Full wwPDB NMR Structure Validation Report (i)

Feb 28, 2022 – 04:42 PM EST

PDB ID	:	2ERR
Title	:	NMR Structure of the RNA Binding Domain of Human Fox-1 in Complex with UGCAUGU
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Deposited on	:	2005-10-25

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 (i) symbol.

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

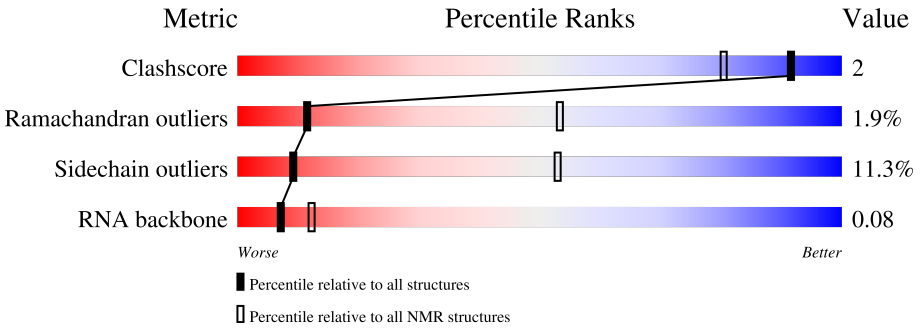
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 <=5%

Mol	Chain	Length	Quality of chain
1	B	7	43% 43% 14%
2	A	109	55% 15% • 10% 19%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:116-A:192 (77)	0.27	7

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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 7, 11, 13, 14, 15, 16, 17, 18, 19, 21, 22, 24, 25, 28
2	6, 8, 10, 20, 30
3	5, 9, 12
4	23, 26
Single-model clusters	27; 29

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1636 atoms, of which 780 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called UGCAUGU.

Mol	Chain	Residues	Atoms						Trace
1	B	7	Total	C	H	N	O	P	0
			221	66	76	24	49	6	

- Molecule 2 is a protein called Ataxin-2-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
2	A	88	Total	C	H	N	O	S	0
			1415	443	704	135	131	2	

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MET	-	expression tag	UNP Q9NWB1
A	89	GLY	-	expression tag	UNP Q9NWB1
A	90	SER	-	expression tag	UNP Q9NWB1
A	91	SER	-	expression tag	UNP Q9NWB1
A	92	HIS	-	expression tag	UNP Q9NWB1
A	93	HIS	-	expression tag	UNP Q9NWB1
A	94	HIS	-	expression tag	UNP Q9NWB1
A	95	HIS	-	expression tag	UNP Q9NWB1
A	96	HIS	-	expression tag	UNP Q9NWB1
A	97	HIS	-	expression tag	UNP Q9NWB1
A	98	SER	-	expression tag	UNP Q9NWB1
A	99	SER	-	expression tag	UNP Q9NWB1
A	100	GLY	-	expression tag	UNP Q9NWB1
A	101	LEU	-	expression tag	UNP Q9NWB1
A	102	VAL	-	expression tag	UNP Q9NWB1
A	103	PRO	-	expression tag	UNP Q9NWB1
A	104	ARG	-	expression tag	UNP Q9NWB1
A	105	GLY	-	expression tag	UNP Q9NWB1
A	106	SER	-	expression tag	UNP Q9NWB1
A	107	HIS	-	expression tag	UNP Q9NWB1
A	108	MET	-	expression tag	UNP Q9NWB1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

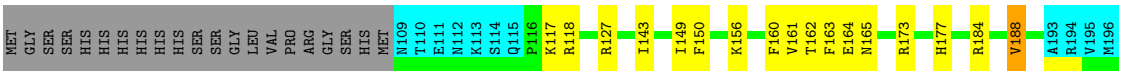
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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: UGCAUGU

Chain B:

• Molecule 2: Ataxin-2-binding protein 1

Chain A:



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

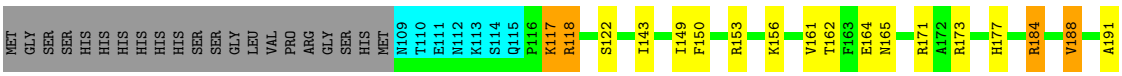
4.2.1 Score per residue for model 1

• Molecule 1: UGCAUGU

Chain B:

• Molecule 2: Ataxin-2-binding protein 1

Chain A:



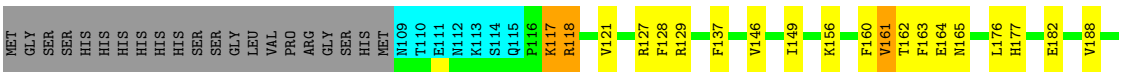
4.2.2 Score per residue for model 2

• Molecule 1: UGCAUGU

Chain B:

• Molecule 2: Ataxin-2-binding protein 1

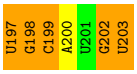
Chain A:



4.2.3 Score per residue for model 3

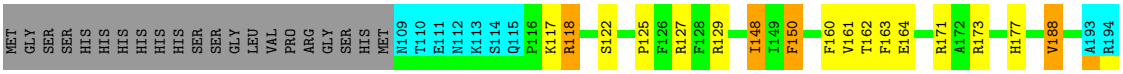
• Molecule 1: UGCAUGU

Chain B:



• Molecule 2: Ataxin-2-binding protein 1

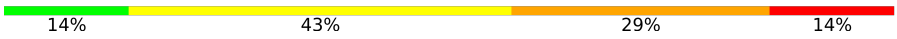
Chain A:

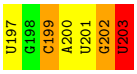


4.2.4 Score per residue for model 4

• Molecule 1: UGCAUGU

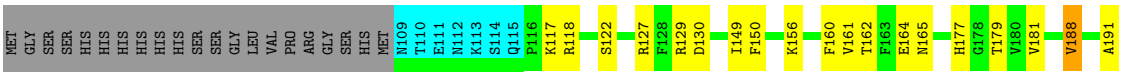
Chain B:





• Molecule 2: Ataxin-2-binding protein 1

Chain A:



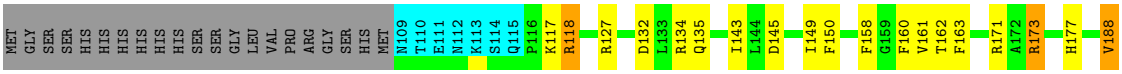
4.2.5 Score per residue for model 5

• Molecule 1: UGCAUGU

Chain B:

• Molecule 2: Ataxin-2-binding protein 1

Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: UGCAUGU

Chain B:

• Molecule 2: Ataxin-2-binding protein 1

Chain A:

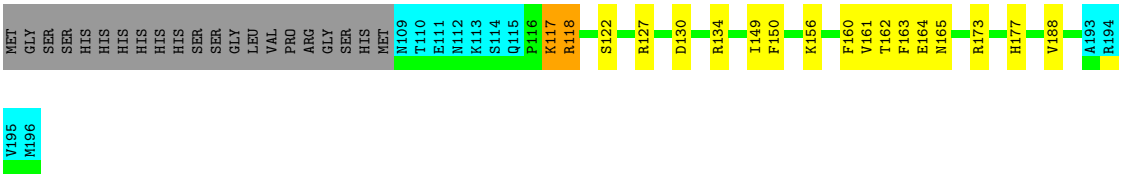
4.2.7 Score per residue for model 7 (medoid)

• Molecule 1: UGCAUGU

Chain B:

• Molecule 2: Ataxin-2-binding protein 1

Chain A:



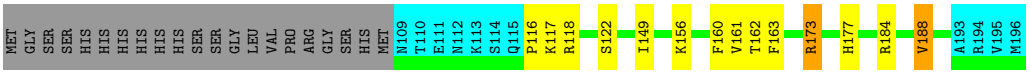
4.2.8 Score per residue for model 8

• Molecule 1: UGCAUGU

Chain B:

• Molecule 2: Ataxin-2-binding protein 1

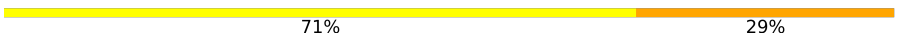
Chain A:



4.2.9 Score per residue for model 9

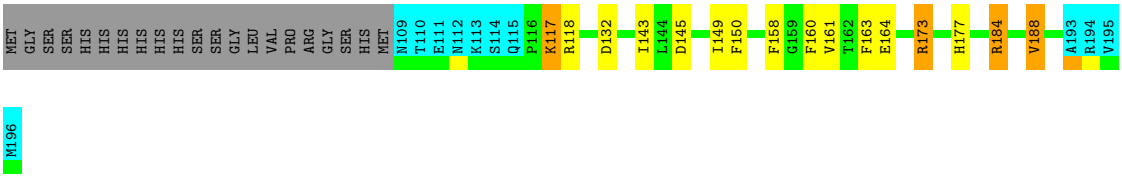
• Molecule 1: UGCAUGU

Chain B:



• Molecule 2: Ataxin-2-binding protein 1

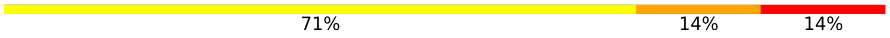
Chain A:



4.2.10 Score per residue for model 10

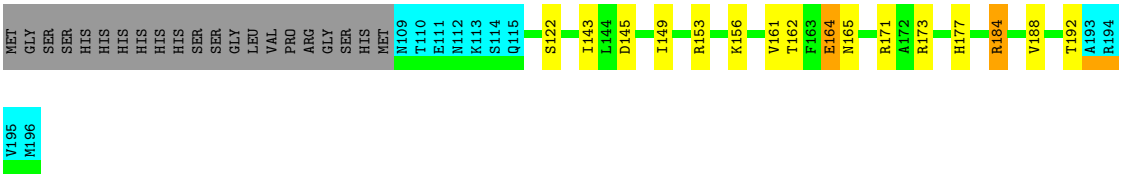
• Molecule 1: UGCAUGU

Chain B:



• Molecule 2: Ataxin-2-binding protein 1

Chain A:



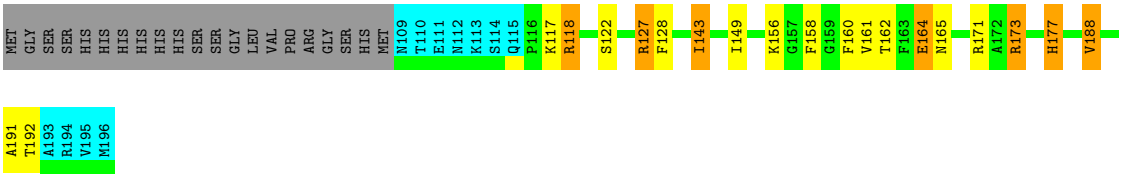
4.2.11 Score per residue for model 11

• Molecule 1: UGCAUGU

Chain B:

• Molecule 2: Ataxin-2-binding protein 1

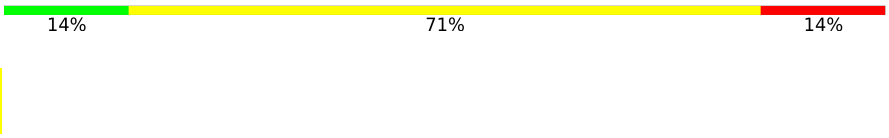
Chain A:



4.2.12 Score per residue for model 12

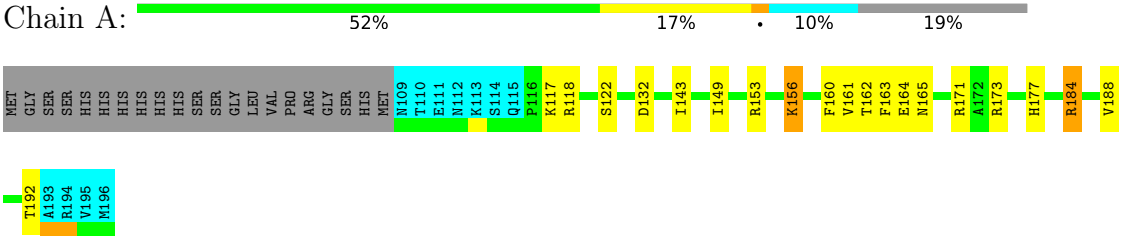
• Molecule 1: UGCAUGU

Chain B:



• Molecule 2: Ataxin-2-binding protein 1

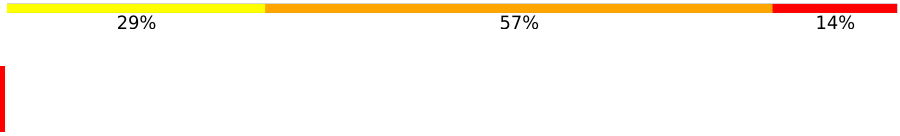
Chain A:



4.2.13 Score per residue for model 13

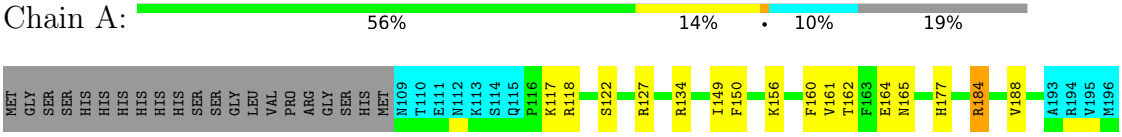
• Molecule 1: UGCAUGU

Chain B:



• Molecule 2: Ataxin-2-binding protein 1

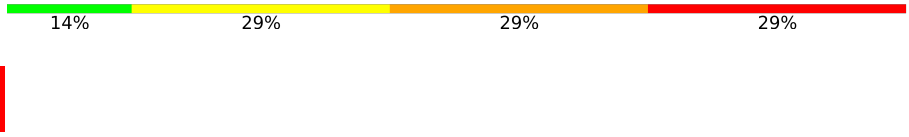
Chain A:



4.2.14 Score per residue for model 14

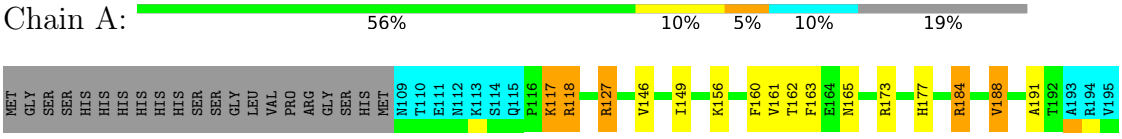
• Molecule 1: UGCAUGU

Chain B:



• Molecule 2: Ataxin-2-binding protein 1

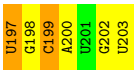
Chain A:



4.2.15 Score per residue for model 15

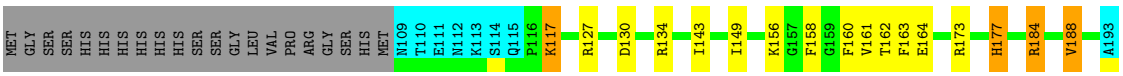
• Molecule 1: UGCAUGU

Chain B:



• Molecule 2: Ataxin-2-binding protein 1

Chain A:



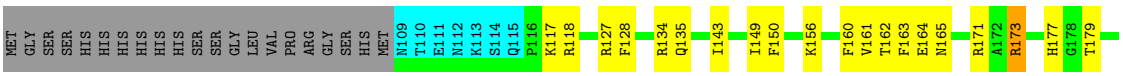
4.2.16 Score per residue for model 16

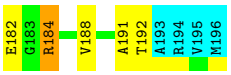
• Molecule 1: UGCAUGU

Chain B:

• Molecule 2: Ataxin-2-binding protein 1

Chain A:

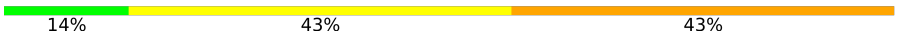


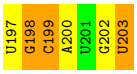


4.2.17 Score per residue for model 17

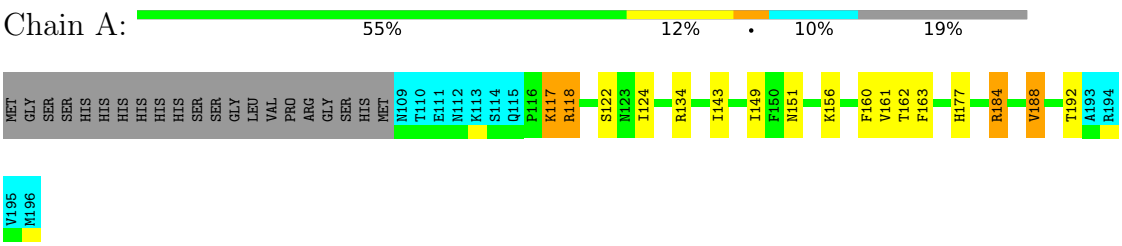
• Molecule 1: UGCAUGU

Chain B:



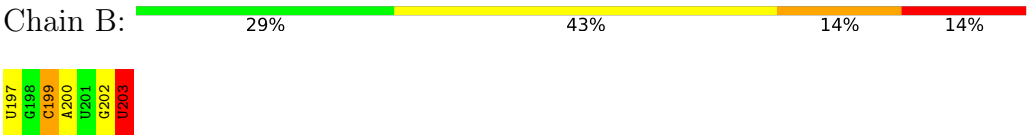


• Molecule 2: Ataxin-2-binding protein 1

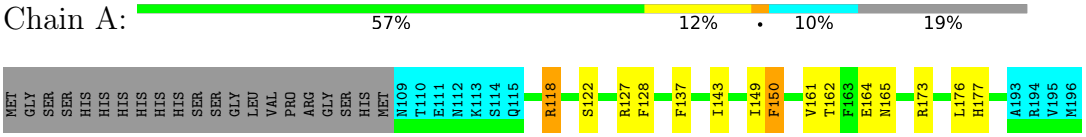


4.2.18 Score per residue for model 18

• Molecule 1: UGCAUGU

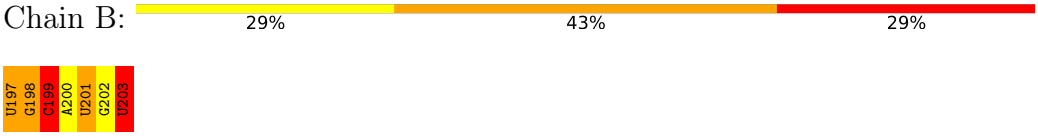


• Molecule 2: Ataxin-2-binding protein 1

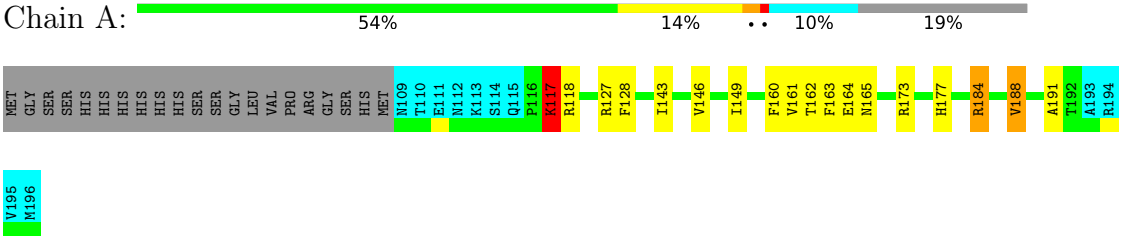


4.2.19 Score per residue for model 19

• Molecule 1: UGCAUGU



• Molecule 2: Ataxin-2-binding protein 1



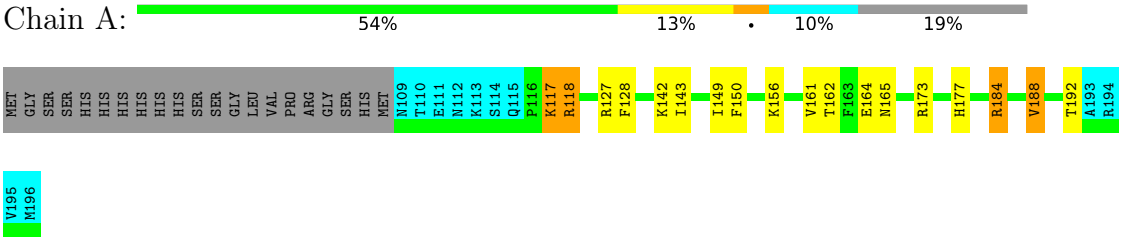
4.2.20 Score per residue for model 20

• Molecule 1: UGCAUGU

Chain B:

• Molecule 2: Ataxin-2-binding protein 1

Chain A:



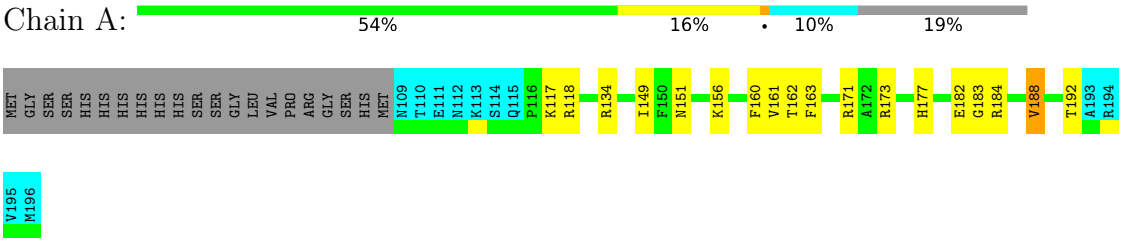
4.2.21 Score per residue for model 21

• Molecule 1: UGCAUGU

Chain B:

• Molecule 2: Ataxin-2-binding protein 1

Chain A:



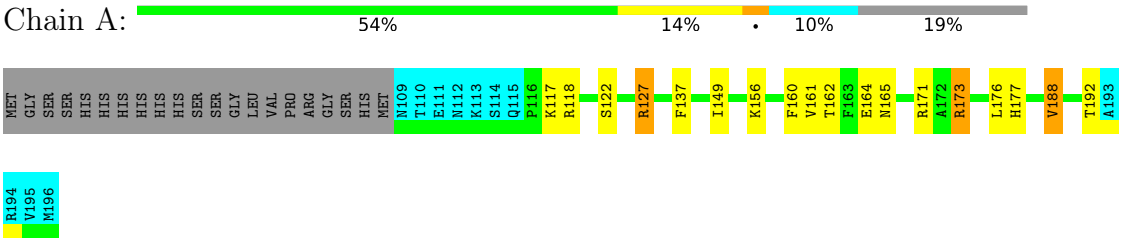
4.2.22 Score per residue for model 22

• Molecule 1: UGCAUGU

Chain B:

• Molecule 2: Ataxin-2-binding protein 1

Chain A:



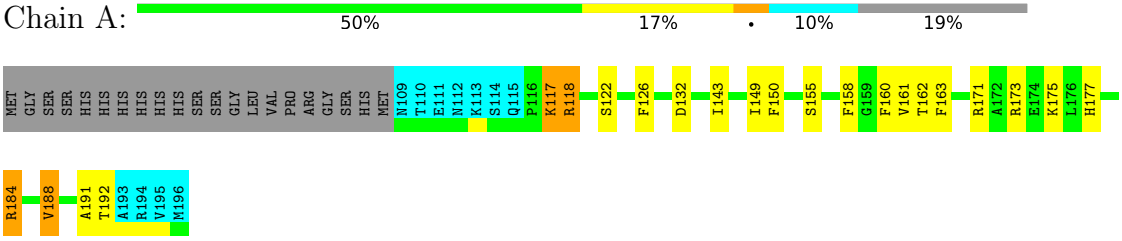
4.2.23 Score per residue for model 23

- Molecule 1: UGCAUGU

Chain B:

- Molecule 2: Ataxin-2-binding protein 1

Chain A:



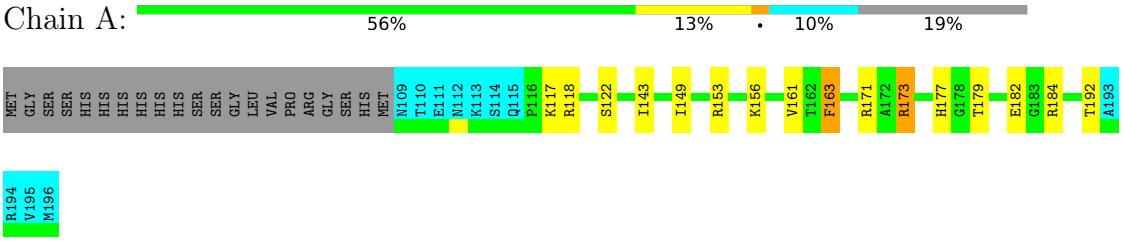
4.2.24 Score per residue for model 24

- Molecule 1: UGCAUGU

Chain B:

- Molecule 2: Ataxin-2-binding protein 1

Chain A:



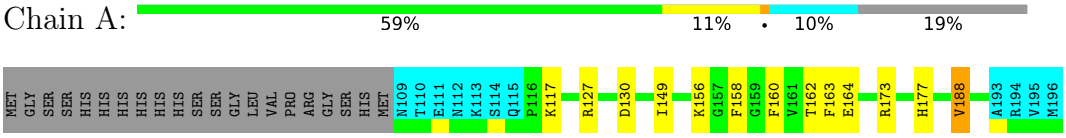
4.2.25 Score per residue for model 25

• Molecule 1: UGCAUGU

Chain B:

• Molecule 2: Ataxin-2-binding protein 1

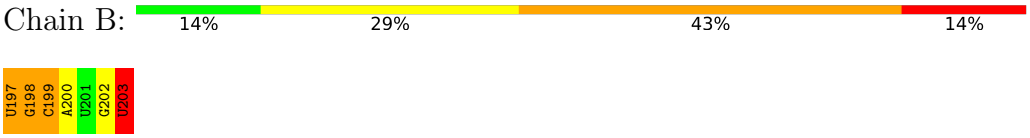
Chain A:



4.2.26 Score per residue for model 26

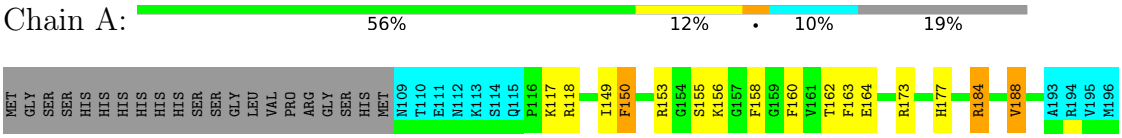
• Molecule 1: UGCAUGU

Chain B:



• Molecule 2: Ataxin-2-binding protein 1

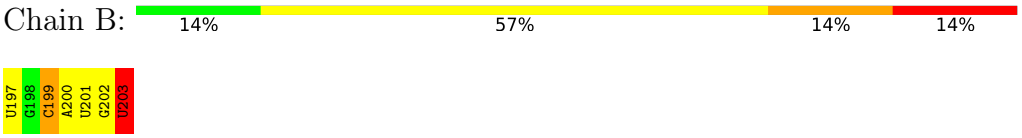
Chain A:



4.2.27 Score per residue for model 27

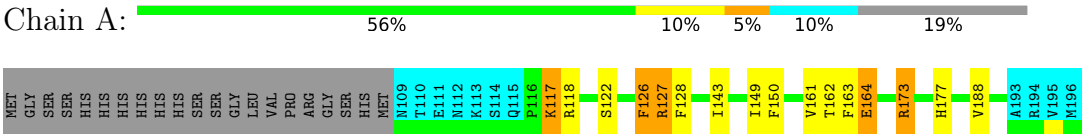
• Molecule 1: UGCAUGU

Chain B:



• Molecule 2: Ataxin-2-binding protein 1

Chain A:



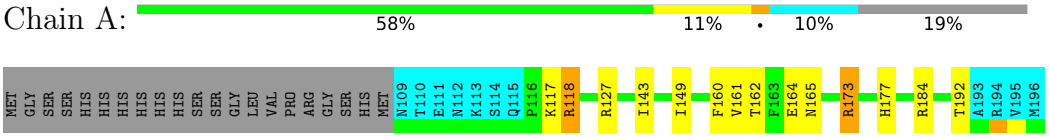
4.2.28 Score per residue for model 28

• Molecule 1: UGCAUGU

Chain B:

• Molecule 2: Ataxin-2-binding protein 1

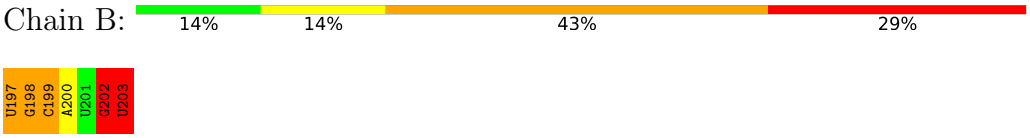
Chain A:



4.2.29 Score per residue for model 29

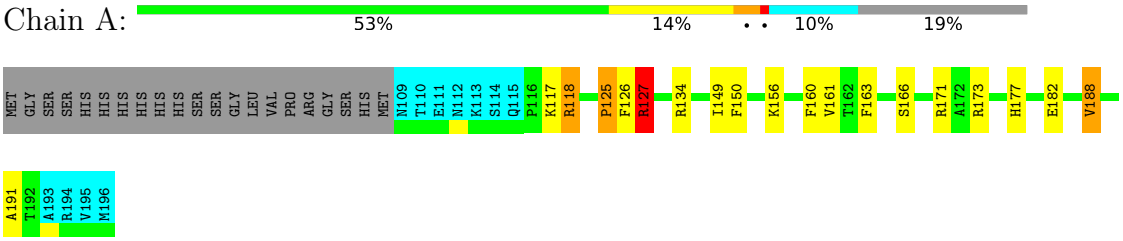
• Molecule 1: UGCAUGU

Chain B:



• Molecule 2: Ataxin-2-binding protein 1

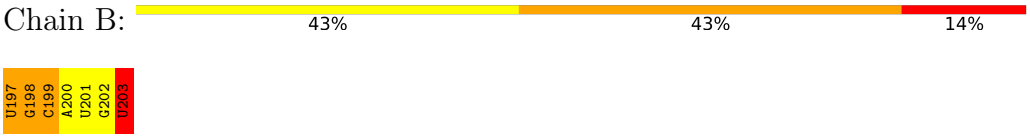
Chain A:



4.2.30 Score per residue for model 30

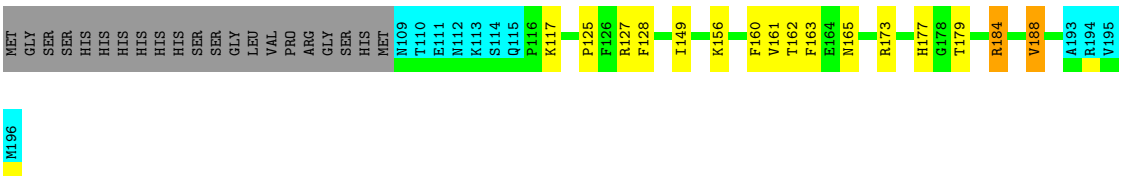
• Molecule 1: UGCAUGU

Chain B:



• Molecule 2: Ataxin-2-binding protein 1

Chain A:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET
N109 T110 E111 N112 K113 S114 Q115 P116 K117
P125 F126 R127 F128
I149
K156
F160 V161 T162 F163 E164 N165
R173
H177 G178 T179
R184
V188
A193 R194 V195
M196

5 Refinement protocol and experimental data overview

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

Of the 30 calculated structures, 30 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CYANA	structure solution	2.0
Amber	refinement	7.0

No chemical shift data was provided.

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	B	1.40±0.03	0±0/161 (0.0± 0.1%)	2.29±0.04	11±2/249 (4.2± 0.8%)
2	A	0.73±0.01	0±0/636 (0.0± 0.0%)	1.28±0.03	6±2/852 (0.6± 0.2%)
All	All	0.91	1/23910 (0.0%)	1.56	481/33030 (1.5%)

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
1	B	0.0±0.0	1.8±1.0
2	A	0.0±0.0	4.0±1.4
All	All	0	173

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	202	G	C2-N2	-5.27	1.29	1.34	15	1

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	A	173	ARG	NE-CZ-NH1	9.68	125.14	120.30	1	22
1	B	202	G	O4'-C1'-N9	8.65	115.12	108.20	11	28
2	A	118	ARG	NE-CZ-NH1	8.43	124.52	120.30	3	16
1	B	200	A	N1-C6-N6	-8.38	113.57	118.60	5	12
1	B	200	A	C5-C6-N1	8.15	121.78	117.70	25	30
1	B	203	U	O4'-C1'-N1	8.12	114.69	108.20	27	26
2	A	134	ARG	NE-CZ-NH1	7.49	124.05	120.30	16	6
1	B	197	U	N3-C2-O2	-7.46	116.98	122.20	18	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	199	C	N3-C2-O2	-7.28	116.81	121.90	9	30
1	B	200	A	P-O3'-C3'	7.26	128.41	119.70	16	3
2	A	173	ARG	NE-CZ-NH2	-7.21	116.70	120.30	5	9
2	A	171	ARG	NE-CZ-NH1	7.09	123.84	120.30	3	12
2	A	184	ARG	NE-CZ-NH1	6.91	123.76	120.30	13	15
1	B	200	A	C4-C5-C6	-6.84	113.58	117.00	20	27
1	B	202	G	N1-C6-O6	-6.51	115.99	119.90	11	15
1	B	202	G	N3-C2-N2	-6.43	115.40	119.90	5	5
2	A	127	ARG	NE-CZ-NH1	6.36	123.48	120.30	11	16
1	B	203	U	C5'-C4'-C3'	6.29	126.06	116.00	4	5
1	B	199	C	O4'-C1'-N1	6.23	113.18	108.20	19	10
2	A	188	VAL	CA-CB-CG2	6.13	120.09	110.90	5	20
2	A	161	VAL	CA-CB-CG1	6.02	119.93	110.90	17	6
1	B	198	G	O4'-C1'-N9	5.97	112.97	108.20	17	10
2	A	153	ARG	NE-CZ-NH1	5.91	123.26	120.30	10	4
1	B	197	U	C3'-C2'-C1'	5.88	106.20	101.50	9	2
1	B	201	U	O4'-C1'-N1	5.87	112.89	108.20	11	1
1	B	202	G	C4'-C3'-C2'	-5.86	96.75	102.60	7	10
2	A	161	VAL	CG1-CB-CG2	-5.82	101.58	110.90	13	26
1	B	198	G	N1-C6-O6	-5.80	116.42	119.90	13	13
2	A	149	ILE	C-N-CA	5.77	136.12	121.70	18	3
2	A	121	VAL	CA-CB-CG1	5.74	119.52	110.90	2	1
1	B	199	C	N3-C4-C5	5.74	124.19	121.90	15	5
1	B	202	G	C5-C6-N1	5.71	114.35	111.50	4	13
1	B	197	U	N1-C1'-C2'	5.71	121.42	114.00	3	3
2	A	173	ARG	CD-NE-CZ	5.64	131.49	123.60	30	3
1	B	199	C	N3-C4-N4	-5.53	114.13	118.00	15	1
1	B	202	G	O4'-C4'-C3'	5.50	110.50	106.10	15	13
1	B	201	U	N3-C2-O2	-5.50	118.35	122.20	14	11
1	B	201	U	C5'-C4'-O4'	5.48	115.67	109.10	27	4
2	A	129	ARG	NE-CZ-NH1	5.44	123.02	120.30	2	3
1	B	198	G	C8-N9-C4	-5.43	104.23	106.40	15	1
1	B	199	C	N1-C2-O2	5.41	122.15	118.90	10	13
2	A	134	ARG	CD-NE-CZ	5.27	130.97	123.60	21	1
1	B	202	G	N3-C4-C5	-5.24	125.98	128.60	11	1
1	B	201	U	N1-C2-N3	5.17	118.00	114.90	4	2
1	B	200	A	O4'-C1'-N9	5.13	112.30	108.20	7	1
1	B	203	U	N3-C2-O2	-5.12	118.61	122.20	4	1
2	A	184	ARG	CD-NE-CZ	5.09	130.72	123.60	15	1
1	B	197	U	O4'-C1'-C2'	-5.05	100.75	105.80	18	1
2	A	117	LYS	C-N-CA	5.02	134.24	121.70	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	198	G	N3-C4-C5	-5.02	126.09	128.60	15	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	A	162	THR	Peptide	27
2	A	117	LYS	Peptide	20
2	A	164	GLU	Peptide	20
2	A	163	PHE	Peptide	20
2	A	118	ARG	Peptide	19
1	B	203	U	Sidechain	16
1	B	197	U	Sidechain	15
2	A	191	ALA	Peptide	8
1	B	201	U	Sidechain	8
1	B	199	C	Sidechain	6
1	B	198	G	Sidechain	5
1	B	200	A	Sidechain	2
2	A	177	HIS	Sidechain	2
1	B	202	G	Sidechain	2
2	A	192	THR	Peptide	1
2	A	150	PHE	Sidechain	1
2	A	125	PRO	Peptide	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	B	145	76	76	0±1
2	A	623	617	617	2±1
All	All	23040	20790	20788	66

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:149:ILE:HG22	2:A:156:LYS:CE	0.72	2.15	10	9
2:A:149:ILE:HG22	2:A:156:LYS:HE2	0.69	1.63	10	1
2:A:149:ILE:HG22	2:A:156:LYS:HE3	0.66	1.67	14	16
2:A:143:ILE:HD12	2:A:143:ILE:H	0.64	1.53	11	16
1:B:202:G:H1'	2:A:149:ILE:HD12	0.47	1.87	21	2
2:A:137:PHE:CE2	2:A:176:LEU:HD12	0.45	2.47	18	1
1:B:203:U:H5'	1:B:203:U:C6	0.44	2.48	23	7
2:A:177:HIS:HB2	2:A:188:VAL:HG22	0.44	1.88	11	1
2:A:148:ILE:CG2	2:A:150:PHE:CD1	0.44	3.01	3	1
2:A:149:ILE:HG13	2:A:158:PHE:CE2	0.43	2.49	25	7
2:A:143:ILE:H	2:A:143:ILE:HD12	0.41	1.75	28	1
2:A:137:PHE:CE1	2:A:176:LEU:HD12	0.41	2.51	2	2
1:B:203:U:C6	1:B:203:U:H5'	0.40	2.52	4	1
1:B:201:U:H4'	1:B:202:G:H5'	0.40	1.92	14	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	
2	A	77/109 (71%)	67±2 (88±3%)	8±2 (10±2%)	1±1 (2±2%)	11	53
All	All	2310/3270 (71%)	2024 (88%)	242 (10%)	44 (2%)	11	53

All 16 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	A	117	LYS	11
2	A	182	GLU	5
2	A	150	PHE	3
2	A	125	PRO	3
2	A	127	ARG	3
2	A	126	PHE	3
2	A	156	LYS	2
2	A	164	GLU	2
2	A	192	THR	2

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Mol	Chain	Res	Type	Models (Total)
2	A	118	ARG	2
2	A	149	ILE	2
2	A	155	SER	2
2	A	116	PRO	1
2	A	183	GLY	1
2	A	128	PHE	1
2	A	166	SER	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	
2	A	66/94 (70%)	59±2 (89±3%)	7±2 (11±3%)	9	53
All	All	1980/2820 (70%)	1756 (89%)	224 (11%)	9	53

All 33 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	A	177	HIS	29
2	A	188	VAL	25
2	A	160	PHE	24
2	A	165	ASN	17
2	A	184	ARG	17
2	A	122	SER	15
2	A	150	PHE	13
2	A	173	ARG	13
2	A	192	THR	9
2	A	117	LYS	8
2	A	128	PHE	8
2	A	127	ARG	6
2	A	130	ASP	4
2	A	179	THR	4
2	A	132	ASP	4
2	A	146	VAL	3
2	A	145	ASP	3
2	A	164	GLU	3

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Mol	Chain	Res	Type	Models (Total)
2	A	135	GLN	2
2	A	134	ARG	2
2	A	118	ARG	2
2	A	151	ASN	2
2	A	161	VAL	1
2	A	148	ILE	1
2	A	181	VAL	1
2	A	171	ARG	1
2	A	143	ILE	1
2	A	153	ARG	1
2	A	124	ILE	1
2	A	142	LYS	1
2	A	175	LYS	1
2	A	163	PHE	1
2	A	126	PHE	1

6.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	B	7/7 (100%)	3±1 (40±9%)	1±1 (20±14%)	0.08±0.04
All	All	192/210 (91%)	85 (44%)	41 (21%)	0.08

The overall RNA backbone suiteness is 0.08.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	199	C	30
1	B	203	U	30
1	B	198	G	17
1	B	201	U	8

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	199	C	16
1	B	197	U	12
1	B	198	G	11
1	B	200	A	2

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 monosaccharides 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

No chemical shift data were provided