



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 09:23 pm BST

PDB ID : 2BN5
Title : P-Element Somatic Inhibitor Protein Complex with U1-70k proline-rich peptide
Authors : Ignjatovic, T.; Yang, J.-C.; Butler, P.J.G.; Neuhaus, D.; Nagai, K.
Deposited on : 2005-03-21

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

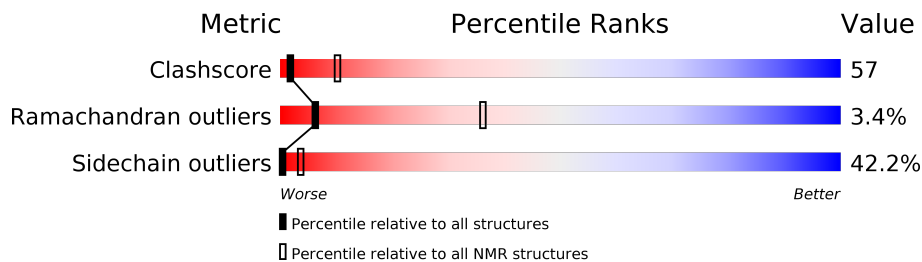
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 73%.

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

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	33	
2	B	21	

2 Ensemble composition and analysis i

This entry contains 28 models. Model 20 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:654-A:679 (26)	0.12	20

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 3 single-model clusters were found.

Cluster number	Models
1	4, 5, 6, 7, 9, 11, 13, 14, 15, 18, 19, 21, 24, 25
2	1, 2, 3, 8, 10, 12, 16, 20, 22, 26, 27
Single-model clusters	17; 23; 28

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 847 atoms, of which 418 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PSI.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	33	523	167	255	45	56	0

- Molecule 2 is a protein called U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA.

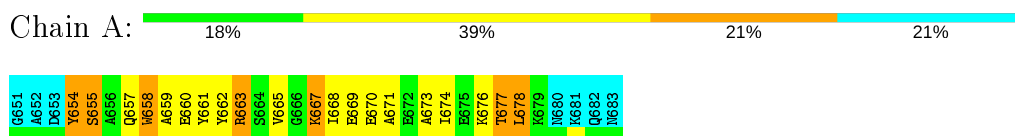
Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
2	B	21	324	104	163	32	24	1	0

4 Residue-property plots [i](#)

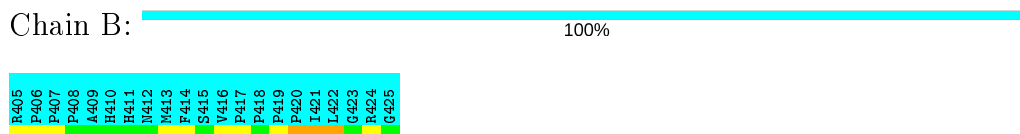
4.1 Average score per residue in the NMR ensemble

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: PSI



- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

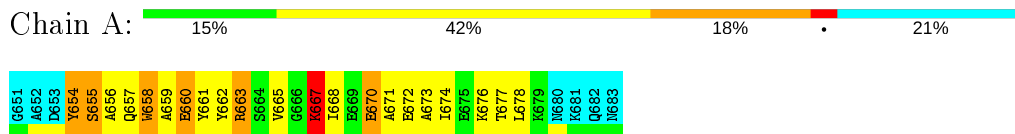


4.2 Scores per residue for each member of the ensemble

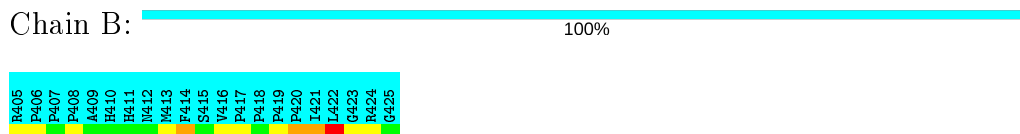
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: PSI

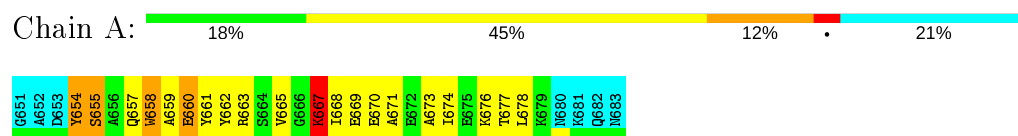


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

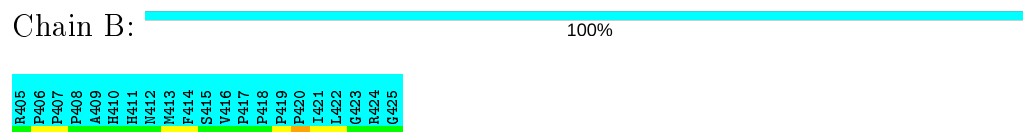


4.2.2 Score per residue for model 2

- Molecule 1: PSI

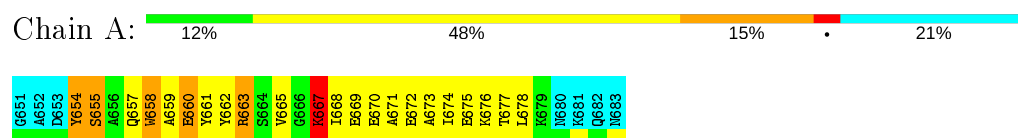


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

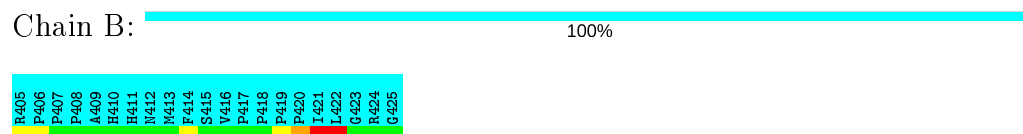


4.2.3 Score per residue for model 3

- Molecule 1: PSI

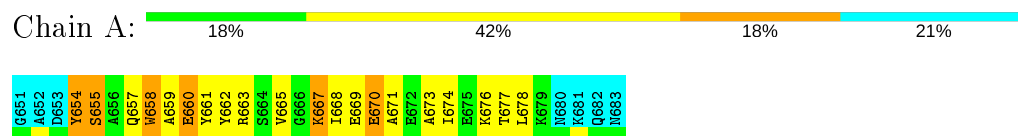


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

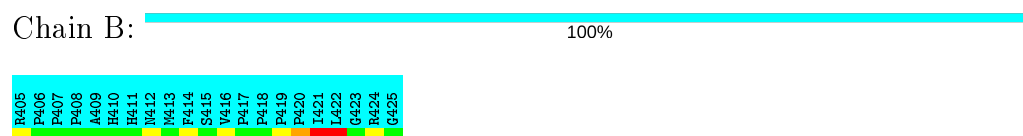


4.2.4 Score per residue for model 4

- Molecule 1: PSI

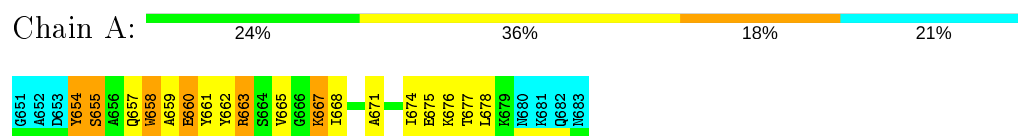


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

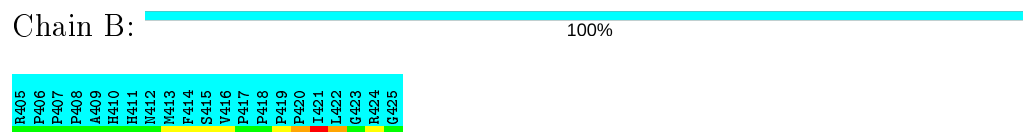


4.2.5 Score per residue for model 5

- Molecule 1: PSI

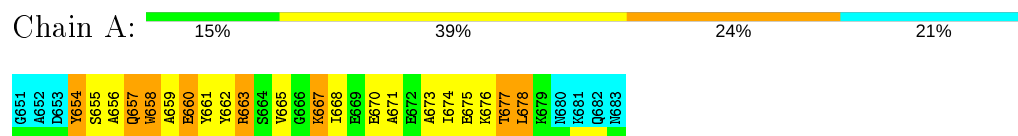


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

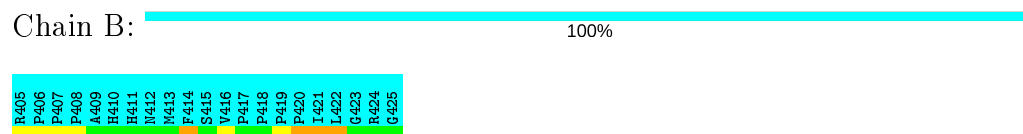


4.2.6 Score per residue for model 6

- Molecule 1: PSI

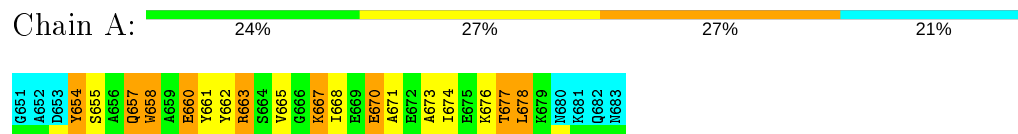


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

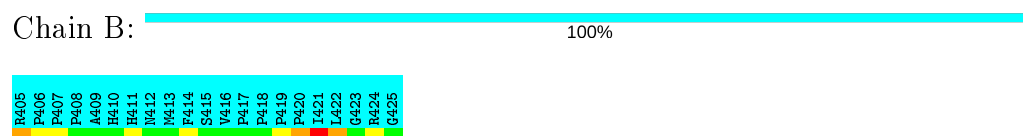


4.2.7 Score per residue for model 7

- Molecule 1: PSI

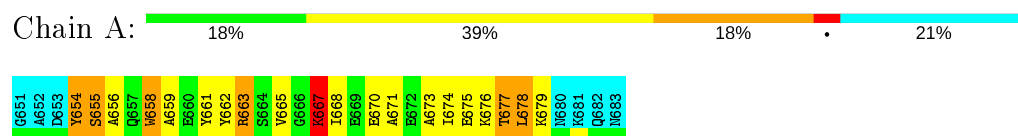


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

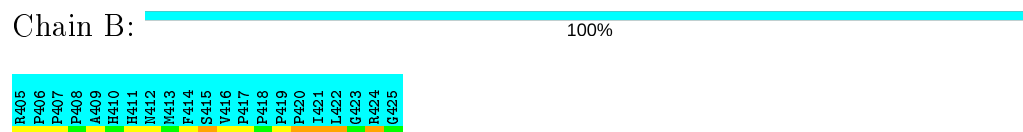


4.2.8 Score per residue for model 8

- Molecule 1: PSI

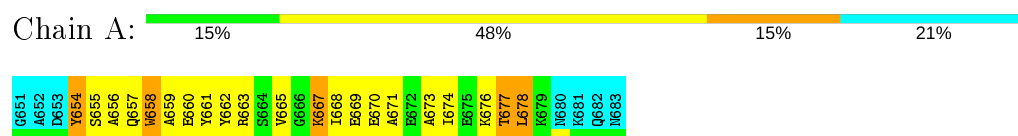


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

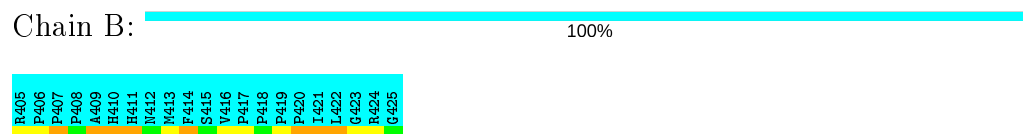


4.2.9 Score per residue for model 9

- Molecule 1: PSI

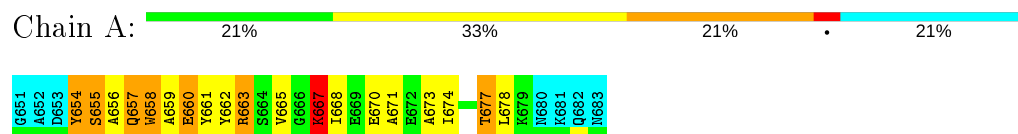


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

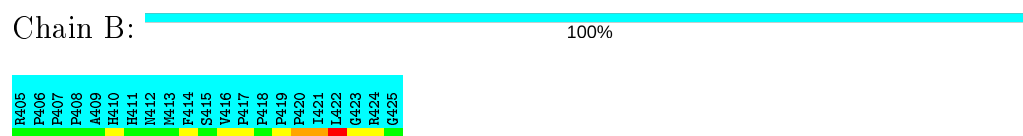


4.2.10 Score per residue for model 10

- Molecule 1: PSI

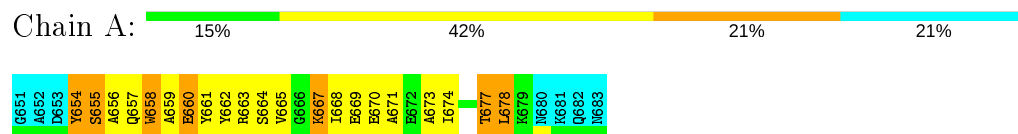


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

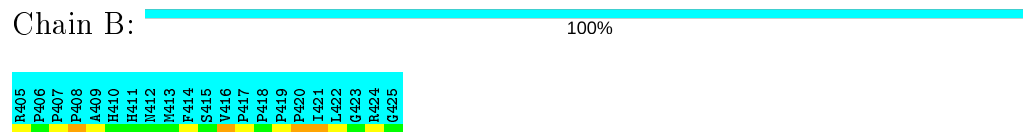


4.2.11 Score per residue for model 11

- Molecule 1: PSI

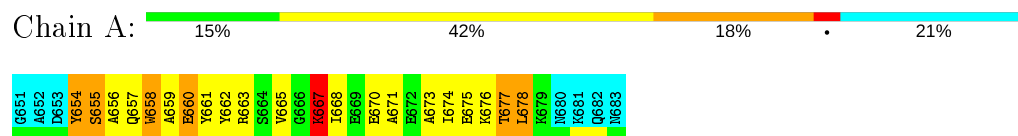


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

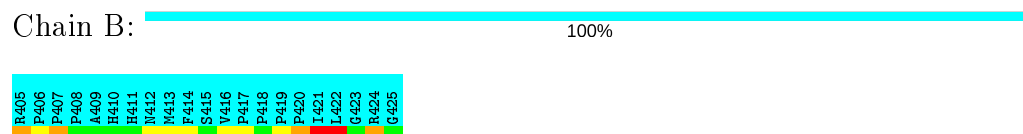


4.2.12 Score per residue for model 12

- Molecule 1: PSI

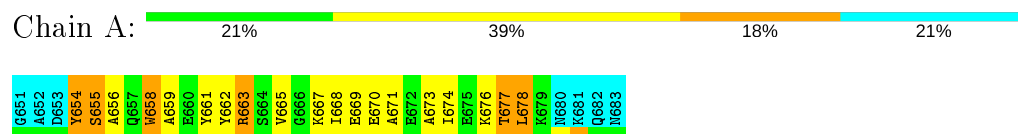


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

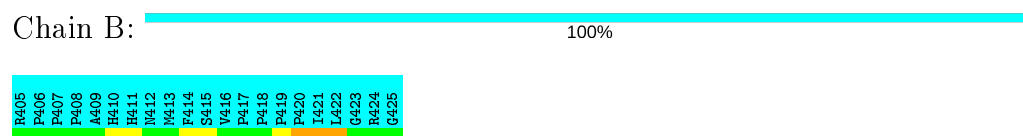


4.2.13 Score per residue for model 13

- Molecule 1: PSI

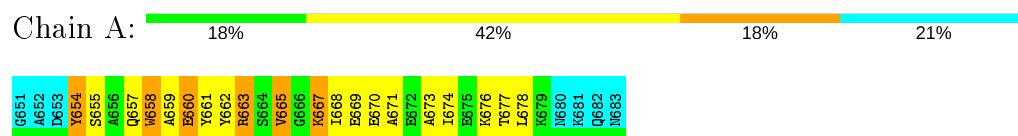


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

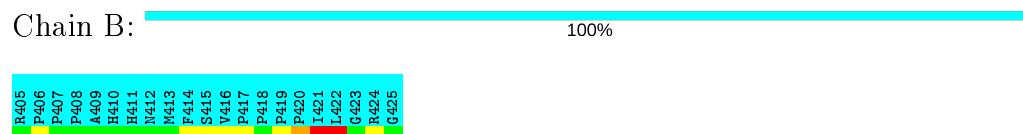


4.2.14 Score per residue for model 14

- Molecule 1: PSI

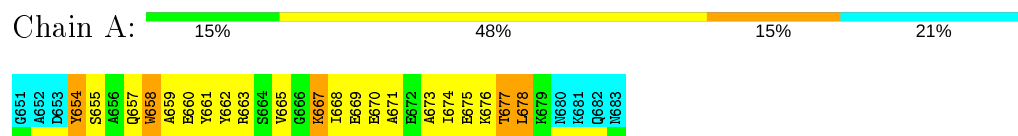


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

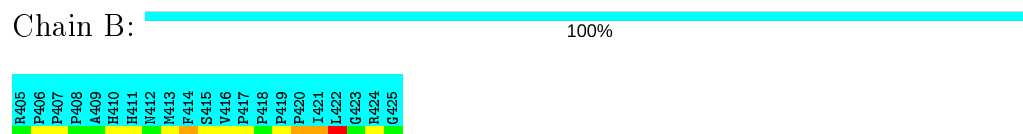


4.2.15 Score per residue for model 15

- Molecule 1: PSI

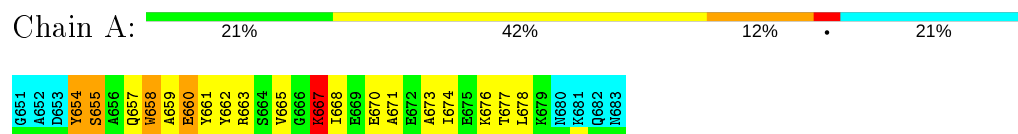


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

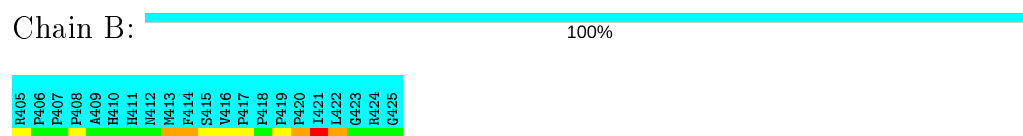


4.2.16 Score per residue for model 16

- Molecule 1: PSI

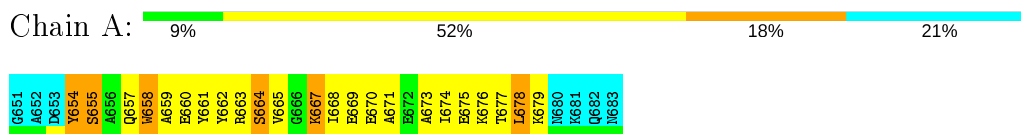


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

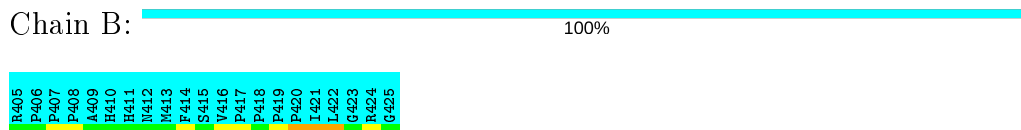


4.2.17 Score per residue for model 17

- Molecule 1: PSI

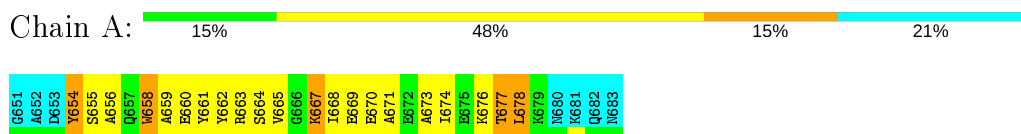


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

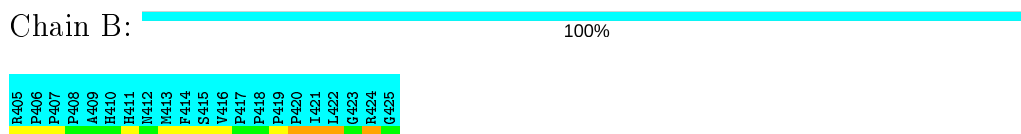


4.2.18 Score per residue for model 18

- Molecule 1: PSI

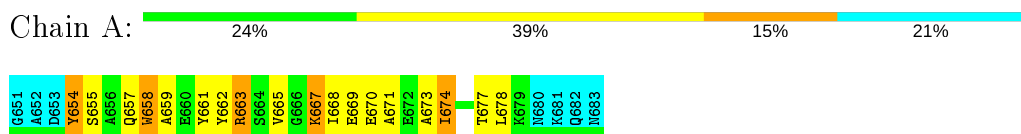


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

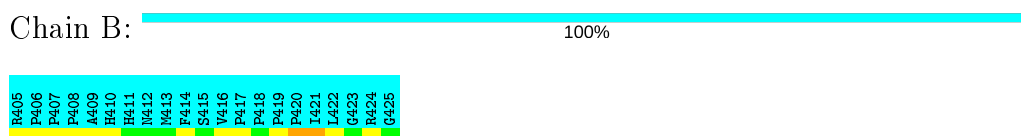


4.2.19 Score per residue for model 19

- Molecule 1: PSI

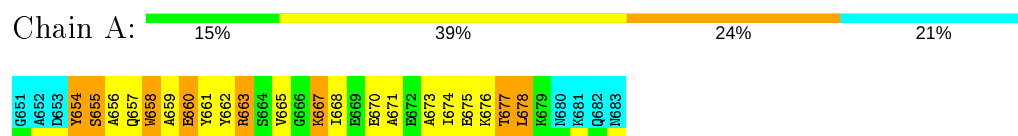


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

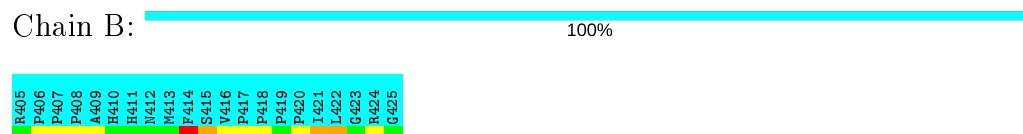


4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: PSI

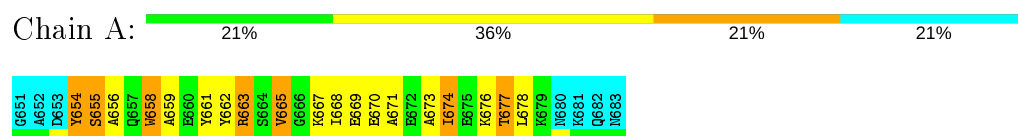


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

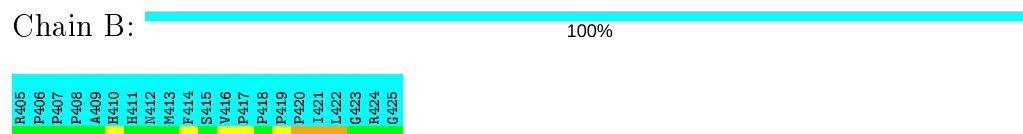


4.2.21 Score per residue for model 21

- Molecule 1: PSI

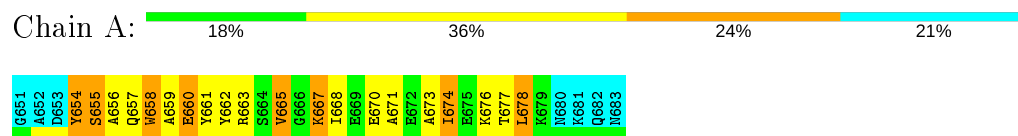


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

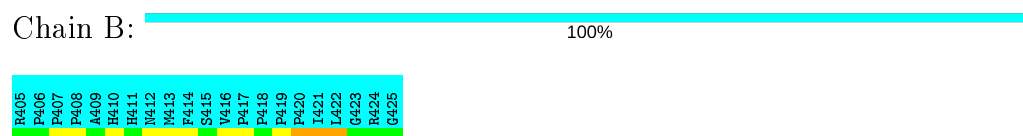


4.2.22 Score per residue for model 22

- Molecule 1: PSI

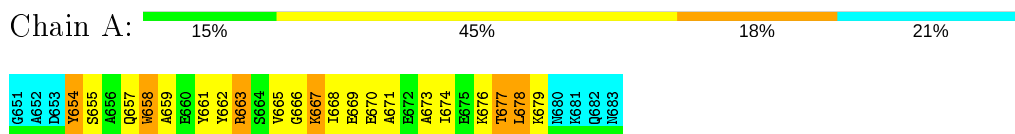


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

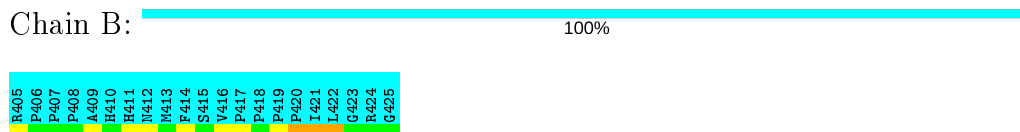


4.2.23 Score per residue for model 23

- Molecule 1: PSI

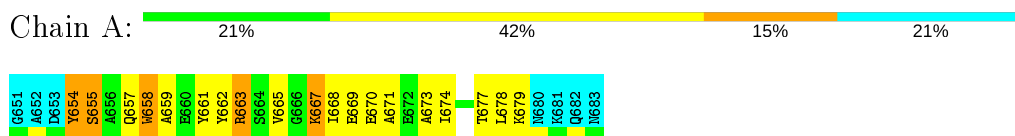


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

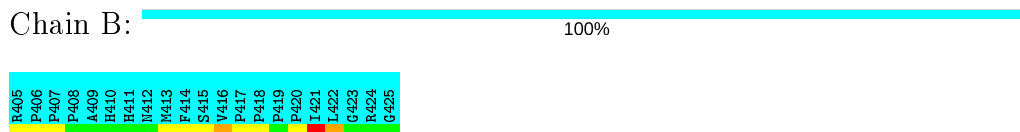


4.2.24 Score per residue for model 24

- Molecule 1: PSI

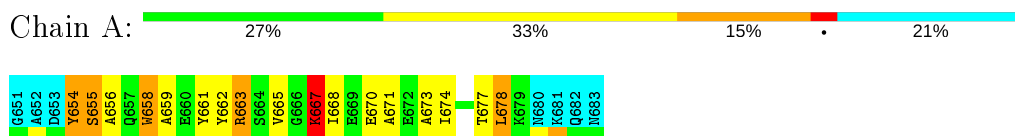


