Full wwPDB NMR Structure Validation Report (i)

Mar 5, 2022 – 09:58 AM EST

PDB ID	:	2JWN
Title	:	Solution NMR structure of the protease-resistent domain of Xenopus laevis ePABP2
Authors	:	Song, J.; Markley, J.L.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on	:	2007-10-16

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:

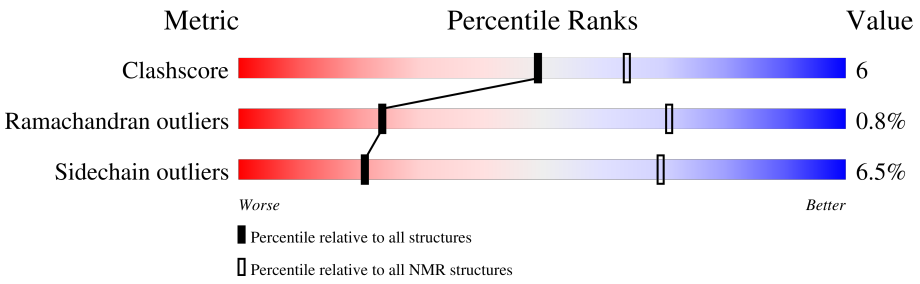
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

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

Mol	Chain	Length	Quality of chain
1	A	124	56% 8% 35%
1	B	124	60% 13% • 26%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 5 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:33-A:112, B:21-B:112 (172)	0.58	8

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 3 clusters and 7 single-model clusters were found.

Cluster number	Models
1	9, 11, 13, 14, 20
2	3, 5, 7, 12
3	4, 6, 8, 10
Single-model clusters	1; 2; 15; 16; 17; 18; 19

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3757 atoms, of which 1864 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Embryonic polyadenylate-binding protein 2-B.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	124	1879	586	933	166	187	7	0
1	B	124	1878	586	931	166	188	7	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP Q6TY21
A	2	ILE	-	expression tag	UNP Q6TY21
A	3	ALA	-	expression tag	UNP Q6TY21
B	1	ALA	-	expression tag	UNP Q6TY21
B	2	ILE	-	expression tag	UNP Q6TY21
B	3	ALA	-	expression tag	UNP Q6TY21

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A: 56% 8% 35%

A1 I2 A3 P4 C5 M6 Q7 T8 T9 H10 S11 K12 M13 T14 A15 G16 A17 Y18 T19 E20 G21 P22 P23 Q24 P25 L26 S27 A28 E29 E30 K31 K32 Y40 L69 F73 R88 V91 D98 K108 V109 L110 P111 K112 R113 T114 N115 M116 P117 G118 I119 S120 S121 T122

D123 R124

• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain B: 60% 13% • 26%

A1 I2 A3 P4 C5 M6 Q7 T8 T9 H10 S11 K12 M13 T14 A15 G16 A17 Y18 T19 E20 G21 P22 L26 E30 K31 K32 Y40 Y46 N64 R65 D71 P77 Y82 R88 V91 K108 V109 L110 P111 K112 R113 T114 N115 M116 P117 G118 I119 S120 S121

T122 D123 R124

4.2 Scores per residue for each member of the ensemble

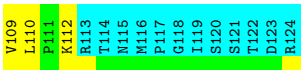
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Embryonic polyadenylate-binding protein 2-B

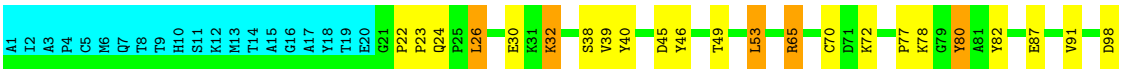
Chain A: 48% 15% • 35%

A1 I2 A3 P4 C5 M6 Q7 T8 T9 H10 S11 K12 M13 T14 A15 G16 A17 Y18 T19 E20 G21 P22 P23 Q24 P25 L26 S27 A28 E29 E30 K31 K32 E33 R37 S38 V39 Y40 Q51 N64 R65 L69 C70 F73 K78 G79 Y80 E84 V91 D98 K108



• Molecule 1: Embryonic polyadenylate-binding protein 2-B

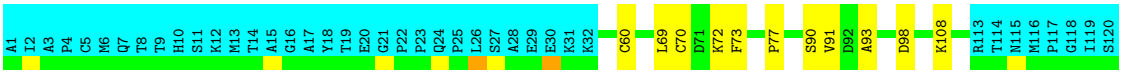
Chain B:



4.2.2 Score per residue for model 2

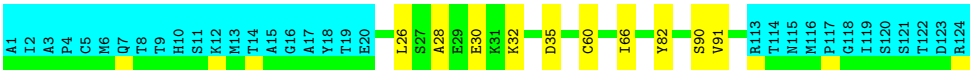
• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A:



• Molecule 1: Embryonic polyadenylate-binding protein 2-B

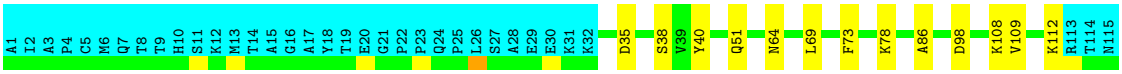
Chain B:

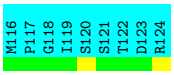


4.2.3 Score per residue for model 3

• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A:





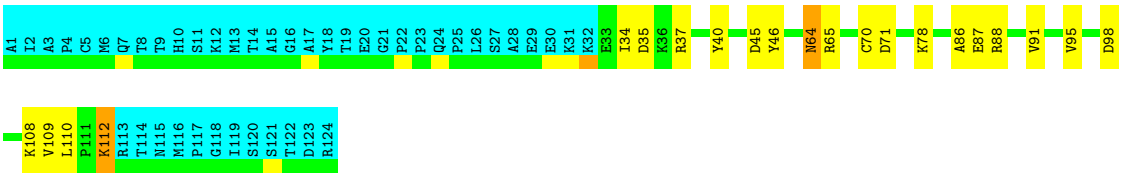
• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain B:

4.2.4 Score per residue for model 4

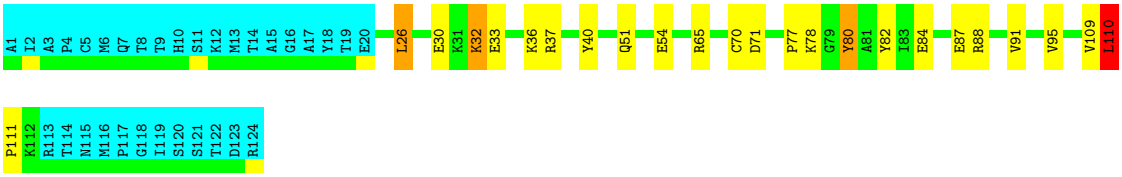
• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A:



• Molecule 1: Embryonic polyadenylate-binding protein 2-B

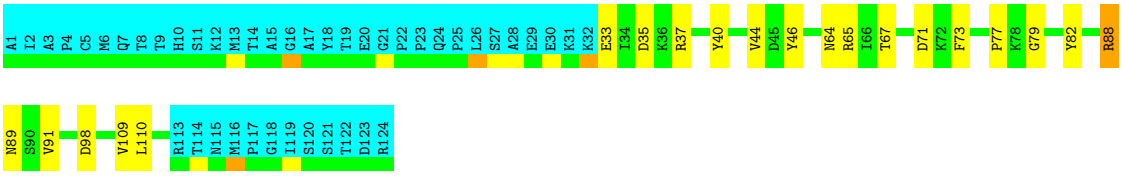
Chain B:



4.2.5 Score per residue for model 5

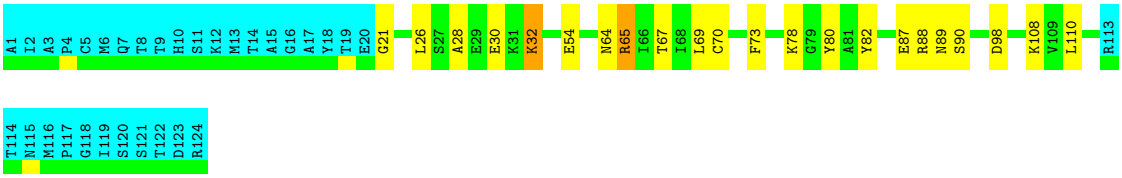
• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A:



• Molecule 1: Embryonic polyadenylate-binding protein 2-B

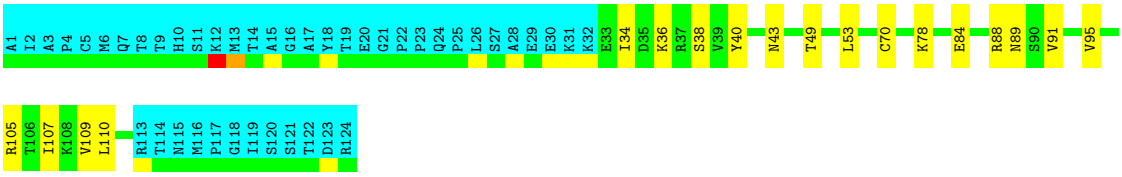
Chain B:



4.2.6 Score per residue for model 6

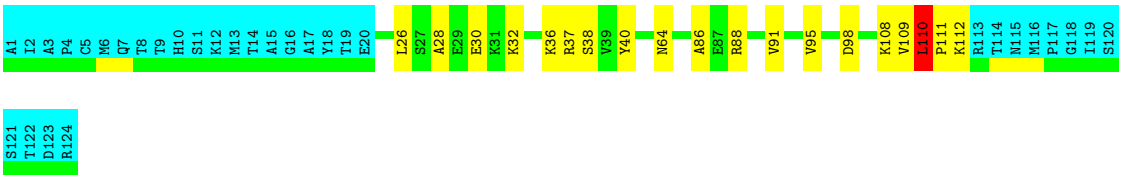
- Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A: 50% 15% 35%



- Molecule 1: Embryonic polyadenylate-binding protein 2-B

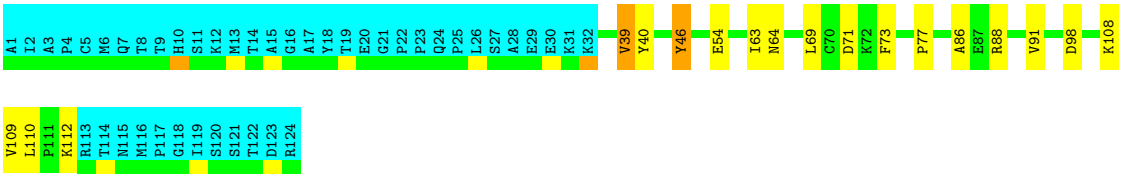
Chain B: 59% 15% • 26%



4.2.7 Score per residue for model 7

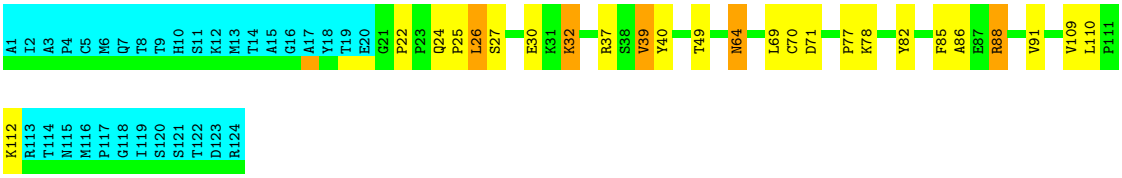
- Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A: 50% 13% • 35%



- Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain B: 54% 16% • 26%



4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A: 56% 8% 35%

A1 I2 A3 P4 C5 M6 Q7 T8 T9 H10 S11 K12 M13 T14 A15 G16 A17 Y18 T19 E20 G21 P22 P23 Q24 P25 L26 S27 A28 E29 E30 K31 K32 K36 R37 Y40 E54 A86 E87 R88 M97 T100 V109 L110 R113 T114 N115 M116 P117 G118 I119 S120 S121

T122 D123 R124

• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain B: 60% 13% • 26%

A1 I2 A3 P4 C5 M6 Q7 T8 T9 H10 S11 K12 M13 T14 A15 G16 A17 Y18 T19 E20 L26 E30 K31 K32 E33 I34 D35 K36 R37 Y40 Y46 D71 S74 F77 A86 E87 R88 D98 K108 V109 L110 P111 K112 R113 T114 N115 M116 P117 G118 I119

S120 S121 T122 D123 R124

4.2.9 Score per residue for model 9

• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A: 56% 9% 35%

A1 I2 A3 P4 C5 M6 Q7 T8 T9 H10 S11 K12 M13 T14 A15 G16 A17 Y18 T19 E20 G21 P22 P23 Q24 P25 L26 S27 A28 E29 E30 K31 K32 V39 Y40 V41 L69 V91 M97 D98 E99 T100 K108 V109 L110 R113 T114 N115 M116 P117 G118 I119 S120 S121 T122

D123 R124

• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain B: 63% 10% • 26%

A1 I2 A3 P4 C5 M6 Q7 T8 T9 H10 S11 K12 M13 T14 A15 G16 A17 Y18 T19 E20 G21 P22 P25 L26 E30 E33 R37 Y40 N43 Y46 A50 I66 P77 V109 L110 R113 T114 N115 M116 P117 G118 I119 S120 S121 T122 D123 R124

4.2.10 Score per residue for model 10

• Molecule 1: Embryonic polyadenylate-binding protein 2-B

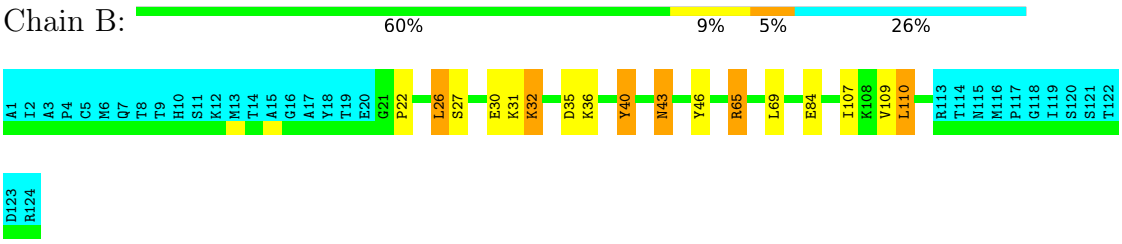
Chain A: 54% 9% • 35%

A1 I2 A3 P4 C5 M6 Q7 T8 T9 H10 S11 K12 M13 T14 A15 G16 A17 Y18 T19 E20 G21 P22 P23 Q24 P25 L26 S27 A28 E29 E30 K31 K32 K36 Y40 M43 Y46 N64 R65 L69 Y82 A86 I107 K108 V109 L110 P111 K112 R113 T114 N115 M116

P117 G118 I119 S120 S121 T122 D123 R124

• Molecule 1: Embryonic polyadenylate-binding protein 2-B

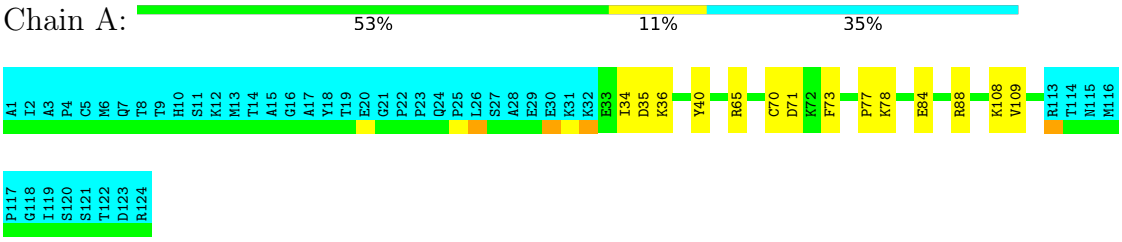
Chain B:



4.2.11 Score per residue for model 11

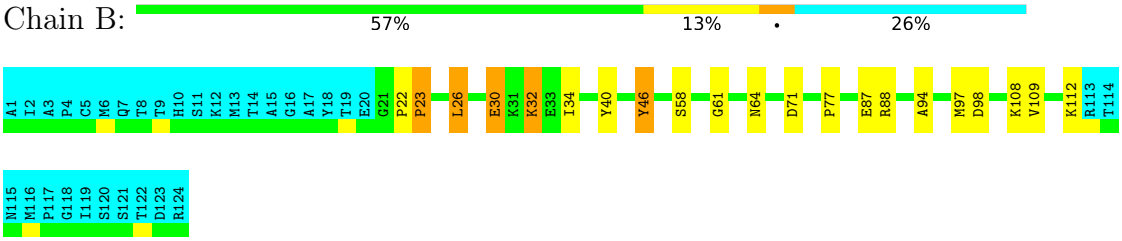
• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A:



• Molecule 1: Embryonic polyadenylate-binding protein 2-B

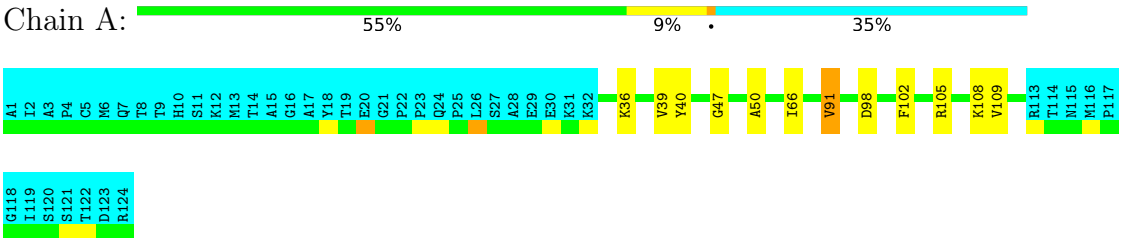
Chain B:



4.2.12 Score per residue for model 12

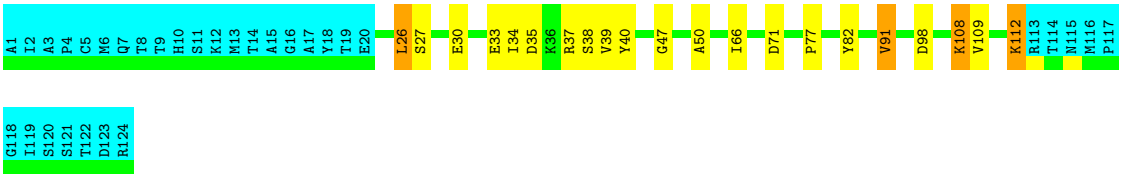
• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A:



• Molecule 1: Embryonic polyadenylate-binding protein 2-B

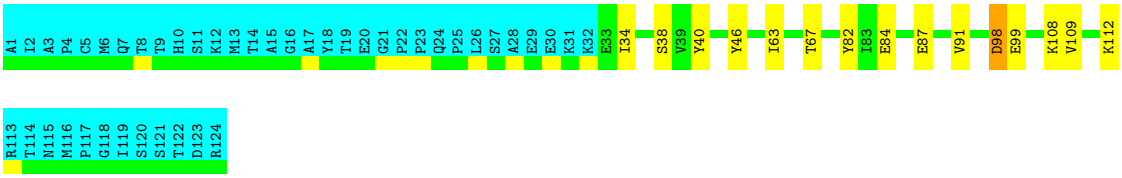
Chain B:



4.2.13 Score per residue for model 13

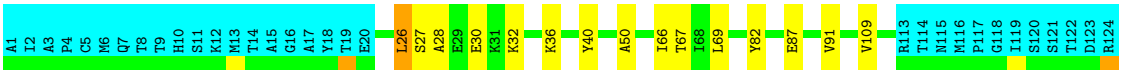
• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A:



• Molecule 1: Embryonic polyadenylate-binding protein 2-B

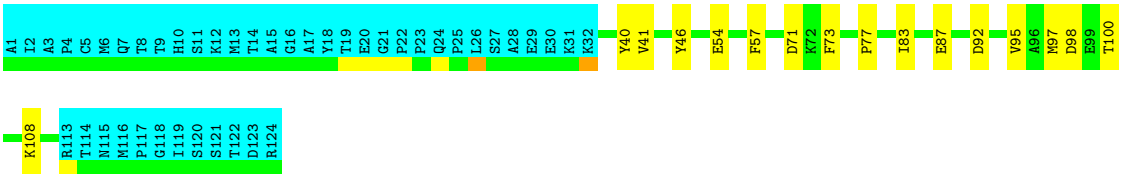
Chain B:



4.2.14 Score per residue for model 14

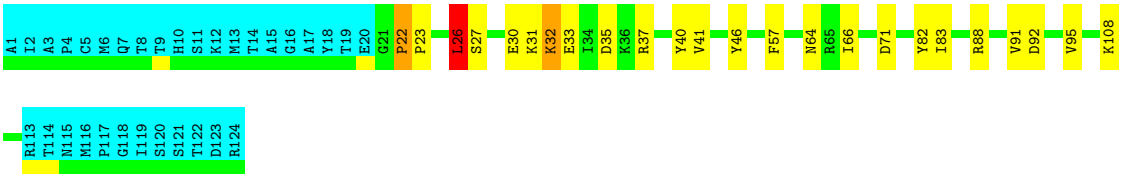
• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A:



• Molecule 1: Embryonic polyadenylate-binding protein 2-B

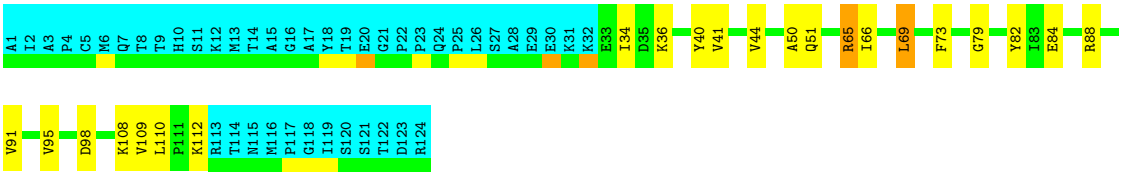
Chain B:



4.2.15 Score per residue for model 15

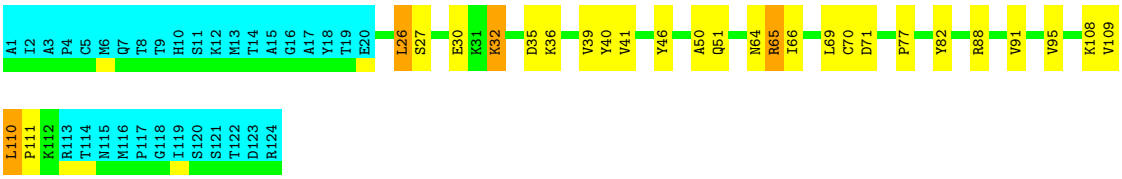
- Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A: 47% 16% • 35%



- Molecule 1: Embryonic polyadenylate-binding protein 2-B

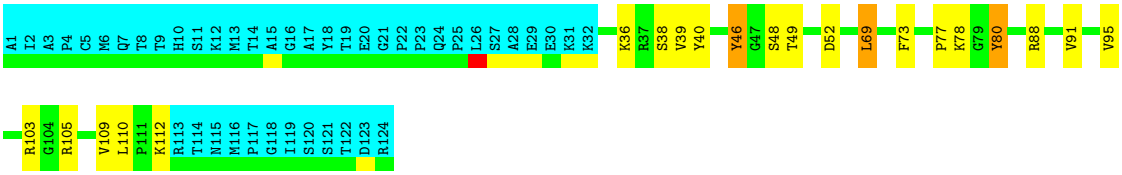
Chain B: 52% 19% • 26%



4.2.16 Score per residue for model 16

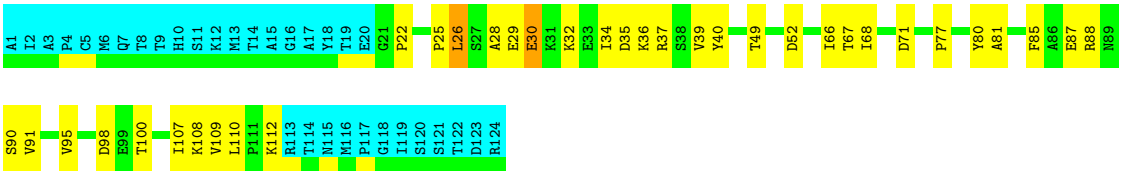
- Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A: 48% 15% • 35%



- Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain B: 46% 27% • 26%



4.2.17 Score per residue for model 17

- Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A: 51% 14% 35%

A1 I2 A3 P4 C5 M6 Q7 T8 T9 H10 S11 K12 M13 T14 A15 G16 A17 Y18 T19 E20 G21 P22 P23 Q24 P25 L26 S27 A28 E29 E30 K31 K32 E33 I34 S38 V39 Y40 Q51 E54 C60 L69 C70 D71 P77 R88 N89 S90 V91 V95 A96 M97

V109 L110 P111 K112 R113 T114 N115 M116 P117 G118 I119 S120 S121 T122 D123 R124

- Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain B: 59% 14% • 26%

A1 I2 A3 P4 C5 M6 Q7 T8 T9 H10 S11 K12 M13 T14 A15 G16 A17 Y18 T19 E20 G21 P22 P25 L26 E30 K31 K32 Y40 V41 Y46 G47 E54 R65 D71 P77 R88 V91 V95 K108 V109 L110 R113 T114 N115 M116 P117 G118

I119 S120 S121 T122 D123 R124

4.2.18 Score per residue for model 18

- Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A: 53% 11% 35%

A1 I2 A3 P4 C5 M6 Q7 T8 T9 H10 S11 K12 M13 T14 A15 G16 A17 Y18 T19 E20 G21 P22 P23 Q24 P25 L26 S27 A28 E29 E30 K31 K32 E33 I34 R37 Y40 T49 A50 Q51 L69 F73 Y82 F85 A86 E87 V91 V109 L110 P111 K112 R113

T114 N115 M116 P117 G118 I119 S120 S121 T122 D123 R124

- Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain B: 55% 16% • 26%

A1 I2 A3 P4 C5 M6 Q7 T8 T9 H10 S11 K12 M13 T14 A15 G16 A17 Y18 T19 E20 G21 P22 P23 Q24 P25 L26 K32 S38 V39 Y40 Y46 T49 A50 Q51 E54 I63 N64 L69 C70 D71 P77 Y80 A81 Y82 V91 D98 K108 V109

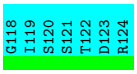
L110 P111 K112 R113 T114 N115 M116 P117 G118 I119 S120 S121 T122 D123 R124

4.2.19 Score per residue for model 19

- Molecule 1: Embryonic polyadenylate-binding protein 2-B

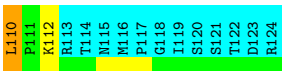
Chain A: 53% 10% • 35%

A1 I2 A3 P4 C5 M6 Q7 T8 T9 H10 S11 K12 M13 T14 A15 G16 A17 Y18 T19 E20 G21 P22 P23 Q24 P25 L26 S27 A28 E29 E30 K31 K32 V39 Y40 D45 N64 R65 K72 A86 E87 R88 V91 D98 K108 V109 L110 R113 T114 N115 M116 P117



• Molecule 1: Embryonic polyadenylate-binding protein 2-B

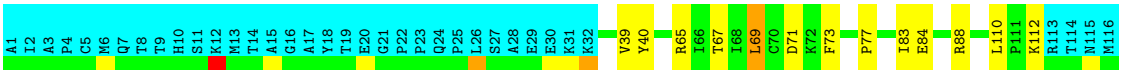
Chain B:

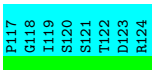


4.2.20 Score per residue for model 20

• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain A:





• Molecule 1: Embryonic polyadenylate-binding protein 2-B

Chain B:

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Torsion Angle Dynamics, Simulated Annealing.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
Xplor-NIH	refinement	2.17.0

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.85±0.04	0±0/634 (0.0± 0.0%)	0.77±0.03	0±0/856 (0.0± 0.0%)
1	B	0.85±0.04	0±0/726 (0.0± 0.0%)	0.78±0.03	0±1/981 (0.1± 0.1%)
All	All	0.85	0/27200 (0.0%)	0.78	10/36740 (0.0%)

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	A	0.0±0.0	0.2±0.4
1	B	0.0±0.0	0.2±0.4
All	All	0	9

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	110	LEU	CA-CB-CG	5.49	127.92	115.30	9	7
1	B	110	LEU	N-CA-CB	-5.20	100.01	110.40	9	3

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)
1	B	65	ARG	Sidechain	4
1	A	65	ARG	Sidechain	3
1	A	37	ARG	Sidechain	1
1	A	105	ARG	Sidechain	1

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	622	609	607	8±3
1	B	711	700	698	10±3
All	All	26660	26180	26100	322

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:CYS:SG	1:A:90:SER:HA	0.75	2.21	2	1
1:B:82:TYR:CD1	1:B:112:LYS:HD3	0.67	2.25	18	2
1:B:46:TYR:CE1	1:B:77:PRO:HB2	0.65	2.27	8	3
1:A:82:TYR:CD1	1:A:112:LYS:HD2	0.63	2.28	15	1
1:B:82:TYR:CD1	1:B:112:LYS:HE2	0.62	2.29	12	1
1:A:40:TYR:O	1:A:109:VAL:HA	0.61	1.94	17	17
1:B:71:ASP:O	1:B:77:PRO:HA	0.61	1.96	20	11
1:B:38:SER:OG	1:B:112:LYS:HD3	0.60	1.95	19	1
1:A:41:VAL:HA	1:A:108:LYS:O	0.60	1.96	14	3
1:A:70:CYS:HA	1:A:78:LYS:O	0.60	1.97	1	4
1:B:28:ALA:O	1:B:32:LYS:HG2	0.60	1.96	13	3
1:B:98:ASP:O	1:B:108:LYS:HA	0.60	1.96	12	7
1:B:40:TYR:O	1:B:109:VAL:HA	0.59	1.98	18	16
1:A:82:TYR:OH	1:B:21:GLY:HA3	0.59	1.97	5	1
1:B:32:LYS:O	1:B:36:LYS:HG3	0.58	1.99	6	5
1:B:32:LYS:N	1:B:32:LYS:HE2	0.58	2.13	7	7
1:A:43:ASN:OD1	1:A:105:ARG:HG3	0.58	1.98	6	1
1:B:26:LEU:H	1:B:26:LEU:HD13	0.57	1.59	14	9
1:A:98:ASP:HA	1:A:109:VAL:HG22	0.57	1.77	3	3
1:B:26:LEU:HD13	1:B:26:LEU:H	0.57	1.59	18	2
1:A:35:ASP:OD1	1:A:112:LYS:HE3	0.56	2.01	3	1
1:B:110:LEU:HB3	1:B:111:PRO:HD2	0.56	1.78	4	3
1:A:37:ARG:HG3	1:A:85:PHE:O	0.56	2.00	18	1
1:A:39:VAL:HG22	1:A:91:VAL:HG23	0.55	1.78	16	2
1:B:33:GLU:O	1:B:37:ARG:HG2	0.55	2.00	14	2
1:A:33:GLU:O	1:A:37:ARG:HG2	0.55	2.02	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:ASP:O	1:A:108:LYS:HA	0.55	2.02	19	7
1:A:73:PHE:HB3	1:B:64:ASN:OD1	0.55	2.02	14	4
1:A:71:ASP:O	1:A:77:PRO:HA	0.54	2.03	5	5
1:B:92:ASP:O	1:B:95:VAL:HG22	0.54	2.02	14	1
1:A:46:TYR:CE1	1:A:77:PRO:HB2	0.54	2.37	5	2
1:A:82:TYR:CD2	1:A:112:LYS:HD3	0.54	2.37	18	2
1:A:64:ASN:OD1	1:B:73:PHE:HB3	0.53	2.03	5	1
1:B:64:ASN:ND2	1:B:86:ALA:HA	0.53	2.19	3	1
1:A:98:ASP:HA	1:A:109:VAL:HB	0.53	1.81	13	2
1:B:37:ARG:HD2	1:B:85:PHE:O	0.52	2.04	7	1
1:A:92:ASP:O	1:A:95:VAL:HG22	0.52	2.05	14	1
1:A:40:TYR:CZ	1:B:22:PRO:HG3	0.52	2.38	16	3
1:A:49:THR:O	1:A:53:LEU:HB2	0.52	2.05	6	1
1:B:37:ARG:HD3	1:B:86:ALA:O	0.52	2.04	6	2
1:B:70:CYS:HA	1:B:78:LYS:O	0.52	2.05	1	4
1:B:39:VAL:HG13	1:B:91:VAL:CG2	0.51	2.36	7	2
1:B:58:SER:HA	1:B:61:GLY:O	0.51	2.05	11	1
1:A:73:PHE:CE2	1:B:65:ARG:HD2	0.50	2.40	1	1
1:B:39:VAL:HG22	1:B:91:VAL:HG23	0.50	1.82	16	2
1:B:27:SER:HB3	1:B:30:GLU:OE1	0.50	2.06	13	4
1:A:57:PHE:CD2	1:A:83:ILE:HG12	0.50	2.42	14	1
1:A:39:VAL:HG13	1:A:91:VAL:CG2	0.50	2.37	7	2
1:B:46:TYR:HB3	1:B:70:CYS:SG	0.50	2.46	19	1
1:A:43:ASN:HB3	1:A:107:ILE:HA	0.50	1.83	6	2
1:A:73:PHE:CE2	1:B:64:ASN:HB3	0.50	2.42	15	1
1:B:32:LYS:HE2	1:B:32:LYS:N	0.50	2.22	18	2
1:A:98:ASP:HA	1:A:109:VAL:CG2	0.49	2.37	3	2
1:A:60:CYS:SG	1:A:93:ALA:HB3	0.49	2.47	2	1
1:A:98:ASP:HB2	1:A:109:VAL:O	0.49	2.07	13	1
1:A:40:TYR:CE1	1:B:22:PRO:HG3	0.49	2.42	9	2
1:B:22:PRO:N	1:B:23:PRO:HD2	0.49	2.23	11	2
1:B:87:GLU:HB3	1:B:90:SER:OG	0.49	2.07	5	1
1:B:46:TYR:CD2	1:B:77:PRO:HB2	0.49	2.42	17	1
1:B:27:SER:HB2	1:B:30:GLU:OE1	0.49	2.08	10	1
1:B:38:SER:OG	1:B:112:LYS:HE2	0.49	2.07	18	1
1:A:69:LEU:HG	1:A:80:TYR:CE1	0.49	2.42	16	1
1:A:40:TYR:OH	1:B:22:PRO:HD3	0.48	2.08	17	1
1:B:32:LYS:O	1:B:36:LYS:HB2	0.48	2.09	4	1
1:B:88:ARG:O	1:B:91:VAL:HG22	0.48	2.08	6	2
1:B:41:VAL:HA	1:B:108:LYS:O	0.48	2.08	14	4
1:B:91:VAL:O	1:B:95:VAL:HG13	0.48	2.07	4	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:100:THR:HB	1:B:107:ILE:HG12	0.48	1.85	16	1
1:B:26:LEU:HD23	1:B:30:GLU:HB3	0.48	1.86	14	1
1:B:100:THR:HB	1:B:107:ILE:CG1	0.48	2.38	16	1
1:A:40:TYR:CZ	1:B:22:PRO:HD3	0.47	2.43	17	1
1:A:88:ARG:O	1:A:91:VAL:HG12	0.47	2.09	19	1
1:B:38:SER:HB2	1:B:112:LYS:O	0.47	2.08	12	1
1:B:60:CYS:O	1:B:90:SER:HA	0.47	2.09	2	1
1:A:69:LEU:HD12	1:B:65:ARG:NH2	0.47	2.25	15	2
1:B:43:ASN:HB3	1:B:107:ILE:HA	0.47	1.87	10	1
1:B:32:LYS:O	1:B:36:LYS:HG2	0.47	2.09	13	1
1:A:34:ILE:HD12	1:A:65:ARG:NH2	0.47	2.25	4	1
1:B:67:THR:OG1	1:B:82:TYR:HB2	0.47	2.10	5	2
1:A:97:MET:HA	1:A:100:THR:OG1	0.47	2.09	14	2
1:B:57:PHE:CD2	1:B:83:ILE:HG13	0.47	2.45	14	1
1:A:50:ALA:HB1	1:A:66:ILE:HD11	0.47	1.86	12	2
1:A:69:LEU:HA	1:B:66:ILE:O	0.47	2.10	20	1
1:B:88:ARG:O	1:B:91:VAL:HG12	0.47	2.10	19	2
1:A:46:TYR:CZ	1:A:77:PRO:HB2	0.46	2.45	5	1
1:B:26:LEU:HD23	1:B:30:GLU:HB2	0.46	1.87	11	2
