Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 04:35 PM BST

PDB ID	:	1RW2
Title	:	Three-dimensional structure of Ku80 CTD
Authors	:	Zhang, Z.; Hu, W.; Cano, L.; Lee, T.D.; Chen, D.J.; Chen, Y.
Deposited on	:	2003-12-15

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

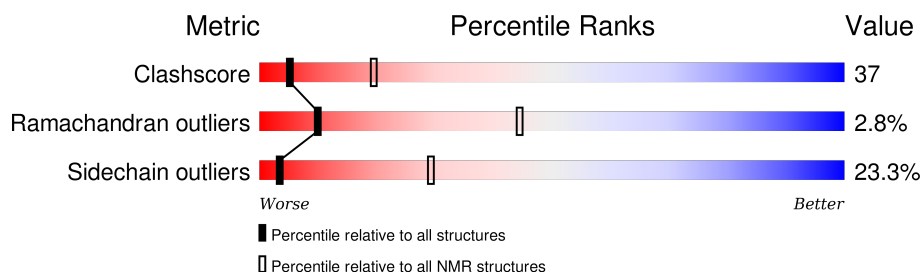|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
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 (i)

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

The overall completeness of chemical shifts assignment is 86%.

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	Percentile Ranks	Value
Clashscore		37
Ramachandran outliers		2.8%
Sidechain outliers		23.3%

Worse   *Better*

▮ Percentile relative to all structures

❑ Percentile relative to all NMR structures

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	152	17% 35% 7% • 39%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 9 is the overall representative, medoid model (most similar to other models).

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:36-A:127 (92)	0.19	9

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 1 single-model cluster was found.

Cluster number	Models
1	1, 3, 4, 7, 8, 9, 10
2	2, 5
Single-model clusters	6

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2433 atoms, of which 1210 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ATP-dependent DNA helicase II, 80 kDa subunit.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	152	2433	772	1210	214	234	3	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP P13010
A	2	HIS	-	EXPRESSION TAG	UNP P13010
A	3	HIS	-	EXPRESSION TAG	UNP P13010
A	4	HIS	-	EXPRESSION TAG	UNP P13010
A	5	HIS	-	EXPRESSION TAG	UNP P13010
A	6	HIS	-	EXPRESSION TAG	UNP P13010
A	7	HIS	-	EXPRESSION TAG	UNP P13010

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: ATP-dependent DNA helicase II, 80 kDa subunit

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: ATP-dependent DNA helicase II, 80 kDa subunit
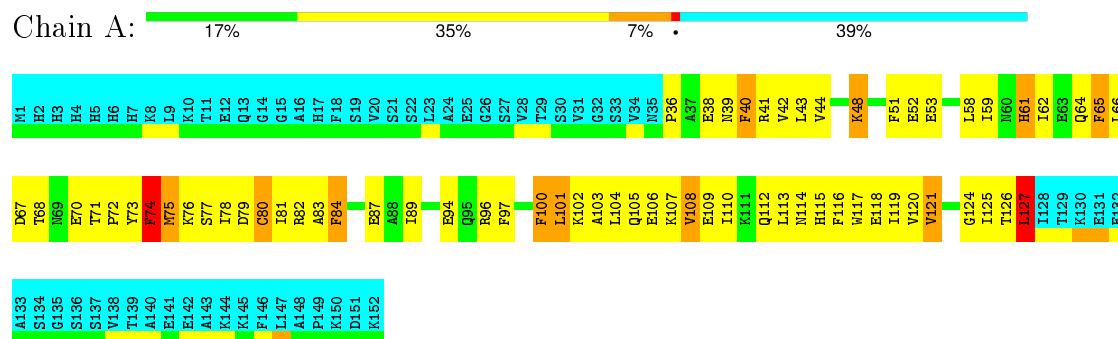
4.2.2 Score per residue for model 2

• Molecule 1: ATP-dependent DNA helicase II, 80 kDa subunit

Chain A: 22% 30% 7% • 39%
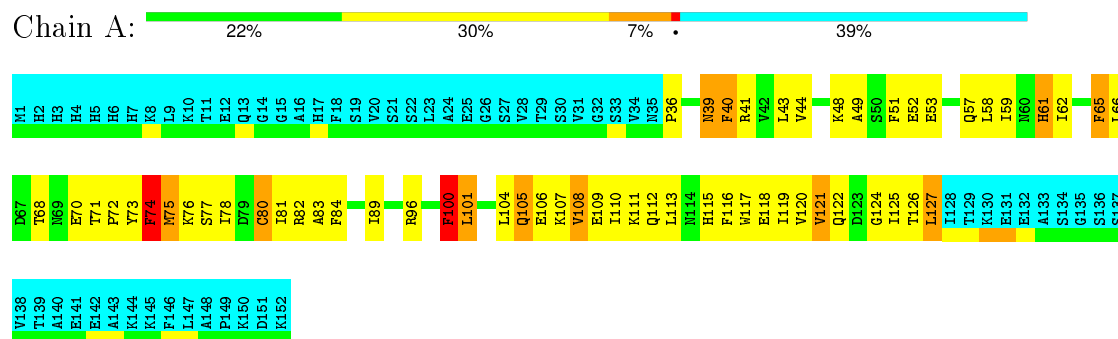
4.2.3 Score per residue for model 3

• Molecule 1: ATP-dependent DNA helicase II, 80 kDa subunit

Chain A: 19% 32% 8% • 39%

4.2.4 Score per residue for model 4

• Molecule 1: ATP-dependent DNA helicase II, 80 kDa subunit

Chain A: 16% 33% 10% • 39%

4.2.5 Score per residue for model 5

• Molecule 1: ATP-dependent DNA helicase II, 80 kDa subunit

Chain A: 20% 31% 9% • 39%

4.2.6 Score per residue for model 6

• Molecule 1: ATP-dependent DNA helicase II, 80 kDa subunit

Chain A: 22% 33% 5% • 39%

4.2.7 Score per residue for model 7

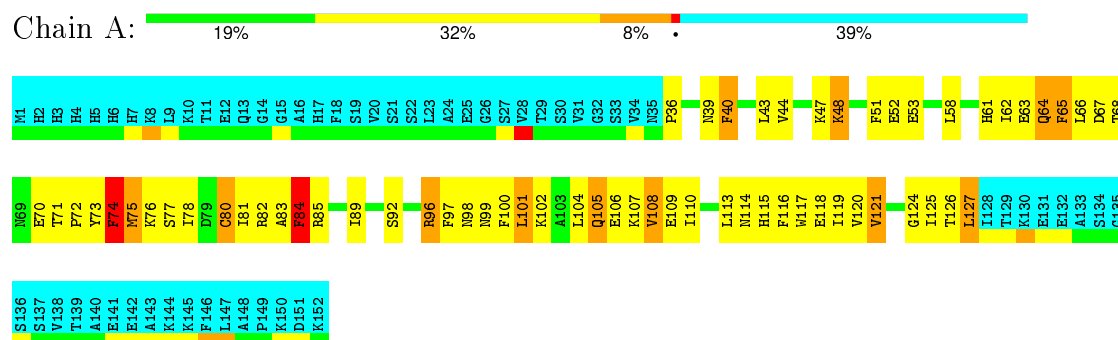• Molecule 1: ATP-dependent DNA helicase II, 80 kDa subunit

Chain A: 16% 36% 8% • 39%

4.2.8 Score per residue for model 8

• Molecule 1: ATP-dependent DNA helicase II, 80 kDa subunit

4.2.9 Score per residue for model 9 (medoid)

• Molecule 1: ATP-dependent DNA helicase II, 80 kDa subunit
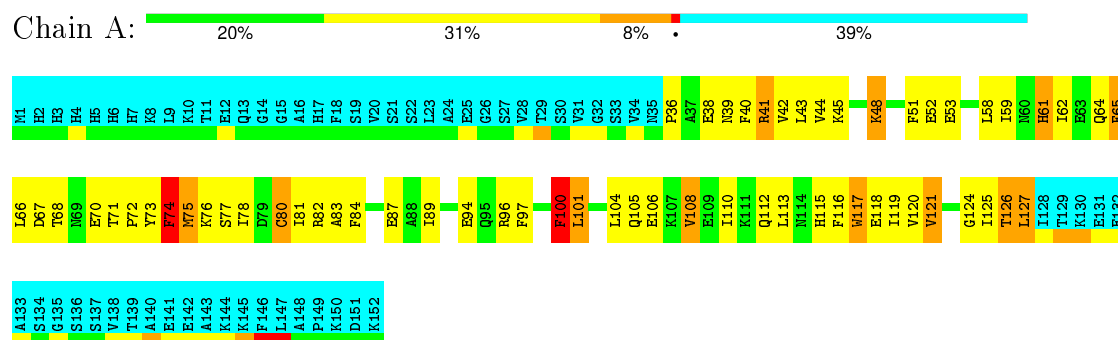
4.2.10 Score per residue for model 10

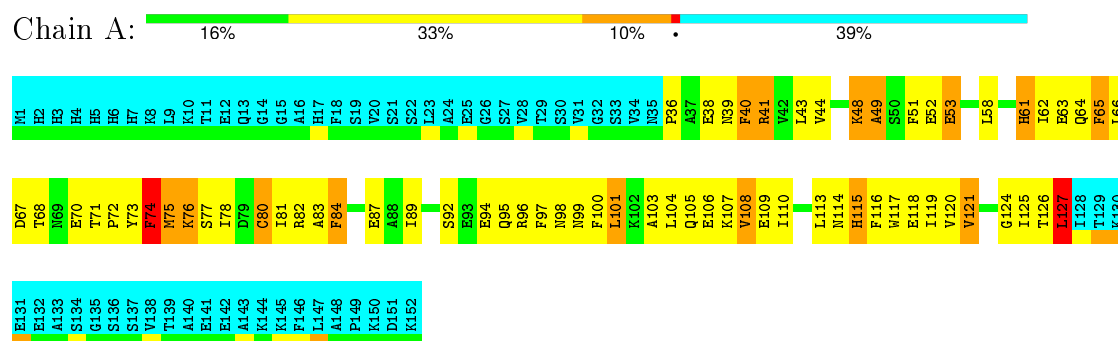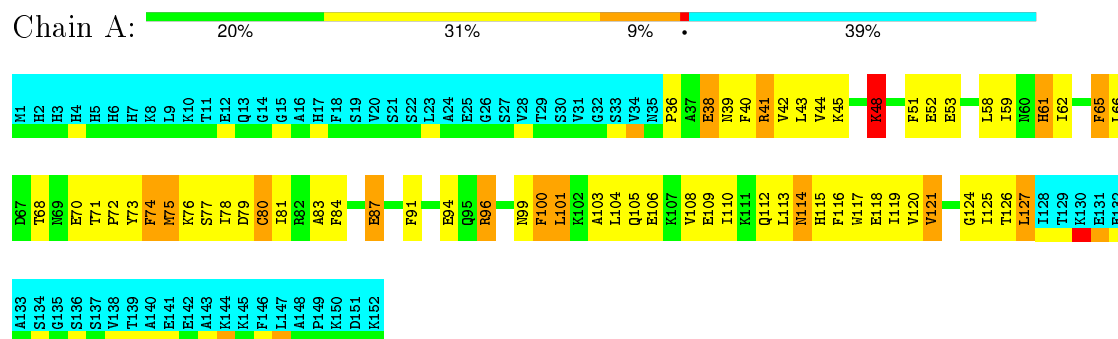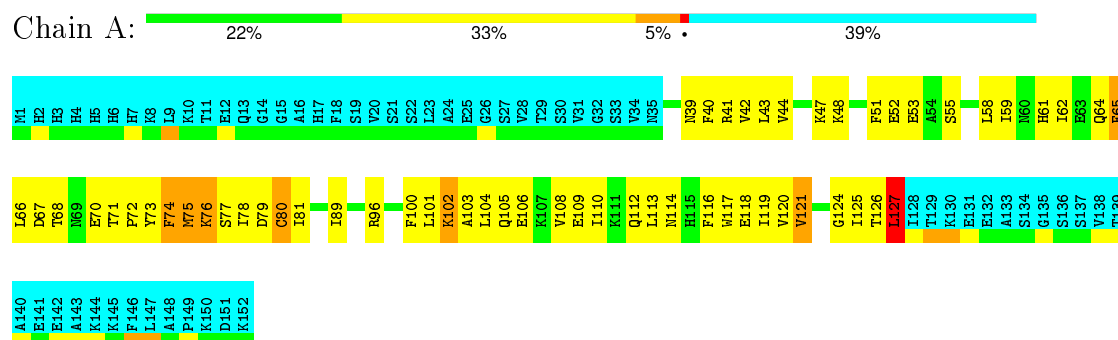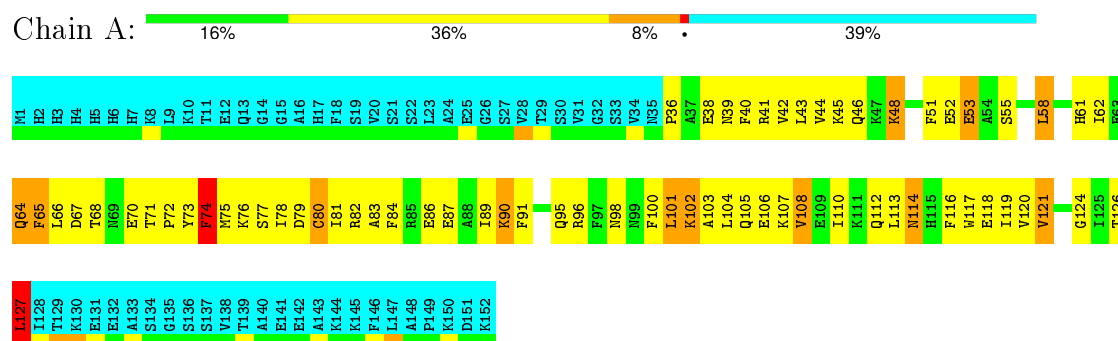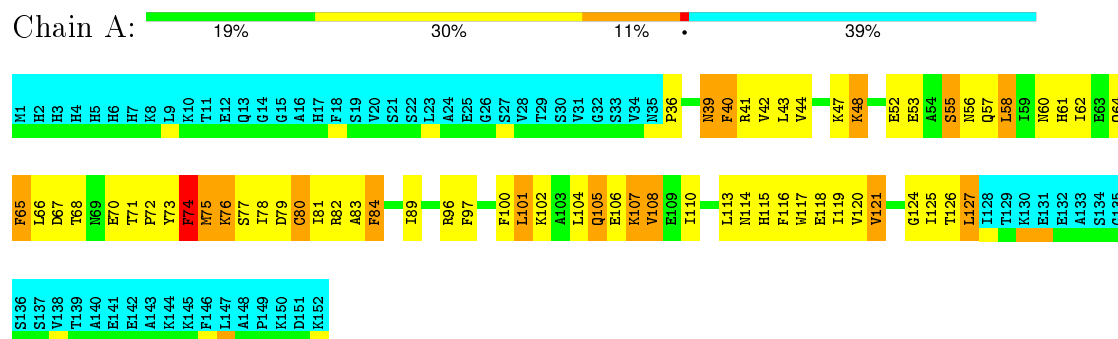• Molecule 1: ATP-dependent DNA helicase II, 80 kDa subunit
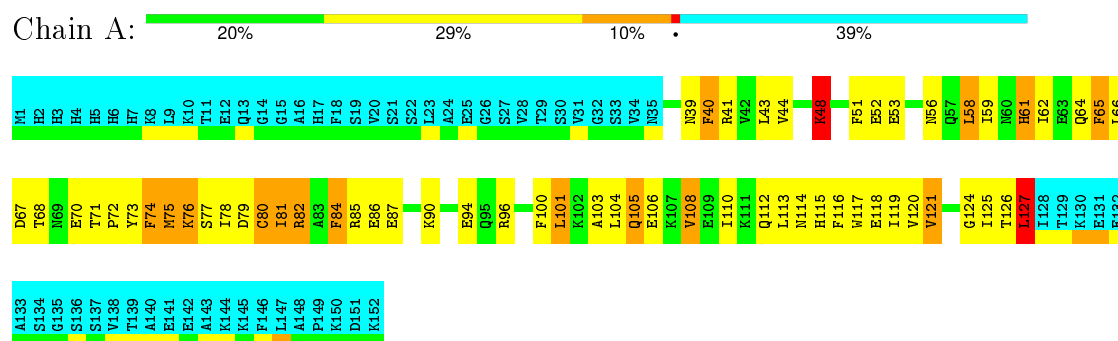
5   Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 40 calculated structures, 10 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
DIANA	structure solution	1.5
ARIA	refinement	1.2

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 5907
Number of chemical shift lists	1
Total number of shifts	1733
Number of shifts mapped to atoms	1733
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.54±0.16	2±2/790 (0.3±0.2%)	0.50±0.02	0±0/1062 (0.0±0.0%)
All	All	0.56	20/7900 (0.3%)	0.50	0/10620 (0.0%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models Worst	Models Total
1	A	74	PHE	CE1-CZ	12.51	1.61	1.37	7	6
1	A	74	PHE	CE2-CZ	-10.94	1.16	1.37	7	6
1	A	100	PHE	CE1-CZ	9.48	1.55	1.37	2	3
1	A	100	PHE	CE2-CZ	-8.61	1.21	1.37	2	3
1	A	84	PHE	CE1-CZ	6.20	1.49	1.37	3	1
1	A	84	PHE	CE2-CZ	-5.08	1.27	1.37	3	1

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	774	766	764	57±6
All	All	7740	7660	7640	568

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 37.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:GLN:C	1:A:113:LEU:HD22	0.80	1.95	2	2
1:A:126:THR:C	1:A:127:LEU:HD23	0.79	1.97	3	3
1:A:65:PHE:O	1:A:68:THR:HG22	0.74	1.82	8	10
1:A:101:LEU:HD21	1:A:126:THR:HA	0.71	1.59	6	9
1:A:68:THR:HG23	1:A:70:GLU:H	0.70	1.46	9	10
1:A:125:ILE:HG22	1:A:125:ILE:O	0.70	1.86	1	1
1:A:44:VAL:HG12	1:A:51:PHE:HA	0.69	1.64	6	9
1:A:39:ASN:O	1:A:43:LEU:HD12	0.67	1.89	8	10
1:A:101:LEU:HD21	1:A:127:LEU:H	0.67	1.48	8	1
1:A:74:PHE:CE1	1:A:75:MET:HG2	0.65	2.26	8	9
1:A:105:GLN:O	1:A:108:VAL:HG22	0.64	1.93	5	8
1:A:125:ILE:CG2	1:A:125:ILE:O	0.62	2.46	1	1
1:A:101:LEU:HD11	1:A:126:THR:C	0.62	2.14	8	1
1:A:71:THR:N	1:A:72:PRO:CD	0.61	2.64	8	10
1:A:74:PHE:CD1	1:A:75:MET:N	0.61	2.69	3	10
1:A:116:PHE:O	1:A:119:ILE:HG12	0.61	1.96	3	9
1:A:59:ILE:HG23	1:A:100:PHE:CE1	0.60	2.30	2	2
1:A:66:LEU:O	1:A:113:LEU:HD11	0.59	1.96	7	8
1:A:101:LEU:HD21	1:A:126:THR:CA	0.59	2.27	1	9
1:A:104:LEU:O	1:A:108:VAL:HG13	0.59	1.98	1	10
1:A:80:CYS:SG	1:A:81:ILE:N	0.59	2.75	8	9
1:A:62:ILE:HG13	1:A:80:CYS:SG	0.58	2.39	1	9
1:A:106:GLU:O	1:A:110:ILE:HD13	0.58	1.99	6	10
1:A:102:LYS:N	1:A:102:LYS:HE3	0.57	2.14	7	2
1:A:58:LEU:HB3	1:A:84:PHE:CZ	0.57	2.34	10	1
1:A:101:LEU:HD11	1:A:127:LEU:N	0.57	2.14	8	1
1:A:40:PHE:CD1	1:A:40:PHE:C	0.57	2.78	8	1
1:A:77:SER:HA	1:A:80:CYS:SG	0.57	2.40	10	1
1:A:114:ASN:HD22	1:A:114:ASN:N	0.56	1.98	7	1
1:A:126:THR:O	1:A:127:LEU:HD23	0.56	2.01	2	2
1:A:55:SER:O	1:A:59:ILE:HD12	0.56	2.01	6	1
1:A:102:LYS:HE3	1:A:102:LYS:N	0.56	2.15	6	1
1:A:100:PHE:CD1	1:A:104:LEU:HD23	0.55	2.36	9	1
1:A:113:LEU:HD22	1:A:113:LEU:N	0.55	2.17	10	7
1:A:117:TRP:O	1:A:121:VAL:HG13	0.55	2.02	3	10
1:A:126:THR:HG22	1:A:127:LEU:N	0.54	2.18	2	4
1:A:108:VAL:HG21	1:A:117:TRP:HB2	0.54	1.79	5	1
1:A:73:TYR:O	1:A:77:SER:N	0.54	2.41	10	10
1:A:113:LEU:N	1:A:113:LEU:HD22	0.54	2.18	7	3
1:A:71:THR:O	1:A:74:PHE:CD1	0.53	2.62	7	8
1:A:77:SER:O	1:A:81:ILE:HD12	0.53	2.03	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:PHE:HD1	1:A:100:PHE:O	0.53	1.87	2	1
1:A:65:PHE:CD1	1:A:73:TYR:HB2	0.53	2.38	4	10
1:A:126:THR:O	1:A:127:LEU:HG	0.52	2.04	8	5
1:A:104:LEU:HD12	1:A:105:GLN:N	0.52	2.20	9	10
1:A:116:PHE:O	1:A:120:VAL:HG23	0.52	2.04	1	1
1:A:40:PHE:CD2	1:A:58:LEU:HG	0.52	2.40	7	1
1:A:75:MET:O	1:A:78:ILE:HG22	0.52	2.05	10	9
1:A:39:ASN:O	1:A:42:VAL:HB	0.52	2.05	7	4
1:A:38:GLU:HA	1:A:41:ARG:NE	0.52	2.20	4	3
1:A:120:VAL:HB	1:A:125:ILE:HB	0.51	1.82	3	5
1:A:86:GLU:HG3	1:A:87:GLU:N	0.51	2.21	7	1
1:A:62:ILE:HD11	1:A:80:CYS:SG	0.51	2.47	10	1
1:A:73:TYR:O	1:A:77:SER:HB3	0.50	2.05	8	4
1:A:80:CYS:O	1:A:83:ALA:HB3	0.50	2.07	1	6
1:A:112:GLN:O	1:A:113:LEU:HD13	0.50	2.06	5	1
1:A:84:PHE:HB2	1:A:96:ARG:NH1	0.50	2.21	3	1
1:A:101:LEU:HD21	1:A:126:THR:C	0.50	2.26	5	3
1:A:74:PHE:CE1	1:A:75:MET:CG	0.50	2.95	7	1
1:A:101:LEU:HD21	1:A:127:LEU:N	0.50	2.19	8	1
1:A:114:ASN:HD22	1:A:114:ASN:H	0.49	1.49	7	1
1:A:66:LEU:HD13	1:A:107:LYS:NZ	0.49	2.22	8	1
1:A:74:PHE:HE1	1:A:75:MET:HG2	0.49	1.65	8	5
1:A:87:GLU:O	1:A:91:PHE:N	0.49	2.45	7	2
1:A:95:GLN:HA	1:A:98:ASN:HD21	0.49	1.67	7	2
1:A:58:LEU:HD12	1:A:84:PHE:HD2	0.49	1.67	8	1
1:A:74:PHE:HD1	1:A:75:MET:N	0.49	2.05	7	4
1:A:114:ASN:N	1:A:114:ASN:HD22	0.49	2.05	5	1
1:A:71:THR:N	1:A:72:PRO:HD2	0.49	2.21	4	4
1:A:81:ILE:HA	1:A:84:PHE:CZ	0.49	2.43	4	3
1:A:82:ARG:NH1	1:A:85:ARG:NH1	0.48	2.62	10	1
1:A:120:VAL:O	1:A:124:GLY:N	0.48	2.46	7	9
1:A:100:PHE:CD1	1:A:100:PHE:O	0.48	2.66	2	1
1:A:43:LEU:HD23	1:A:48:LYS:HB3	0.48	1.85	10	6
1:A:65:PHE:CD1	1:A:65:PHE:C	0.48	2.86	10	8
1:A:65:PHE:CZ	1:A:74:PHE:HA	0.48	2.44	3	10
1:A:104:LEU:HD12	1:A:104:LEU:C	0.48	2.28	4	3
1:A:40:PHE:CG	1:A:41:ARG:N	0.48	2.82	8	1
1:A:96:ARG:NH2	1:A:99:ASN:HD22	0.47	2.07	5	1
1:A:116:PHE:O	1:A:120:VAL:HG13	0.47	2.09	4	5
1:A:52:GLU:CG	1:A:53:GLU:N	0.47	2.77	4	10
1:A:76:LYS:NZ	1:A:76:LYS:HB3	0.47	2.25	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ILE:O	1:A:85:ARG:HB2	0.47	2.07	3	1
1:A:40:PHE:CE1	1:A:44:VAL:HG11	0.47	2.44	4	4
1:A:100:PHE:C	1:A:100:PHE:CD1	0.47	2.88	1	2
1:A:126:THR:O	1:A:127:LEU:O	0.47	2.32	3	5
1:A:41:ARG:O	1:A:44:VAL:HG22	0.47	2.09	10	5
1:A:100:PHE:CD1	1:A:100:PHE:C	0.47	2.88	4	3
1:A:40:PHE:CE1	1:A:84:PHE:CE2	0.47	3.03	8	1
1:A:76:LYS:HB3	1:A:76:LYS:NZ	0.47	2.25	4	1
1:A:96:ARG:C	1:A:96:ARG:HE	0.47	2.13	3	1
1:A:78:ILE:HG13	1:A:82:ARG:NH1	0.46	2.25	7	1
1:A:59:ILE:HG12	1:A:100:PHE:CD1	0.46	2.45	5	3
1:A:81:ILE:HG23	1:A:100:PHE:CE1	0.46	2.45	7	2
1:A:101:LEU:HD23	1:A:102:LYS:N	0.46	2.26	8	1
1:A:61:HIS:ND1	1:A:62:ILE:HG13	0.46	2.25	10	1
1:A:85:ARG:NH1	1:A:125:ILE:HG23	0.46	2.26	3	1
1:A:51:PHE:O	1:A:55:SER:OG	0.46	2.34	7	1
1:A:36:PRO:HG3	1:A:76:LYS:HD2	0.46	1.87	1	6
1:A:100:PHE:O	1:A:100:PHE:HD1	0.45	1.94	9	1
1:A:113:LEU:N	1:A:113:LEU:CD2	0.45	2.79	8	5
1:A:127:LEU:HD12	1:A:127:LEU:C	0.45	2.32	10	1
1:A:81:ILE:O	1:A:84:PHE:HB2	0.45	2.11	10	1
1:A:74:PHE:HD1	1:A:75:MET:H	0.45	1.55	9	5
1:A:101:LEU:O	1:A:105:GLN:HB3	0.45	2.11	10	2
1:A:68:THR:HG23	1:A:70:GLU:N	0.45	2.25	10	5
1:A:104:LEU:C	1:A:104:LEU:HD12	0.45	2.32	5	1
1:A:66:LEU:HD13	1:A:107:LYS:HZ1	0.45	1.72	8	1
1:A:38:GLU:HA	1:A:41:ARG:HE	0.45	1.72	4	3
1:A:81:ILE:HA	1:A:84:PHE:CE1	0.45	2.47	4	2
1:A:113:LEU:CD2	1:A:113:LEU:N	0.44	2.80	6	4
1:A:76:LYS:HZ3	1:A:76:LYS:HB3	0.44	1.71	8	2
1:A:58:LEU:HD12	1:A:84:PHE:CD1	0.44	2.48	7	1
1:A:65:PHE:CG	1:A:66:LEU:N	0.44	2.84	10	8
1:A:105:GLN:NE2	1:A:108:VAL:HG22	0.44	2.28	6	1
1:A:40:PHE:CZ	1:A:84:PHE:HB3	0.44	2.48	3	1
1:A:41:ARG:HA	1:A:44:VAL:HG22	0.44	1.90	8	2
1:A:81:ILE:HG13	1:A:100:PHE:CZ	0.44	2.47	5	2
1:A:73:TYR:O	1:A:76:LYS:NZ	0.44	2.51	8	3
1:A:101:LEU:HD11	1:A:126:THR:CA	0.44	2.43	8	1
1:A:36:PRO:HB2	1:A:61:HIS:NE2	0.44	2.28	2	4
1:A:64:GLN:O	1:A:67:ASP:HB3	0.43	2.13	8	7
1:A:65:PHE:C	1:A:65:PHE:CD1	0.43	2.88	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:82:ARG:HE	1:A:125:ILE:HD11	0.43	1.73	1	1
1:A:55:SER:HA	1:A:84:PHE:CE2	0.43	2.48	8	1
1:A:118:GLU:O	1:A:121:VAL:HG22	0.43	2.12	6	2
1:A:58:LEU:O	1:A:62:ILE:HG12	0.43	2.14	7	1
1:A:115:HIS:O	1:A:118:GLU:HB2	0.43	2.14	8	8
1:A:55:SER:CB	1:A:84:PHE:CZ	0.43	3.01	8	1
1:A:114:ASN:O	1:A:118:GLU:HG2	0.43	2.14	4	6
1:A:79:ASP:O	1:A:82:ARG:HB2	0.43	2.14	10	1
1:A:41:ARG:HG2	1:A:87:GLU:HG3	0.43	1.91	7	1
1:A:41:ARG:NH2	1:A:83:ALA:HA	0.43	2.29	7	1
1:A:65:PHE:O	1:A:68:THR:N	0.43	2.52	10	3
1:A:100:PHE:O	1:A:104:LEU:HD23	0.43	2.14	8	1
1:A:81:ILE:O	1:A:85:ARG:HG3	0.43	2.14	10	1
1:A:111:LYS:HB3	1:A:113:LEU:HD23	0.43	1.91	2	1
1:A:126:THR:HG22	1:A:127:LEU:H	0.43	1.73	5	1
1:A:117:TRP:O	1:A:120:VAL:HB	0.43	2.14	1	1
1:A:104:LEU:HD13	1:A:116:PHE:CE2	0.42	2.49	1	2
1:A:41:ARG:HH21	1:A:83:ALA:HA	0.42	1.73	2	1
1:A:59:ILE:HG12	1:A:100:PHE:CE1	0.42	2.48	5	1
1:A:101:LEU:HD11	1:A:126:THR:HA	0.42	1.90	3	2
1:A:97:PHE:O	1:A:101:LEU:HB3	0.42	2.14	8	1
1:A:101:LEU:HD11	1:A:125:ILE:O	0.42	2.14	4	1
1:A:96:ARG:HH21	1:A:97:PHE:HA	0.42	1.73	3	1
1:A:73:TYR:HA	1:A:76:LYS:HB3	0.42	1.90	10	5
1:A:36:PRO:HG3	1:A:76:LYS:HE3	0.42	1.92	8	1
1:A:82:ARG:O	1:A:86:GLU:HG2	0.42	2.15	7	1
1:A:42:VAL:O	1:A:46:GLN:N	0.42	2.53	7	1
1:A:86:GLU:O	1:A:90:LYS:HE2	0.42	2.15	10	1
1:A:100:PHE:HD1	1:A:104:LEU:HD23	0.42	1.74	4	1
1:A:103:ALA:HA	1:A:106:GLU:HG2	0.42	1.92	4	5
1:A:40:PHE:O	1:A:44:VAL:HG13	0.42	2.15	10	2
1:A:104:LEU:HA	1:A:107:LYS:NZ	0.42	2.30	7	1
1:A:59:ILE:HG12	1:A:100:PHE:CG	0.42	2.49	9	1
1:A:63:GLU:HG2	1:A:107:LYS:NZ	0.41	2.30	3	2
1:A:124:GLY:O	1:A:125:ILE:HD13	0.41	2.15	6	2
1:A:114:ASN:N	1:A:114:ASN:ND2	0.41	2.68	7	1
1:A:78:ILE:O	1:A:82:ARG:HD3	0.41	2.16	10	1
1:A:42:VAL:HA	1:A:45:LYS:HG2	0.41	1.93	7	3
1:A:126:THR:CG2	1:A:127:LEU:N	0.41	2.83	2	1
1:A:81:ILE:HG21	1:A:125:ILE:CG2	0.41	2.46	2	1
1:A:40:PHE:CE2	1:A:41:ARG:HG3	0.41	2.50	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:101:LEU:HD23	1:A:102:LYS:HD2	0.41	1.92	8	1
1:A:74:PHE:CD2	1:A:119:ILE:HD13	0.41	2.51	3	1
1:A:106:GLU:O	1:A:109:GLU:HB3	0.41	2.16	3	1
1:A:100:PHE:O	1:A:100:PHE:CD1	0.41	2.73	5	1
1:A:40:PHE:CD1	1:A:84:PHE:CE2	0.41	3.08	8	1
1:A:89:ILE:HG22	1:A:90:LYS:HD3	0.41	1.91	7	1
1:A:59:ILE:HG12	1:A:100:PHE:CD2	0.41	2.50	9	1
1:A:127:LEU:C	1:A:127:LEU:HD12	0.41	2.35	8	1
1:A:59:ILE:HG13	1:A:84:PHE:CE2	0.41	2.51	10	1
1:A:97:PHE:HA	1:A:100:PHE:CE2	0.41	2.51	1	1
1:A:56:ASN:O	1:A:60:ASN:HB2	0.41	2.16	8	1
1:A:49:ALA:HB1	1:A:53:GLU:HB2	0.41	1.92	4	1
1:A:42:VAL:O	1:A:46:GLN:HG2	0.40	2.16	7	1
1:A:97:PHE:HA	1:A:100:PHE:CD2	0.40	2.51	4	1
1:A:66:LEU:CD2	1:A:113:LEU:HD12	0.40	2.46	3	1
1:A:98:ASN:O	1:A:102:LYS:HG2	0.40	2.16	3	1
1:A:74:PHE:HE1	1:A:75:MET:CG	0.40	2.28	7	1
1:A:59:ILE:O	1:A:62:ILE:HB	0.40	2.16	9	1
1:A:96:ARG:NH2	1:A:100:PHE:CD2	0.40	2.89	3	1
1:A:40:PHE:HB2	1:A:84:PHE:CE1	0.40	2.51	7	1
1:A:112:GLN:O	1:A:113:LEU:HB2	0.40	2.17	6	1
1:A:95:GLN:HA	1:A:98:ASN:OD1	0.40	2.17	4	1
1:A:51:PHE:CE2	1:A:96:ARG:NH1	0.40	2.90	3	1

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	92/152 (61%)	82±2 (89±2%)	8±1 (9±1%)	3±1 (3±1%)	10	44
All	All	920/1520 (61%)	815 (89%)	79 (9%)	26 (3%)	10	44

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	127	LEU	10
1	A	48	LYS	9
1	A	112	GLN	3
1	A	49	ALA	2
1	A	92	SER	2

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	85/134 (63%)	65±2 (77±2%)	20±2 (23±2%)	3	29
All	All	850/1340 (63%)	652 (77%)	198 (23%)	3	29

All 45 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	74	PHE	10
1	A	61	HIS	10
1	A	65	PHE	10
1	A	121	VAL	10
1	A	80	CYS	10
1	A	96	ARG	10
1	A	58	LEU	10
1	A	40	PHE	9
1	A	101	LEU	9
1	A	75	MET	9
1	A	108	VAL	8
1	A	84	PHE	8
1	A	89	ILE	7
1	A	82	ARG	6
1	A	79	ASP	5
1	A	127	LEU	5
1	A	109	GLU	4
1	A	87	GLU	4
1	A	47	LYS	4
1	A	105	GLN	4
1	A	76	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	48	LYS	3
1	A	64	GLN	3
1	A	100	PHE	3
1	A	41	ARG	3
1	A	102	LYS	3
1	A	107	LYS	2
1	A	39	ASN	2
1	A	53	GLU	2
1	A	57	GLN	2
1	A	99	ASN	2
1	A	94	GLU	2
1	A	38	GLU	2
1	A	114	ASN	2
1	A	81	ILE	1
1	A	117	TRP	1
1	A	90	LYS	1
1	A	97	PHE	1
1	A	56	ASN	1
1	A	93	GLU	1
1	A	126	THR	1
1	A	125	ILE	1
1	A	122	GLN	1
1	A	55	SER	1
1	A	115	HIS	1

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 86% for the well-defined parts and 82% for the entire structure.

7.1   Chemical shift list 1

File name: BMRB entry 5907

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	1733
Number of shifts mapped to atoms	1733
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2   Chemical shift referencing   ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	146	-0.91 ± 0.10	Should be applied
$^{13}C_\beta$	140	-0.19 ± 0.15	None needed (< 0.5 ppm)
$^{13}C'$	146	-0.47 ± 0.13	None needed (< 0.5 ppm)
^{15}N	139	0.43 ± 0.25	None needed (< 0.5 ppm)

7.1.3   Completeness of resonance assignments   ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 86%, i.e. 1059 atoms were assigned a chemical shift out of a possible 1233. 10 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	453/456 (99%)	181/182 (99%)	184/184 (100%)	88/90 (98%)
Sidechain	575/660 (87%)	354/387 (91%)	207/239 (87%)	14/34 (41%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	31/117 (26%)	31/63 (49%)	0/49 (0%)	0/5 (0%)
Overall	1059/1233 (86%)	566/632 (90%)	391/472 (83%)	102/129 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1581 atoms were assigned a chemical shift out of a possible 1924. 13 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	718/754 (95%)	287/301 (95%)	292/304 (96%)	139/149 (93%)
Sidechain	826/979 (84%)	508/575 (88%)	302/361 (84%)	16/43 (37%)
Aromatic	37/191 (19%)	37/101 (37%)	0/71 (0%)	0/19 (0%)
Overall	1581/1924 (82%)	832/977 (85%)	594/736 (81%)	155/211 (73%)

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	25	GLU	HG2	0.00	3.33 − 1.23	-10.9
1	A	25	GLU	HG3	0.00	3.31 − 1.21	-10.8
1	A	93	GLU	HB3	0.51	3.10 − 0.90	-6.8

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: