

Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	8H0U
BMRB ID	:	36513
Title	:	AQEE-30 in a DPC solution
Authors	:	Park, OS.; Jeon, Y.H.; Cheong, C.
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This is a Full wwPDB NMR Structure Validation 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:

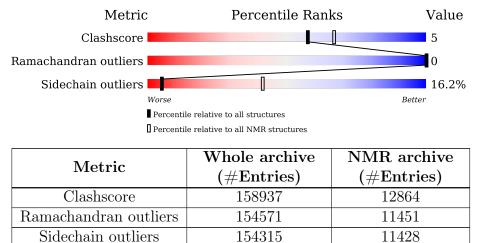
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.31.3
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 71%.

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.



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	31	68%	19%	13%						



2 Ensemble composition and analysis (i)

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:586-A:600 (15)	0.48	1						
2	A:601-A:612 (12)	0.10	17						

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 3 clusters and 2 single-model clusters were found.

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



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 515 atoms, of which 249 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called AQEE-30.

Mol	Chain	Residues		Trace				
1	А	31	Total	С	Η	Ν	0	0
1	11	01	515	160	249	49	57	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	585	SER	-	expression tag	UNP O15240



4 Residue-property plots (i)

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: AQEE-30

Chain A:	68%	19%	13%
S585 L603 E604 N605 Y606 1607 L611 L612 L613 R613 R613 R613 P615 P615			

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)



4.2.2 Score per residue for model 2

• Molecule 1: AQEE-30

• Molecule 1: AQEE-30





4.2.3 Score per residue for model 3

• Molecule 1: AQEE-30



4.2.4 Score per residue for model 4

• Molecule 1: AQEE-30

Chain A:	58%	29%	13%
SS85 L557 L557 C558 C558 C558 C558 C558 C558 C558 C			

4.2.5 Score per residue for model 5

 \bullet Molecule 1: AQEE-30

Chain A:	68%	 19%	13%
S585 R595 R595 L603 F604 N605 Y605 N605 N605 N605 R613 R613 P615			

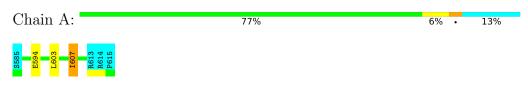
4.2.6 Score per residue for model 6

• Molecule 1: AQEE-30

Chain A: 65% 16% 6% 13%

4.2.7 Score per residue for model 7

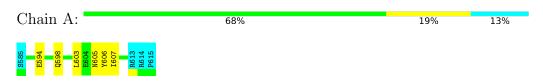
 \bullet Molecule 1: AQEE-30





4.2.8 Score per residue for model 8

• Molecule 1: AQEE-30



4.2.9 Score per residue for model 9

• Molecule 1: AQEE-30

Cl	nai	in	A	.:					68%	16%	·	13%
S585	<mark>0600</mark>	NGO5	Y606	1607	 V610	LO12 B613	DE 1A	TO 14 D6 15				

4.2.10 Score per residue for model 10

 \bullet Molecule 1: AQEE-30

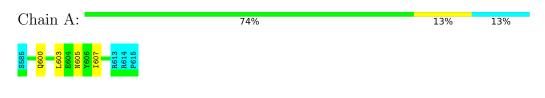
Chain A:	68%	16%	•	13%
S585 L603 E604 N605 N605 H609 H609 H609 R613 R613 R613 P615				

- 4.2.11 Score per residue for model 11
- Molecule 1: AQEE-30



4.2.12 Score per residue for model 12

 \bullet Molecule 1: AQEE-30





4.2.13 Score per residue for model 13

• Molecule 1: AQEE-30



4.2.14 Score per residue for model 14

• Molecule 1: AQEE-30

C	bε	aiı	n	A	:	-						68%	19	9%	13%
S585	D600		L603	E604	N605	Y606	1607	VR 10	R613	R614	P615				

4.2.15 Score per residue for model 15

 \bullet Molecule 1: AQEE-30

Chain A:	65%	19% •	13%
S585 E593 E593 E593 P600 F600 F600 F600 F600 F600 F613 F613 F613 F614 F615			

4.2.16 Score per residue for model 16

• Molecule 1: AQEE-30

Chain A: 58% 26% 13%

4.2.17 Score per residue for model 17

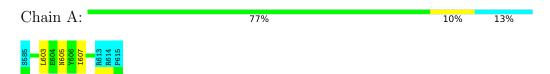
• Molecule 1: AQEE-30





4.2.18 Score per residue for model 18

• Molecule 1: AQEE-30



4.2.19 Score per residue for model 19

 \bullet Molecule 1: AQEE-30

Chain A:	65%	19% •	13%
Image: Second state Second			

4.2.20 Score per residue for model 20

 \bullet Molecule 1: AQEE-30

Chain A:	68%	19%	13%
8585 8585 1603 1604 1605 1605 1607 1611 1611 1611 1611 1611 1611 1611			



5 Refinement protocol and experimental data overview (i)

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CYANA	structure calculation	

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	319
Number of shifts mapped to atoms	319
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%



6 Model quality (i)

6.1 Standard geometry (i)

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 (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	А	231	211	211	2 ± 1
All	All	4620	4220	4220	44

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 5.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:606:TYR:O	1:A:610:VAL:HG23	0.55	2.02	14	13
1:A:611:LEU:HD23	1:A:611:LEU:O	0.53	2.03	20	1
1:A:608:GLU:O	1:A:612:LEU:HD12	0.53	2.04	13	4
1:A:600:GLN:OE1	1:A:603:LEU:HD23	0.50	2.06	14	5
1:A:600:GLN:NE2	1:A:603:LEU:HD23	0.47	2.25	1	1
1:A:603:LEU:HD12	1:A:603:LEU:O	0.46	2.10	5	11
1:A:611:LEU:O	1:A:611:LEU:HD13	0.46	2.11	1	3
1:A:597:LEU:HD13	1:A:597:LEU:O	0.42	2.14	2	1
1:A:607:ILE:N	1:A:607:ILE:HD13	0.42	2.30	7	3
1:A:603:LEU:O	1:A:603:LEU:HD12	0.40	2.17	16	2

All unique clashes are listed below, sorted by their clash magnitude.



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	Perce	ntiles
1	А	27/31~(87%)	$25 \pm 1 (92 \pm 4\%)$	2 ± 1 (8 $\pm4\%$)	0±0 (0±0%)	100	100
All	All	540/620~(87%)	499 (92%)	41 (8%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Per	$\operatorname{centiles}$
1	А	24/28~(86%)	20 ± 1 (84 $\pm5\%$)	$4\pm1~(16\pm5\%)$	5	41
All	All	480/560~(86%)	402 (84%)	78 (16%)	5	41

All 16 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	А	607	ILE	20
1	А	605	ASN	18
1	А	606	TYR	8
1	А	611	LEU	7
1	А	595	ARG	4
1	А	600	GLN	4
1	А	597	LEU	3
1	А	608	GLU	3
1	А	604	GLU	2
1	А	598	GLN	2
1	А	594	GLU	2
1	А	603	LEU	1
1	А	609	HIS	1

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Mol	Chain	Res	Type	Models (Total)
1	А	593	GLU	1
1	А	587	GLN	1
1	А	596	ARG	1

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 (i)

The completeness of assignment taking into account all chemical shift lists is 71% for the well-defined parts and 69% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: AQEE-30_DPC_CS_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	319
Number of shifts mapped to atoms	319
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	${\rm Correction}\pm{\rm precision},ppm$	Suggested action
$^{13}C_{\alpha}$	30	0.51 ± 0.16	Should be applied
$^{13}C_{\beta}$	30	0.94 ± 0.08	Should be applied
$^{13}C'$	0		None (insufficient data)
¹⁵ N	28	-0.02 ± 0.68	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 71%, i.e. 254 atoms were assigned a chemical shift out of a possible 356. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	106/135~(79%)	53/54~(98%)	27/54~(50%)	26/27~(96%)
Sidechain	148/206~(72%)	82/119~(69%)	60/77~(78%)	6/10~(60%)

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	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Aromatic	0/15~(0%)	0/8~(0%)	0/6~(0%)	0/1~(0%)
Overall	254/356 (71%)	135/181~(75%)	87/137 (64%)	32/38~(84%)

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The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 290 atoms were assigned a chemical shift out of a possible 422. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	15 N
Backbone	116/153~(76%)	58/61~(95%)	30/62~(48%)	28/30~(93%)
Sidechain	174/254~(69%)	97/149~(65%)	69/89~(78%)	8/16~(50%)
Aromatic	0/15~(0%)	0/8~(0%)	0/6~(0%)	0/1~(0%)
Overall	290/422~(69%)	155/218~(71%)	99/157~(63%)	36/47~(77%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (1)

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:



