wwPDB NMR Structure Validation Summary Report (i)

Apr 26, 2016 – 08:22 PM BST

PDB ID	:	2FVF
Title	:	Structure of 10:0-ACP (protein with docked fatty acid)
Authors	:	Zornetzer, G.A.; Fox, B.G.; Markley, J.L.
Deposited on	:	2006-01-30

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
http://wwpdb.org/validation/2016/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:

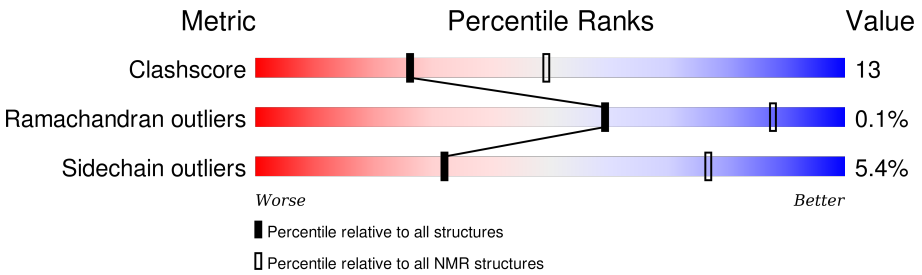
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	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 (i)

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

The overall completeness of chemical shifts assignment is 83%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	82	78% 17% 5%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 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:1-A:78 (78)	0.20	3

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 1 single-model cluster was found.

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

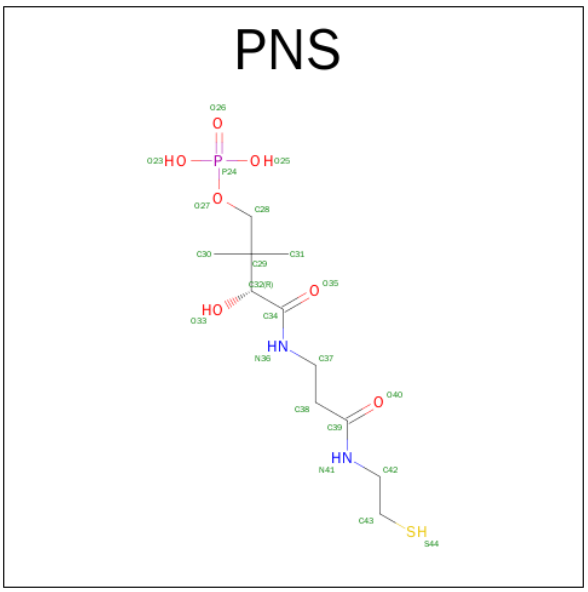
3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1316 atoms, of which 665 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Acyl Carrier Protein.

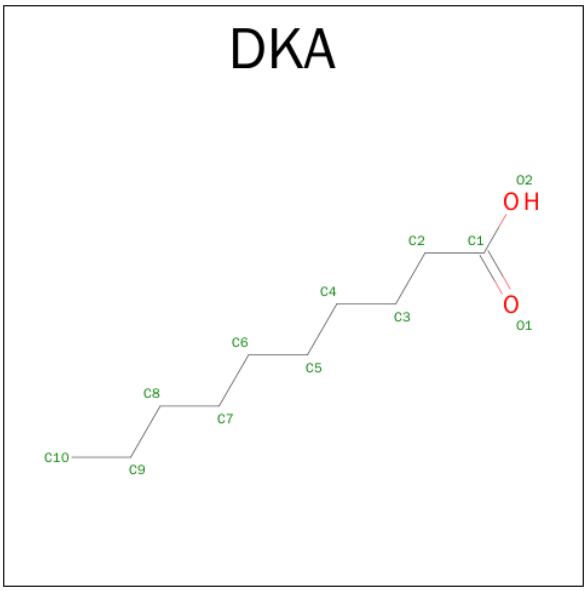
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	82	1244	385	626	96	136	1	0

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



Mol	Chain	Residues	Atoms						
			Total	C	H	N	O	P	S
2	A	1	42	11	20	2	7	1	1

- Molecule 3 is DECANOIC ACID (three-letter code: DKA) (formula: $C_{10}H_{20}O_2$).



Mol	Chain	Residues	Atoms			
			Total	C	H	O
3	A	1	30	10	19	1

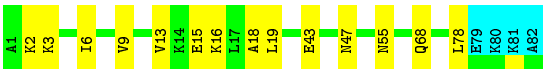
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

Chain A:

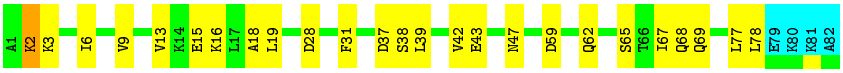


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 3. Colouring as in section 4.1 above.

- Molecule 1: Acyl Carrier Protein

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Initial structure from torsion angle dynamics (in CYANA). Fatty acid and phosphopantetheine were added and docked using ambiguous distance restraints in XPLOR-NIH.*

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with lowest energy in a clustering of the fatty acid structures.*

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

Software name	Classification	Version
CYANA	structure solution	2.1
XPLOR-NIH	refinement	2.12

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 6790
Number of chemical shift lists	1
Total number of shifts	920
Number of shifts mapped to atoms	896
Number of unparsed shifts	0
Number of shifts with mapping errors	24
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PNS, DKA

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	585	589	587	16±4
2	A	22	20	20	1±1
All	All	12360	12560	12520	331

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 13.

5 of 139 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:GLN:NE2	1:A:62:GLN:H	0.84	1.68	6	1
1:A:59:ASP:O	1:A:62:GLN:NE2	0.70	2.25	6	2
1:A:16:LYS:NZ	1:A:47:ASN:ND2	0.65	2.45	7	8
1:A:6:ILE:HD11	1:A:68:GLN:NE2	0.63	2.08	5	13
1:A:16:LYS:NZ	1:A:47:ASN:HD21	0.61	1.92	7	7

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	77/82 (94%)	73±1 (95±2%)	4±1 (5±2%)	0±0 (0±0%)	59 88
All	All	1540/1640 (94%)	1463 (95%)	76 (5%)	1 (0%)	59 88

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	18	ALA	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	65/69 (94%)	62±1 (95±2%)	4±1 (5±2%)	32 77
All	All	1300/1380 (94%)	1230 (95%)	70 (5%)	32 77

5 of 14 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	2	LYS	19
1	A	3	LYS	18
1	A	16	LYS	8
1	A	55	ASN	7
1	A	68	GLN	5

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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	PNS	A	101	1,3	18,21,21	0.75±0.01	0±0 (0±0%)
3	DKA	A	102	2	10,10,11	0.34±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	PNS	A	101	1,3	22,29,29	0.91±0.01	0±0 (0±0%)
3	DKA	A	102	2	9,9,11	0.87±0.01	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PNS	A	101	1,3	-	0±0,27,27,27	0±0,0,0,0
3	DKA	A	102	2	-	0±0,7,8,9	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 83% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6790

Chemical shift list name: *assigned_chem_shift_list_1*

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	920
Number of shifts mapped to atoms	896
Number of unparsed shifts	0
Number of shifts with mapping errors	24
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.

- Chain not found in structure. First 5 (of 24) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	STE	H181	0.738	0.005	9
UNMAPPED	1	PNS	H41	8.29	0.016	1
UNMAPPED	1	PNS	H313	0.88	0.005	4
UNMAPPED	1	PNS	H36	8.108	0.007	1
UNMAPPED	1	PNS	H432	3.009	0.013	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	73	-0.62 ± 0.22	Should be applied
$^{13}C_{\beta}$	69	0.26 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	62	-0.31 ± 0.19	None needed (< 0.5 ppm)

Continued on next page...

Continued from previous page...

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
^{15}N	78	0.47 ± 0.36	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 83%, i.e. 733 atoms were assigned a chemical shift out of a possible 887. 11 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	343/390 (88%)	141/156 (90%)	128/156 (82%)	74/78 (95%)
Sidechain	382/479 (80%)	231/270 (86%)	146/197 (74%)	5/12 (42%)
Aromatic	8/18 (44%)	8/10 (80%)	0/8 (0%)	0/0 (—%)
Overall	733/887 (83%)	380/436 (87%)	274/361 (76%)	79/90 (88%)

7.1.4 Statistically unusual chemical shifts (i)

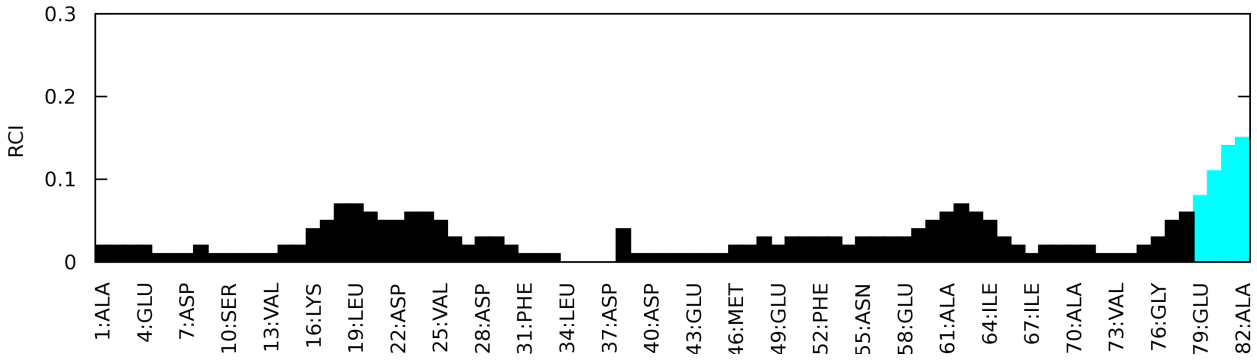
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	1	ALA	N	98.05	141.07 – 105.37	-7.0

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:


RCI
0.3
0.2
0.1
0
1:ALA
4:GLU
7:ASP
10:SER
13:VAL
16:LYS
19:LEU
22:ASP
25:VAL
28:ASP
31:PHE
34:LEU
37:ASP
40:ASP
43:GLU
46:MET
49:GLU
52:PHE
55:ASN
58:GLU
61:ALA
64:ILE
67:ILE
70:ALA
73:VAL
76:GLY
79:GLU
82:ALA