Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 11:33 PM BST

PDB ID	:	2KH9
Title	:	Solution structure of yeast Prp24-RRM2 bound to a fragment of U6 RNA
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Deposited on	:	2009-03-27

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 (i) symbol.

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

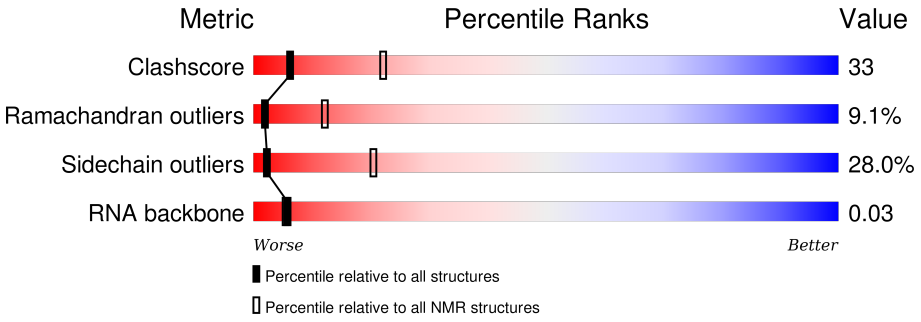
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 82%.

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
RNA backbone	3027	600

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	92	28% 32% 15% 18% 7%
2	B	6	33% 67%

2 Ensemble composition and analysis

This entry contains 10 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:117-A:150, A:159-A:193 (69)	0.25	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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1612 atoms, of which 782 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called U4/U6 snRNA-associated-splicing factor PRP24.

Mol	Chain	Residues	Atoms						Trace
1	A	86	Total	C	H	N	O	S	0
			1416	445	715	120	132	4	

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	MET	-	EXPRESSION TAG	UNP P49960
A	198	LEU	-	EXPRESSION TAG	UNP P49960
A	199	GLU	-	EXPRESSION TAG	UNP P49960
A	200	HIS	-	EXPRESSION TAG	UNP P49960
A	201	HIS	-	EXPRESSION TAG	UNP P49960
A	202	HIS	-	EXPRESSION TAG	UNP P49960
A	203	HIS	-	EXPRESSION TAG	UNP P49960
A	204	HIS	-	EXPRESSION TAG	UNP P49960
A	205	HIS	-	EXPRESSION TAG	UNP P49960

- Molecule 2 is a RNA chain called 5'-R(*AP*GP*AP*GP*AP*U)-3'.

Mol	Chain	Residues	Atoms						Trace
2	B	6	Total	C	H	N	O	P	0
			196	59	67	27	38	5	

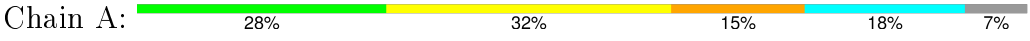
4 Residue-property plots (i)

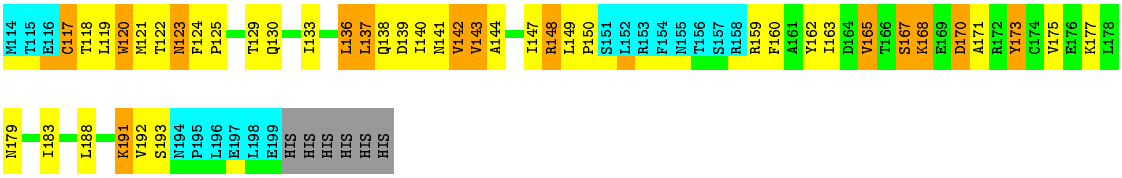
4.1 Average score per residue in the NMR ensemble

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: U4/U6 snRNA-associated-splicing factor PRP24

Chain A:





- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'

Chain B:

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: U4/U6 snRNA-associated-splicing factor PRP24

Chain A:

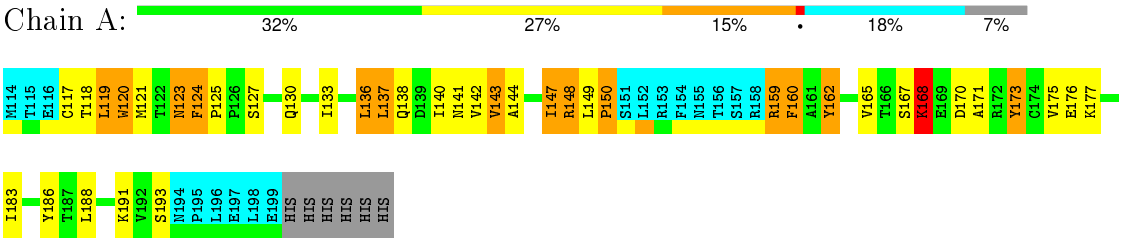
- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'

Chain B:

4.2.2 Score per residue for model 2

- Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24

Chain A:



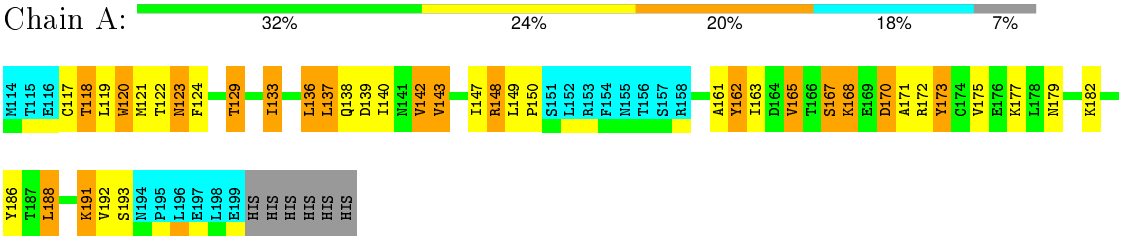
- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'

Chain B:

4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24

Chain A:



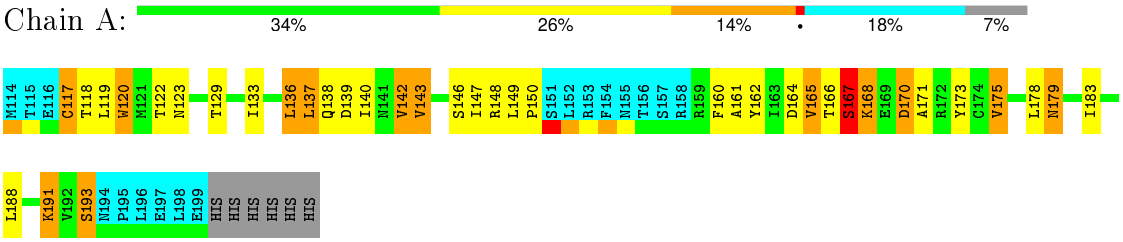
- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'

Chain B:

4.2.4 Score per residue for model 4

- Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24

Chain A:



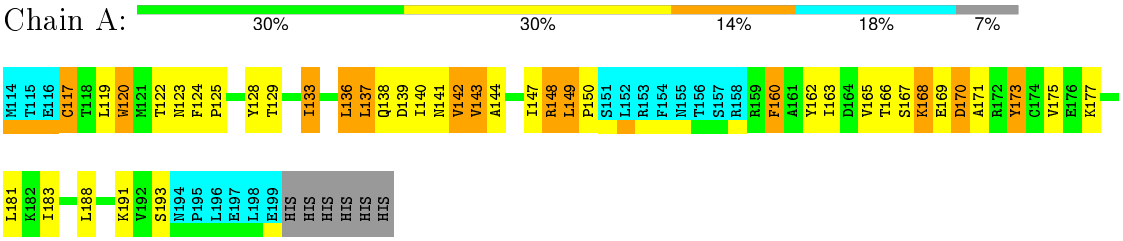
• Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'

Chain B:

4.2.5 Score per residue for model 5

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24

Chain A:



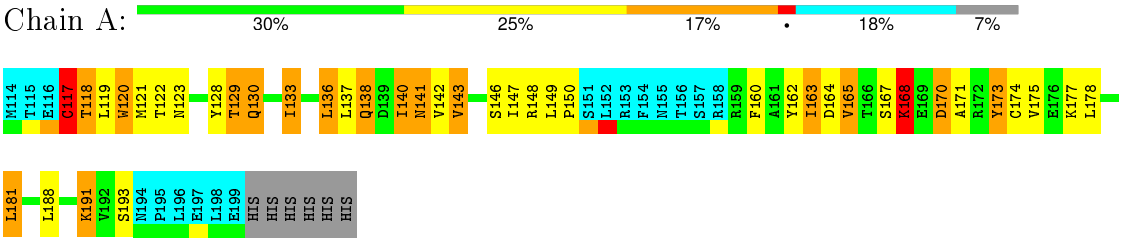
• Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'

Chain B:

4.2.6 Score per residue for model 6

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24

Chain A:



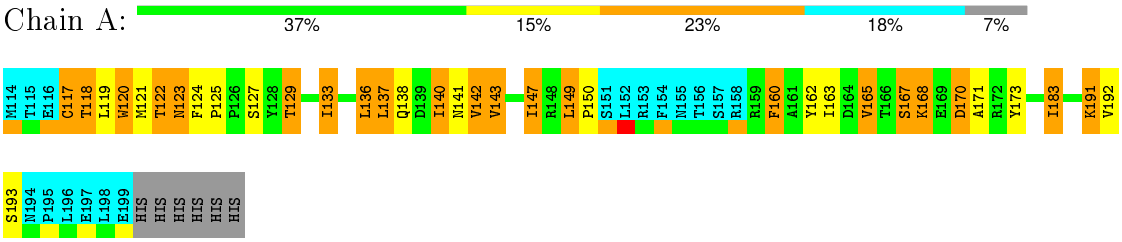
• Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'

Chain B:

4.2.7 Score per residue for model 7

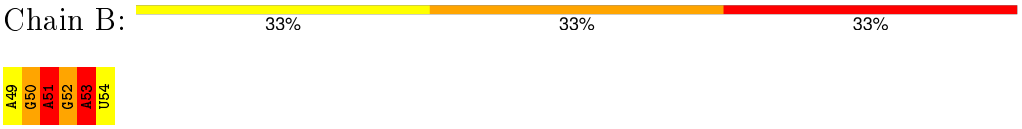
- Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24

Chain A:



- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'

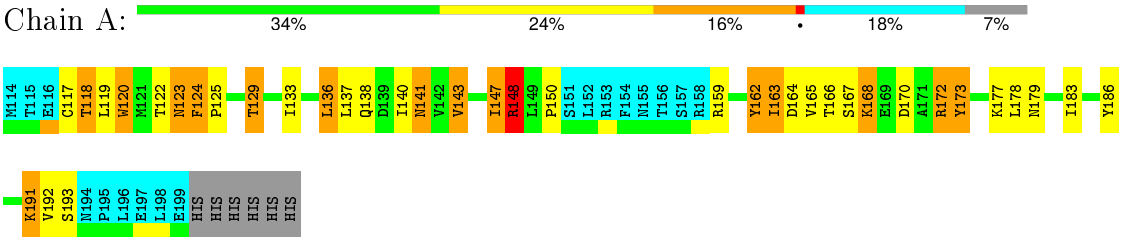
Chain B:



4.2.8 Score per residue for model 8

- Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24

Chain A:

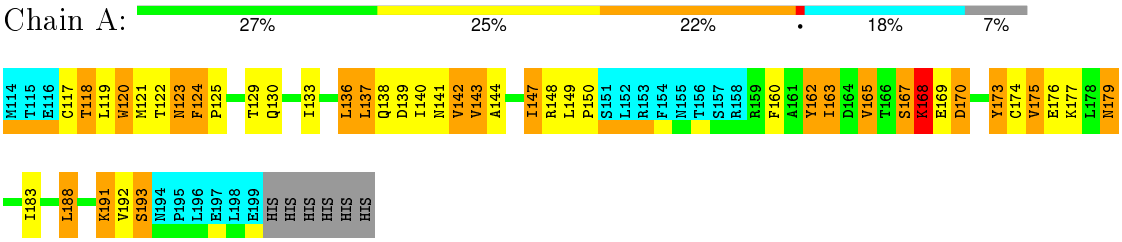


- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'

Chain B:

4.2.9 Score per residue for model 9

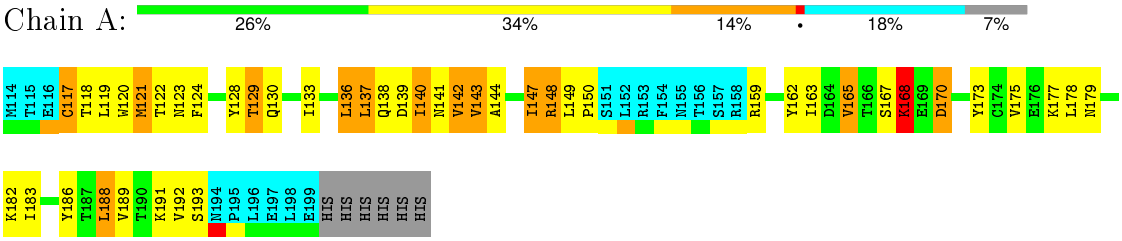
- Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



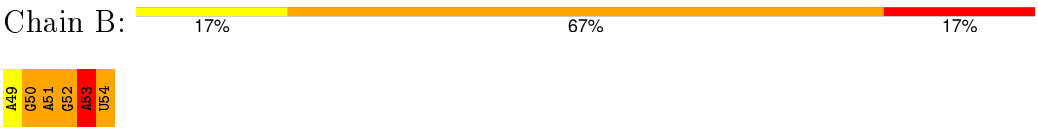
- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'

4.2.10 Score per residue for model 10

- Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, torsion angle dynamics*.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
AMBER	refinement	
AtnosCandid	structure solution	
CNS	structure solution	
HADDOCK	refinement	2
HADDOCK	structure solution	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 16243, BMRB entry 16230, BMRB entry 162
Number of chemical shift lists	
Total number of shifts	
Number of shifts mapped to atoms	
Number of unparsed shifts	
Number of shifts with mapping errors	
Number of shifts with mapping warnings	
Assignment completeness (well-defined parts)	

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

6 Model quality

6.1 Standard geometry

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	0.57±0.03	0±0/571 (0.0±0.0%)	0.79±0.04	1±1/777 (0.1±0.1%)
2	B	0.54±0.08	0±0/145 (0.0±0.0%)	1.16±0.11	1±1/225 (0.5±0.6%)
All	All	0.57	0/7160 (0.0%)	0.89	17/10020 (0.2%)

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
2	B	0.0±0.0	0.4±0.7
All	All	0	4

There are no bond-length outliers.

All unique angle 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	52	G	C3'-C2'-C1'	-9.59	93.83	101.50	3	1
2	B	51	A	C3'-C2'-C1'	-7.02	95.88	101.50	9	3
1	A	162	TYR	CB-CG-CD2	-6.77	116.94	121.00	8	4
2	B	51	A	O4'-C1'-N9	6.21	113.17	108.20	7	2
2	B	52	G	C5'-C4'-C3'	-5.75	106.80	116.00	8	1
1	A	148	ARG	NE-CZ-NH1	5.51	123.06	120.30	8	1
2	B	53	A	O4'-C1'-C2'	-5.37	100.43	105.80	10	1
2	B	51	A	C4-N9-C1'	-5.35	116.67	126.30	7	1
2	B	51	A	O4'-C1'-C2'	-5.34	100.46	105.80	9	1
1	A	162	TYR	CB-CG-CD1	5.19	124.11	121.00	8	1
2	B	51	A	C8-N9-C1'	5.18	137.03	127.70	7	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	53	A	Sidechain	3
2	B	54	U	Sidechain	1

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	560	575	575	36±5
2	B	129	67	67	12±5
All	All	6890	6420	6420	442

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 33.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:52:G:H3'	2:B:53:A:O4'	0.97	1.59	3	1
2:B:53:A:O3'	2:B:54:U:H2'	0.96	1.59	3	1
2:B:52:G:H5'	2:B:53:A:N7	0.91	1.79	8	1
1:A:138:GLN:HB2	1:A:143:VAL:HA	0.85	1.46	6	10
1:A:137:LEU:HD13	1:A:163:ILE:HG21	0.84	1.48	7	5
1:A:120:TRP:CZ2	1:A:193:SER:HA	0.80	2.12	9	9
2:B:53:A:O2'	2:B:54:U:C5	0.78	2.36	9	1
1:A:138:GLN:HA	1:A:143:VAL:N	0.78	1.92	9	8
1:A:150:PRO:HG3	1:A:162:TYR:CE2	0.77	2.13	4	6
2:B:52:G:H2'	2:B:54:U:O4	0.76	1.80	3	1
2:B:52:G:O2'	2:B:54:U:H5	0.76	1.64	2	1
1:A:138:GLN:CB	1:A:143:VAL:HA	0.75	2.11	8	10
2:B:53:A:N3	2:B:54:U:C4	0.75	2.55	9	1
2:B:51:A:C2	2:B:52:G:N7	0.74	2.56	8	7
1:A:138:GLN:HB2	1:A:143:VAL:CA	0.74	2.12	6	2
1:A:150:PRO:HG2	1:A:160:PHE:CE2	0.71	2.20	4	2
1:A:129:THR:O	1:A:133:ILE:HB	0.70	1.87	7	7
2:B:52:G:H4'	2:B:53:A:C4	0.70	2.20	3	1
1:A:136:LEU:O	1:A:140:ILE:HB	0.70	1.85	2	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:PRO:HB2	2:B:53:A:C6	0.70	2.21	2	1
1:A:148:ARG:HG3	2:B:52:G:C5	0.68	2.23	2	3
1:A:125:PRO:HD2	1:A:183:ILE:CG2	0.68	2.19	2	3
2:B:52:G:C3'	2:B:53:A:O4'	0.68	2.40	3	1
2:B:52:G:H4'	2:B:54:U:O4	0.68	1.89	7	1
2:B:51:A:H2	2:B:52:G:N7	0.68	1.87	6	8
1:A:150:PRO:HG2	1:A:160:PHE:CE1	0.67	2.24	5	1
1:A:138:GLN:HB2	1:A:143:VAL:N	0.67	2.05	6	2
1:A:165:VAL:HG11	1:A:170:ASP:HB2	0.67	1.67	9	8
1:A:137:LEU:HD12	1:A:141:ASN:OD1	0.67	1.90	2	1
1:A:165:VAL:CG1	1:A:170:ASP:HB2	0.66	2.20	9	9
2:B:51:A:O2'	2:B:52:G:H5'	0.66	1.91	10	1
1:A:148:ARG:HG2	2:B:52:G:C8	0.66	2.25	10	2
1:A:167:SER:O	1:A:168:LYS:HB2	0.66	1.90	1	6
1:A:141:ASN:O	1:A:170:ASP:HB3	0.64	1.91	7	7
1:A:149:LEU:HG	1:A:149:LEU:O	0.63	1.93	6	2
1:A:148:ARG:O	1:A:150:PRO:HD3	0.63	1.94	4	5
1:A:119:LEU:HD21	1:A:171:ALA:O	0.62	1.95	5	7
2:B:52:G:O5'	2:B:53:A:C5	0.62	2.52	7	1
1:A:133:ILE:O	1:A:137:LEU:HB2	0.61	1.95	5	8
1:A:148:ARG:HG3	2:B:52:G:C4	0.60	2.30	3	2
1:A:138:GLN:HA	1:A:142:VAL:C	0.60	2.16	5	7
1:A:136:LEU:HD21	1:A:178:LEU:HD11	0.60	1.73	4	1
2:B:52:G:C5'	2:B:53:A:N7	0.60	2.62	8	1
1:A:150:PRO:HA	2:B:53:A:C2	0.59	2.31	4	3
2:B:53:A:C2	2:B:54:U:C4	0.59	2.90	9	1
1:A:167:SER:O	1:A:168:LYS:HE3	0.59	1.97	6	1
1:A:119:LEU:HD11	1:A:171:ALA:HA	0.59	1.74	2	3
1:A:125:PRO:HD2	1:A:183:ILE:HG23	0.59	1.73	2	2
1:A:130:GLN:NE2	1:A:149:LEU:HD22	0.59	2.13	9	1
1:A:150:PRO:O	2:B:53:A:N6	0.59	2.36	3	1
1:A:148:ARG:CG	1:A:148:ARG:HH11	0.58	2.11	8	1
1:A:138:GLN:HA	1:A:143:VAL:H	0.58	1.57	8	2
1:A:138:GLN:HB2	1:A:143:VAL:H	0.58	1.58	6	1
1:A:136:LEU:HD11	1:A:178:LEU:HD11	0.58	1.75	10	1
2:B:52:G:O3'	2:B:53:A:C8	0.58	2.56	3	2
2:B:52:G:H3'	2:B:53:A:C1'	0.58	2.27	3	1
1:A:137:LEU:CD1	1:A:163:ILE:HG21	0.58	2.28	6	2
1:A:137:LEU:HB3	1:A:144:ALA:HB2	0.58	1.75	2	5
1:A:175:VAL:O	1:A:179:ASN:HB3	0.58	1.98	4	2
1:A:150:PRO:HB2	2:B:54:U:O4	0.58	1.99	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:ILE:O	1:A:137:LEU:HG	0.57	1.98	8	1
1:A:150:PRO:HD2	1:A:160:PHE:O	0.57	2.00	4	3
1:A:148:ARG:HD3	2:B:53:A:N6	0.56	2.14	4	3
1:A:120:TRP:CD1	1:A:191:LYS:HB3	0.56	2.35	9	5
2:B:52:G:H5'	2:B:53:A:C8	0.56	2.35	8	1
1:A:160:PHE:HZ	1:A:162:TYR:CE1	0.55	2.18	9	2
2:B:53:A:O2'	2:B:54:U:C2'	0.54	2.55	3	1
2:B:52:G:C5'	2:B:53:A:C5	0.54	2.90	7	1
1:A:149:LEU:H	1:A:149:LEU:HD23	0.54	1.61	5	3
1:A:148:ARG:HD2	2:B:52:G:C4	0.54	2.38	4	3
1:A:125:PRO:CD	1:A:183:ILE:HG23	0.53	2.33	2	2
1:A:165:VAL:HG21	1:A:171:ALA:HA	0.53	1.79	6	2
1:A:138:GLN:CA	1:A:143:VAL:H	0.53	2.16	6	2
1:A:150:PRO:HG2	1:A:160:PHE:CZ	0.53	2.39	4	2
1:A:124:PHE:O	1:A:159:ARG:HD2	0.53	2.04	1	2
1:A:137:LEU:O	1:A:141:ASN:N	0.53	2.39	8	2
2:B:52:G:H5"	2:B:53:A:C5	0.52	2.39	7	1
2:B:51:A:O2'	2:B:52:G:OP2	0.52	2.26	9	1
1:A:137:LEU:O	1:A:141:ASN:HB2	0.52	2.04	7	4
1:A:148:ARG:HD2	2:B:52:G:C5	0.52	2.39	1	2
1:A:168:LYS:HE3	1:A:192:VAL:HG21	0.52	1.81	8	2
1:A:160:PHE:CZ	1:A:162:TYR:CE1	0.52	2.97	9	2
1:A:147:ILE:O	1:A:147:ILE:HG13	0.52	2.05	7	3
1:A:162:TYR:CG	2:B:51:A:C2	0.52	2.98	5	4
1:A:173:TYR:O	1:A:177:LYS:HG2	0.52	2.05	10	7
1:A:183:ILE:HG22	1:A:186:TYR:O	0.51	2.05	8	2
1:A:149:LEU:H	1:A:149:LEU:CD2	0.51	2.18	7	1
1:A:138:GLN:CA	1:A:143:VAL:N	0.51	2.74	5	8
1:A:169:GLU:O	1:A:173:TYR:HB2	0.51	2.04	9	3
1:A:192:VAL:HG22	1:A:193:SER:H	0.51	1.65	10	1
2:B:49:A:C2'	2:B:50:G:O5'	0.51	2.59	2	9
1:A:149:LEU:O	1:A:149:LEU:HG	0.51	2.07	9	2
1:A:138:GLN:CB	1:A:143:VAL:H	0.51	2.18	6	1
1:A:128:TYR:O	1:A:129:THR:CB	0.51	2.58	6	1
1:A:162:TYR:CD2	2:B:51:A:C2	0.50	2.99	5	6
1:A:118:THR:O	1:A:193:SER:HB2	0.50	2.06	7	3
1:A:119:LEU:HD13	1:A:174:CYS:SG	0.50	2.45	9	2
1:A:148:ARG:HH11	1:A:148:ARG:CG	0.50	2.20	5	1
1:A:150:PRO:HB3	2:B:52:G:H5'	0.50	1.82	7	1
2:B:52:G:C5'	2:B:53:A:C6	0.50	2.95	7	1
1:A:118:THR:HG21	2:B:51:A:N1	0.50	2.22	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:LEU:CB	1:A:144:ALA:HB2	0.50	2.37	2	1
1:A:148:ARG:CG	1:A:162:TYR:HB2	0.50	2.36	1	1
1:A:149:LEU:HD23	1:A:149:LEU:H	0.50	1.67	1	2
2:B:52:G:O5'	2:B:53:A:C6	0.50	2.65	7	1
1:A:191:LYS:HE2	1:A:192:VAL:O	0.50	2.07	9	2
1:A:138:GLN:O	1:A:142:VAL:HA	0.49	2.07	9	5
2:B:52:G:H2'	2:B:54:U:C4	0.49	2.41	3	1
2:B:53:A:O2'	2:B:54:U:O2'	0.49	2.30	3	1
1:A:124:PHE:CE1	1:A:128:TYR:HB2	0.49	2.42	10	2
1:A:133:ILE:O	1:A:137:LEU:HD22	0.49	2.07	2	2
1:A:123:ASN:O	1:A:124:PHE:HB3	0.49	2.07	9	5
1:A:192:VAL:HG22	1:A:193:SER:N	0.49	2.23	10	2
1:A:150:PRO:HA	2:B:53:A:N3	0.49	2.22	5	1
1:A:122:THR:HG23	1:A:160:PHE:HB2	0.48	1.84	1	1
2:B:53:A:O3'	2:B:54:U:C2'	0.48	2.49	3	1
1:A:130:GLN:O	1:A:133:ILE:HG22	0.48	2.07	2	1
1:A:137:LEU:HD12	1:A:163:ILE:HG21	0.48	1.84	6	1
1:A:147:ILE:HG22	1:A:163:ILE:HG23	0.48	1.85	10	1
2:B:52:G:P	2:B:53:A:N7	0.48	2.87	2	1
2:B:52:G:O5'	2:B:53:A:N7	0.48	2.47	7	2
1:A:183:ILE:HG23	1:A:183:ILE:O	0.48	2.09	2	1
2:B:53:A:C2	2:B:54:U:N3	0.48	2.81	9	1
2:B:53:A:O2'	2:B:54:U:C6	0.47	2.48	7	2
2:B:52:G:O2'	2:B:54:U:C5	0.47	2.48	2	1
1:A:138:GLN:HG3	1:A:139:ASP:N	0.47	2.21	9	5
2:B:54:U:C2'	2:B:54:U:O2	0.47	2.63	2	1
1:A:167:SER:O	1:A:168:LYS:CB	0.47	2.63	1	1
1:A:121:MET:HA	1:A:189:VAL:O	0.47	2.10	10	1
1:A:160:PHE:HE2	1:A:162:TYR:HH	0.47	1.53	1	1
1:A:130:GLN:HA	1:A:147:ILE:HD11	0.46	1.85	10	1
1:A:117:CYS:HB3	1:A:167:SER:O	0.46	2.10	5	1
1:A:129:THR:HG22	1:A:130:GLN:N	0.46	2.25	6	1
1:A:129:THR:CG2	1:A:149:LEU:HD13	0.46	2.41	6	1
1:A:148:ARG:HG3	1:A:148:ARG:HH11	0.46	1.70	8	1
2:B:52:G:H1'	2:B:53:A:C5	0.46	2.46	1	1
1:A:148:ARG:HH11	1:A:148:ARG:HG3	0.46	1.71	5	1
1:A:124:PHE:HB3	1:A:188:LEU:HG	0.46	1.88	9	3
2:B:53:A:C2	2:B:54:U:O4	0.46	2.69	9	1
1:A:146:SER:H	1:A:164:ASP:HB3	0.46	1.71	6	2
2:B:51:A:O3'	2:B:53:A:N6	0.45	2.49	7	1
1:A:165:VAL:HG12	1:A:166:THR:N	0.45	2.26	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:51:A:C3'	2:B:53:A:N6	0.45	2.79	7	1
1:A:136:LEU:O	1:A:140:ILE:HG12	0.45	2.12	10	1
1:A:118:THR:CB	2:B:51:A:H61	0.45	2.25	9	1
1:A:125:PRO:HD2	1:A:183:ILE:HD12	0.44	1.89	9	2
2:B:52:G:C8	2:B:52:G:OP2	0.44	2.70	7	1
1:A:117:CYS:O	1:A:165:VAL:HG23	0.44	2.13	7	1
1:A:148:ARG:NE	2:B:53:A:N6	0.44	2.65	10	1
1:A:182:LYS:HA	1:A:186:TYR:O	0.44	2.13	10	2
1:A:136:LEU:HD12	1:A:140:ILE:HD12	0.44	1.88	5	1
2:B:53:A:C3'	2:B:54:U:H2'	0.44	2.41	3	1
1:A:141:ASN:C	1:A:141:ASN:HD22	0.44	2.16	6	1
1:A:183:ILE:HD13	1:A:188:LEU:HD11	0.44	1.88	2	1
1:A:136:LEU:HD23	1:A:137:LEU:HD13	0.44	1.89	4	1
1:A:162:TYR:CZ	2:B:51:A:H1'	0.44	2.48	5	2
1:A:130:GLN:HG2	1:A:147:ILE:HD11	0.43	1.91	2	1
1:A:144:ALA:HB1	1:A:163:ILE:CG2	0.43	2.43	10	1
1:A:162:TYR:CE2	2:B:51:A:N3	0.43	2.86	4	2
1:A:122:THR:HG23	1:A:160:PHE:CD1	0.43	2.49	7	1
2:B:53:A:O2'	2:B:54:U:H6	0.43	1.97	10	1
2:B:52:G:OP1	2:B:53:A:N6	0.43	2.51	9	1
1:A:137:LEU:O	1:A:141:ASN:C	0.43	2.57	5	1
2:B:53:A:P	2:B:53:A:O4'	0.43	2.76	3	1
1:A:133:ILE:O	1:A:137:LEU:HD12	0.43	2.14	1	1
1:A:191:LYS:HD3	2:B:50:G:N7	0.43	2.29	3	3
2:B:53:A:O2'	2:B:54:U:O4'	0.43	2.37	7	1
1:A:130:GLN:HA	1:A:147:ILE:CD1	0.43	2.43	10	1
1:A:121:MET:SD	1:A:133:ILE:HD11	0.43	2.54	3	2
2:B:53:A:O2'	2:B:54:U:H5	0.42	1.93	9	1
1:A:147:ILE:HB	1:A:163:ILE:HG23	0.42	1.91	9	1
2:B:53:A:N3	2:B:54:U:N3	0.42	2.67	9	1
1:A:168:LYS:O	1:A:172:ARG:HB2	0.42	2.13	8	1
1:A:136:LEU:CD1	1:A:178:LEU:HD21	0.42	2.44	8	2
2:B:51:A:H3'	2:B:53:A:H62	0.42	1.73	7	1
1:A:148:ARG:NH1	1:A:148:ARG:CG	0.42	2.82	5	1
1:A:138:GLN:CB	1:A:143:VAL:CA	0.42	2.91	8	1
1:A:149:LEU:HG	1:A:161:ALA:HB2	0.42	1.91	3	1
2:B:53:A:O5'	2:B:53:A:H8	0.42	1.98	3	1
1:A:160:PHE:HE2	1:A:162:TYR:OH	0.42	1.98	1	1
1:A:141:ASN:O	1:A:142:VAL:HB	0.41	2.15	9	2
1:A:136:LEU:HD11	1:A:178:LEU:HD21	0.41	1.92	8	1
2:B:53:A:O2'	2:B:54:U:H2'	0.41	2.14	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:ARG:HD3	2:B:52:G:H1'	0.41	1.92	9	1
2:B:52:G:O2'	2:B:53:A:C8	0.41	2.72	10	2
1:A:141:ASN:ND2	1:A:141:ASN:C	0.41	2.74	6	1
1:A:148:ARG:O	1:A:162:TYR:N	0.41	2.45	4	1
1:A:128:TYR:O	1:A:129:THR:HB	0.41	2.14	6	1
1:A:168:LYS:HE2	1:A:172:ARG:HB2	0.41	1.92	1	1
2:B:51:A:O2'	2:B:52:G:P	0.41	2.78	9	1
1:A:137:LEU:HD11	1:A:163:ILE:HD13	0.41	1.92	6	1
1:A:183:ILE:HG21	1:A:188:LEU:CD1	0.41	2.45	2	1
1:A:165:VAL:HG11	1:A:170:ASP:CB	0.41	2.45	8	1
1:A:148:ARG:CB	2:B:52:G:C8	0.41	3.04	3	1
1:A:133:ILE:O	1:A:137:LEU:N	0.41	2.53	4	1
1:A:148:ARG:CG	1:A:148:ARG:NH1	0.41	2.79	8	1
1:A:150:PRO:HD2	1:A:161:ALA:HA	0.41	1.91	4	1
2:B:52:G:N3	2:B:54:U:O4	0.40	2.54	2	1
1:A:150:PRO:CD	1:A:161:ALA:HA	0.40	2.46	4	1
1:A:125:PRO:HD2	1:A:183:ILE:HG21	0.40	1.92	2	1
2:B:49:A:H2'	2:B:50:G:O5'	0.40	2.15	9	1
1:A:183:ILE:O	1:A:183:ILE:HG23	0.40	2.16	8	1
1:A:181:LEU:O	1:A:188:LEU:HD12	0.40	2.17	6	1
1:A:162:TYR:CD2	2:B:51:A:N3	0.40	2.90	2	1
1:A:140:ILE:HG21	1:A:177:LYS:HG3	0.40	1.94	2	1
1:A:168:LYS:O	1:A:172:ARG:N	0.40	2.48	8	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	69/92 (75%)	57±1 (82±2%)	6±1 (9±2%)	6±1 (9±2%)	2	12
All	All	690/920 (75%)	565 (82%)	62 (9%)	63 (9%)	2	12

All 10 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	117	CYS	10
1	A	143	VAL	10
1	A	123	ASN	10
1	A	168	LYS	10
1	A	142	VAL	9
1	A	167	SER	5
1	A	124	PHE	4
1	A	159	ARG	3
1	A	150	PRO	1
1	A	129	THR	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	64/87 (74%)	46±2 (72±3%)	18±2 (28±3%)	2 20
All	All	640/870 (74%)	461 (72%)	179 (28%)	2 20

All 37 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	136	LEU	10
1	A	191	LYS	10
1	A	120	TRP	10
1	A	147	ILE	10
1	A	173	TYR	9
1	A	122	THR	9
1	A	175	VAL	8
1	A	170	ASP	8
1	A	118	THR	8
1	A	165	VAL	8
1	A	137	LEU	8
1	A	188	LEU	6
1	A	129	THR	6
1	A	179	ASN	6
1	A	168	LYS	5
1	A	148	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	149	LEU	4
1	A	160	PHE	4
1	A	133	ILE	4
1	A	121	MET	4
1	A	140	ILE	3
1	A	119	LEU	3
1	A	183	ILE	3
1	A	193	SER	3
1	A	163	ILE	3
1	A	166	THR	2
1	A	176	GLU	2
1	A	130	GLN	2
1	A	181	LEU	2
1	A	117	CYS	2
1	A	172	ARG	2
1	A	141	ASN	2
1	A	167	SER	2
1	A	164	ASP	2
1	A	127	SER	2
1	A	138	GLN	1
1	A	159	ARG	1

6.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	5/6 (83%)	5±1 (90±10%)	2±1 (34±13%)	0.03±0.05
All	All	51/60 (85%)	45 (88%)	17 (33%)	0.03

The overall RNA backbone suiteness is 0.03.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	53	A	10
2	B	50	G	10
2	B	51	A	10
2	B	52	G	10
2	B	54	U	5

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	50	G	10
2	B	52	G	4
2	B	53	A	2
2	B	49	A	1

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

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 16230

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	1100
Number of shifts mapped to atoms	1100
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
$^{13}C_{\alpha}$	84	-0.81 ± 0.08	Should be applied
$^{13}C_{\beta}$	83	-0.01 ± 0.18	None needed (< 0.5 ppm)
$^{13}C'$	79	-0.29 ± 0.13	None needed (< 0.5 ppm)
^{15}N	83	0.66 ± 0.23	Should be applied

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 80%, i.e. 802 atoms were assigned a chemical shift out of a possible 999. 1 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	329/339 (97%)	133/135 (99%)	130/138 (94%)	66/66 (100%)
Sidechain	382/484 (79%)	234/282 (83%)	142/177 (80%)	6/25 (24%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	27/62 (44%)	27/32 (84%)	0/29 (0%)	0/1 (0%)
Overall	802/999 (80%)	436/515 (85%)	294/384 (77%)	72/100 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 973 atoms were assigned a chemical shift out of a possible 1223. 1 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	405/422 (96%)	163/168 (97%)	161/172 (94%)	81/82 (99%)
Sidechain	473/616 (77%)	291/360 (81%)	174/223 (78%)	8/33 (24%)
Aromatic	31/71 (44%)	31/37 (84%)	0/33 (0%)	0/1 (0%)
Overall	973/1223 (80%)	527/631 (84%)	357/468 (76%)	89/124 (72%)

7.1.4 Statistically unusual chemical shifts (i)

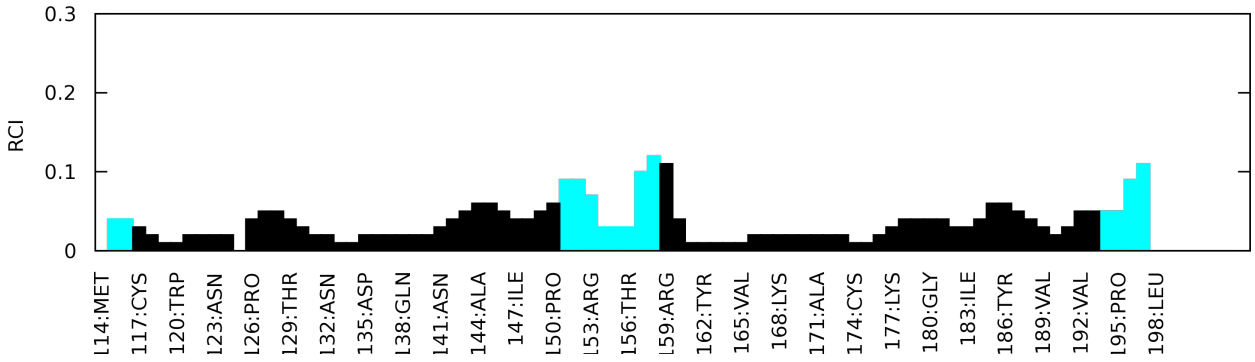
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	198	LEU	HD21	23.45	2.14 – -0.66	81.1
1	A	198	LEU	HD23	23.45	2.14 – -0.66	81.1
1	A	198	LEU	HD22	23.45	2.14 – -0.66	81.1

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:



7.2 Chemical shift list 2

File name: BMRB entry 16243

Chemical shift list name: *assigned_chem_shift_list_1*

7.2.1 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	316
Number of shifts mapped to atoms	148
Number of unparsed shifts	2
Number of shifts with mapping errors	166
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 2 occurences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
315	A	177	LYS	H	8.314	0.02	1
316	A	177	LYS	N	123.82	0.4	1

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

- Residue not found in structure. All 166 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	92	ALA	N	124.707	0.4	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	153	ALA	H	6.514	0.02	1
A	121	PHE	N	116.963	0.4	1
A	102	ARG	H	9.215	0.02	1
A	133	GLN	N	118.252	0.4	1
A	147	PHE	N	126.672	0.4	1
A	135	GLU	H	8.772	0.02	1
A	149	ASN	N	112.147	0.4	1
A	175	ASP	H	8.319	0.02	1
A	168	GLU	N	122.947	0.4	1
A	112	ASN	H	8.215	0.02	1
A	135	GLU	N	119.171	0.4	1
A	175	ASP	N	120.081	0.4	1
A	157	LEU	H	7.216	0.02	1
A	165	GLY	H	8.84	0.02	1
A	139	ASN	N	118.214	0.4	1
A	129	ILE	N	126.72	0.4	1
A	134	LYS	H	8.252	0.02	1
A	128	ASN	H	9.135	0.02	1
A	98	GLU	H	8.081	0.02	1
A	167	ARG	N	119.539	0.4	1
A	172	SER	H	8.517	0.02	1
A	99	ILE	N	120.819	0.4	1
A	117	SER	H	7.816	0.02	1
A	108	LEU	N	117.948	0.4	1
A	174	ALA	N	126.496	0.4	1
A	104	LEU	N	115.328	0.4	1
A	158	GLN	H	7.763	0.02	1
A	123	SER	N	110.269	0.4	1
A	87	LYS	N	122.914	0.4	1
A	153	ALA	N	122.063	0.4	1
A	166	ASN	N	120.314	0.4	1
A	121	PHE	H	7.821	0.02	1
A	85	LYS	H	8.286	0.02	1
A	176	LYS	N	120.864	0.4	1
A	149	ASN	H	8.249	0.02	1
A	172	SER	N	119.04	0.4	1
A	156	ALA	H	7.515	0.02	1
A	151	ASP	N	119.409	0.4	1
A	160	ASN	N	118.938	0.4	1
A	140	ASN	H	8.006	0.02	1
A	132	GLY	H	8.63	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	91	SER	H	8.223	0.02	1
A	144	PHE	H	8.84	0.02	1
A	164	LEU	H	9.062	0.02	1
A	148	GLU	N	119.193	0.4	1
A	106	THR	H	8.93	0.02	1
A	129	ILE	H	8.944	0.02	1
A	118	PHE	H	7.845	0.02	1
A	98	GLU	N	121.953	0.4	1
A	120	GLY	H	8.61	0.02	1
A	108	LEU	H	7.242	0.02	1
A	152	SER	N	116.046	0.4	1
A	165	GLY	N	114.518	0.4	1
A	126	LYS	H	7.468	0.02	1
A	87	LYS	H	8.224	0.02	1
A	89	THR	N	114.991	0.4	1
A	141	CYS	H	8.896	0.02	1
A	155	ARG	H	7.749	0.02	1
A	169	ILE	H	8.631	0.02	1
A	162	SER	N	114.844	0.4	1
A	101	ILE	H	8.98	0.02	1
A	141	CYS	N	121.085	0.4	1
A	107	GLU	N	119.637	0.4	1
A	110	ASP	N	124.638	0.4	1
A	105	SER	H	6.511	0.02	1
A	100	MET	N	122.078	0.4	1
A	154	GLU	N	113.512	0.4	1
A	93	THR	H	7.947	0.02	1
A	144	PHE	N	117.855	0.4	1
A	106	THR	N	112.867	0.4	1
A	146	VAL	H	8.874	0.02	1
A	105	SER	N	114.219	0.4	1
A	93	THR	N	112.512	0.4	1
A	173	LEU	N	122.184	0.4	1
A	163	LEU	N	120.019	0.4	1
A	120	GLY	N	108.607	0.4	1
A	109	LEU	H	6.966	0.02	1
A	150	LYS	H	9.024	0.02	1
A	117	SER	N	111.609	0.4	1
A	126	LYS	N	115.754	0.4	1
A	88	ARG	N	122.372	0.4	1
A	86	SER	N	116.393	0.4	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	110	ASP	H	7.807	0.02	1
A	152	SER	H	7.648	0.02	1
A	122	GLY	H	7.472	0.02	1
A	111	GLU	H	9.475	0.02	1
A	139	ASN	H	8.41	0.02	1
A	166	ASN	H	8.381	0.02	1
A	86	SER	H	8.243	0.02	1
A	127	ILE	N	123.999	0.4	1
A	170	SER	N	115.983	0.4	1
A	142	CYS	H	9.616	0.02	1
A	133	GLN	H	8.114	0.02	1
A	131	ALA	H	8.627	0.02	1
A	160	ASN	H	7.866	0.02	1
A	137	SER	H	8.009	0.02	1
A	155	ARG	N	119.546	0.4	1
A	163	LEU	H	8.163	0.02	1
A	145	MET	N	121.578	0.4	1
A	90	ASP	H	8.38	0.02	1
A	99	ILE	H	9.415	0.02	1
A	176	LYS	H	8.227	0.02	1
A	104	LEU	H	8.011	0.02	1
A	167	ARG	H	8.015	0.02	1
A	119	GLU	H	8.772	0.02	1
A	123	SER	H	7.94	0.02	1
A	90	ASP	N	122.418	0.4	1
A	97	ARG	N	121.213	0.4	1
A	171	VAL	H	8.983	0.02	1
A	111	GLU	N	126.61	0.4	1
A	170	SER	H	8.025	0.02	1
A	138	PHE	H	7.873	0.02	1
A	85	LYS	N	122.632	0.4	1
A	124	ILE	N	129.603	0.4	1
A	131	ALA	N	126.699	0.4	1
A	137	SER	N	114.754	0.4	1
A	156	ALA	N	120.957	0.4	1
A	151	ASP	H	8.614	0.02	1
A	159	MET	N	114.408	0.4	1
A	118	PHE	N	116.473	0.4	1
A	132	GLY	N	107.991	0.4	1
A	91	SER	N	115.772	0.4	1
A	103	ASN	H	8.273	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	97	ARG	H	7.997	0.02	1
A	113	LEU	N	122.837	0.4	1
A	148	GLU	H	8.347	0.02	1
A	159	MET	H	7.698	0.02	1
A	127	ILE	H	8.601	0.02	1
A	146	VAL	N	125.799	0.4	1
A	173	LEU	H	8.886	0.02	1
A	150	LYS	N	122.213	0.4	1
A	142	CYS	N	118.264	0.4	1
A	138	PHE	N	119.613	0.4	1
A	119	GLU	N	120.92	0.4	1
A	128	ASN	N	125.983	0.4	1
A	147	PHE	H	9.098	0.02	1
A	169	ILE	N	122.999	0.4	1
A	89	THR	H	8.3	0.02	1
A	92	ALA	H	8.205	0.02	1
A	157	LEU	N	115.42	0.4	1
A	107	GLU	H	8.354	0.02	1
A	140	ASN	N	118.438	0.4	1
A	143	ALA	N	119.647	0.4	1
A	102	ARG	N	123.152	0.4	1
A	154	GLU	H	7.689	0.02	1
A	171	VAL	N	126.259	0.4	1
A	113	LEU	H	7.963	0.02	1
A	161	ARG	H	8.908	0.02	1
A	162	SER	H	7.853	0.02	1
A	101	ILE	N	128.857	0.4	1
A	168	GLU	H	8.435	0.02	1
A	134	LYS	N	117.997	0.4	1
A	122	GLY	N	106.891	0.4	1
A	100	MET	H	9.338	0.02	1
A	103	ASN	N	114.309	0.4	1
A	164	LEU	N	128.785	0.4	1
A	109	LEU	N	118.384	0.4	1
A	124	ILE	H	8.982	0.02	1
A	161	ARG	N	121.126	0.4	1
A	88	ARG	H	8.322	0.02	1
A	174	ALA	H	8.504	0.02	1
A	143	ALA	H	8.531	0.02	1
A	145	MET	H	8.807	0.02	1
A	158	GLN	N	118.632	0.4	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	112	ASN	N	116.864	0.4	1

7.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	—
$^{13}C_{\beta}$	0	—	—
$^{13}C'$	0	—	—
^{15}N	157	0.52 ± 0.36	None needed (imprecise)

7.2.3 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 12%, i.e. 122 atoms were assigned a chemical shift out of a possible 999. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	122/339 (36%)	61/135 (45%)	0/138 (0%)	61/66 (92%)
Sidechain	0/484 (0%)	0/282 (0%)	0/177 (0%)	0/25 (0%)
Aromatic	0/62 (0%)	0/32 (0%)	0/29 (0%)	0/1 (0%)
Overall	122/999 (12%)	61/515 (12%)	0/384 (0%)	61/100 (61%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 12%, i.e. 146 atoms were assigned a chemical shift out of a possible 1223. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	146/422 (35%)	73/168 (43%)	0/172 (0%)	73/82 (89%)
Sidechain	0/616 (0%)	0/360 (0%)	0/223 (0%)	0/33 (0%)
Aromatic	0/71 (0%)	0/37 (0%)	0/33 (0%)	0/1 (0%)
Overall	146/1223 (12%)	73/631 (12%)	0/468 (0%)	73/124 (59%)

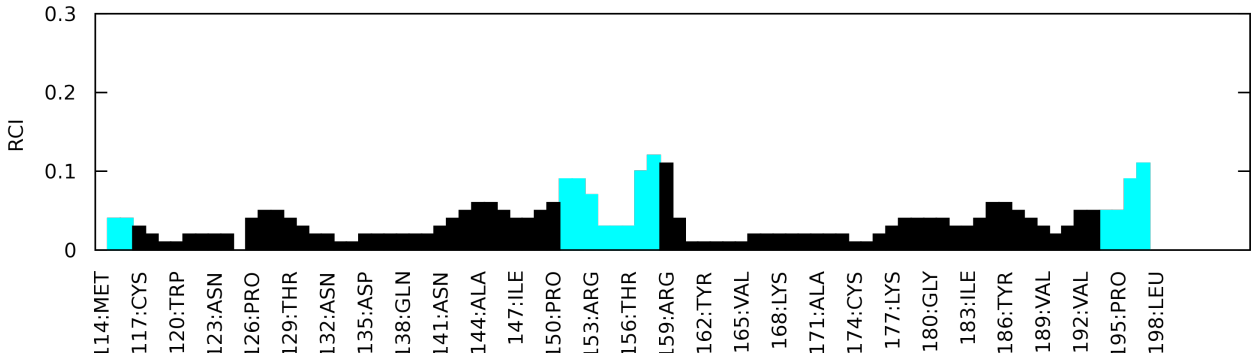
7.2.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots

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:



7.3 Chemical shift list 3

File name: BMRB entry 16244

Chemical shift list name: *assigned_chem_shift_list_1*

7.3.1 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	262
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	262
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chain not found in structure. All 262 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	148	GLU	H	8.349	0.02	1
UNMAPPED	36	LEU	H	8.674	0.02	1
UNMAPPED	65	LEU	H	8.389	0.02	1
UNMAPPED	66	ASN	N	116.316	0.4	1
UNMAPPED	122	GLY	H	7.559	0.02	1
UNMAPPED	155	ARG	H	7.803	0.02	1
UNMAPPED	128	ASN	N	125.673	0.4	1
UNMAPPED	49	TYR	N	117.275	0.4	1
UNMAPPED	104	LEU	H	8.021	0.02	1
UNMAPPED	20	ILE	N	119.086	0.4	1
UNMAPPED	127	ILE	N	124.085	0.4	1
UNMAPPED	76	VAL	H	8.032	0.02	1
UNMAPPED	64	LYS	H	7.954	0.02	1
UNMAPPED	6	LEU	N	127.03	0.4	1
UNMAPPED	40	ARG	H	8.533	0.02	1
UNMAPPED	176	LYS	H	8.233	0.02	1
UNMAPPED	63	GLU	H	7.946	0.02	1
UNMAPPED	175	ASP	H	8.508	0.02	1
UNMAPPED	39	LEU	N	124.152	0.4	1
UNMAPPED	108	LEU	H	7.254	0.02	1
UNMAPPED	149	ASN	N	112.244	0.4	1
UNMAPPED	19	ASN	N	114.78	0.4	1
UNMAPPED	34	ILE	N	125.352	0.4	1
UNMAPPED	146	VAL	N	125.906	0.4	1
UNMAPPED	59	ARG	N	117.214	0.4	1
UNMAPPED	17	GLN	N	118.81	0.4	1
UNMAPPED	126	LYS	H	7.497	0.02	1
UNMAPPED	62	VAL	N	119.483	0.4	1
UNMAPPED	69	LYS	H	8.248	0.02	1
UNMAPPED	134	LYS	H	8.15	0.02	1
UNMAPPED	158	GLN	N	119.19	0.4	1
UNMAPPED	89	THR	N	115.42	0.4	1
UNMAPPED	159	MET	H	7.727	0.02	1
UNMAPPED	145	MET	H	8.758	0.02	1
UNMAPPED	154	GLU	H	7.675	0.02	1
UNMAPPED	104	LEU	N	115.432	0.4	1
UNMAPPED	91	SER	N	116.806	0.4	1
UNMAPPED	16	THR	N	112.665	0.4	1
UNMAPPED	177	LYS	H	8.361	0.02	1
UNMAPPED	105	SER	H	6.463	0.02	1
UNMAPPED	169	ILE	H	8.612	0.02	1
UNMAPPED	101	ILE	N	129.043	0.4	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	136	HIS	N	115.101	0.4	1
UNMAPPED	23	LEU	N	121.274	0.4	1
UNMAPPED	177	LYS	N	124.58	0.4	1
UNMAPPED	147	PHE	H	9.152	0.02	1
UNMAPPED	38	SER	N	116.597	0.4	1
UNMAPPED	113	LEU	N	122.826	0.4	1
UNMAPPED	164	LEU	N	129.3	0.4	1
UNMAPPED	28	ASN	H	8.15	0.02	1
UNMAPPED	176	LYS	N	121.113	0.4	1
UNMAPPED	173	LEU	H	8.885	0.02	1
UNMAPPED	165	GLY	N	114.429	0.4	1
UNMAPPED	9	THR	N	115.912	0.4	1
UNMAPPED	110	ASP	N	124.773	0.4	1
UNMAPPED	174	ALA	H	8.573	0.02	1
UNMAPPED	51	ASP	H	8.786	0.02	1
UNMAPPED	136	HIS	H	7.266	0.02	1
UNMAPPED	20	ILE	H	7.187	0.02	1
UNMAPPED	143	ALA	H	8.436	0.02	1
UNMAPPED	120	GLY	H	8.57	0.02	1
UNMAPPED	113	LEU	H	7.893	0.02	1
UNMAPPED	32	LEU	H	8.835	0.02	1
UNMAPPED	48	ALA	H	8.836	0.02	1
UNMAPPED	6	LEU	H	10.03	0.02	1
UNMAPPED	40	ARG	N	121.883	0.4	1
UNMAPPED	109	LEU	N	118.341	0.4	1
UNMAPPED	30	VAL	N	127.453	0.4	1
UNMAPPED	166	ASN	H	8.347	0.02	1
UNMAPPED	39	LEU	H	8.341	0.02	1
UNMAPPED	51	ASP	N	127.508	0.4	1
UNMAPPED	24	LEU	N	117.656	0.4	1
UNMAPPED	149	ASN	H	8.293	0.02	1
UNMAPPED	168	GLU	N	122.767	0.4	1
UNMAPPED	71	GLU	N	123.956	0.4	1
UNMAPPED	50	ILE	H	9.087	0.02	1
UNMAPPED	112	ASN	N	116.892	0.4	1
UNMAPPED	111	GLU	N	126.614	0.4	1
UNMAPPED	126	LYS	N	116.093	0.4	1
UNMAPPED	159	MET	N	114.882	0.4	1
UNMAPPED	157	LEU	N	115.404	0.4	1
UNMAPPED	162	SER	H	7.828	0.02	1
UNMAPPED	68	LEU	N	123.752	0.4	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	129	ILE	N	127.462	0.4	1
UNMAPPED	160	ASN	N	119.181	0.4	1
UNMAPPED	16	THR	H	8.727	0.02	1
UNMAPPED	111	GLU	H	9.465	0.02	1
UNMAPPED	132	GLY	H	8.608	0.02	1
UNMAPPED	23	LEU	H	7.407	0.02	1
UNMAPPED	158	GLN	H	7.849	0.02	1
UNMAPPED	53	THR	N	111.634	0.4	1
UNMAPPED	60	TYR	H	8.157	0.02	1
UNMAPPED	172	SER	N	119.093	0.4	1
UNMAPPED	73	TYR	N	123.175	0.4	1
UNMAPPED	28	ASN	N	116.891	0.4	1
UNMAPPED	33	SER	H	7.206	0.02	1
UNMAPPED	10	ASN	H	7.921	0.02	1
UNMAPPED	121	PHE	N	117.216	0.4	1
UNMAPPED	103	ASN	N	114.267	0.4	1
UNMAPPED	94	LEU	H	8.114	0.02	1
UNMAPPED	19	ASN	H	7.032	0.02	1
UNMAPPED	14	SER	N	109.306	0.4	1
UNMAPPED	135	GLU	H	8.797	0.02	1
UNMAPPED	90	ASP	N	122.956	0.4	1
UNMAPPED	120	GLY	N	108.716	0.4	1
UNMAPPED	150	LYS	H	9.023	0.02	1
UNMAPPED	74	THR	N	119.064	0.4	1
UNMAPPED	71	GLU	H	9.203	0.02	1
UNMAPPED	32	LEU	N	123.986	0.4	1
UNMAPPED	48	ALA	N	119.877	0.4	1
UNMAPPED	31	ALA	H	8.427	0.02	1
UNMAPPED	103	ASN	H	8.327	0.02	1
UNMAPPED	171	VAL	N	126.282	0.4	1
UNMAPPED	27	ILE	H	7.232	0.02	1
UNMAPPED	153	ALA	H	6.537	0.02	1
UNMAPPED	72	GLY	H	8.273	0.02	1
UNMAPPED	61	CYS	H	8.298	0.02	1
UNMAPPED	112	ASN	H	8.245	0.02	1
UNMAPPED	67	GLY	H	8.968	0.02	1
UNMAPPED	35	ARG	H	9.447	0.02	1
UNMAPPED	140	ASN	N	118.496	0.4	1
UNMAPPED	171	VAL	H	8.968	0.02	1
UNMAPPED	129	ILE	H	8.901	0.02	1
UNMAPPED	107	GLU	H	8.315	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	119	GLU	H	8.751	0.02	1
UNMAPPED	123	SER	H	8.212	0.02	1
UNMAPPED	151	ASP	H	8.613	0.02	1
UNMAPPED	52	VAL	H	8.98	0.02	1
UNMAPPED	142	CYS	N	118.094	0.4	1
UNMAPPED	118	PHE	N	116.635	0.4	1
UNMAPPED	29	VAL	H	8.09	0.02	1
UNMAPPED	75	LEU	H	9.096	0.02	1
UNMAPPED	73	TYR	H	8.452	0.02	1
UNMAPPED	74	THR	H	8.277	0.02	1
UNMAPPED	152	SER	H	7.708	0.02	1
UNMAPPED	10	ASN	N	119.108	0.4	1
UNMAPPED	121	PHE	H	7.755	0.02	1
UNMAPPED	122	GLY	N	106.468	0.4	1
UNMAPPED	11	PHE	H	5.965	0.02	1
UNMAPPED	131	ALA	N	126.97	0.4	1
UNMAPPED	90	ASP	H	8.388	0.02	1
UNMAPPED	75	LEU	N	131.261	0.4	1
UNMAPPED	36	LEU	N	126.29	0.4	1
UNMAPPED	21	ARG	N	120.805	0.4	1
UNMAPPED	99	ILE	H	9.444	0.02	1
UNMAPPED	163	LEU	H	8.148	0.02	1
UNMAPPED	64	LYS	N	114.002	0.4	1
UNMAPPED	65	LEU	N	115.567	0.4	1
UNMAPPED	66	ASN	H	7.97	0.02	1
UNMAPPED	166	ASN	N	120.308	0.4	1
UNMAPPED	63	GLU	N	118.564	0.4	1
UNMAPPED	168	GLU	H	8.383	0.02	1
UNMAPPED	163	LEU	N	120.168	0.4	1
UNMAPPED	92	ALA	H	8.361	0.02	1
UNMAPPED	7	TRP	H	9.321	0.02	1
UNMAPPED	72	GLY	N	103.599	0.4	1
UNMAPPED	61	CYS	N	115.67	0.4	1
UNMAPPED	17	GLN	H	9.241	0.02	1
UNMAPPED	156	ALA	H	7.522	0.02	1
UNMAPPED	35	ARG	N	127.354	0.4	1
UNMAPPED	170	SER	N	115.898	0.4	1
UNMAPPED	141	CYS	H	8.914	0.02	1
UNMAPPED	7	TRP	N	122.74	0.4	1
UNMAPPED	146	VAL	H	8.923	0.02	1
UNMAPPED	59	ARG	H	8.127	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	144	PHE	H	8.756	0.02	1
UNMAPPED	52	VAL	N	115.456	0.4	1
UNMAPPED	101	ILE	H	8.911	0.02	1
UNMAPPED	100	MET	N	122.222	0.4	1
UNMAPPED	134	LYS	N	117.586	0.4	1
UNMAPPED	161	ARG	N	121.292	0.4	1
UNMAPPED	141	CYS	N	121.161	0.4	1
UNMAPPED	154	GLU	N	113.296	0.4	1
UNMAPPED	133	GLN	N	118.267	0.4	1
UNMAPPED	160	ASN	H	7.922	0.02	1
UNMAPPED	9	THR	H	8.47	0.02	1
UNMAPPED	119	GLU	N	120.594	0.4	1
UNMAPPED	143	ALA	N	119.328	0.4	1
UNMAPPED	132	GLY	N	107.887	0.4	1
UNMAPPED	38	SER	H	8.488	0.02	1
UNMAPPED	167	ARG	H	8.083	0.02	1
UNMAPPED	102	ARG	N	123.126	0.4	1
UNMAPPED	21	ARG	H	8.206	0.02	1
UNMAPPED	173	LEU	N	122.153	0.4	1
UNMAPPED	91	SER	H	8.247	0.02	1
UNMAPPED	58	ALA	N	122.919	0.4	1
UNMAPPED	26	ASP	H	7.765	0.02	1
UNMAPPED	156	ALA	N	120.919	0.4	1
UNMAPPED	30	VAL	H	8.46	0.02	1
UNMAPPED	110	ASP	H	7.819	0.02	1
UNMAPPED	24	LEU	H	7.309	0.02	1
UNMAPPED	15	TYR	N	124.542	0.4	1
UNMAPPED	25	GLN	N	119.939	0.4	1
UNMAPPED	92	ALA	N	124.797	0.4	1
UNMAPPED	50	ILE	N	121.686	0.4	1
UNMAPPED	109	LEU	H	6.936	0.02	1
UNMAPPED	100	MET	H	9.297	0.02	1
UNMAPPED	140	ASN	H	8.13	0.02	1
UNMAPPED	117	SER	N	111.887	0.4	1
UNMAPPED	170	SER	H	8.028	0.02	1
UNMAPPED	133	GLN	H	7.947	0.02	1
UNMAPPED	68	LEU	H	7.439	0.02	1
UNMAPPED	106	THR	H	8.952	0.02	1
UNMAPPED	144	PHE	N	117.783	0.4	1
UNMAPPED	70	ILE	N	126.322	0.4	1
UNMAPPED	169	ILE	N	122.928	0.4	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	89	THR	H	8.243	0.02	1
UNMAPPED	161	ARG	H	8.915	0.02	1
UNMAPPED	60	TYR	N	121.497	0.4	1
UNMAPPED	106	THR	N	112.809	0.4	1
UNMAPPED	162	SER	N	114.939	0.4	1
UNMAPPED	174	ALA	N	126.929	0.4	1
UNMAPPED	175	ASP	N	120.161	0.4	1
UNMAPPED	70	ILE	H	9.032	0.02	1
UNMAPPED	93	THR	N	112.673	0.4	1
UNMAPPED	14	SER	H	7.52	0.02	1
UNMAPPED	135	GLU	N	119.486	0.4	1
UNMAPPED	53	THR	H	9.297	0.02	1
UNMAPPED	157	LEU	H	7.158	0.02	1
UNMAPPED	167	ARG	N	119.633	0.4	1
UNMAPPED	102	ARG	H	9.189	0.02	1
UNMAPPED	150	LYS	N	122.32	0.4	1
UNMAPPED	148	GLU	N	119.357	0.4	1
UNMAPPED	33	SER	N	110.433	0.4	1
UNMAPPED	58	ALA	H	7.919	0.02	1
UNMAPPED	26	ASP	N	119.486	0.4	1
UNMAPPED	94	LEU	N	123.404	0.4	1
UNMAPPED	49	TYR	H	8.758	0.02	1
UNMAPPED	172	SER	H	8.492	0.02	1
UNMAPPED	164	LEU	H	9.086	0.02	1
UNMAPPED	124	ILE	N	129.599	0.4	1
UNMAPPED	127	ILE	H	8.587	0.02	1
UNMAPPED	76	VAL	N	125.277	0.4	1
UNMAPPED	15	TYR	H	7.979	0.02	1
UNMAPPED	25	GLN	H	8.51	0.02	1
UNMAPPED	31	ALA	N	128.827	0.4	1
UNMAPPED	67	GLY	N	116.989	0.4	1
UNMAPPED	128	ASN	H	9.211	0.02	1
UNMAPPED	27	ILE	N	110.26	0.4	1
UNMAPPED	153	ALA	N	122.136	0.4	1
UNMAPPED	108	LEU	N	118.157	0.4	1
UNMAPPED	124	ILE	H	9.026	0.02	1
UNMAPPED	117	SER	H	7.821	0.02	1
UNMAPPED	34	ILE	H	8.375	0.02	1
UNMAPPED	123	SER	N	110.838	0.4	1
UNMAPPED	151	ASP	N	119.694	0.4	1
UNMAPPED	62	VAL	H	7.848	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	29	VAL	N	119.61	0.4	1
UNMAPPED	165	GLY	H	8.896	0.02	1
UNMAPPED	145	MET	N	121.312	0.4	1
UNMAPPED	118	PHE	H	7.835	0.02	1
UNMAPPED	99	ILE	N	120.993	0.4	1
UNMAPPED	152	SER	N	116.086	0.4	1
UNMAPPED	155	ARG	N	119.839	0.4	1
UNMAPPED	107	GLU	N	119.606	0.4	1
UNMAPPED	105	SER	N	114.278	0.4	1
UNMAPPED	93	THR	H	7.897	0.02	1
UNMAPPED	11	PHE	N	108.63	0.4	1
UNMAPPED	131	ALA	H	8.729	0.02	1
UNMAPPED	69	LYS	N	125.634	0.4	1
UNMAPPED	142	CYS	H	9.617	0.02	1
UNMAPPED	147	PHE	N	126.73	0.4	1

7.3.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	—
$^{13}C_{\beta}$	0	—	—
$^{13}C'$	0	—	—
^{15}N	131	0.00 ± 0.00	None needed (< 0.5 ppm)

7.3.3 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 999. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/339 (0%)	0/135 (0%)	0/138 (0%)	0/66 (0%)
Sidechain	0/484 (0%)	0/282 (0%)	0/177 (0%)	0/25 (0%)
Aromatic	0/62 (0%)	0/32 (0%)	0/29 (0%)	0/1 (0%)
Overall	0/999 (0%)	0/515 (0%)	0/384 (0%)	0/100 (0%)

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 1223.

0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/422 (0%)	0/168 (0%)	0/172 (0%)	0/82 (0%)
Sidechain	0/616 (0%)	0/360 (0%)	0/223 (0%)	0/33 (0%)
Aromatic	0/71 (0%)	0/37 (0%)	0/33 (0%)	0/1 (0%)
Overall	0/1223 (0%)	0/631 (0%)	0/468 (0%)	0/124 (0%)

7.3.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.3.5 Random Coil Index (RCI) plots

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.

7.4 Chemical shift list 4

File name: BMRB entry 16246

Chemical shift list name: *assigned_chem_shift_list_1*

7.4.1 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	861
Number of shifts mapped to atoms	861
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.4.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	82	-0.55 ± 0.24	Should be applied
$^{13}C_{\beta}$	80	0.15 ± 0.15	None needed (< 0.5 ppm)

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C'$	0	—	—
^{15}N	77	0.45 ± 0.55	None needed (< 0.5 ppm)

7.4.3 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 64%, i.e. 637 atoms were assigned a chemical shift out of a possible 999. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	264/339 (78%)	130/135 (96%)	68/138 (49%)	66/66 (100%)
Sidechain	372/484 (77%)	225/282 (80%)	141/177 (80%)	6/25 (24%)
Aromatic	1/62 (2%)	1/32 (3%)	0/29 (0%)	0/1 (0%)
Overall	637/999 (64%)	356/515 (69%)	209/384 (54%)	72/100 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 61%, i.e. 751 atoms were assigned a chemical shift out of a possible 1223. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	310/422 (73%)	151/168 (90%)	82/172 (48%)	77/82 (94%)
Sidechain	440/616 (71%)	266/360 (74%)	168/223 (75%)	6/33 (18%)
Aromatic	1/71 (1%)	1/37 (3%)	0/33 (0%)	0/1 (0%)
Overall	751/1223 (61%)	418/631 (66%)	250/468 (53%)	83/124 (67%)

7.4.4 Statistically unusual chemical shifts

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	153	ARG	CD	36.16	47.57 – 38.77	-8.0

7.4.5 Random Coil Index (RCI) plots

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: