



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1HY8
Title : SOLUTION STRUCTURE OF B. SUBTILIS ACYL CARRIER PROTEIN
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Deposited on : 2001-01-18

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

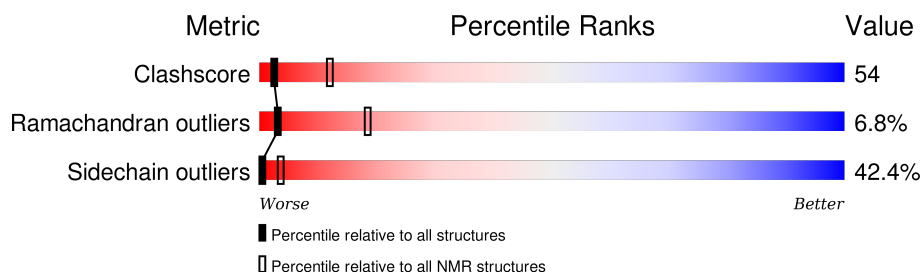
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	76	

2 Ensemble composition and analysis ⓘ

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 1158 atoms, of which 566 are hydrogens and 0 are deuteriums.

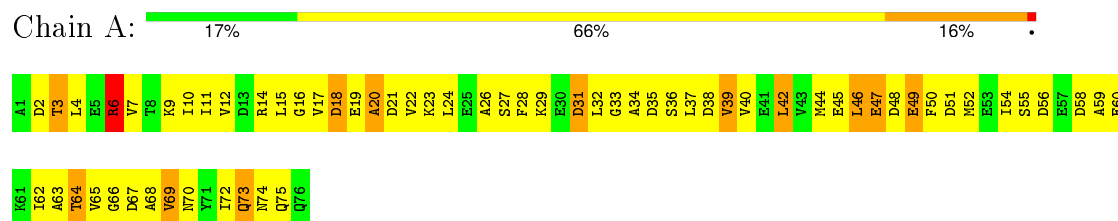
- Molecule 1 is a protein called ACYL CARRIER PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1158	364	566	91	135	2	

4 Residue-property plots

These plots are provided for all protein, RNA and DNA 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: ACYL CARRIER PROTEIN



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Distance geometry, Simulated annealing, molecular dynamics*.

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

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

Software name	Classification	Version
X-PLOR	structure solution	98.0
X-PLOR	refinement	98.0

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)	BMRB entry 4989
Number of chemical shift lists	1
Total number of shifts	904
Number of shifts mapped to atoms	861
Number of unparsed shifts	0
Number of shifts with mapping errors	43
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

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	2
All	All	0	2

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	14	ARG	Sidechain
1	A	6	ARG	Sidechain

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	592	566	568	63
All	All	592	566	568	63

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 54.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:40:VAL:HG13	1:A:59:ALA:HB3	1.03	1.08
1:A:40:VAL:HG13	1:A:59:ALA:CB	0.87	1.99

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:40:VAL:CG1	1:A:59:ALA:HB3	0.81	2.01
1:A:11:ILE:HG21	1:A:22:VAL:HG23	0.76	1.57
1:A:24:LEU:HD23	1:A:66:GLY:CA	0.75	2.11
1:A:15:LEU:HD12	1:A:34:ALA:HB1	0.73	1.58
1:A:63:ALA:O	1:A:64:THR:HG23	0.73	1.84
1:A:21:ASP:O	1:A:32:LEU:HD22	0.73	1.83
1:A:46:LEU:HD11	1:A:72:ILE:HD11	0.71	1.63
1:A:24:LEU:HD23	1:A:66:GLY:HA3	0.69	1.64
1:A:28:PHE:CZ	1:A:65:VAL:HG11	0.66	2.26
1:A:11:ILE:CG2	1:A:22:VAL:HG23	0.65	2.21
1:A:28:PHE:CD2	1:A:65:VAL:HG21	0.65	2.26
1:A:7:VAL:HG13	1:A:46:LEU:CD1	0.64	2.23
1:A:28:PHE:CG	1:A:65:VAL:HG21	0.63	2.28
1:A:7:VAL:HG22	1:A:46:LEU:HD12	0.62	1.72
1:A:15:LEU:HD12	1:A:34:ALA:CB	0.59	2.27
1:A:35:ASP:O	1:A:39:VAL:HG23	0.57	1.99
1:A:69:VAL:HA	1:A:72:ILE:HD12	0.57	1.77
1:A:54:ILE:HG23	1:A:58:ASP:CB	0.57	2.30
1:A:65:VAL:O	1:A:68:ALA:HB3	0.57	2.00
1:A:46:LEU:HD23	1:A:54:ILE:HD12	0.55	1.78
1:A:7:VAL:HG22	1:A:46:LEU:CD1	0.54	2.32
1:A:12:VAL:HG13	1:A:19:GLU:HA	0.54	1.79
1:A:15:LEU:CD1	1:A:34:ALA:HB1	0.54	2.31
1:A:21:ASP:HB3	1:A:32:LEU:HD13	0.54	1.78
1:A:28:PHE:O	1:A:39:VAL:HG21	0.53	2.03
1:A:54:ILE:HG23	1:A:58:ASP:HB3	0.52	1.80
1:A:24:LEU:HD23	1:A:66:GLY:HA2	0.52	1.80
1:A:19:GLU:O	1:A:20:ALA:HB2	0.52	2.05
1:A:15:LEU:N	1:A:15:LEU:CD2	0.51	2.73
1:A:15:LEU:HD22	1:A:15:LEU:N	0.51	2.21
1:A:26:ALA:HB1	1:A:31:ASP:CB	0.50	2.36
1:A:6:ARG:CG	1:A:50:PHE:CZ	0.49	2.95
1:A:62:ILE:CD1	1:A:68:ALA:N	0.49	2.76
1:A:28:PHE:CE1	1:A:65:VAL:HB	0.48	2.43
1:A:7:VAL:HG13	1:A:46:LEU:HD12	0.48	1.84
1:A:15:LEU:HD23	1:A:42:LEU:HD22	0.48	1.86
1:A:15:LEU:HD23	1:A:42:LEU:CD2	0.47	2.39
1:A:46:LEU:CD2	1:A:54:ILE:CD1	0.47	2.93
1:A:7:VAL:CG1	1:A:46:LEU:CD1	0.46	2.93
1:A:62:ILE:CD1	1:A:68:ALA:CA	0.46	2.93
1:A:62:ILE:HD11	1:A:68:ALA:N	0.46	2.26
1:A:28:PHE:CD2	1:A:39:VAL:HG13	0.45	2.46

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:28:PHE:CE2	1:A:65:VAL:HG21	0.45	2.46
1:A:44:MET:O	1:A:47:GLU:CG	0.44	2.65
1:A:6:ARG:HG2	1:A:50:PHE:CE1	0.43	2.48
1:A:10:ILE:HD11	1:A:49:GLU:HG2	0.43	1.89
1:A:16:GLY:O	1:A:18:ASP:N	0.43	2.51
1:A:3:THR:HG23	1:A:72:ILE:HG21	0.43	1.91
1:A:3:THR:CG2	1:A:72:ILE:HG21	0.43	2.44
1:A:3:THR:CG2	1:A:72:ILE:CG2	0.42	2.98
1:A:28:PHE:CD1	1:A:65:VAL:HG21	0.42	2.49
1:A:22:VAL:O	1:A:23:LYS:CG	0.42	2.68
1:A:22:VAL:HG13	1:A:22:VAL:O	0.42	2.13
1:A:3:THR:HG21	1:A:72:ILE:HB	0.41	1.91
1:A:28:PHE:CD1	1:A:65:VAL:CG2	0.41	3.03
1:A:28:PHE:CG	1:A:65:VAL:CG2	0.41	3.02
1:A:12:VAL:HG22	1:A:22:VAL:HG11	0.41	1.93
1:A:69:VAL:O	1:A:73:GLN:NE2	0.40	2.55
1:A:11:ILE:HG12	1:A:42:LEU:HD11	0.40	1.93
1:A:28:PHE:CE1	1:A:65:VAL:CB	0.40	3.05
1:A:4:LEU:HD12	1:A:69:VAL:HG21	0.40	1.91

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	74/76 (97%)	59 (80%)	10 (14%)	5 (7%)	3	18
All	All	74/76 (97%)	59 (80%)	10 (14%)	5 (7%)	3	18

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

Mol	Chain	Res	Type
1	A	29	LYS
1	A	33	GLY
1	A	17	VAL
1	A	39	VAL

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Mol	Chain	Res	Type
1	A	20	ALA

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	66/66 (100%)	38 (58%)	28 (42%)	0	3
All	All	66/66 (100%)	38 (58%)	28 (42%)	0	3

All 28 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	70	ASN
1	A	38	ASP
1	A	3	THR
1	A	46	LEU
1	A	27	SER
1	A	9	LYS
1	A	55	SER
1	A	69	VAL
1	A	18	ASP
1	A	6	ARG
1	A	51	ASP
1	A	52	MET
1	A	36	SER
1	A	49	GLU
1	A	42	LEU
1	A	2	ASP
1	A	75	GLN
1	A	48	ASP
1	A	64	THR
1	A	45	GLU
1	A	31	ASP
1	A	60	GLU
1	A	56	ASP
1	A	47	GLU

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Mol	Chain	Res	Type
1	A	74	ASN
1	A	67	ASP
1	A	37	LEU
1	A	73	GLN

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 carbohydrates 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 84% for the well-defined parts and 84% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4989

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	904
Number of shifts mapped to atoms	861
Number of unparsed shifts	0
Number of shifts with mapping errors	43
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- Residue not found in structure. All 43 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	3	LEU	CD1	25.05	-1.0	1
A	2	PRO	HA	4.53	-1.0	1
A	2	PRO	HB3	2.3178	-1.0	1
A	1	GLY	HA2	4.04	-1.0	1
A	3	LEU	HD21	0.9565	-1.0	1
A	1	GLY	CA	43.53	-1.0	1
A	5	SER	HA	4.3522	-1.0	1
A	2	PRO	HD2	3.62	-1.0	1
A	5	SER	CA	59.4	-1.0	1
A	2	PRO	CB	32.37	-1.0	1
A	2	PRO	HG3	2.04	-1.0	1
A	2	PRO	HD3	3.62	-1.0	1
A	4	GLY	HA2	4.077	-1.0	1
A	5	SER	N	116.84	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	3	LEU	CA	55.25	-1.0	1
A	4	GLY	N	110.2	-1.0	1
A	3	LEU	CG	27.07	-1.0	1
A	2	PRO	HG2	2.04	-1.0	1
A	3	LEU	HD23	0.9565	-1.0	1
A	3	LEU	HD11	0.9565	-1.0	1
A	4	GLY	H	8.52	-1.0	1
A	4	GLY	HA3	4.077	-1.0	1
A	3	LEU	CB	42.34	-1.0	1
A	5	SER	H	8.4	-1.0	1
A	3	LEU	HD12	0.9565	-1.0	1
A	5	SER	HB3	3.9247	-1.0	1
A	3	LEU	HD22	0.9565	-1.0	1
A	3	LEU	H	8.62	-1.0	1
A	5	SER	HB2	3.9247	-1.0	1
A	3	LEU	HA	4.4363	-1.0	1
A	3	LEU	HG	1.6317	-1.0	1
A	5	SER	CB	63.346	-1.0	1
A	3	LEU	HB2	1.7309	-1.0	1
A	2	PRO	CG	27.05	-1.0	1
A	2	PRO	CA	63.2	-1.0	1
A	3	LEU	CD2	23.5	-1.0	1
A	2	PRO	HB2	2.3178	-1.0	1
A	4	GLY	CA	45.25	-1.0	1
A	3	LEU	HD13	0.9565	-1.0	1
A	3	LEU	N	122.61	-1.0	1
A	3	LEU	HB3	1.7309	-1.0	1
A	2	PRO	CD	49.63	-1.0	1
A	1	GLY	HA3	4.04	-1.0	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	81	-0.64 ± 0.19	Should be applied
$^{13}\text{C}_\beta$	76	0.27 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	79	0.47 ± 0.33	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 84%, i.e. 744 atoms were assigned a chemical shift out of a possible 885. 16 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	304/380 (80%)	152/152 (100%)	76/152 (50%)	76/76 (100%)
Sidechain	422/479 (88%)	256/270 (95%)	161/194 (83%)	5/15 (33%)
Aromatic	18/26 (69%)	12/14 (86%)	6/12 (50%)	0/0 (—%)
Overall	744/885 (84%)	420/436 (96%)	243/358 (68%)	81/91 (89%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 744 atoms were assigned a chemical shift out of a possible 885. 16 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	304/380 (80%)	152/152 (100%)	76/152 (50%)	76/76 (100%)
Sidechain	422/479 (88%)	256/270 (95%)	161/194 (83%)	5/15 (33%)
Aromatic	18/26 (69%)	12/14 (86%)	6/12 (50%)	0/0 (—%)
Overall	744/885 (84%)	420/436 (96%)	243/358 (68%)	81/91 (89%)

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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	49	GLU	HG3	0.99	3.31 – 1.21	-6.0

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.

Random coil index (RCI) for chain A:

