wwPDB NMR Structure Validation Summary Report (i)

Mar 7, 2022 – 06:17 AM EST

PDB ID	:	2YT1
Title	:	Solution structure of the chimera of the C-terminal tail peptide of APP and the C-terminal PID domain of Fe65L
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Deposited on	:	2007-04-05

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 following versions of software and data (see references (i)) were used in the production of this report:

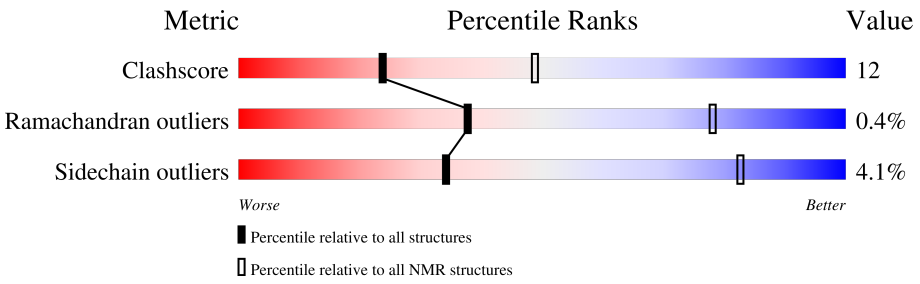
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 was not calculated.

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	185	55% 12% • 32%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:17-A:28, A:70-A:158, A:162-A:185 (125)	0.23	5

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 2 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2718 atoms, of which 1322 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Amyloid beta A4 protein and Amyloid beta A4 precursor protein-binding family B member 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	185	2718	857	1322	240	287	12	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P12023
A	2	SER	-	expression tag	UNP P12023
A	3	SER	-	expression tag	UNP P12023
A	4	GLY	-	expression tag	UNP P12023
A	5	SER	-	expression tag	UNP P12023
A	6	SER	-	expression tag	UNP P12023
A	7	GLY	-	expression tag	UNP P12023
A	40	SER	-	linker	UNP P12023
A	41	GLY	-	linker	UNP P12023
A	42	PRO	-	linker	UNP P12023
A	43	SER	-	linker	UNP P12023
A	44	SER	-	linker	UNP P12023
A	45	GLY	-	linker	UNP P12023
A	46	ILE	-	linker	UNP P12023
A	47	GLU	-	linker	UNP P12023
A	48	GLY	-	linker	UNP P12023
A	49	ARG	-	linker	UNP P12023
A	50	GLY	-	linker	UNP P12023
A	51	SER	-	linker	UNP P12023
A	52	SER	-	linker	UNP P12023
A	53	GLY	-	linker	UNP P12023
A	54	SER	-	linker	UNP P12023
A	55	SER	-	linker	UNP P12023
A	56	GLY	-	linker	UNP P12023
A	57	SER	-	linker	UNP P12023
A	58	SER	-	linker	UNP P12023
A	59	GLY	-	linker	UNP P12023
A	60	SER	-	linker	UNP P12023
A	61	SER	-	linker	UNP P12023
A	62	GLY	-	linker	UNP P12023

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: Amyloid beta A4 protein and Amyloid beta A4 precursor protein-binding family B member 2

Chain A: 55% 12% • 32%

G1 S2 S3 G4 S5 S6 G7 D8 A9 A10 V11 T12 P13 E14 E15 R16 H17 L18 P29 T30 Y31 K32 F33 F34 E35 Q36 M37 Q38 N39 S40 G41 P42 S43 S44 G45 I46 E47 G48 R49 G50 S51 S52 G53 S54 S55 G56 S57 S58 G59 S60 S61 G62 P63 T64 P65 K66 T67 E68 L69

V70 R74 M80 L81 V87 S104 W108 A116 E130 V131 L132 F142 M143 G146 K147 H150 F154 G159 N160 Q161 H166 V167 F168 E171 P172 Q182 C185

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

The representative model is number 5. Colouring as in section 4.1 above.

• Molecule 1: Amyloid beta A4 protein and Amyloid beta A4 precursor protein-binding family B member 2

Chain A: 48% 18% • 32%

G1 S2 S3 G4 S5 S6 G7 D8 A9 A10 V11 T12 P13 E14 E15 R16 H17 L18 P29 T30 Y31 K32 F33 F34 E35 Q36 M37 Q38 N39 S40 G41 P42 S43 S44 G45 I46 E47 G48 R49 G50 S51 S52 G53 S54 S55 G56 S57 S58 G59 S60 S61 G62 P63 T64 P65 K66 T67 E68 L69

V75 M80 L81 P82 V87 N93 S94 A95 T96 E97 N98 T101 S102 S103 V111 E130 V131 L132 R136 V137 R138 F142 G146 K147 D148 V149 H150 A153 G159 N160 Q161 E164 C165 H166 V167 F168 E171 P172 A175 V181 Q182 C185

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

No chemical shift data was provided.

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	A	984	949	948	23±4
All	All	19680	18980	18960	467

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 12.

5 of 178 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:VAL:HG23	1:A:116:ALA:HB2	0.78	1.55	20	10
1:A:87:VAL:HG12	1:A:142:PHE:HB2	0.74	1.57	5	11
1:A:142:PHE:CD1	1:A:143:MET:N	0.68	2.61	13	3
1:A:70:VAL:CG2	1:A:116:ALA:HB2	0.68	2.19	20	4
1:A:87:VAL:HG12	1:A:142:PHE:HB3	0.68	1.66	14	4

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	124/185 (67%)	109±2 (88±2%)	15±3 (12±2%)	0±1 (0±0%)	38 78
All	All	2480/3700 (67%)	2173 (88%)	298 (12%)	9 (0%)	38 78

All 5 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	172	PRO	3
1	A	23	GLN	2
1	A	96	ILE	2
1	A	140	LEU	1
1	A	75	VAL	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	111/157 (71%)	106±2 (96±1%)	5±2 (4±1%)	34 82
All	All	2220/3140 (71%)	2128 (96%)	92 (4%)	34 82

5 of 34 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	81	LEU	19
1	A	74	ARG	8
1	A	147	LYS	6
1	A	157	ASP	5
1	A	24	ASN	4

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)

No chemical shift data were provided