



Full wwPDB NMR Structure Validation Report ⓘ

Nov 20, 2022 – 05:27 pm GMT

PDB ID : 3ZPK
EMDB ID : EMD-2324
BMRB ID : 19157
Title : Atomic-resolution structure of a quadruplet cross-beta amyloid fibril.
Authors : Fitzpatrick, A.W.P.; Debelouchina, G.T.; Bayro, M.J.; Clare, D.K.; Caporini, M.A.; Bajaj, V.S.; Jaroniec, C.P.; Wang, L.; Ladizhansky, V.; Muller, S.A.; MacPhee, C.E.; Waudby, C.A.; Mott, H.R.; de Simone, A.; Knowles, T.P.J.; Saibil, H.R.; Vendruscolo, M.; Orlova, E.V.; Griffin, R.G.; Dobson, C.M.
Deposited on : 2013-02-28

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 ⓘ 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:

EMDB validation analysis : **NOT EXECUTED**
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR, ELECTRON MICROSCOPY

The overall completeness of chemical shifts assignment was not calculated.

There are no overall percentile quality scores available for this entry.

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	11	 100%
1	B	11	 100%
1	C	11	 100%
1	D	11	 100%
1	E	11	 100%
1	F	11	 100%
1	G	11	 100%
1	H	11	 100%
1	I	11	 100%
1	J	11	 100%
1	K	11	 100%
1	L	11	 100%
1	M	11	 100%
1	N	11	 100%
1	O	11	 100%
1	P	11	 100%

2 Ensemble composition and analysis ⓘ

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2752 atoms, of which 1392 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TRANSTHYRETIN.

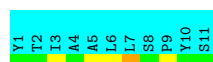
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	11	Total	C	H	N	O	0	
			172	57	87	11	17		
1	B	11	Total	C	H	N	O	0	
			172	57	87	11	17		
1	C	11	Total	C	H	N	O	0	
			172	57	87	11	17		
1	D	11	Total	C	H	N	O	0	
			172	57	87	11	17		
1	E	11	Total	C	H	N	O	0	
			172	57	87	11	17		
1	F	11	Total	C	H	N	O	0	
			172	57	87	11	17		
1	G	11	Total	C	H	N	O	0	
			172	57	87	11	17		
1	H	11	Total	C	H	N	O	0	
			172	57	87	11	17		
1	I	11	Total	C	H	N	O	0	
			172	57	87	11	17		
1	J	11	Total	C	H	N	O	0	
			172	57	87	11	17		
1	K	11	Total	C	H	N	O	0	
			172	57	87	11	17		
1	L	11	Total	C	H	N	O	0	
			172	57	87	11	17		
1	M	11	Total	C	H	N	O	0	
			172	57	87	11	17		
1	N	11	Total	C	H	N	O	0	
			172	57	87	11	17		
1	O	11	Total	C	H	N	O	0	
			172	57	87	11	17		
1	P	11	Total	C	H	N	O	0	
			172	57	87	11	17		

4 Residue-property plots

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: TRANSTHYRETIN

Chain A:  100%



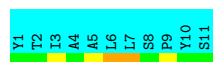
• Molecule 1: TRANSTHYRETIN

Chain B:  100%



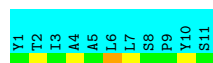
• Molecule 1: TRANSTHYRETIN

Chain C:  100%



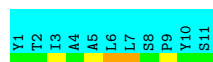
• Molecule 1: TRANSTHYRETIN

Chain D:  100%



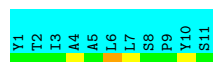
• Molecule 1: TRANSTHYRETIN

Chain E:  100%



• Molecule 1: TRANSTHYRETIN

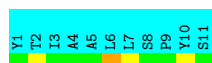
Chain F:  100%



● Molecule 1: TRANSTHYRETIN

Chain G:  100%

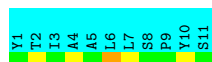
● Molecule 1: TRANSTHYRETIN

Chain H:  100%

● Molecule 1: TRANSTHYRETIN

Chain I:  100%

● Molecule 1: TRANSTHYRETIN

Chain J:  100%

● Molecule 1: TRANSTHYRETIN

Chain K:  100%

● Molecule 1: TRANSTHYRETIN

Chain L:  100%

● Molecule 1: TRANSTHYRETIN

Chain M:  100%

● Molecule 1: TRANSTHYRETIN

Chain N:  100%



● Molecule 1: TRANSTHYRETIN



● Molecule 1: TRANSTHYRETIN



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or 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	66
Number of shifts mapped to atoms	0
Number of unparsed shifts	66
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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	0	0	0	0
1	B	0	0	0	0
1	C	0	0	0	0
1	D	0	0	0	0
1	E	0	0	0	0
1	F	0	0	0	0
1	G	0	0	0	0
1	H	0	0	0	0
1	I	0	0	0	0
1	J	0	0	0	0
1	K	0	0	0	0
1	L	0	0	0	0
1	M	0	0	0	0
1	N	0	0	0	0
1	O	0	0	0	0
1	P	0	0	0	0
All	All	0	0	0	-

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 -.

There are no clashes.

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	0	-	-	-	-
1	B	0	-	-	-	-
1	C	0	-	-	-	-
1	D	0	-	-	-	-
1	E	0	-	-	-	-
1	F	0	-	-	-	-
1	G	0	-	-	-	-
1	H	0	-	-	-	-
1	I	0	-	-	-	-
1	J	0	-	-	-	-
1	K	0	-	-	-	-
1	L	0	-	-	-	-
1	M	0	-	-	-	-
1	N	0	-	-	-	-
1	O	0	-	-	-	-
1	P	0	-	-	-	-
All	All	0	-	-	-	-

There are no Ramachandran outliers.

6.3.2 Protein sidechains

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	0	-	-	-
1	B	0	-	-	-
1	C	0	-	-	-
1	D	0	-	-	-
1	E	0	-	-	-
1	F	0	-	-	-

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	0	-	-	-
1	H	0	-	-	-
1	I	0	-	-	-
1	J	0	-	-	-
1	K	0	-	-	-
1	L	0	-	-	-
1	M	0	-	-	-
1	N	0	-	-	-
1	O	0	-	-	-
1	P	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

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 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *D_1290056000_cs_P1.cif.V1*

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	66
Number of shifts mapped to atoms	0
Number of unparsed shifts	66
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Entity instance (chain) must be specified. All 66 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	1	TYR	C	172.000	0.02	1
2	?	1	TYR	CA	56.300	0.02	1
3	?	1	TYR	CB	36.500	0.02	1
4	?	1	TYR	CG	124.500	0.02	1
5	?	1	TYR	CD1	133.400	0.02	3
6	?	1	TYR	CD2	134.500	0.02	3
7	?	1	TYR	CE1	117.800	0.02	3
8	?	1	TYR	CE2	118.700	0.02	3
9	?	1	TYR	CZ	160.000	0.02	1
10	?	1	TYR	N	39.200	0.02	1
11	?	2	THR	C	173.500	0.02	1
12	?	2	THR	CA	62.600	0.02	1
13	?	2	THR	CB	72.500	0.02	1
14	?	2	THR	CG2	20.000	0.02	1
15	?	2	THR	N	117.000	0.02	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	?	3	ILE	C	174.100	0.02	1
17	?	3	ILE	CA	60.200	0.02	1
18	?	3	ILE	CB	41.800	0.02	1
19	?	3	ILE	CG1	28.200	0.02	1
20	?	3	ILE	CG2	17.000	0.02	1
21	?	3	ILE	CD1	14.600	0.02	1
22	?	3	ILE	N	127.000	0.02	1
23	?	4	ALA	C	174.500	0.02	1
24	?	4	ALA	CA	49.900	0.02	1
25	?	4	ALA	CB	22.100	0.02	1
26	?	4	ALA	N	128.000	0.02	1
27	?	5	ALA	C	173.300	0.02	1
28	?	5	ALA	CA	50.300	0.02	1
29	?	5	ALA	CB	22.900	0.02	1
30	?	5	ALA	N	125.100	0.02	1
31	?	6	LEU	C	174.200	0.02	1
32	?	6	LEU	CA	54.400	0.02	1
33	?	6	LEU	CB	45.500	0.02	1
34	?	6	LEU	CG	29.400	0.02	1
35	?	6	LEU	CD1	23.900	0.02	1
36	?	6	LEU	CD2	28.200	0.02	1
37	?	6	LEU	N	127.000	0.02	1
38	?	7	LEU	C	173.900	0.02	1
39	?	7	LEU	CA	54.100	0.02	1
40	?	7	LEU	CB	44.300	0.02	1
41	?	7	LEU	CG	29.900	0.02	1
42	?	7	LEU	CD1	27.700	0.02	1
43	?	7	LEU	CD2	25.300	0.02	1
44	?	7	LEU	N	127.500	0.02	1
45	?	8	SER	C	173.600	0.02	1
46	?	8	SER	CA	55.400	0.02	1
47	?	8	SER	CB	63.200	0.02	1
48	?	8	SER	N	117.200	0.02	1
49	?	9	PRO	C	174.800	0.02	1
50	?	9	PRO	CA	62.600	0.02	1
51	?	9	PRO	CB	32.600	0.02	1
52	?	9	PRO	CG	28.000	0.02	1
53	?	9	PRO	CD	49.600	0.02	1
54	?	9	PRO	N	135.800	0.02	1
55	?	10	TYR	C	173.600	0.02	1
56	?	10	TYR	CA	57.700	0.02	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
57	?	10	TYR	CB	43.800	0.02	1
58	?	10	TYR	CG	128.700	0.02	1
59	?	10	TYR	CD1	133.600	0.02	1
60	?	10	TYR	CD2	133.600	0.02	1
61	?	10	TYR	CE1	118.300	0.02	1
62	?	10	TYR	CE2	118.300	0.02	1
63	?	10	TYR	CZ	157.400	0.02	1
64	?	10	TYR	N	127.300	0.02	1
65	?	11	SER	C	181.900	0.02	1
66	?	11	SER	CA	57.800	0.02	1

7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 2000. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/848 (0%)	0/336 (0%)	0/352 (0%)	0/160 (0%)
Sidechain	0/896 (0%)	0/528 (0%)	0/368 (0%)	0/0 (—%)
Aromatic	0/256 (0%)	0/128 (0%)	0/128 (0%)	0/0 (—%)
Overall	0/2000 (0%)	0/992 (0%)	0/848 (0%)	0/160 (0%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 2000. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/848 (0%)	0/336 (0%)	0/352 (0%)	0/160 (0%)
Sidechain	0/896 (0%)	0/528 (0%)	0/368 (0%)	0/0 (—%)
Aromatic	0/256 (0%)	0/128 (0%)	0/128 (0%)	0/0 (—%)
Overall	0/2000 (0%)	0/992 (0%)	0/848 (0%)	0/160 (0%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

No *random coil index* (RCI) plot could be generated from the current chemical shift list (D_1290056000_cs_P). RCI is only applicable to proteins.