



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 09:54 pm GMT

PDB ID : 2FQ2  
Title : Solution structure of minor conformation of holo-acyl carrier protein from malaria parasite plasmodium falciparum  
Authors : Sharma, A.K.; Sharma, S.K.; Surolia, A.; Surolia, N.; Sarma, S.P.  
Deposited on : 2006-01-17

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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	:	1.7.2 (RC1), CSD as538be (2017)
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

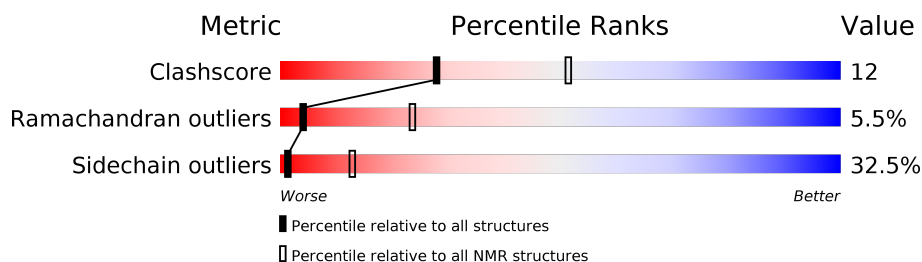
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 93%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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  $\geq 3$ , 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	79	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	A	PNS	137	20	-

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:3-A:77 (75)	0.36	2

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. No single-model clusters were found.

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

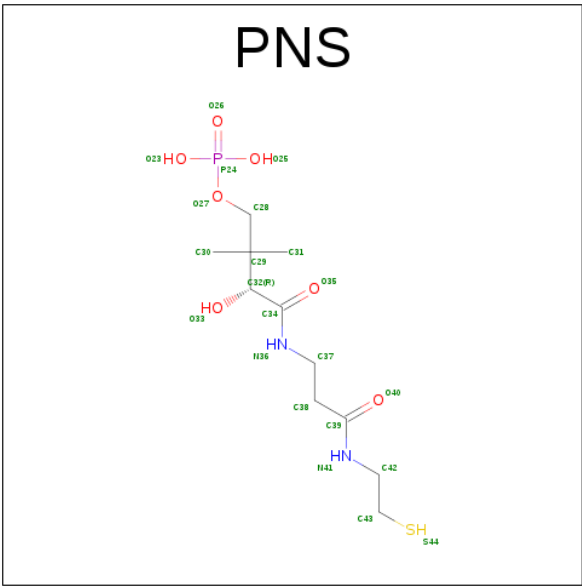
### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1311 atoms, of which 660 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	79	1269	395	639	100	133	2	0

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C<sub>11</sub>H<sub>23</sub>N<sub>2</sub>O<sub>7</sub>PS).



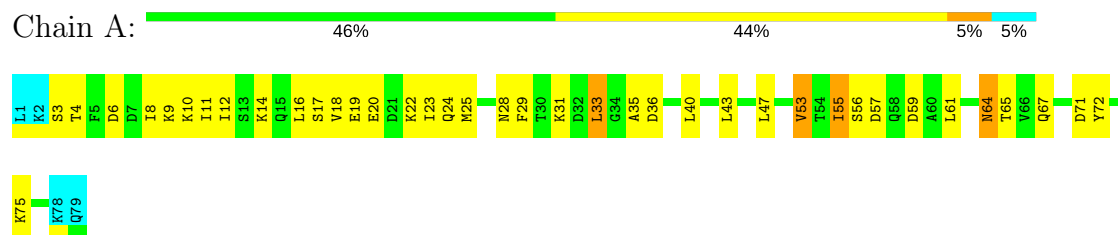
Mol	Chain	Residues	Atoms						
			Total	C	H	N	O	P	S
2	A	1	42	11	21	2	6	1	1

## 4 Residue-property plots

### 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

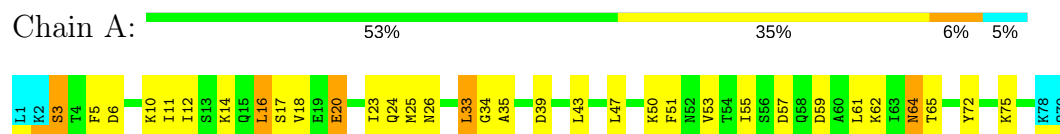


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

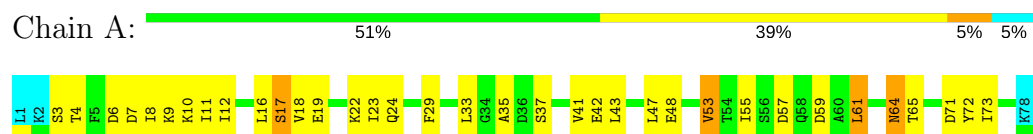
#### 4.2.1 Score per residue for model 1