1:B:50:ALA:HB1	1:B:66:ILE:HD11	0.46	1.86	12	5
1:A:67:THR:OG1	1:A:82:TYR:HB2	0.46	2.10	5	2
1:B:82:TYR:CD2	1:B:112:LYS:HG3	0.46	2.46	7	1
1:B:37:ARG:HD3	1:B:85:PHE:O	0.46	2.09	16	1
1:B:35:ASP:OD1	1:B:112:LYS:HE2	0.46	2.10	19	1
1:A:91:VAL:O	1:A:95:VAL:HG13	0.46	2.11	4	5
1:A:64:ASN:ND2	1:A:86:ALA:HA	0.46	2.26	3	3
1:A:45:ASP:OD2	1:A:78:LYS:HA	0.45	2.11	4	1
1:B:46:TYR:HA	1:B:70:CYS:SG	0.45	2.51	15	1
1:A:102:PHE:O	1:A:105:ARG:HG2	0.45	2.12	12	1
1:B:27:SER:O	1:B:31:LYS:HG3	0.45	2.12	14	1
1:B:33:GLU:O	1:B:37:ARG:HG3	0.45	2.11	9	1
1:A:38:SER:OG	1:A:84:GLU:HG2	0.45	2.11	1	1
1:A:88:ARG:O	1:A:91:VAL:HG22	0.45	2.12	5	3
1:A:49:THR:HG21	1:B:49:THR:HB	0.45	1.89	16	1
1:A:40:TYR:CE2	1:B:22:PRO:HG2	0.45	2.47	10	2
1:B:65:ARG:HD2	1:B:84:GLU:OE1	0.45	2.11	20	2
1:A:98:ASP:HA	1:A:109:VAL:HG12	0.45	1.88	15	1
1:A:38:SER:OG	1:A:112:LYS:HE2	0.45	2.11	16	1
1:A:40:TYR:C	1:A:40:TYR:CD1	0.44	2.90	10	1
1:A:39:VAL:HG13	1:A:91:VAL:HG23	0.44	1.89	7	1
1:B:64:ASN:OD1	1:B:65:ARG:HG3	0.44	2.12	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:ASN:HB3	1:B:73:PHE:CE2	0.44	2.47	19	1
1:A:65:ARG:HD2	1:A:84:GLU:OE1	0.44	2.11	20	1
1:A:38:SER:HB2	1:A:112:LYS:O	0.44	2.13	17	1
1:A:46:TYR:CD2	1:A:77:PRO:HB2	0.43	2.48	16	1
1:B:49:THR:O	1:B:53:LEU:HB2	0.43	2.13	1	1
1:B:98:ASP:HA	1:B:109:VAL:HG22	0.43	1.90	3	2
1:A:44:VAL:O	1:A:79:GLY:HA3	0.43	2.13	5	2
1:B:33:GLU:O	1:B:37:ARG:HD3	0.43	2.13	12	1
1:B:40:TYR:HD1	1:B:82:TYR:CE1	0.43	2.32	12	2
1:A:38:SER:CB	1:A:112:LYS:HE2	0.43	2.43	16	1
1:B:87:GLU:HB2	1:B:90:SER:OG	0.43	2.13	16	1
1:B:65:ARG:HB2	1:B:84:GLU:OE1	0.43	2.14	4	1
1:B:28:ALA:O	1:B:32:LYS:HE2	0.43	2.14	5	1
1:A:39:VAL:HG22	1:A:83:ILE:O	0.43	2.14	20	1
1:B:29:GLU:HA	1:B:32:LYS:CG	0.43	2.43	16	1
1:B:27:SER:HB2	1:B:30:GLU:HG2	0.43	1.89	3	1
1:A:60:CYS:SG	1:A:97:MET:SD	0.43	3.17	17	1
1:B:30:GLU:O	1:B:34:ILE:HG12	0.43	2.13	20	4
1:A:37:ARG:HD3	1:A:86:ALA:O	0.42	2.13	8	1
1:A:51:GLN:HG2	1:B:46:TYR:CE2	0.42	2.49	1	1
1:B:26:LEU:O	1:B:31:LYS:HE3	0.42	2.13	10	1
1:A:39:VAL:HG22	1:A:91:VAL:CG2	0.42	2.44	16	1
1:A:64:ASN:OD1	1:A:65:ARG:HG3	0.42	2.15	1	1
1:A:38:SER:OG	1:A:84:GLU:HG3	0.42	2.13	6	1
1:A:65:ARG:HB2	1:A:84:GLU:OE1	0.42	2.14	11	1
1:A:71:ASP:HB2	1:A:73:PHE:CD2	0.42	2.50	20	2
1:A:65:ARG:HD3	1:A:84:GLU:OE1	0.42	2.15	15	1
1:A:48:SER:OG	1:A:103:ARG:HD3	0.41	2.15	16	1
1:B:38:SER:OG	1:B:112:LYS:HE3	0.41	2.15	6	2
1:A:49:THR:HG22	1:B:49:THR:HG22	0.41	1.91	18	1
1:A:40:TYR:CD2	1:B:22:PRO:HG2	0.41	2.51	20	1
1:A:70:CYS:HB2	1:B:66:ILE:HG12	0.41	1.91	2	1
1:B:64:ASN:ND2	1:B:86:ALA:HB2	0.41	2.29	7	1
1:B:69:LEU:HG	1:B:80:TYR:CE1	0.41	2.50	18	1
1:A:72:LYS:HE2	1:A:77:PRO:HB3	0.41	1.93	2	1
1:A:39:VAL:CG1	1:A:91:VAL:HB	0.41	2.46	9	1
1:B:22:PRO:HG2	1:B:23:PRO:HD3	0.41	1.93	18	1
1:B:39:VAL:HG13	1:B:91:VAL:HG23	0.41	1.93	7	1
1:B:45:ASP:OD1	1:B:103:ARG:HD2	0.41	2.15	1	1
1:B:72:LYS:HE2	1:B:77:PRO:HB3	0.41	1.92	1	1
1:A:71:ASP:HA	1:B:65:ARG:HA	0.41	1.92	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:VAL:CG1	1:A:91:VAL:HG23	0.41	2.46	12	1
1:A:67:THR:HA	1:B:68:ILE:O	0.41	2.16	20	1
1:A:38:SER:OG	1:A:112:LYS:HE3	0.41	2.16	1	1
1:B:28:ALA:O	1:B:32:LYS:HG3	0.41	2.16	2	1
1:A:35:ASP:OD2	1:A:112:LYS:NZ	0.41	2.54	4	1
1:A:71:ASP:HA	1:B:65:ARG:HG2	0.41	1.93	4	1
1:B:69:LEU:HG	1:B:80:TYR:CE2	0.41	2.50	5	1
1:B:39:VAL:CG1	1:B:91:VAL:HG23	0.41	2.45	12	1
1:B:66:ILE:HG22	1:B:83:ILE:HG23	0.41	1.92	20	1
1:A:38:SER:HB2	1:A:84:GLU:HG3	0.41	1.91	13	1
1:B:94:ALA:O	1:B:97:MET:HB2	0.40	2.17	11	1
1:B:82:TYR:CD1	1:B:112:LYS:HG3	0.40	2.52	1	1
1:B:39:VAL:O	1:B:82:TYR:HA	0.40	2.16	15	1
1:A:38:SER:OG	1:A:112:LYS:HB3	0.40	2.16	3	1
1:A:64:ASN:HD21	1:A:86:ALA:HB2	0.40	1.77	4	1
1:A:64:ASN:OD1	1:A:86:ALA:HB2	0.40	2.16	7	1
1:A:97:MET:O	1:A:100:THR:HG22	0.40	2.16	8	1
1:A:54:GLU:HG3	1:B:46:TYR:OH	0.40	2.16	14	1
1:B:67:THR:O	1:B:81:ALA:HA	0.40	2.17	16	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	80/124 (65%)	75±2 (94±2%)	4±2 (5±2%)	0±1 (1±1%)	29	74
1	B	92/124 (74%)	87±2 (95±2%)	4±1 (4±2%)	1±1 (1±1%)	21	69
All	All	3440/4960 (69%)	3251 (95%)	163 (5%)	26 (1%)	24	71

All 12 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	46	TYR	5
1	B	25	PRO	5

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Mol	Chain	Res	Type	Models (Total)
1	B	46	TYR	3
1	B	26	LEU	2
1	A	63	ILE	2
1	B	43	ASN	2
1	B	47	GLY	2
1	A	98	ASP	1
1	A	43	ASN	1
1	B	23	PRO	1
1	A	47	GLY	1
1	B	63	ILE	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	67/103 (65%)	63±2 (95±2%)	4±2 (5±2%)	26	75
1	B	77/103 (75%)	71±2 (92±3%)	6±2 (8±3%)	17	65
All	All	2880/4120 (70%)	2693 (94%)	187 (6%)	21	69

All 51 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	B	26	LEU	18
1	A	110	LEU	13
1	B	110	LEU	13
1	B	32	LYS	12
1	B	30	GLU	10
1	A	69	LEU	10
1	B	88	ARG	9
1	A	88	ARG	8
1	B	69	LEU	6
1	A	87	GLU	5
1	B	54	GLU	5
1	B	87	GLU	4
1	A	91	VAL	4
1	B	91	VAL	4

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Mol	Chain	Res	Type	Models (Total)
1	A	51	GLN	4
1	B	51	GLN	4
1	A	112	LYS	4
1	B	80	TYR	3
1	B	112	LYS	3
1	A	73	PHE	3
1	A	89	ASN	3
1	B	64	ASN	3
1	A	54	GLU	3
1	A	80	TYR	2
1	B	24	GLN	2
1	B	89	ASN	2
1	A	39	VAL	2
1	B	39	VAL	2
1	B	35	ASP	2
1	A	98	ASP	2
1	B	66	ILE	2
1	B	53	LEU	1
1	B	73	PHE	1
1	A	64	ASN	1
1	B	49	THR	1
1	A	40	TYR	1
1	A	65	ARG	1
1	B	40	TYR	1
1	B	65	ARG	1
1	A	108	LYS	1
1	B	108	LYS	1
1	B	22	PRO	1
1	A	46	TYR	1
1	A	52	ASP	1
1	B	52	ASP	1
1	B	68	ILE	1
1	A	45	ASP	1
1	A	72	LYS	1
1	B	33	GLU	1
1	B	98	ASP	1
1	B	107	ILE	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 monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided