chain	Residue	Modelled	Actual	Comment	Reference
A	315	MET	-	expression tag	UNP Q70M91
A	316	LYS	-	expression tag	UNP Q70M91
A	317	HIS	-	expression tag	UNP Q70M91
A	318	HIS	-	expression tag	UNP Q70M91
A	319	HIS	-	expression tag	UNP Q70M91
A	320	HIS	-	expression tag	UNP Q70M91
A	321	HIS	-	expression tag	UNP Q70M91
A	322	HIS	-	expression tag	UNP Q70M91
A	323	PRO	-	expression tag	UNP Q70M91
A	324	MET	-	expression tag	UNP Q70M91
A	325	SER	-	expression tag	UNP Q70M91
A	326	ASP	-	expression tag	UNP Q70M91
A	327	TYR	-	expression tag	UNP Q70M91
A	328	ASP	-	expression tag	UNP Q70M91
A	329	ILE	-	expression tag	UNP Q70M91
A	330	PRO	-	expression tag	UNP Q70M91
A	331	THR	-	expression tag	UNP Q70M91
A	332	THR	-	expression tag	UNP Q70M91
A	333	GLU	-	expression tag	UNP Q70M91
A	334	ASN	-	expression tag	UNP Q70M91
A	335	LEU	-	expression tag	UNP Q70M91
A	336	TYR	-	expression tag	UNP Q70M91
A	337	PHE	-	expression tag	UNP Q70M91
A	338	GLU	-	expression tag	UNP Q70M91
A	339	GLY	-	expression tag	UNP Q70M91
A	340	ALA	-	expression tag	UNP Q70M91
A	341	MET	-	expression tag	UNP Q70M91
A	342	GLY	-	expression tag	UNP Q70M91
A	428	PHE	LEU	variant	UNP Q70M91

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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.

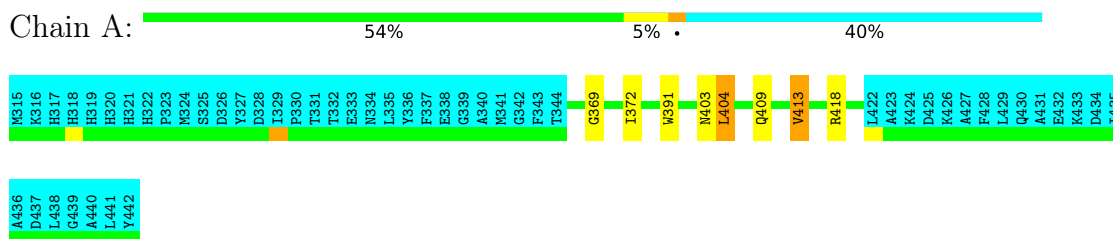
- Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ



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

The representative model is number 1. 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
CYANA	refinement	
TopSpin	structure solution	
CcpNmr Analysis	structure solution	ANALYSIS
CYANA	structure solution	
CNS	structure solution	
TALOS+	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1520
Number of shifts mapped to atoms	1520
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

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	1.14±0.05	1±1/607 (0.2± 0.2%)	0.97±0.04	0±0/819 (0.0± 0.0%)
All	All	1.14	21/12140 (0.2%)	0.97	0/16380 (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	0.2±0.4
All	All	0	4

5 of 11 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	389	VAL	N-CA	-7.62	1.39	1.46	18	2
1	A	388	ASP	C-N	-7.60	1.26	1.33	18	1
1	A	398	VAL	N-CA	-7.17	1.37	1.46	16	6
1	A	413	VAL	N-CA	-5.78	1.39	1.46	11	3
1	A	404	LEU	C-N	-5.75	1.26	1.33	16	3

There are no bond-angle outliers.

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	402	ARG	Sidechain	2
1	A	407	ARG	Sidechain	1
1	A	358	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	602	620	620	4±3
All	All	12040	12400	12400	90

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 4.

5 of 54 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:382:MET:SD	1:A:384:LEU:HG	0.65	2.31	17	2
1:A:395:LEU:HG	1:A:399:MET:SD	0.60	2.36	10	1
1:A:395:LEU:O	1:A:398:VAL:HG22	0.58	1.99	2	2
1:A:362:GLN:HE21	1:A:362:GLN:HA	0.57	1.60	8	1
1:A:375:SER:O	1:A:378:VAL:HG12	0.55	2.01	7	3

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	77/128 (60%)	71±1 (92±2%)	5±2 (6±2%)	1±0 (2±1%)	9	52
All	All	1540/2560 (60%)	1413 (92%)	100 (6%)	27 (2%)	9	52

5 of 8 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	403	ASN	19
1	A	368	SER	2
1	A	353	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	347	LYS	1
1	A	374	ALA	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	68/110 (62%)	66±1 (97±2%)	2±1 (3±2%)	35	84
All	All	1360/2200 (62%)	1317 (97%)	43 (3%)	35	84

5 of 22 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	364	LEU	6
1	A	409	GLN	5
1	A	384	LEU	5
1	A	404	LEU	3
1	A	387	LYS	3

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 oligosaccharides 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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping [i](#)

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	1520
Number of shifts mapped to atoms	1520
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	120	-0.16 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	113	0.23 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	106	0.27 ± 0.15	None needed (< 0.5 ppm)
^{15}N	116	-0.45 ± 0.24	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 93%, i.e. 1000 atoms were assigned a chemical shift out of a possible 1076. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	379/385 (98%)	156/156 (100%)	148/154 (96%)	75/75 (100%)
Sidechain	599/669 (90%)	408/434 (94%)	177/205 (86%)	14/30 (47%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	22/22 (100%)	11/11 (100%)	10/10 (100%)	1/1 (100%)
Overall	1000/1076 (93%)	575/601 (96%)	335/369 (91%)	90/106 (85%)

7.1.4 Statistically unusual chemical shifts [i](#)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	368	SER	HB3	2.15	2.49 – 5.20	-6.3
1	A	392	ASP	HB3	1.00	1.32 – 4.00	-6.2
1	A	368	SER	HB2	2.32	2.61 – 5.13	-6.2

7.1.5 Random Coil Index (RCI) plots [i](#)

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