- Molecule 1: acyl carrier protein



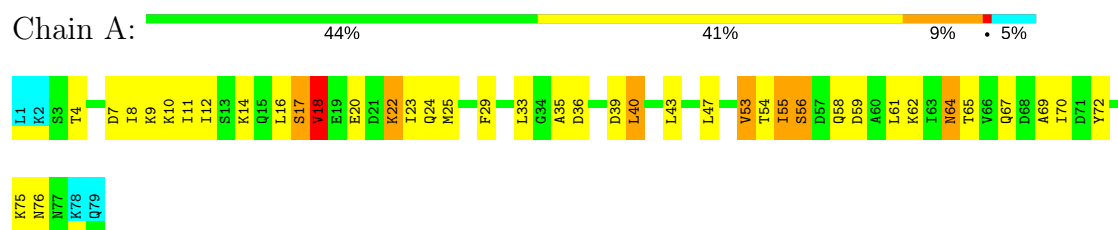
#### 4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: acyl carrier protein



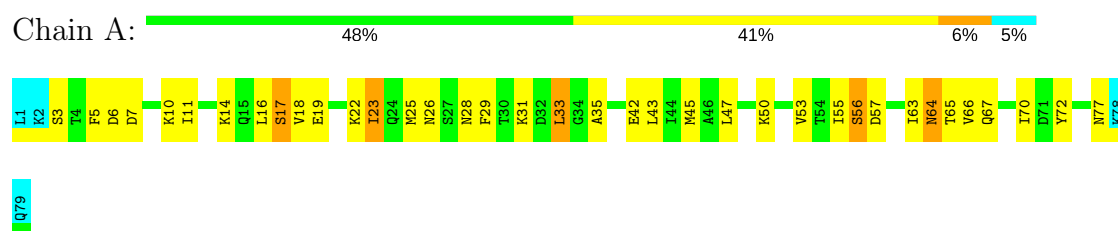
### 4.2.3 Score per residue for model 3

- Molecule 1: acyl carrier protein



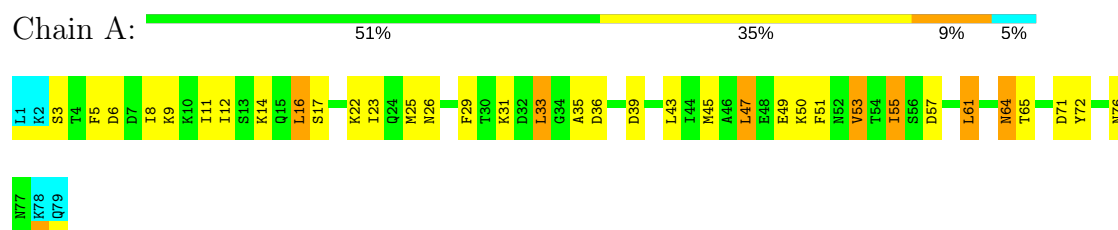
### 4.2.4 Score per residue for model 4

- Molecule 1: acyl carrier protein



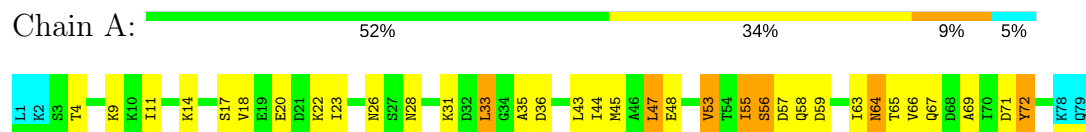
### 4.2.5 Score per residue for model 5

- Molecule 1: acyl carrier protein



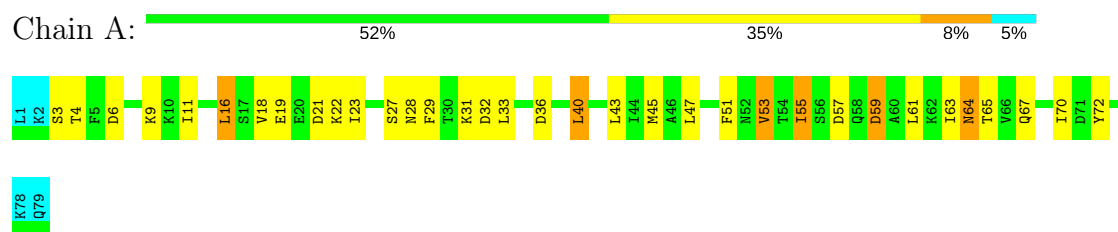
### 4.2.6 Score per residue for model 6

- Molecule 1: acyl carrier protein



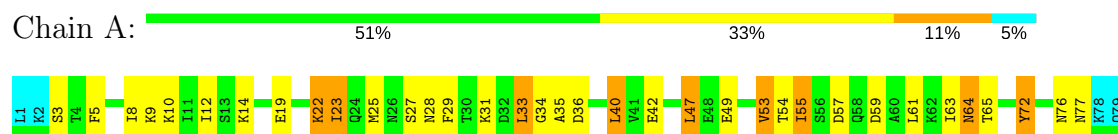
### 4.2.7 Score per residue for model 7

- Molecule 1: acyl carrier protein



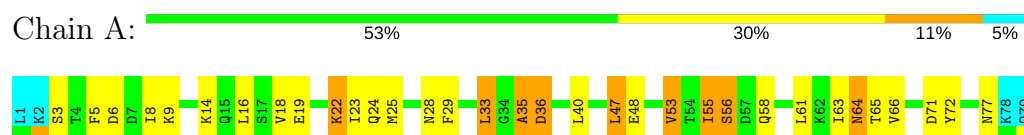
### 4.2.8 Score per residue for model 8

- Molecule 1: acyl carrier protein



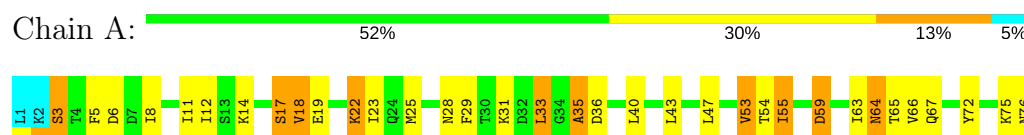
### 4.2.9 Score per residue for model 9

- Molecule 1: acyl carrier protein



### 4.2.10 Score per residue for model 10

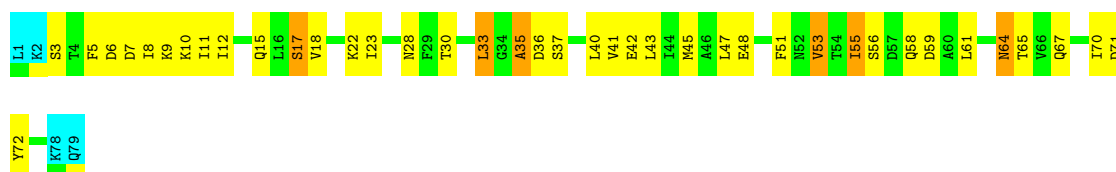
- Molecule 1: acyl carrier protein



### 4.2.11 Score per residue for model 11

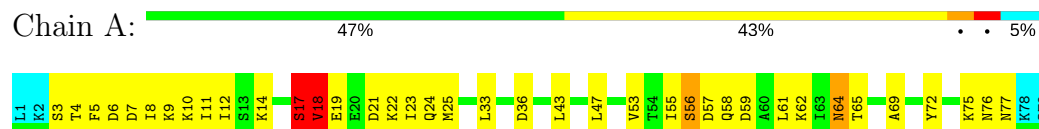
- Molecule 1: acyl carrier protein





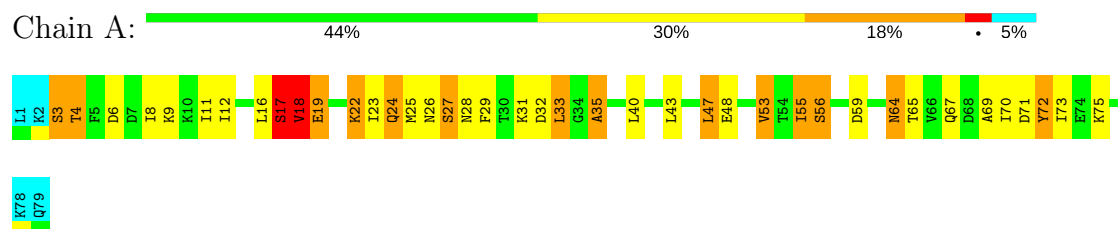
#### 4.2.12 Score per residue for model 12

- Molecule 1: acyl carrier protein



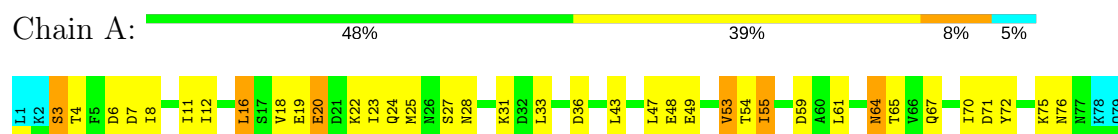
#### 4.2.13 Score per residue for model 13

- Molecule 1: acyl carrier protein



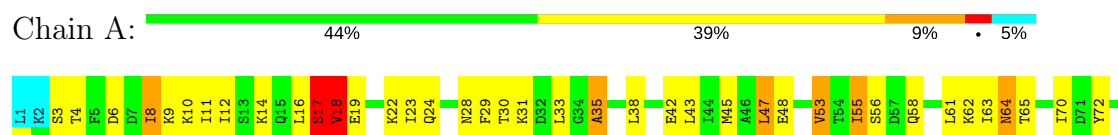
#### 4.2.14 Score per residue for model 14

- Molecule 1: acyl carrier protein



#### 4.2.15 Score per residue for model 15

- Molecule 1: acyl carrier protein

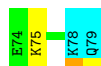
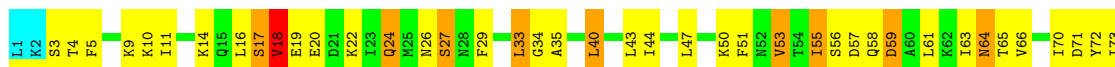




#### 4.2.16 Score per residue for model 16

- Molecule 1: acyl carrier protein

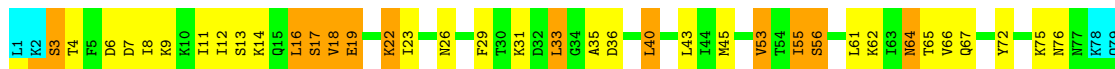
Chain A: 42% 41% 11% 5%



#### 4.2.17 Score per residue for model 17

- Molecule 1: acyl carrier protein

Chain A: 48% 32% 15% 5%



#### 4.2.18 Score per residue for model 18

- Molecule 1: acyl carrier protein

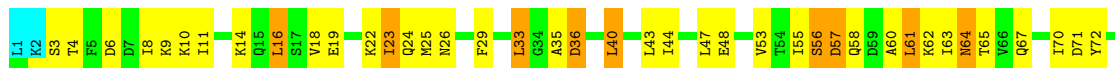
Chain A: 39% 41% 14% 5%



#### 4.2.19 Score per residue for model 19

- Molecule 1: acyl carrier protein

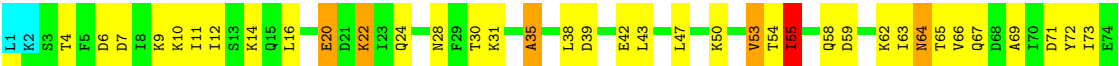
Chain A: 43% 41% 11% 5%





4.2.20 Score per residue for model 20

- Molecule 1: acyl carrier protein



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS, SIMULATED ANNEALING*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

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 6516
Number of chemical shift lists	1
Total number of shifts	1070
Number of shifts mapped to atoms	1029
Number of unparsed shifts	10
Number of shifts with mapping errors	31
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

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

## 6 Model quality

### 6.1 Standard geometry

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

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

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	595	594	594	15±4
All	All	12320	12300	12300	297

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ILE:HD13	1:A:33:LEU:HD21	0.82	1.52	8	2
1:A:23:ILE:HD13	1:A:33:LEU:HD22	0.77	1.54	19	1
1:A:8:ILE:HD12	1:A:47:LEU:HD11	0.69	1.65	18	2
1:A:23:ILE:HD11	1:A:29:PHE:CD2	0.68	2.24	18	5
1:A:23:ILE:HD11	1:A:29:PHE:CE2	0.67	2.25	9	4
1:A:12:ILE:HD11	1:A:20:GLU:HB3	0.64	1.70	20	1
1:A:16:LEU:HD13	1:A:19:GLU:OE1	0.64	1.93	9	1
1:A:33:LEU:HD12	1:A:35:ALA:HB2	0.63	1.70	11	3
1:A:53:VAL:CG2	1:A:55:ILE:HD11	0.63	2.23	18	16
1:A:23:ILE:HD12	1:A:33:LEU:HD21	0.63	1.69	5	2
1:A:29:PHE:HB3	1:A:40:LEU:HD11	0.61	1.73	7	6
1:A:29:PHE:O	1:A:40:LEU:HD11	0.61	1.95	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ILE:HD12	1:A:43:LEU:HD12	0.60	1.73	15	18
1:A:23:ILE:HD12	1:A:33:LEU:CD2	0.60	2.27	5	4
1:A:22:LYS:HE2	1:A:33:LEU:HD13	0.60	1.71	17	1
1:A:12:ILE:HD12	1:A:17:SER:O	0.60	1.97	5	2
1:A:4:THR:HG23	1:A:73:ILE:CG2	0.60	2.27	13	2
1:A:16:LEU:HD13	1:A:19:GLU:OE2	0.59	1.97	4	1
1:A:16:LEU:O	1:A:18:VAL:HG13	0.59	1.98	19	2
1:A:24:GLN:OE1	1:A:66:VAL:HG22	0.59	1.96	20	1
1:A:4:THR:HG22	1:A:70:ILE:HG22	0.59	1.73	7	5
1:A:47:LEU:HD21	1:A:72:TYR:OH	0.59	1.98	6	2
1:A:44:ILE:HG21	1:A:59:ASP:OD1	0.59	1.97	6	1
1:A:12:ILE:HD12	1:A:19:GLU:HG2	0.58	1.75	15	2
1:A:23:ILE:HD12	1:A:33:LEU:HD22	0.58	1.74	6	3
1:A:23:ILE:HD13	1:A:33:LEU:CD2	0.57	2.27	19	2
1:A:4:THR:HG21	1:A:69:ALA:HB1	0.56	1.76	18	5
1:A:17:SER:O	1:A:18:VAL:HG13	0.56	2.00	3	7
1:A:30:THR:HB	1:A:40:LEU:HD12	0.56	1.77	18	1
1:A:47:LEU:HD23	1:A:48:GLU:N	0.56	2.15	6	2
1:A:64:ASN:HD22	1:A:65:THR:HG23	0.55	1.61	14	7
1:A:48:GLU:HG3	1:A:55:ILE:HD12	0.55	1.78	9	4
1:A:35:ALA:HB3	1:A:40:LEU:CD2	0.55	2.32	10	1
1:A:16:LEU:HD22	1:A:19:GLU:OE2	0.54	2.01	16	2
1:A:16:LEU:HD21	1:A:39:ASP:CB	0.53	2.33	20	2
1:A:12:ILE:HD12	1:A:19:GLU:CG	0.53	2.34	15	1
1:A:64:ASN:ND2	1:A:65:THR:HG23	0.53	2.19	1	13
1:A:66:VAL:O	1:A:70:ILE:HG22	0.53	2.04	4	1
1:A:59:ASP:OD1	1:A:63:ILE:HD13	0.53	2.03	16	1
1:A:55:ILE:HD13	1:A:59:ASP:OD2	0.53	2.03	7	2
1:A:23:ILE:CD1	1:A:33:LEU:HD21	0.52	2.31	8	1
1:A:12:ILE:HD13	1:A:19:GLU:CG	0.52	2.33	2	1
1:A:53:VAL:HG23	1:A:55:ILE:HD11	0.52	1.81	18	4
1:A:57:ASP:O	1:A:61:LEU:HD21	0.52	2.05	2	3
1:A:11:ILE:HD12	1:A:43:LEU:CD1	0.52	2.35	19	3
1:A:4:THR:HG23	1:A:73:ILE:HG21	0.51	1.81	13	3
1:A:8:ILE:HG13	1:A:47:LEU:HD11	0.51	1.82	8	3
1:A:8:ILE:HD11	1:A:63:ILE:CG2	0.51	2.35	19	1
1:A:30:THR:HA	1:A:35:ALA:HB3	0.51	1.81	20	2
1:A:54:THR:HG23	1:A:54:THR:O	0.51	2.06	3	4
1:A:4:THR:HG21	1:A:69:ALA:CB	0.51	2.36	6	2
1:A:27:SER:O	1:A:65:THR:HG22	0.51	2.06	14	5
1:A:16:LEU:HD22	1:A:19:GLU:OE1	0.51	2.05	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:VAL:HG11	1:A:76:ASN:HB3	0.51	1.83	18	7
1:A:4:THR:HG22	1:A:70:ILE:CG2	0.50	2.37	19	5
1:A:44:ILE:HD13	1:A:60:ALA:HA	0.50	1.81	19	1
1:A:55:ILE:HG22	1:A:58:GLN:HB2	0.50	1.84	11	1
1:A:4:THR:HG23	1:A:8:ILE:HD12	0.49	1.84	12	1
1:A:54:THR:C	1:A:55:ILE:HD12	0.49	2.27	20	2
1:A:35:ALA:HB3	1:A:40:LEU:HD21	0.48	1.85	10	1
1:A:55:ILE:HG21	1:A:59:ASP:HB3	0.48	1.85	1	1
1:A:37:SER:O	1:A:41:VAL:HG23	0.48	2.09	11	2
1:A:33:LEU:HD12	1:A:34:GLY:N	0.48	2.24	16	3
1:A:29:PHE:O	1:A:40:LEU:HD21	0.48	2.09	19	3
1:A:23:ILE:HD11	1:A:29:PHE:CZ	0.48	2.42	9	1
1:A:22:LYS:NZ	1:A:33:LEU:HD22	0.47	2.23	8	1
1:A:7:ASP:O	1:A:11:ILE:HG23	0.47	2.10	3	2
1:A:53:VAL:HB	1:A:55:ILE:HD11	0.47	1.87	13	6
1:A:30:THR:CB	1:A:40:LEU:HD22	0.47	2.40	11	1
1:A:33:LEU:HD12	1:A:35:ALA:H	0.47	1.68	19	3
1:A:67:GLN:NE2	1:A:70:ILE:HD11	0.47	2.25	19	1
1:A:8:ILE:O	1:A:12:ILE:HG23	0.47	2.09	11	9
1:A:44:ILE:HG23	1:A:59:ASP:OD1	0.46	2.09	16	1
1:A:4:THR:CA	1:A:73:ILE:HD13	0.46	2.40	20	2
1:A:16:LEU:HD13	1:A:19:GLU:CD	0.46	2.31	17	1
1:A:11:ILE:HD13	1:A:47:LEU:HD12	0.46	1.88	18	1
1:A:63:ILE:HG22	1:A:63:ILE:O	0.46	2.10	16	4
1:A:12:ILE:HG22	1:A:43:LEU:HD22	0.46	1.88	13	1
1:A:16:LEU:HD21	1:A:39:ASP:CG	0.46	2.30	1	1
1:A:23:ILE:HG23	1:A:24:GLN:NE2	0.46	2.25	18	2
1:A:4:THR:HG22	1:A:8:ILE:CD1	0.46	2.41	17	2
1:A:12:ILE:HD11	1:A:20:GLU:HG3	0.46	1.88	14	1
1:A:24:GLN:HG2	1:A:66:VAL:HG22	0.45	1.87	16	1
1:A:63:ILE:O	1:A:63:ILE:HG22	0.45	2.12	7	4
1:A:70:ILE:HD12	1:A:71:ASP:N	0.45	2.27	11	4
1:A:59:ASP:O	1:A:63:ILE:HD13	0.45	2.12	8	1
1:A:33:LEU:CD1	1:A:35:ALA:HB2	0.44	2.42	10	2
1:A:23:ILE:HG13	1:A:33:LEU:HD21	0.44	1.87	1	1
1:A:26:ASN:HA	1:A:66:VAL:HG23	0.44	1.89	6	1
1:A:55:ILE:HG22	1:A:59:ASP:N	0.44	2.28	14	2
1:A:30:THR:HB	1:A:40:LEU:HD22	0.44	1.87	11	1
1:A:4:THR:HB	1:A:73:ILE:HD13	0.44	1.90	16	2
1:A:55:ILE:HG22	1:A:59:ASP:HB2	0.44	1.88	2	1
1:A:8:ILE:CD1	1:A:47:LEU:HD11	0.44	2.42	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:THR:CB	1:A:73:ILE:HD13	0.44	2.43	20	1
1:A:44:ILE:HG21	1:A:59:ASP:CG	0.43	2.33	6	1
1:A:16:LEU:HD11	1:A:39:ASP:OD1	0.43	2.12	18	1
1:A:64:ASN:CG	1:A:65:THR:HG23	0.43	2.34	2	9
1:A:16:LEU:HD11	1:A:39:ASP:HB3	0.43	1.89	3	1
1:A:30:THR:HB	1:A:40:LEU:HD13	0.43	1.91	11	1
1:A:61:LEU:O	1:A:61:LEU:HD12	0.42	2.14	16	1
1:A:12:ILE:HD13	1:A:19:GLU:HG3	0.42	1.91	2	1
1:A:4:THR:O	1:A:8:ILE:HD12	0.42	2.15	13	1
1:A:57:ASP:O	1:A:61:LEU:HD12	0.42	2.14	8	1
1:A:12:ILE:HD11	1:A:20:GLU:CG	0.42	2.44	14	1
1:A:20:GLU:HA	1:A:23:ILE:HG22	0.42	1.92	18	3
1:A:23:ILE:HD12	1:A:29:PHE:CE2	0.42	2.50	8	1
1:A:12:ILE:HD12	1:A:19:GLU:HG3	0.42	1.91	12	1
1:A:12:ILE:HD13	1:A:23:ILE:HG13	0.42	1.91	17	1
1:A:63:ILE:HD11	1:A:72:TYR:CE2	0.41	2.50	8	1
1:A:48:GLU:CG	1:A:55:ILE:HD12	0.41	2.46	14	2
1:A:63:ILE:O	1:A:63:ILE:CG2	0.41	2.69	20	1
1:A:55:ILE:HG21	1:A:59:ASP:CG	0.41	2.36	20	1
1:A:53:VAL:CB	1:A:55:ILE:HD11	0.41	2.46	6	1
1:A:18:VAL:O	1:A:18:VAL:HG23	0.41	2.16	1	1
1:A:16:LEU:HB3	1:A:18:VAL:HG22	0.40	1.94	7	1
1:A:4:THR:OG1	1:A:73:ILE:HD13	0.40	2.16	2	1
1:A:55:ILE:HG22	1:A:58:GLN:CB	0.40	2.46	11	1
1:A:12:ILE:HD13	1:A:19:GLU:HG2	0.40	1.94	2	1

## 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	75/79 (95%)	56±2 (75±3%)	15±2 (20±2%)	4±2 (5±3%)	4	23
All	All	1500/1580 (95%)	1119 (75%)	299 (20%)	82 (5%)	4	23

All 12 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	35	ALA	14
1	A	56	SER	11
1	A	17	SER	11
1	A	18	VAL	11
1	A	22	LYS	11
1	A	3	SER	9
1	A	6	ASP	6
1	A	36	ASP	4
1	A	55	ILE	2
1	A	77	ASN	1
1	A	27	SER	1
1	A	19	GLU	1

### 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	70/74 (95%)	47±3 (68±5%)	23±3 (32±5%)	1	13
All	All	1400/1480 (95%)	945 (68%)	455 (32%)	1	13

All 55 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	72	TYR	20
1	A	64	ASN	20
1	A	53	VAL	20
1	A	47	LEU	19
1	A	55	ILE	18
1	A	33	LEU	18
1	A	9	LYS	16
1	A	14	LYS	15
1	A	22	LYS	14
1	A	61	LEU	13
1	A	3	SER	13
1	A	25	MET	12
1	A	36	ASP	12
1	A	10	LYS	12

*Continued on next page...*

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Mol	Chain	Res	Type	Models (Total)
1	A	28	ASN	11
1	A	75	LYS	11
1	A	24	GLN	11
1	A	31	LYS	11
1	A	67	GLN	10
1	A	56	SER	9
1	A	6	ASP	9
1	A	58	GLN	8
1	A	5	PHE	8
1	A	16	LEU	8
1	A	45	MET	8
1	A	57	ASP	8
1	A	40	LEU	8
1	A	71	ASP	7
1	A	17	SER	7
1	A	62	LYS	7
1	A	18	VAL	7
1	A	26	ASN	7
1	A	59	ASP	7
1	A	50	LYS	6
1	A	51	PHE	6
1	A	77	ASN	6
1	A	23	ILE	6
1	A	19	GLU	6
1	A	42	GLU	6
1	A	7	ASP	6
1	A	20	GLU	5
1	A	49	GLU	4
1	A	32	ASP	2
1	A	8	ILE	2
1	A	21	ASP	2
1	A	38	LEU	2
1	A	48	GLU	2
1	A	4	THR	2
1	A	29	PHE	2
1	A	27	SER	1
1	A	15	GLN	1
1	A	13	SER	1
1	A	43	LEU	1
1	A	70	ILE	1
1	A	76	ASN	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry ⓘ

1 ligand is 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	137	1	15,20,21	0.84±0.01	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	137	1	17,26,29	1.45±0.00	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	137	1	1±0,1,7,7	1±0,24,26,27	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	137	PNS	C32	20

All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	137	PNS	C32-C34-N36-C37	20

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

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 93% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 6516

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	1070
Number of shifts mapped to atoms	1029
Number of unparsed shifts	10
Number of shifts with mapping errors	31
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chemical shift has been reported more than once. All 10 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1061	A	41	VAL	H	7.311	0.01	1
1062	A	41	VAL	N	119.32	0.25	1
1063	A	60	ALA	H	8.610	0.01	1
1064	A	60	ALA	N	123.48	0.25	1
1065	A	61	LEU	H	7.126	0.01	1
1066	A	61	LEU	N	115.72	0.25	1
1067	UNMAPPED	1	PNS	H36	7.998	0.01	1
1068	UNMAPPED	1	PNS	N36	121.16	0.25	1
1069	UNMAPPED	1	PNS	H41	8.184	0.01	1
1070	UNMAPPED	1	PNS	N41	124.19	0.25	1

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

- Chain not found in structure. All 31 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	PNS	C34	177.57	0.3	1
UNMAPPED	1	PNS	H41	8.233	0.01	1
UNMAPPED	1	PNS	C39	176.5	0.3	1
UNMAPPED	1	PNS	N36	121.12	0.25	1
UNMAPPED	1	PNS	1H38	2.487	0.01	2
UNMAPPED	1	PNS	N41	123.93	0.25	1
UNMAPPED	1	PNS	C42	38.08	0.3	2
UNMAPPED	1	PNS	C43	39.33	0.3	2
UNMAPPED	1	PNS	C28	74.24	0.3	1
UNMAPPED	1	PNS	2H37	3.487	0.01	2
UNMAPPED	1	PNS	C32	76.78	0.3	1
UNMAPPED	1	PNS	1H28	3.383	0.01	2
UNMAPPED	1	PNS	2H38	2.487	0.01	2
UNMAPPED	1	PNS	1H42	3.463	0.01	2
UNMAPPED	1	PNS	2H43	2.79	0.01	2
UNMAPPED	1	PNS	1H30	0.843	0.01	2
UNMAPPED	1	PNS	C38	41.18	0.3	2
UNMAPPED	1	PNS	2H42	3.463	0.01	2
UNMAPPED	1	PNS	C37	38.17	0.3	2
UNMAPPED	1	PNS	C31	22.55	0.3	2
UNMAPPED	1	PNS	H32	4.003	0.01	1
UNMAPPED	1	PNS	2H31	0.941	0.01	2
UNMAPPED	1	PNS	1H31	0.941	0.01	2
UNMAPPED	1	PNS	C30	20.53	0.3	2
UNMAPPED	1	PNS	1H37	3.487	0.01	2
UNMAPPED	1	PNS	3H30	0.843	0.01	2
UNMAPPED	1	PNS	2H30	0.843	0.01	2
UNMAPPED	1	PNS	H36	8.062	0.01	1
UNMAPPED	1	PNS	1H43	2.79	0.01	2
UNMAPPED	1	PNS	3H31	0.941	0.01	2
UNMAPPED	1	PNS	2H28	3.788	0.01	2

### 7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	79	$-0.55 \pm 0.15$	Should be applied
$^{13}\text{C}_\beta$	78	$0.19 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	77	$-0.26 \pm 0.16$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	79	$0.56 \pm 0.46$	None needed (imprecise)

### 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 93%, i.e. 855 atoms were assigned a chemical shift out of a possible 916. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	374/375 (100%)	150/150 (100%)	149/150 (99%)	75/75 (100%)
Sidechain	464/506 (92%)	286/290 (99%)	168/198 (85%)	10/18 (56%)
Aromatic	17/35 (49%)	17/19 (89%)	0/16 (0%)	0/0 (—%)
Overall	855/916 (93%)	453/459 (99%)	317/364 (87%)	85/93 (91%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 916 atoms were assigned a chemical shift out of a possible 981. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	393/395 (99%)	158/158 (100%)	156/158 (99%)	79/79 (100%)
Sidechain	506/551 (92%)	313/317 (99%)	182/213 (85%)	11/21 (52%)
Aromatic	17/35 (49%)	17/19 (89%)	0/16 (0%)	0/0 (—%)
Overall	916/981 (93%)	488/494 (99%)	338/387 (87%)	90/100 (90%)

### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

### 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:

