



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:47 pm BST

PDB ID : 2KXN
Title : NMR structure of human Tra2beta1 RRM in complex with AAGAAC RNA
Authors : Clery, A.; Jayne, S.; Benderska, N.; Dominguez, C.; Stamm, S.; Allain, F.H.-T.
Deposited on : 2010-05-10

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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

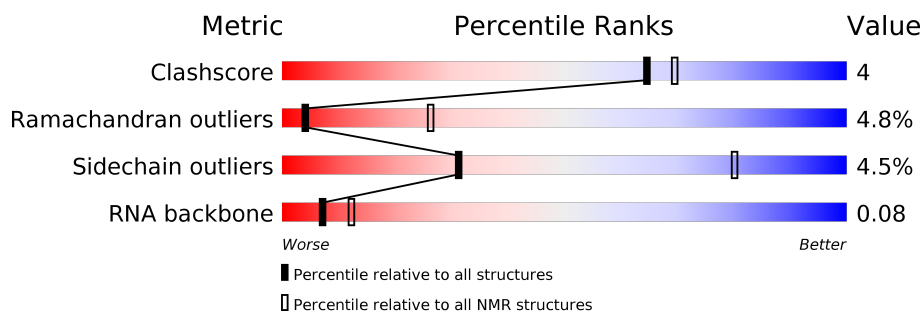
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 76%.

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	6	 17% 17% 50% 17%
2	B	129	 51% 5% 16% 26%

2 Ensemble composition and analysis

This entry contains 12 models. Model 9 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	B:118-B:150, B:159-B:199 (74)	0.41	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. No single-model clusters were found.

Cluster number	Models
1	2, 3, 4, 5, 6, 8, 9, 10, 12
2	1, 7, 11

3 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 1712 atoms, of which 814 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 5'-R(*AP*AP*GP*AP*AP*C)-3'.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		P
1	A	6	196	59	68	28	36	5	0

- Molecule 2 is a protein called Transformer-2 protein homolog beta.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
2	B	95	1516	477	746	146	144	3	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	72	MET	-	expression tag	UNP P62995
B	73	GLY	-	expression tag	UNP P62995
B	74	SER	-	expression tag	UNP P62995
B	75	SER	-	expression tag	UNP P62995
B	76	HIS	-	expression tag	UNP P62995
B	77	HIS	-	expression tag	UNP P62995
B	78	HIS	-	expression tag	UNP P62995
B	79	HIS	-	expression tag	UNP P62995
B	80	HIS	-	expression tag	UNP P62995
B	81	HIS	-	expression tag	UNP P62995
B	82	SER	-	expression tag	UNP P62995
B	83	SER	-	expression tag	UNP P62995
B	84	GLY	-	expression tag	UNP P62995
B	85	LEU	-	expression tag	UNP P62995
B	86	VAL	-	expression tag	UNP P62995
B	87	PRO	-	expression tag	UNP P62995
B	88	ARG	-	expression tag	UNP P62995
B	89	GLY	-	expression tag	UNP P62995
B	90	SER	-	expression tag	UNP P62995
B	91	HIS	-	expression tag	UNP P62995
B	92	MET	-	expression tag	UNP P62995
B	93	ALA	-	expression tag	UNP P62995
B	94	SER	-	expression tag	UNP P62995
B	95	MET	-	expression tag	UNP P62995
B	96	THR	-	expression tag	UNP P62995

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Chain	Residue	Modelled	Actual	Comment	Reference
B	97	GLY	-	expression tag	UNP P62995
B	98	GLY	-	expression tag	UNP P62995
B	99	GLN	-	expression tag	UNP P62995
B	100	GLN	-	expression tag	UNP P62995
B	101	MET	-	expression tag	UNP P62995
B	102	GLY	-	expression tag	UNP P62995
B	103	ARG	-	expression tag	UNP P62995
B	104	GLY	-	expression tag	UNP P62995
B	105	SER	-	expression tag	UNP P62995

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.

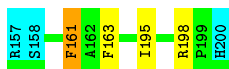
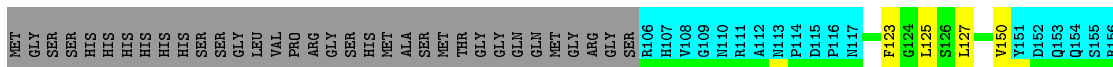
- Molecule 1: 5'-R(*AP*AP*GP*AP*AP*C)-3'

Chain A: 



- Molecule 2: Transformer-2 protein homolog beta

Chain B: 



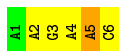
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

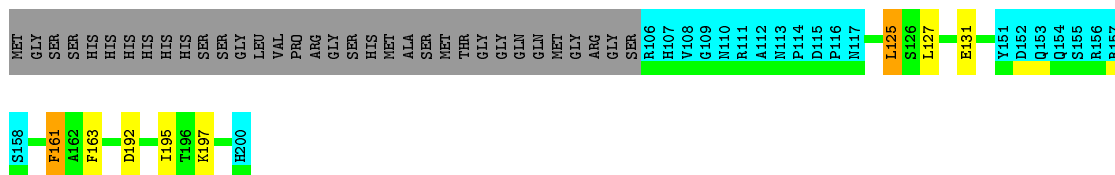
- Molecule 1: 5'-R(*AP*AP*GP*AP*AP*C)-3'

Chain A: 



- Molecule 2: Transformer-2 protein homolog beta

Chain B: 

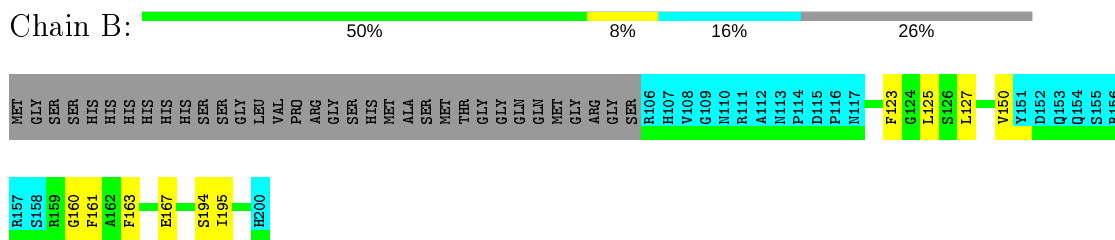


4.2.2 Score per residue for model 2

- Molecule 1: 5'-R(*AP*AP*GP*AP*AP*C)-3'



- Molecule 2: Transformer-2 protein homolog beta

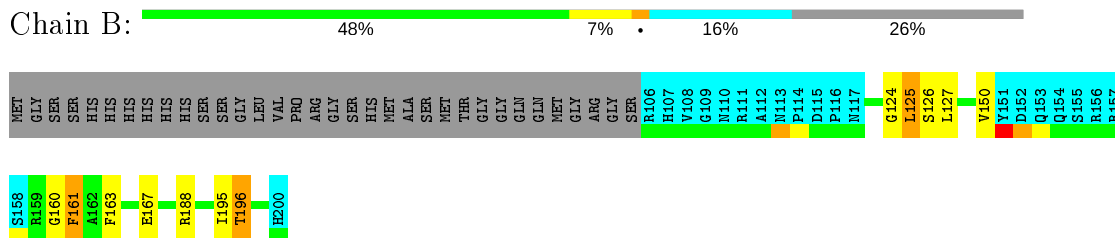


4.2.3 Score per residue for model 3

- Molecule 1: 5'-R(*AP*AP*GP*AP*AP*C)-3'



- Molecule 2: Transformer-2 protein homolog beta



4.2.4 Score per residue for model 4

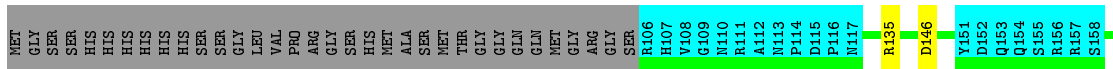
- Molecule 1: 5'-R(*AP*AP*GP*AP*AP*C)-3'

Chain A: 



- Molecule 2: Transformer-2 protein homolog beta

Chain B: 



4.2.5 Score per residue for model 5

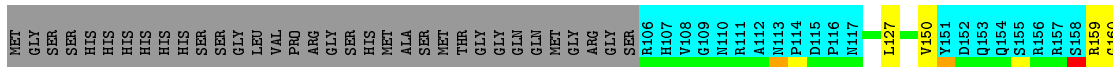
- Molecule 1: 5'-R(*AP*AP*GP*AP*AP*C)-3'

Chain A: 



- Molecule 2: Transformer-2 protein homolog beta

Chain B: 



4.2.6 Score per residue for model 6

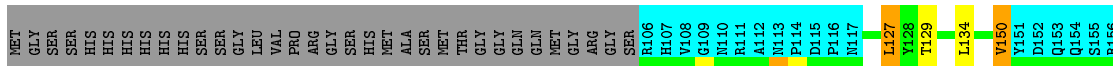
- Molecule 1: 5'-R(*AP*AP*GP*AP*AP*C)-3'

Chain A: 



- Molecule 2: Transformer-2 protein homolog beta

Chain B: 



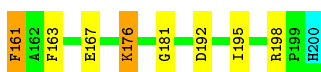
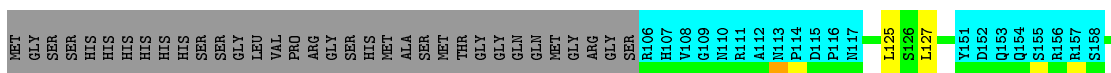


4.2.7 Score per residue for model 7

- Molecule 1: 5'-R(*AP*AP*GP*AP*AP*C)-3'

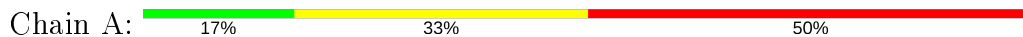


- Molecule 2: Transformer-2 protein homolog beta

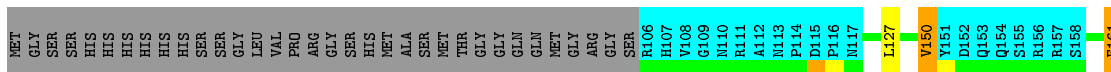


4.2.8 Score per residue for model 8

- Molecule 1: 5'-R(*AP*AP*GP*AP*AP*C)-3'



- Molecule 2: Transformer-2 protein homolog beta



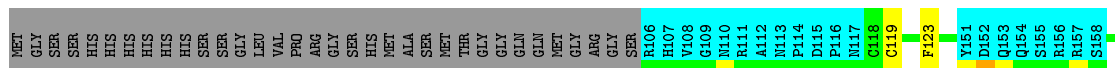
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: 5'-R(*AP*AP*GP*AP*AP*C)-3'





- Molecule 2: Transformer-2 protein homolog beta

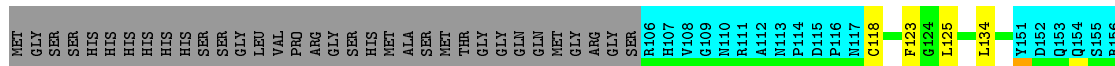


4.2.10 Score per residue for model 10

- Molecule 1: 5'-R(*AP*AP*GP*AP*AP*C)-3'

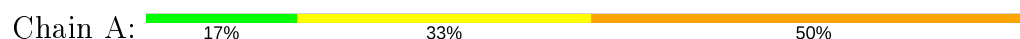


- Molecule 2: Transformer-2 protein homolog beta

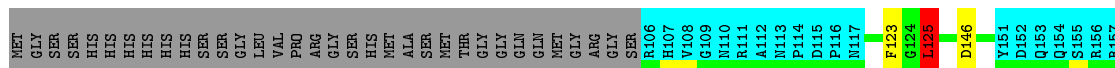


4.2.11 Score per residue for model 11

- Molecule 1: 5'-R(*AP*AP*GP*AP*AP*C)-3'



- Molecule 2: Transformer-2 protein homolog beta



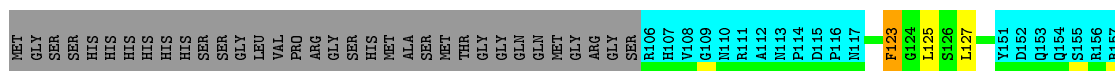


4.2.12 Score per residue for model 12

- Molecule 1: 5'-R(*AP*AP*GP*AP*AP*C)-3'



- Molecule 2: Transformer-2 protein homolog beta



5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 12 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	8
CYANA	structure solution	2.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1025
Number of shifts mapped to atoms	1025
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	128	68	68	3±2
2	B	593	588	588	4±2
All	All	8652	7872	7872	70

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:123:PHE:CE2	2:B:161:PHE:CE2	0.66	2.83	10	1
1:A:4:A:N3	1:A:4:A:H2'	0.63	2.09	12	2
1:A:5:A:H1'	1:A:6:C:C5	0.58	2.33	10	1
2:B:123:PHE:CD2	2:B:161:PHE:CD2	0.54	2.95	10	1
1:A:5:A:H62	2:B:196:THR:HG23	0.52	1.65	3	1
1:A:4:A:H2'	1:A:4:A:N3	0.51	2.18	9	3
2:B:176:LYS:HE3	2:B:192:ASP:HA	0.51	1.83	7	1
1:A:3:G:C2	2:B:123:PHE:CZ	0.50	3.00	10	1
1:A:5:A:C5	2:B:163:PHE:CZ	0.50	2.99	2	4
2:B:123:PHE:CZ	2:B:161:PHE:CE2	0.48	3.01	10	1
2:B:119:CYS:SG	2:B:165:TYR:CE1	0.48	3.05	9	1
1:A:5:A:C5	2:B:163:PHE:CE2	0.47	3.02	8	5
2:B:161:PHE:CZ	2:B:163:PHE:CZ	0.47	3.02	4	4
2:B:150:VAL:CG1	2:B:161:PHE:CE1	0.47	2.98	6	2
2:B:123:PHE:CZ	2:B:194:SER:HA	0.46	2.45	2	2
1:A:5:A:HO2'	1:A:6:C:H6	0.45	1.50	12	3
1:A:5:A:C4	2:B:163:PHE:CZ	0.45	3.05	2	1
2:B:150:VAL:HG23	2:B:161:PHE:CD1	0.45	2.47	3	1
2:B:150:VAL:HG13	2:B:161:PHE:CE1	0.45	2.47	6	1
1:A:5:A:C4	2:B:163:PHE:CE1	0.44	3.05	5	1
2:B:195:ILE:HG22	2:B:196:THR:H	0.44	1.72	6	1
2:B:127:LEU:HD12	2:B:127:LEU:N	0.44	2.27	7	1
2:B:123:PHE:CE2	2:B:161:PHE:CD2	0.43	3.05	10	1
2:B:161:PHE:CE2	2:B:163:PHE:CZ	0.43	3.06	10	2
2:B:127:LEU:N	2:B:127:LEU:HD12	0.43	2.28	1	1
1:A:5:A:C4	2:B:163:PHE:CE2	0.43	3.06	4	1
2:B:198:ARG:CB	2:B:199:PRO:HD2	0.43	2.43	11	4
1:A:2:A:H1'	1:A:3:G:OP1	0.43	2.13	8	1
1:A:3:G:N2	1:A:4:A:C8	0.43	2.86	2	1
2:B:195:ILE:HG12	2:B:196:THR:H	0.43	1.73	11	1
1:A:3:G:C6	2:B:123:PHE:CG	0.43	3.07	10	3
1:A:1:A:C2	1:A:2:A:C5	0.42	3.07	2	1
1:A:2:A:C1'	1:A:3:G:OP1	0.42	2.68	8	2
2:B:129:THR:HG22	2:B:134:LEU:CD2	0.42	2.44	6	1
2:B:123:PHE:C	2:B:125:LEU:H	0.42	2.18	11	1
2:B:150:VAL:HG12	2:B:159:ARG:H	0.42	1.75	5	1
2:B:150:VAL:HG11	2:B:161:PHE:CE2	0.42	2.50	2	1
1:A:5:A:H1'	1:A:6:C:C6	0.42	2.50	10	1
2:B:150:VAL:CG1	2:B:159:ARG:H	0.42	2.28	5	1
2:B:150:VAL:HG13	2:B:161:PHE:CD1	0.41	2.50	8	1
1:A:1:A:C2	1:A:2:A:C4	0.41	3.09	10	1
1:A:4:A:N3	1:A:4:A:H5''	0.41	2.30	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:A:H62	2:B:196:THR:CG2	0.40	2.29	3	1
1:A:4:A:C5'	1:A:4:A:N3	0.40	2.83	5	1
2:B:124:GLY:C	2:B:126:SER:H	0.40	2.19	3	1
2:B:134:LEU:H	2:B:134:LEU:HD22	0.40	1.77	10	1

5.2 Torsion angles [i](#)

5.2.1 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	
2	B	74/129 (57%)	59±2 (80±3%)	11±2 (15±2%)	4±1 (5±1%)	4	26
All	All	888/1548 (57%)	712 (80%)	133 (15%)	43 (5%)	4	26

All 13 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	195	ILE	12
2	B	127	LEU	6
2	B	198	ARG	4
2	B	125	LEU	4
2	B	160	GLY	4
2	B	181	GLY	3
2	B	192	ASP	3
2	B	197	LYS	2
2	B	188	ARG	1
2	B	159	ARG	1
2	B	118	CYS	1
2	B	196	THR	1
2	B	185	ASP	1

5.2.2 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	
2	B	63/108 (58%)	60±1 (96±2%)	3±1 (4±2%)	31	80
All	All	756/1296 (58%)	722 (96%)	34 (4%)	31	80

All 13 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)
2	B	161	PHE	9
2	B	125	LEU	6
2	B	167	GLU	5
2	B	188	ARG	3
2	B	150	VAL	2
2	B	146	ASP	2
2	B	198	ARG	1
2	B	176	LYS	1
2	B	196	THR	1
2	B	123	PHE	1
2	B	127	LEU	1
2	B	135	ARG	1
2	B	131	GLU	1

5.2.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	5/6 (83%)	4±0 (85±9%)	2±1 (40±12%)	0.28±0.22
All	All	60/72 (83%)	51 (85%)	24 (40%)	0.23

The overall RNA backbone suiteness is 0.08.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	4	A	12
1	A	5	A	12
1	A	6	C	12
1	A	3	G	12
1	A	2	A	3

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	2	A	12
1	A	3	G	7
1	A	5	A	3
1	A	4	A	2

5.3 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

There are no ligands in this entry.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 76% for the well-defined parts and 71% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

6.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1025
Number of shifts mapped to atoms	1025
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

6.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	82	-0.23 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	82	0.13 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	83	0.73 ± 0.20	Should be applied

6.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 76%, i.e. 794 atoms were assigned a chemical shift out of a possible 1051. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	281/366 (77%)	141/146 (97%)	70/148 (47%)	70/72 (97%)
Sidechain	392/492 (80%)	241/288 (84%)	145/174 (83%)	6/30 (20%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	77/78 (99%)	41/42 (98%)	36/36 (100%)	0/0 (—%)
Overall	794/1051 (76%)	467/543 (86%)	251/399 (63%)	76/109 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 71%, i.e. 945 atoms were assigned a chemical shift out of a possible 1336. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	333/467 (71%)	168/186 (90%)	82/190 (43%)	83/91 (91%)
Sidechain	481/654 (74%)	302/386 (78%)	170/221 (77%)	9/47 (19%)
Aromatic	87/100 (87%)	46/54 (85%)	41/44 (93%)	0/2 (0%)
Overall	945/1336 (71%)	560/693 (81%)	293/496 (59%)	92/147 (63%)

6.1.4 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
2	B	187	ARG	NE	118.93	92.63 – 76.73	21.5
2	B	135	ARG	NE	118.27	92.63 – 76.73	21.1
2	B	190	ARG	NE	118.20	92.63 – 76.73	21.1
2	B	159	ARG	NE	117.64	92.63 – 76.73	20.7
1	A	4	A	H2'	5.91	5.50 – 3.70	7.3

6.1.5 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 B:

