wwPDB NMR Structure Validation Summary Report

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Title	:	Structural insight into host recognition and biofilm formation by aggregative adherence fimbriae of enteroaggregative Escherichia coli
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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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
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:

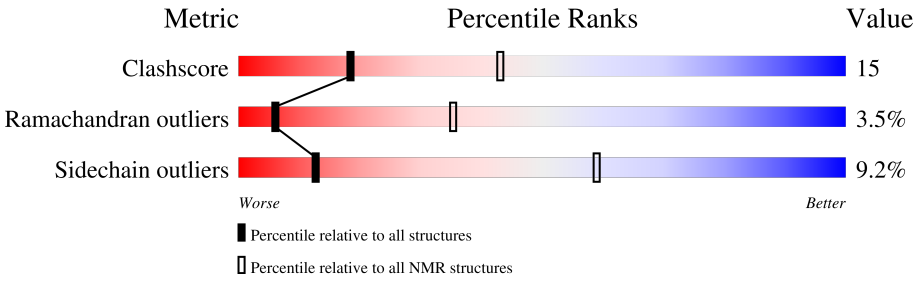
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	145	63% 33% .

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2187 atoms, of which 1095 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major fimbrial subunit of aggregative adherence fimbria II AafA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	145	2187	682	1095	196	209	5	0

There are 20 discrepancies between the modelled and reference sequences:

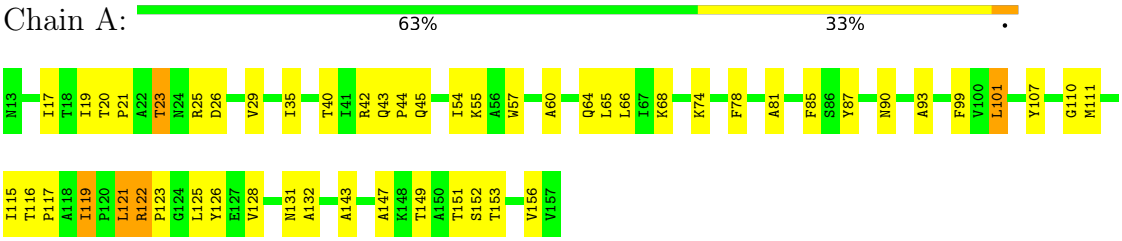
Chain	Residue	Modelled	Actual	Comment	Reference
A	138	ASP	-	expression tag	UNP O30595
A	139	ASN	-	expression tag	UNP O30595
A	140	LYS	-	expression tag	UNP O30595
A	141	GLN	-	expression tag	UNP O30595
A	142	ASN	-	expression tag	UNP O30595
A	143	ALA	-	expression tag	UNP O30595
A	144	THR	-	expression tag	UNP O30595
A	145	ALA	-	expression tag	UNP O30595
A	146	VAL	-	expression tag	UNP O30595
A	147	ALA	-	expression tag	UNP O30595
A	148	LYS	-	expression tag	UNP O30595
A	149	THR	-	expression tag	UNP O30595
A	150	ALA	-	expression tag	UNP O30595
A	151	THR	-	expression tag	UNP O30595
A	152	SER	-	expression tag	UNP O30595
A	153	THR	-	expression tag	UNP O30595
A	154	ILE	-	expression tag	UNP O30595
A	155	THR	-	expression tag	UNP O30595
A	156	VAL	-	expression tag	UNP O30595
A	157	VAL	-	expression tag	UNP O30595

4 Residue-property plots (i)

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: Major fimbrial subunit of aggregative adherence fimbria II AafA

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry, simulated annealing.*

Of the 20 calculated structures, 1 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
ARIA	structure solution	
ARIA	structure solution	
ARIA	refinement	

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	1652
Number of shifts mapped to atoms	1651
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	1092	1095	1094	32
All	All	1092	1095	1094	32

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 15.

5 of 32 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:126:TYR:CZ	1:A:156:VAL:HG11	0.65	2.25
1:A:19:ILE:HA	1:A:40:THR:O	0.62	1.94
1:A:23:THR:HB	1:A:152:SER:OG	0.61	1.94
1:A:122:ARG:N	1:A:123:PRO:HD2	0.59	2.12
1:A:45:GLN:HG2	1:A:107:TYR:CE2	0.56	2.35

6.3 Torsion angles

6.3.1 Protein backbone

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	143/145 (99%)	122 (85%)	16 (11%)	5 (3%)	6 35
All	All	143/145 (99%)	122 (85%)	16 (11%)	5 (3%)	6 35

All 5 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	26	ASP
1	A	65	LEU
1	A	81	ALA
1	A	90	ASN
1	A	122	ARG

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	119/119 (100%)	108 (91%)	11 (9%)	13 59
All	All	119/119 (100%)	108 (91%)	11 (9%)	13 59

5 of 11 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	23	THR
1	A	29	VAL
1	A	54	ILE
1	A	64	GLN
1	A	68	LYS

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 monosaccharides 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

The completeness of assignment taking into account all chemical shift lists is 86% 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_1*

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	1652
Number of shifts mapped to atoms	1651
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	13	ASN	H	8.524	.	.

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	144	0.06 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	133	-0.20 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	129	0.32 ± 0.10	None needed (< 0.5 ppm)
^{15}N	133	-0.34 ± 0.30	None needed (< 0.5 ppm)

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 86%, i.e. 1652 atoms were assigned a chemical shift out of a possible 1912. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	694/716 (97%)	288/291 (99%)	273/290 (94%)	133/135 (99%)
Sidechain	879/1099 (80%)	595/718 (83%)	284/333 (85%)	0/48 (0%)
Aromatic	79/97 (81%)	40/47 (85%)	38/47 (81%)	1/3 (33%)
Overall	1652/1912 (86%)	923/1056 (87%)	595/670 (89%)	134/186 (72%)

7.1.4 Statistically unusual chemical shifts

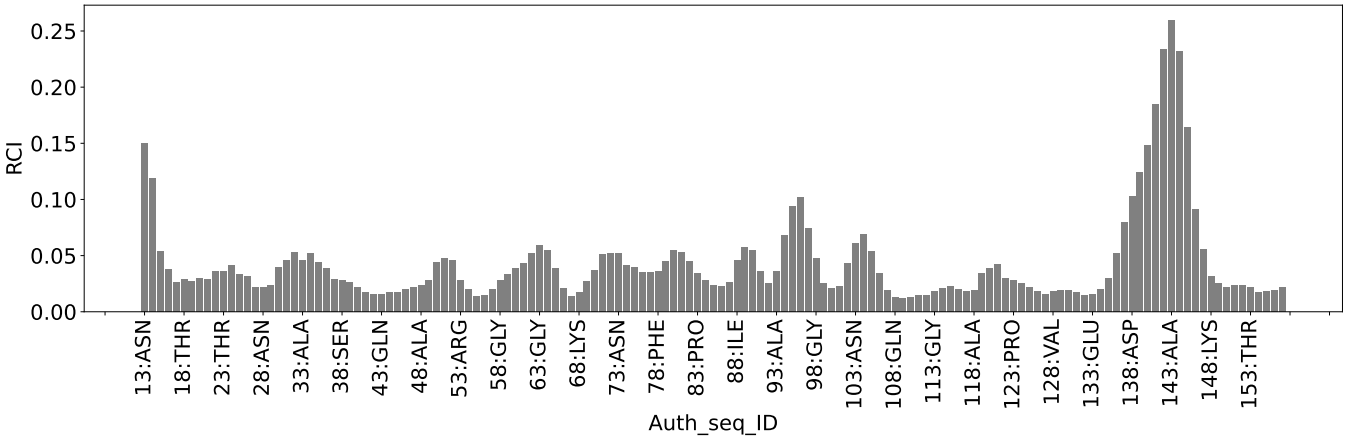
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	43	GLN	CG	51.08	28.36 – 39.21	15.9
1	A	43	GLN	HG3	4.44	0.91 – 3.68	7.7
1	A	131	ASN	HB2	0.48	1.27 – 4.34	-7.5
1	A	43	GLN	HG2	3.69	1.01 – 3.62	5.3
1	A	131	ASN	HB3	1.09	1.12 – 4.38	-5.1

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.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:


RCI
0.25
0.20
0.15
0.10
0.05
0.00
13:ASN
18:THR
23:THR
28:ASN
33:ALA
38:SER
43:GLN
48:ALA
53:ARG
58:GLY
63:GLY
68:LYS
73:ASN
78:PHE
83:PRO
88:ILE
93:ALA
98:GLY
103:ASN
108:GLN
113:GLY
118:ALA
123:PRO
128:VAL
133:GLU
138:ASP
143:ALA
148:LYS
153:THR
Auth_seq_ID