



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2022 – 01:04 PM EST

PDB ID : 2KH9
Title : Solution structure of yeast Prp24-RRM2 bound to a fragment of U6 RNA
Authors : Martin-Tumasz, S.A.; Butcher, S.E.
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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.27
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

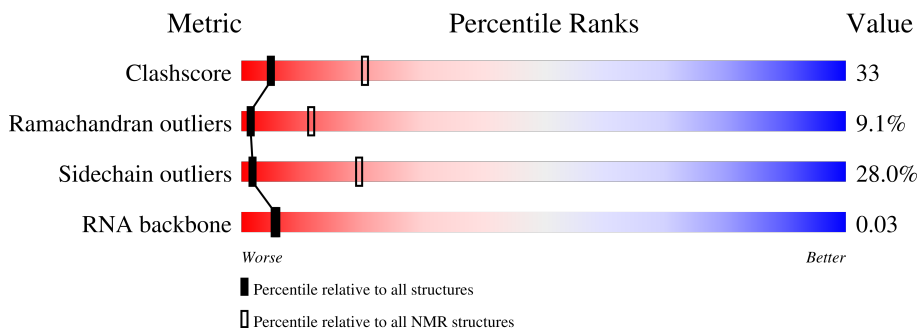
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428
RNA backbone	4643	676

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	92	
2	B	6	

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 [i](#)

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
			Total	C	H	N	O	S	
1	A	86	1416	445	715	120	132	4	0

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'.

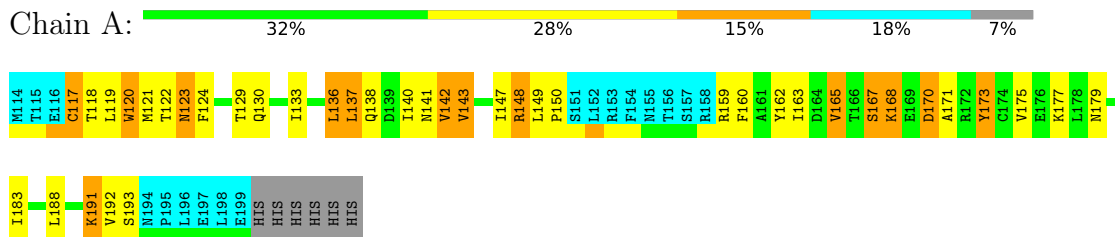
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	6	196	59	67	27	38	5	0

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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



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

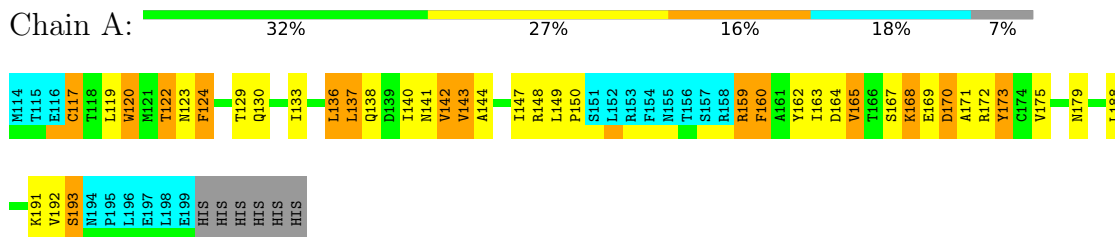


4.2 Scores per residue for each member of the ensemble

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

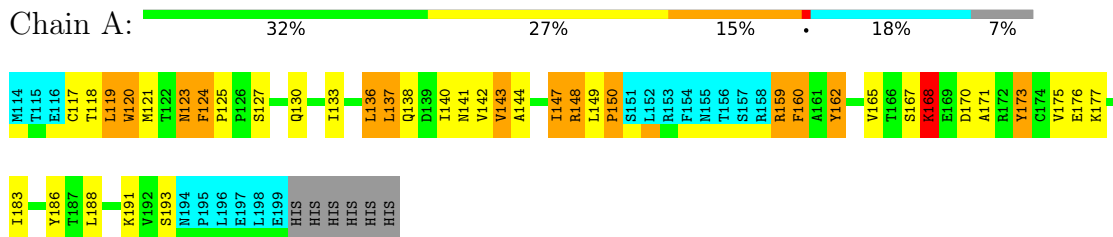


- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'



4.2.2 Score per residue for model 2

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

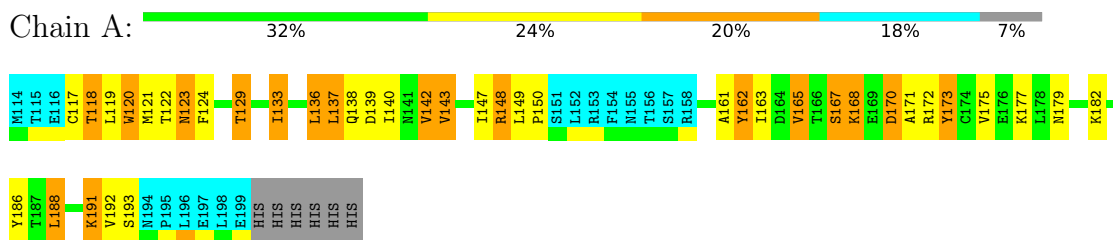


- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'

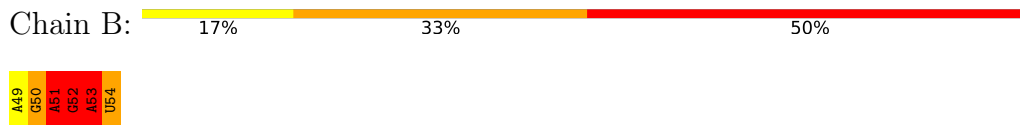


4.2.3 Score per residue for model 3 (medoid)

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

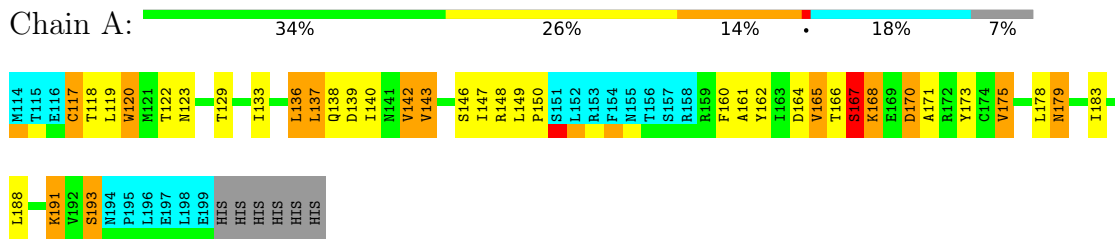


- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'



4.2.4 Score per residue for model 4

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

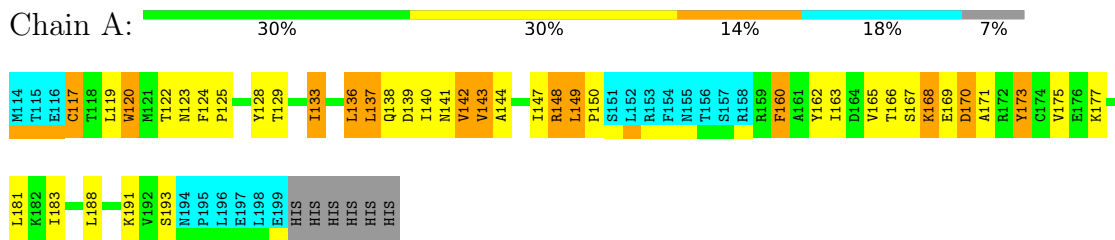


- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'



4.2.5 Score per residue for model 5

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

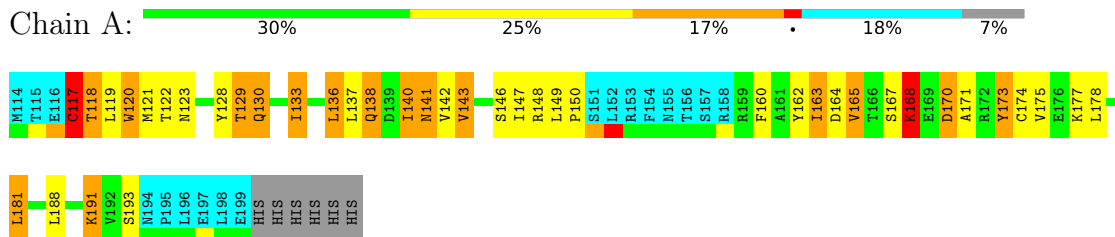


- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'



4.2.6 Score per residue for model 6

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

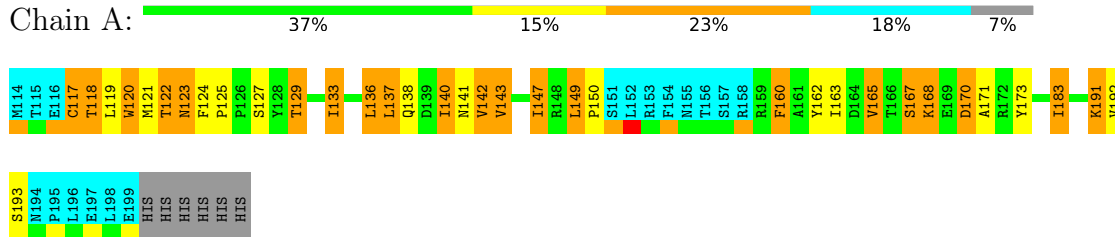


- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'

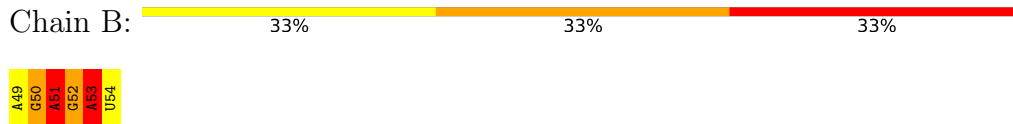


4.2.7 Score per residue for model 7

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

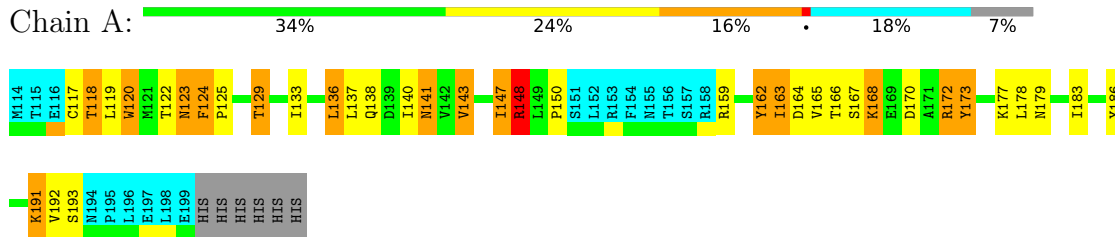


- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'



4.2.8 Score per residue for model 8

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

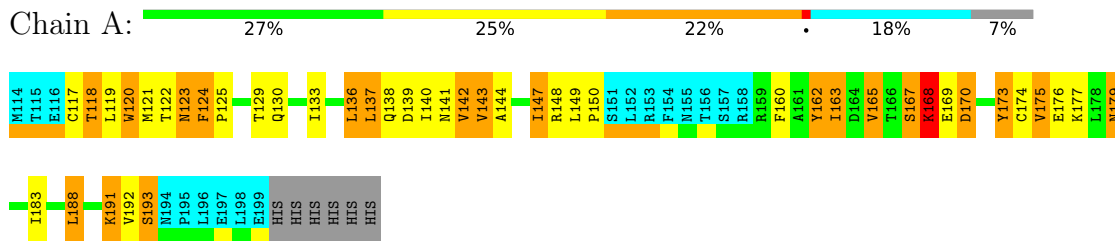


- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'

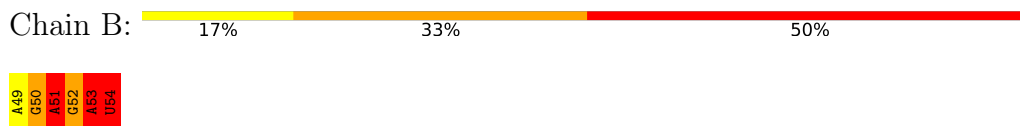


4.2.9 Score per residue for model 9

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

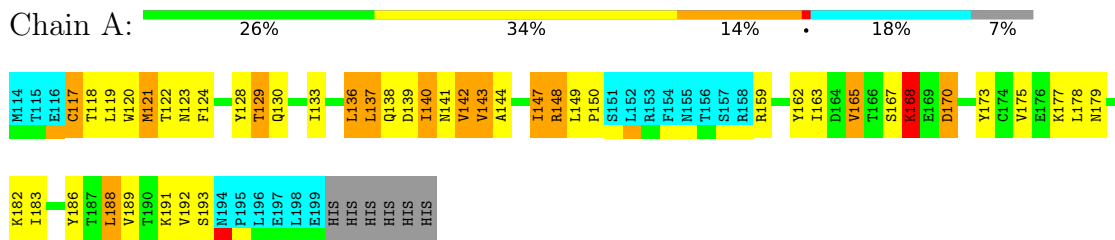


- Molecule 2: 5'-R(*AP*GP*AP*GP*AP*U)-3'

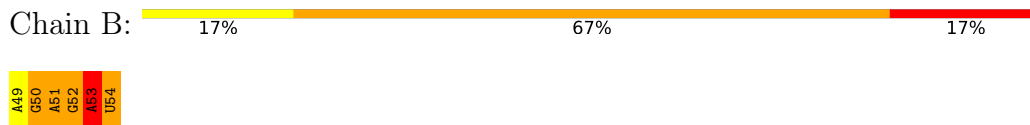


4.2.10 Score per residue for model 10

- 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

No chemical shift data was provided.

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	0.57±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(°)	Ideal(°)	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	4
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:138:GLN:HA	1:A:142:VAL:C	0.60	2.16	5	7
1:A:148:ARG:HG3	2:B:52:G:C4	0.60	2.30	3	2
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:150:PRO:O	2:B:53:A:N6	0.59	2.36	3	1
1:A:130:GLN:NE2	1:A:149:LEU:HD22	0.59	2.13	9	1
1:A:148:ARG:HH11	1:A:148:ARG:CG	0.58	2.11	8	2
1:A:138:GLN:HB2	1:A:143:VAL:H	0.58	1.58	6	1
1:A:138:GLN:HA	1:A:143:VAL:H	0.58	1.57	8	2
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	5
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:HG13	1:A:147:ILE:O	0.52	2.05	7	2
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:128:TYR:O	1:A:129:THR:CB	0.51	2.58	6	1
1:A:138:GLN:CB	1:A:143:VAL:H	0.51	2.18	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: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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:LYS:HE2	1:A:192:VAL:O	0.50	2.07	9	2
2:B:52:G:O5'	2:B:53:A:C6	0.50	2.65	7	1
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:123:ASN:O	1:A:124:PHE:HB3	0.49	2.07	9	5
1:A:133:ILE:O	1:A:137:LEU:HD22	0.49	2.07	2	2
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	2
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
1:A:167:SER:O	1:A:168:LYS:CB	0.47	2.63	1	1
2:B:54:U:O2	2:B:54:U:C2'	0.47	2.63	2	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:117:CYS:HB3	1:A:167:SER:O	0.46	2.10	5	1
1:A:129:THR:CG2	1:A:149:LEU:HD13	0.46	2.41	6	1
1:A:129:THR:HG22	1:A:130:GLN:N	0.46	2.25	6	1
1:A:130:GLN:HA	1:A:147:ILE:HD11	0.46	1.85	10	1
1:A:148:ARG:HH11	1:A:148:ARG:HG3	0.46	1.70	8	2
2:B:52:G:H1'	2:B:53:A:C5	0.46	2.46	1	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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:182:LYS:HA	1:A:186:TYR:O	0.44	2.13	10	2
2:B:53:A:C3'	2:B:54:U:H2'	0.44	2.41	3	1
1:A:136:LEU:HD12	1:A:140:ILE:HD12	0.44	1.88	5	1
1:A:148:ARG:NE	2:B:53:A:N6	0.44	2.65	10	1
1:A:141:ASN:HD22	1:A:141:ASN:C	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:53:A:O4'	2:B:53:A:P	0.43	2.76	3	1
1:A:137:LEU:O	1:A:141:ASN:C	0.43	2.57	5	1
2:B:52:G:OP1	2:B:53:A:N6	0.43	2.51	9	1
1:A:133:ILE:O	1:A:137:LEU:HD12	0.43	2.14	1	1
1:A:121:MET:SD	1:A:133:ILE:HD11	0.43	2.54	3	2
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
2:B:53:A:O2'	2:B:54:U:H5	0.42	1.93	9	1
1:A:136:LEU:CD1	1:A:178:LEU:HD21	0.42	2.44	8	2
1:A:168:LYS:O	1:A:172:ARG:HB2	0.42	2.13	8	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
2:B:51:A:H3'	2:B:53:A:H62	0.42	1.73	7	1
1:A:148:ARG:CG	1:A:148:ARG:NH1	0.42	2.82	5	2
1:A:149:LEU:HG	1:A:161:ALA:HB2	0.42	1.91	3	1
1:A:138:GLN:CB	1:A:143:VAL:CA	0.42	2.91	8	1
2:B:53:A:H8	2:B:53:A:O5'	0.42	1.98	3	1
1:A:160:PHE:HE2	1:A:162:TYR:OH	0.42	1.98	1	1
2:B:53:A:O2'	2:B:54:U:H2'	0.41	2.14	3	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
1:A:148:ARG:HD3	2:B:52:G:H1'	0.41	1.92	9	1
1:A:141:ASN:C	1:A:141:ASN:ND2	0.41	2.74	6	1
2:B:52:G:O2'	2:B:53:A:C8	0.41	2.72	10	2
1:A:148:ARG:O	1:A:162:TYR:N	0.41	2.45	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:137:LEU:HD11	1:A:163:ILE:HD13	0.41	1.92	6	1
2:B:51:A:O2'	2:B:52:G:P	0.41	2.78	9	1
1:A:183:ILE:HG21	1:A:188:LEU:CD1	0.41	2.45	2	1
1:A:148:ARG:CB	2:B:52:G:C8	0.41	3.04	3	1
1:A:147:ILE:O	1:A:147:ILE:HG13	0.41	2.16	8	1
1:A:165:VAL:HG11	1:A:170:ASP:CB	0.41	2.45	8	1
1:A:133:ILE:O	1:A:137:LEU:N	0.41	2.53	4	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:181:LEU:O	1:A:188:LEU:HD12	0.40	2.17	6	1
1:A:140:ILE:HG21	1:A:177:LYS:HG3	0.40	1.94	2	1
1:A:162:TYR:CD2	2:B:51:A:N3	0.40	2.90	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%)	56±1 (82±2%)	6±1 (9±2%)	6±1 (9±2%)	1	11
All	All	690/920 (75%)	565 (82%)	62 (9%)	63 (9%)	1	11

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	123	ASN	10
1	A	143	VAL	10
1	A	168	LYS	10

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Mol	Chain	Res	Type	Models (Total)
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 19
All	All	640/870 (74%)	461 (72%)	179 (28%)	2 19

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	120	TRP	10
1	A	136	LEU	10
1	A	147	ILE	10
1	A	191	LYS	10
1	A	122	THR	9
1	A	173	TYR	9
1	A	137	LEU	8
1	A	165	VAL	8
1	A	170	ASP	8
1	A	175	VAL	8
1	A	118	THR	8
1	A	129	THR	6
1	A	179	ASN	6
1	A	188	LEU	6
1	A	148	ARG	5
1	A	168	LYS	5
1	A	160	PHE	4
1	A	121	MET	4
1	A	149	LEU	4

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

6.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	5/6 (83%)	4±0 (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	50	G	10
2	B	51	A	10
2	B	52	G	10
2	B	53	A	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

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Mol	Chain	Res	Type	Models (Total)
2	B	53	A	2
2	B	49	A	1

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 monosaccharides 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

No chemical shift data were provided