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

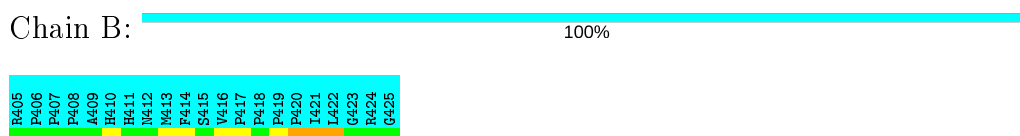


4.2.25 Score per residue for model 25

- Molecule 1: PSI

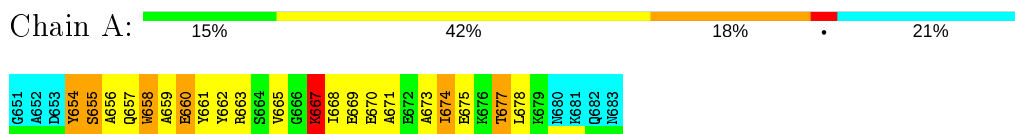


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

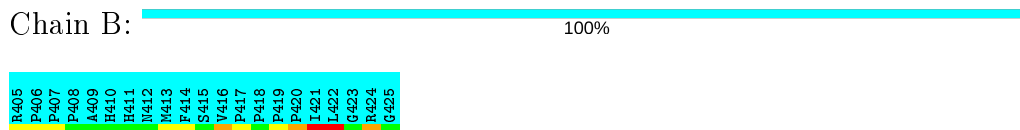


4.2.26 Score per residue for model 26

- Molecule 1: PSI

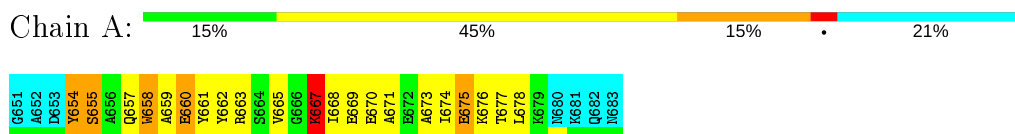


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

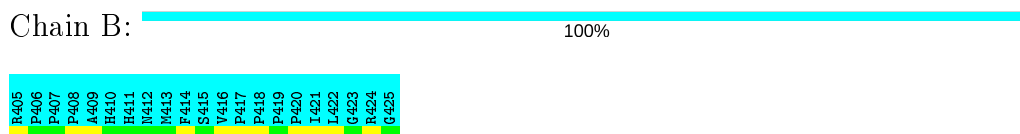


4.2.27 Score per residue for model 27

- Molecule 1: PSI

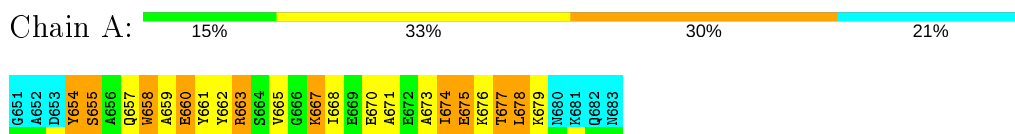


- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA

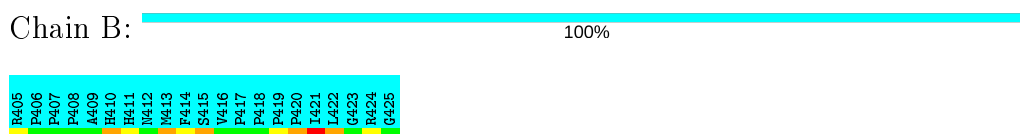


4.2.28 Score per residue for model 28

- Molecule 1: PSI



- Molecule 2: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN 70 KDA



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING*.

Of the 50 calculated structures, 28 were deposited, based on the following criterion: *LOW NOE ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
CNS	structure solution	

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	451
Number of shifts mapped to atoms	365
Number of unparsed shifts	0
Number of shifts with mapping errors	86
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	73%

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

6 Model quality i

6.1 Standard geometry i

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts 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	216	209	209	24±3
2	B	0	0	0	0±0
All	All	6048	5852	5852	678

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 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:661:TYR:O	1:A:665:VAL:HG13	0.86	1.71	16	8
1:A:662:TYR:HA	1:A:665:VAL:HG12	0.75	1.58	28	20
1:A:659:ALA:HB2	1:A:674:ILE:HB	0.74	1.56	21	9
1:A:655:SER:CB	1:A:678:LEU:HD12	0.73	2.14	27	19
1:A:675:GLU:O	1:A:678:LEU:HD22	0.71	1.86	28	1
1:A:665:VAL:HG23	1:A:667:LYS:HE3	0.69	1.64	8	1
1:A:655:SER:OG	1:A:678:LEU:HD13	0.69	1.87	19	1
1:A:663:ARG:CZ	1:A:668:ILE:HG23	0.68	2.18	2	1
1:A:662:TYR:CD2	1:A:674:ILE:HD12	0.68	2.24	26	3
1:A:655:SER:HA	1:A:674:ILE:CG2	0.68	2.19	17	16
1:A:659:ALA:HB2	1:A:674:ILE:CG2	0.68	2.19	28	23
1:A:662:TYR:HA	1:A:665:VAL:HG22	0.68	1.66	15	8
1:A:656:ALA:N	1:A:678:LEU:HD21	0.68	2.02	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:671:ALA:O	1:A:674:ILE:HG12	0.67	1.89	22	3
1:A:655:SER:HB2	1:A:678:LEU:HD12	0.67	1.65	27	12
1:A:665:VAL:HG23	1:A:667:LYS:HE2	0.66	1.67	16	2
1:A:655:SER:OG	1:A:678:LEU:HD12	0.66	1.90	5	11
1:A:671:ALA:HA	1:A:674:ILE:HD13	0.66	1.65	23	8
1:A:675:GLU:HA	1:A:678:LEU:HD13	0.64	1.69	28	2
1:A:662:TYR:HB2	1:A:671:ALA:HB2	0.64	1.68	22	25
1:A:665:VAL:HG23	1:A:667:LYS:CE	0.64	2.23	16	3
1:A:662:TYR:CD2	1:A:674:ILE:HD13	0.63	2.28	11	17
1:A:663:ARG:HD2	1:A:671:ALA:HB1	0.62	1.71	8	4
1:A:662:TYR:CD2	1:A:674:ILE:CD1	0.62	2.83	11	28
1:A:661:TYR:O	1:A:665:VAL:N	0.60	2.33	19	20
1:A:659:ALA:HA	1:A:674:ILE:HG13	0.60	1.73	21	3
1:A:665:VAL:HG13	1:A:667:LYS:HE3	0.60	1.74	12	1
1:A:655:SER:HB2	1:A:678:LEU:HD13	0.60	1.72	14	1
1:A:654:TYR:O	1:A:658:TRP:HB2	0.59	1.96	7	20
1:A:663:ARG:HA	1:A:668:ILE:HG13	0.59	1.74	22	25
1:A:656:ALA:H	1:A:678:LEU:HD21	0.58	1.59	1	1
1:A:675:GLU:O	1:A:678:LEU:CD2	0.58	2.51	28	1
1:A:678:LEU:HD23	1:A:679:LYS:N	0.58	2.13	28	1
1:A:663:ARG:HD3	1:A:671:ALA:HB1	0.57	1.77	19	8
1:A:655:SER:OG	1:A:674:ILE:O	0.57	2.23	28	6
1:A:665:VAL:HG13	1:A:667:LYS:CE	0.56	2.29	1	2
1:A:659:ALA:HB2	1:A:674:ILE:HG22	0.56	1.76	28	2
1:A:671:ALA:HA	1:A:674:ILE:CG1	0.56	2.31	21	3
1:A:675:GLU:OE1	1:A:678:LEU:HD13	0.56	2.01	27	1
1:A:678:LEU:C	1:A:678:LEU:HD23	0.56	2.22	28	1
1:A:662:TYR:HB2	1:A:671:ALA:CB	0.55	2.32	27	9
1:A:670:GLU:O	1:A:673:ALA:HB3	0.54	2.03	23	27
1:A:662:TYR:CE2	1:A:674:ILE:HD12	0.54	2.38	22	2
1:A:665:VAL:HG13	1:A:667:LYS:HE2	0.53	1.78	1	1
1:A:661:TYR:O	1:A:665:VAL:HG22	0.53	2.02	25	2
1:A:655:SER:HB2	1:A:678:LEU:HB3	0.53	1.80	28	1
1:A:655:SER:OG	1:A:678:LEU:HD22	0.53	2.04	19	1
1:A:654:TYR:N	1:A:654:TYR:CD1	0.52	2.77	11	12
1:A:667:LYS:O	1:A:671:ALA:N	0.52	2.42	21	13
1:A:668:ILE:O	1:A:671:ALA:HB3	0.52	2.04	22	5
1:A:655:SER:HB3	1:A:674:ILE:HG22	0.52	1.80	14	1
1:A:655:SER:O	1:A:674:ILE:CG2	0.52	2.57	27	6
1:A:678:LEU:CD2	1:A:679:LYS:N	0.52	2.73	28	1
1:A:661:TYR:O	1:A:665:VAL:HB	0.52	2.05	26	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:654:TYR:CD2	1:A:658:TRP:CD1	0.51	2.98	6	11
1:A:655:SER:HB2	1:A:678:LEU:N	0.51	2.20	28	1
1:A:659:ALA:O	1:A:663:ARG:HG2	0.51	2.05	26	3
1:A:656:ALA:HB2	1:A:678:LEU:HD11	0.51	1.81	12	6
1:A:658:TRP:O	1:A:662:TYR:CD2	0.51	2.64	19	25
1:A:654:TYR:CE2	1:A:658:TRP:CD1	0.51	2.99	19	5
1:A:663:ARG:HA	1:A:668:ILE:HA	0.51	1.82	18	3
1:A:657:GLN:O	1:A:660:GLU:HG2	0.50	2.06	9	3
1:A:662:TYR:CB	1:A:671:ALA:HB2	0.50	2.35	27	4
1:A:662:TYR:C	1:A:671:ALA:HB2	0.50	2.26	17	4
1:A:654:TYR:CD1	1:A:654:TYR:N	0.50	2.80	7	10
1:A:656:ALA:N	1:A:678:LEU:HD13	0.50	2.22	10	1
1:A:663:ARG:NE	1:A:668:ILE:HG23	0.49	2.21	27	1
1:A:654:TYR:CD2	1:A:658:TRP:NE1	0.49	2.81	20	4
1:A:665:VAL:HG13	1:A:667:LYS:HD3	0.48	1.83	27	1
1:A:654:TYR:HD1	1:A:654:TYR:H	0.48	1.52	24	7
1:A:678:LEU:C	1:A:678:LEU:CD2	0.48	2.80	28	1
1:A:655:SER:HA	1:A:674:ILE:HG23	0.48	1.84	28	7
1:A:654:TYR:H	1:A:654:TYR:HD1	0.48	1.51	8	9
1:A:656:ALA:N	1:A:678:LEU:HD11	0.48	2.23	8	2
1:A:659:ALA:N	1:A:674:ILE:HG21	0.48	2.23	17	3
1:A:655:SER:HB2	1:A:674:ILE:O	0.48	2.08	19	2
1:A:655:SER:CA	1:A:674:ILE:CG2	0.48	2.92	15	7
1:A:674:ILE:O	1:A:677:THR:OG1	0.47	2.29	18	6
1:A:655:SER:CB	1:A:674:ILE:O	0.47	2.62	26	12
1:A:674:ILE:O	1:A:677:THR:N	0.47	2.47	20	7
1:A:656:ALA:N	1:A:678:LEU:CD1	0.46	2.78	12	10
1:A:655:SER:HB2	1:A:678:LEU:CD1	0.46	2.40	9	2
1:A:661:TYR:O	1:A:665:VAL:CG1	0.46	2.59	23	3
1:A:662:TYR:CD2	1:A:674:ILE:HD11	0.46	2.46	17	2
1:A:665:VAL:HG23	1:A:667:LYS:HD3	0.46	1.87	10	1
1:A:655:SER:OG	1:A:677:THR:CB	0.46	2.64	15	6
1:A:655:SER:CB	1:A:678:LEU:HD13	0.46	2.41	19	1
1:A:668:ILE:N	1:A:668:ILE:CD1	0.46	2.79	17	4
1:A:662:TYR:CE2	1:A:674:ILE:HG12	0.46	2.46	18	5
1:A:659:ALA:HB2	1:A:674:ILE:CB	0.45	2.38	21	2
1:A:655:SER:OG	1:A:678:LEU:N	0.45	2.50	1	4
1:A:657:GLN:O	1:A:660:GLU:CG	0.45	2.65	22	17
1:A:662:TYR:CD2	1:A:674:ILE:HG12	0.45	2.47	14	5
1:A:655:SER:O	1:A:659:ALA:N	0.45	2.47	19	7
1:A:662:TYR:O	1:A:668:ILE:N	0.44	2.51	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:663:ARG:HE	1:A:668:ILE:HG23	0.44	1.72	27	1
1:A:655:SER:O	1:A:659:ALA:CB	0.44	2.66	6	7
1:A:658:TRP:O	1:A:662:TYR:CE2	0.44	2.70	25	3
1:A:671:ALA:HA	1:A:674:ILE:HG12	0.43	1.90	21	2
1:A:668:ILE:HD12	1:A:668:ILE:N	0.43	2.28	13	5
1:A:659:ALA:HB1	1:A:663:ARG:NH1	0.43	2.29	12	1
1:A:657:GLN:C	1:A:660:GLU:HG2	0.43	2.34	15	1
1:A:675:GLU:OE2	1:A:678:LEU:HD13	0.43	2.13	8	1
1:A:663:ARG:HD3	1:A:671:ALA:CB	0.43	2.43	16	1
1:A:671:ALA:C	1:A:674:ILE:HG12	0.43	2.34	21	3
1:A:655:SER:OG	1:A:678:LEU:HD23	0.42	2.14	1	1
1:A:663:ARG:O	1:A:668:ILE:HD11	0.42	2.14	12	2
1:A:668:ILE:N	1:A:668:ILE:HD12	0.42	2.29	6	6
1:A:661:TYR:C	1:A:665:VAL:HG13	0.42	2.34	24	3
1:A:655:SER:HB3	1:A:674:ILE:O	0.42	2.14	22	1
1:A:655:SER:HB3	1:A:677:THR:HG1	0.42	1.74	26	1
1:A:674:ILE:HD12	1:A:674:ILE:N	0.41	2.30	25	1
1:A:658:TRP:CE3	1:A:658:TRP:HA	0.41	2.50	21	1
1:A:656:ALA:N	1:A:678:LEU:HD12	0.41	2.31	18	1
1:A:655:SER:HB2	1:A:677:THR:CB	0.41	2.45	21	1
1:A:659:ALA:CB	1:A:674:ILE:HB	0.41	2.45	17	1
1:A:666:GLY:O	1:A:667:LYS:CG	0.41	2.69	23	1
1:A:655:SER:CB	1:A:678:LEU:N	0.41	2.84	25	1
1:A:658:TRP:HA	1:A:658:TRP:CE3	0.41	2.51	20	2
1:A:660:GLU:HG3	1:A:661:TYR:N	0.40	2.31	16	2
1:A:668:ILE:O	1:A:671:ALA:N	0.40	2.54	17	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	26/33 (79%)	20±1 (78±3%)	5±1 (19±4%)	1±1 (3±2%)	6	36
2	B	0	-	-	-	-	-
All	All	728/1512 (48%)	566 (78%)	137 (19%)	25 (3%)	6	36

All 2 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	667	LYS	22
1	A	664	SER	3

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	21/26 (81%)	12±1 (58±5%)	9±1 (42±5%)	0 4
2	B	0	-	-	-
All	All	588/1232 (48%)	340 (58%)	248 (42%)	0 4

All 18 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	658	TRP	28
1	A	677	THR	28
1	A	654	TYR	28
1	A	667	LYS	24
1	A	676	LYS	22
1	A	655	SER	20
1	A	660	GLU	18
1	A	669	GLU	16
1	A	663	ARG	16
1	A	678	LEU	15
1	A	675	GLU	9
1	A	657	GLN	6
1	A	674	ILE	5
1	A	679	LYS	4
1	A	670	GLU	3
1	A	665	VAL	3
1	A	672	GLU	2
1	A	664	SER	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 73% for the well-defined parts and 50% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

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	451
Number of shifts mapped to atoms	365
Number of unparsed shifts	0
Number of shifts with mapping errors	86
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- Residue not found in structure. All 86 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	14	MET	CA	56.026	0.2	1
A	16	SER	N	115.843	0.2	1
A	29	ALA	H	7.919	0.01	1
A	13	GLN	N	119.116	0.2	1
A	23	ILE	N	121.205	0.2	1
A	30	LYS	CB	32.683	0.2	1
A	11	TYR	N	118.875	0.2	1
A	27	MET	N	119.69	0.2	1
A	28	LYS	H	8.005	0.01	1
A	32	ALA	CA	52.837	0.2	1
A	24	GLU	CA	54.252	0.2	1
A	22	MET	N	119.82	0.2	1
A	22	MET	CA	57.438	0.2	1
A	16	SER	CA	58.575	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	10	TYR	H	7.938	0.01	1
A	11	TYR	H	8.151	0.01	1
A	9	GLU	HB2	1.975	0.01	2
A	29	ALA	N	122.784	0.2	1
A	30	LYS	CA	57.088	0.2	1
A	8	ILE	N	120.235	0.2	1
A	13	GLN	H	8.098	0.01	1
A	26	GLN	N	120.023	0.2	1
A	23	ILE	H	7.948	0.01	1
A	10	TYR	CA	60.889	0.2	1
A	13	GLN	HA	4.052	0.01	1
A	12	LYS	H	8.028	0.01	1
A	34	GLY	N	108.751	0.2	1
A	25	GLN	N	118.662	0.2	1
A	15	GLY	CA	45.698	0.2	1
A	18	ARG	CA	57.123	0.2	1
A	9	GLU	HA	3.998	0.01	1
A	12	LYS	CA	58.731	0.2	1
A	10	TYR	CB	38.301	0.2	1
A	13	GLN	CB	32.488	0.2	1
A	29	ALA	CA	53.412	0.2	1
A	8	ILE	CA	63.969	0.2	1
A	10	TYR	N	120.884	0.2	1
A	31	GLN	N	120.191	0.2	1
A	27	MET	H	8.215	0.01	1
A	34	GLY	H	8.215	0.01	1
A	20	ALA	CA	54.368	0.2	1
A	26	GLN	H	8.113	0.01	1
A	33	GLY	N	107.968	0.2	1
A	14	MET	N	117.606	0.2	1
A	19	GLU	H	8.323	0.01	1
A	20	ALA	H	8.097	0.01	1
A	24	GLU	H	8.179	0.01	1
A	21	GLU	H	8.153	0.01	1
A	13	GLN	CA	57.718	0.2	1
A	23	ILE	CA	63.386	0.2	1
A	11	TYR	CA	60.486	0.2	1
A	32	ALA	N	124.505	0.2	1
A	32	ALA	CB	18.972	0.2	1
A	20	ALA	N	122.303	0.2	1
A	31	GLN	H	8.074	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	24	GLU	N	121.818	0.2	1
A	21	GLU	N	118.611	0.2	1
A	17	HIS	N	120.044	0.2	1
A	32	ALA	H	8.193	0.01	1
A	30	LYS	N	119.239	0.2	1
A	26	GLN	CA	57.817	0.2	1
A	31	GLN	CB	29.04	0.2	1
A	19	GLU	CA	58.544	0.2	1
A	19	GLU	N	121.122	0.2	1
A	8	ILE	H	7.86	0.01	1
A	28	LYS	CA	57.878	0.2	1
A	16	SER	H	8.105	0.01	1
A	21	GLU	CA	58.271	0.2	1
A	27	MET	CA	57.176	0.2	1
A	17	HIS	H	8.154	0.01	1
A	14	MET	H	7.856	0.01	1
A	25	GLN	CA	57.994	0.2	1
A	13	GLN	HB2	1.995	0.01	2
A	18	ARG	N	121.096	0.2	1
A	15	GLY	N	108.578	0.2	1
A	12	LYS	N	120.763	0.2	1
A	25	GLN	H	8.209	0.01	1
A	22	MET	H	8.025	0.01	1
A	29	ALA	CB	18.574	0.2	1
A	31	GLN	CA	56.154	0.2	1
A	33	GLY	H	8.273	0.01	1
A	30	LYS	H	7.94	0.01	1
A	15	GLY	H	8.011	0.01	1
A	28	LYS	N	120.609	0.2	1
A	18	ARG	H	8.241	0.01	1
A	28	LYS	CB	32.422	0.2	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	55	-0.65 ± 0.37	None needed (imprecise)
$^{13}\text{C}_\beta$	36	0.59 ± 0.15	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	59	-0.52 ± 0.53	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 73%, i.e. 242 atoms were assigned a chemical shift out of a possible 331. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	104/130 (80%)	52/52 (100%)	26/52 (50%)	26/26 (100%)
Sidechain	108/165 (65%)	67/97 (69%)	41/61 (67%)	0/7 (0%)
Aromatic	30/36 (83%)	14/18 (78%)	16/17 (94%)	0/1 (0%)
Overall	242/331 (73%)	133/167 (80%)	83/130 (64%)	26/34 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 50%, i.e. 337 atoms were assigned a chemical shift out of a possible 677. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	149/256 (58%)	84/101 (83%)	32/108 (30%)	33/47 (70%)
Sidechain	153/360 (42%)	103/217 (47%)	50/125 (40%)	0/18 (0%)
Aromatic	35/61 (57%)	19/31 (61%)	16/25 (64%)	0/5 (0%)
Overall	337/677 (50%)	206/349 (59%)	98/258 (38%)	33/70 (47%)

7.1.4 Statistically unusual chemical shifts [i](#)

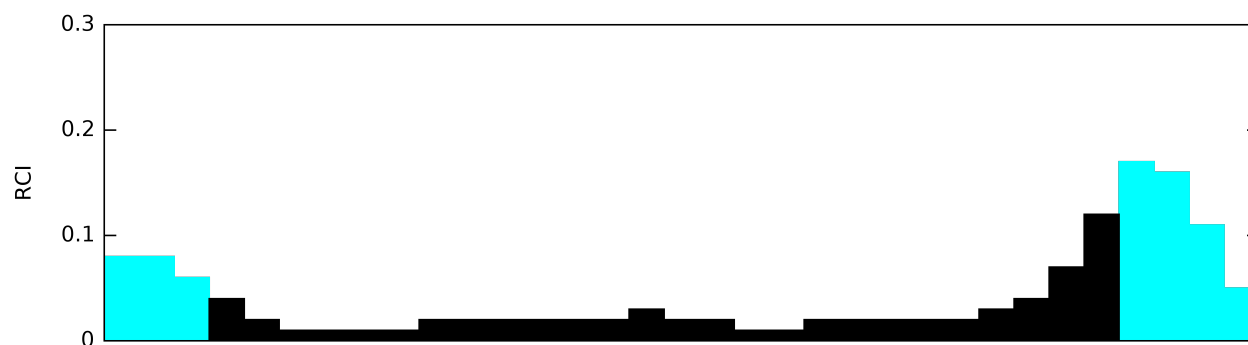
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	670	GLU	HB2	0.97	3.08 – 0.98	-5.1

7.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *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:



Random coil index (RCI) for chain B:

