



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:41 PM BST

PDB ID : 1E91
Title : STRUCTURE OF THE COMPLEX OF THE MAD1-SIN3B INTERACTION DOMAINS
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Deposited on : 2000-10-04

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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

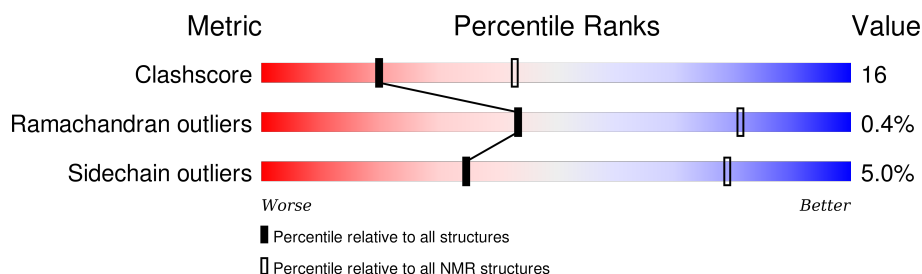
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	85	
2	B	13	

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 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:10-A:37, A:57-A:77, B:2-B:13 (61)	0.21	19

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1615 atoms, of which 795 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B.

Mol	Chain	Residues	Atoms						Trace
1	A	85	Total	C	H	N	O	S	0
			1405	454	691	122	137	1	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	GLY	CONFLICT	UNP Q62141

- Molecule 2 is a protein called MAD PROTEIN (MAX DIMERIZER).

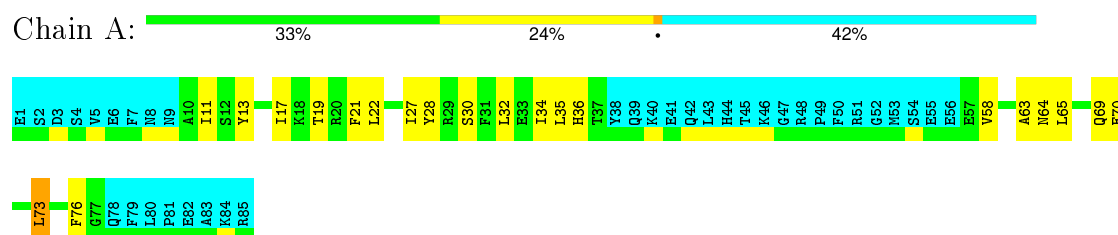
Mol	Chain	Residues	Atoms						Trace
2	B	13	Total	C	H	N	O	S	0
			210	67	104	15	23	1	

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: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B



- Molecule 2: MAD PROTEIN (MAX DIMERIZER)

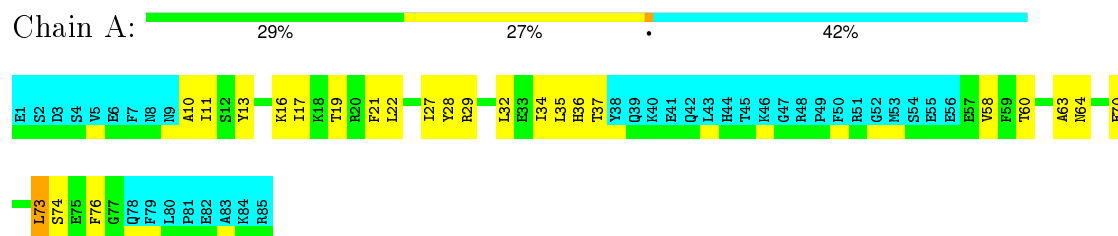


4.2 Scores per residue for each member of the ensemble

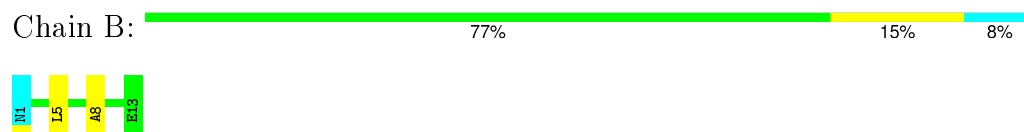
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B

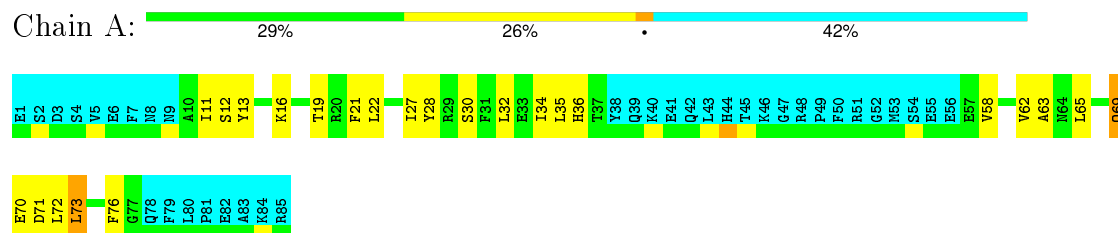


- Molecule 2: MAD PROTEIN (MAX DIMERIZER)

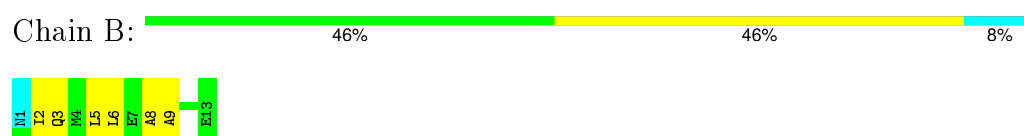


4.2.2 Score per residue for model 2

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B

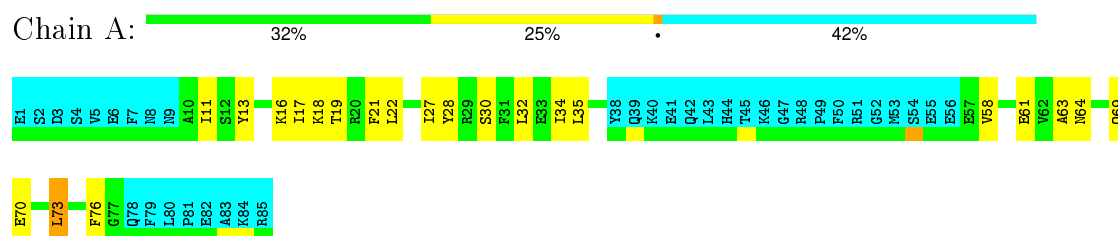


- Molecule 2: MAD PROTEIN (MAX DIMERIZER)

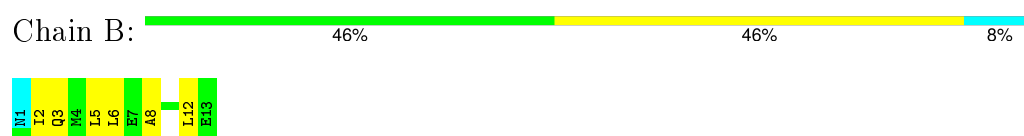


4.2.3 Score per residue for model 3

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B

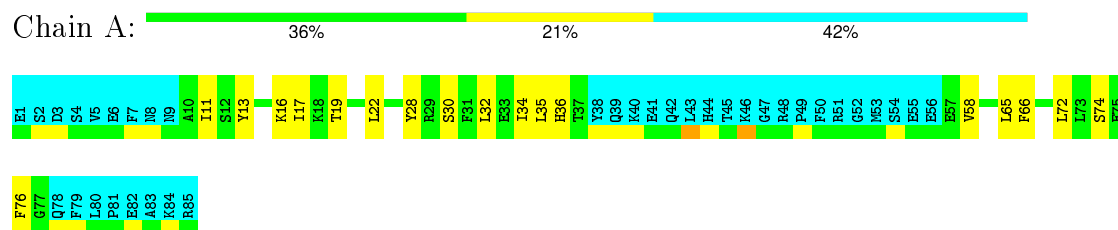


- Molecule 2: MAD PROTEIN (MAX DIMERIZER)

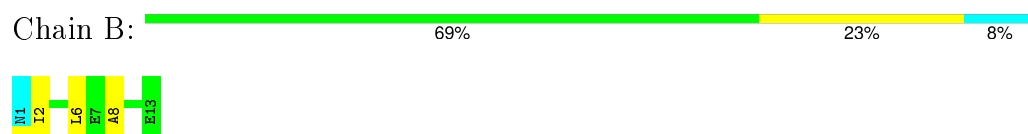


4.2.4 Score per residue for model 4

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B

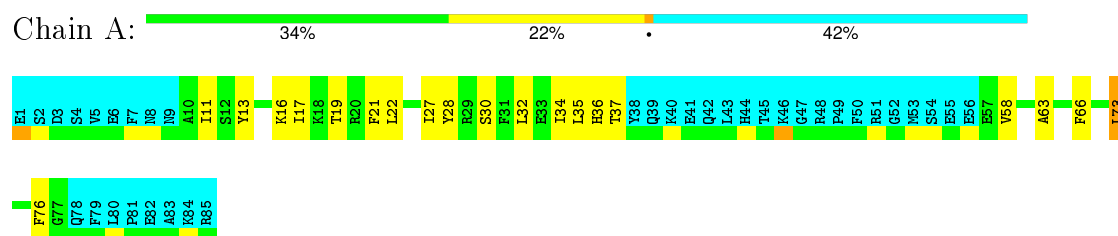


- Molecule 2: MAD PROTEIN (MAX DIMERIZER)



4.2.5 Score per residue for model 5

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B

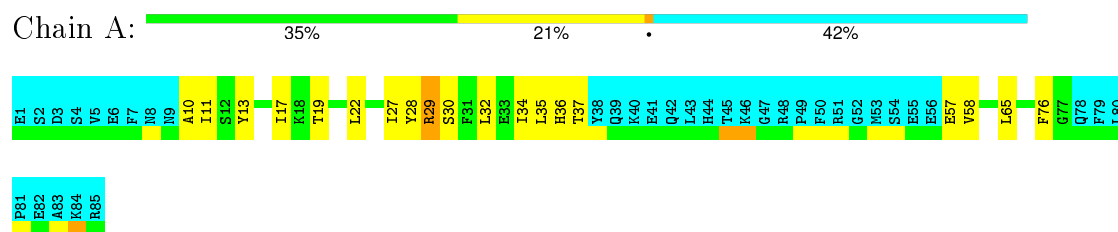


- Molecule 2: MAD PROTEIN (MAX DIMERIZER)



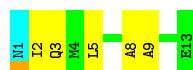
4.2.6 Score per residue for model 6

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B



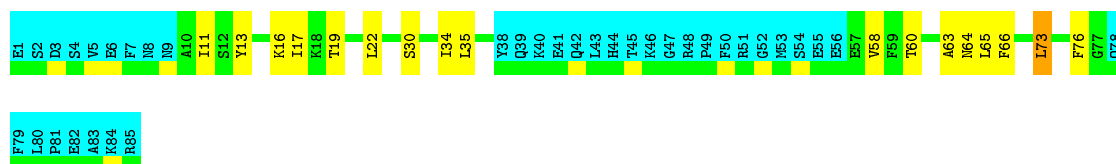
- Molecule 2: MAD PROTEIN (MAX DIMERIZER)





4.2.7 Score per residue for model 7

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B

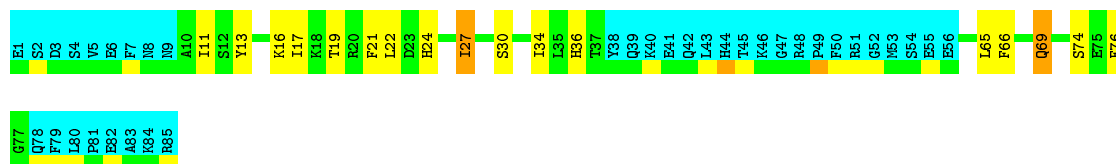


- Molecule 2: MAD PROTEIN (MAX DIMERIZER)



4.2.8 Score per residue for model 8

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B

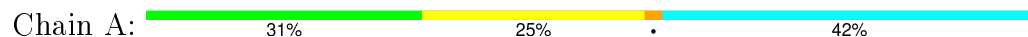


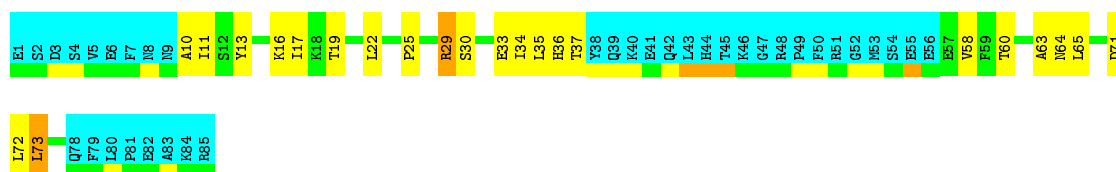
- Molecule 2: MAD PROTEIN (MAX DIMERIZER)



4.2.9 Score per residue for model 9

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B



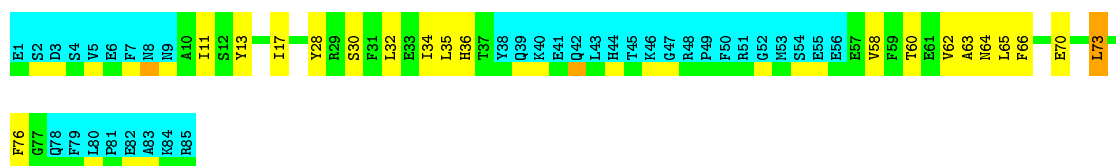


- Molecule 2: MAD PROTEIN (MAX DIMERIZER)



4.2.10 Score per residue for model 10

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B

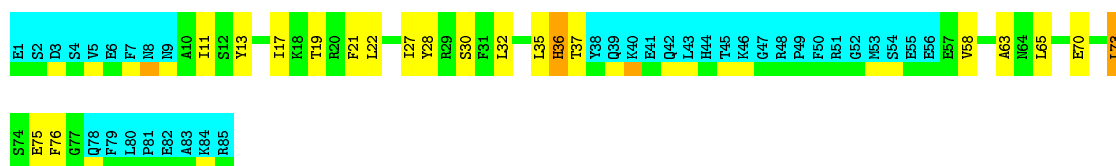
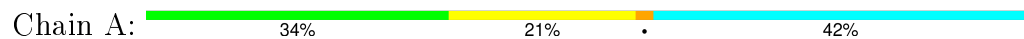


- Molecule 2: MAD PROTEIN (MAX DIMERIZER)



4.2.11 Score per residue for model 11

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B



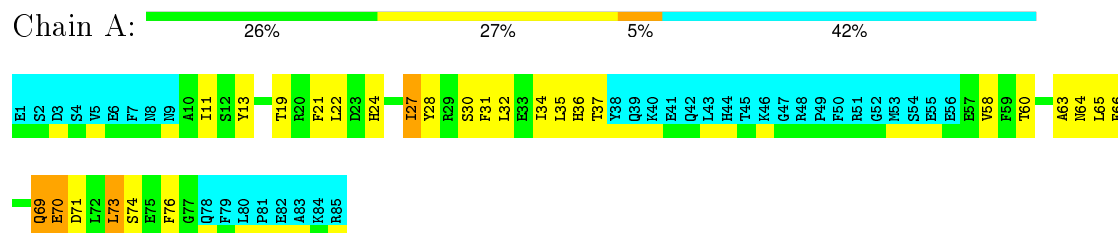
- Molecule 2: MAD PROTEIN (MAX DIMERIZER)





4.2.12 Score per residue for model 12

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B

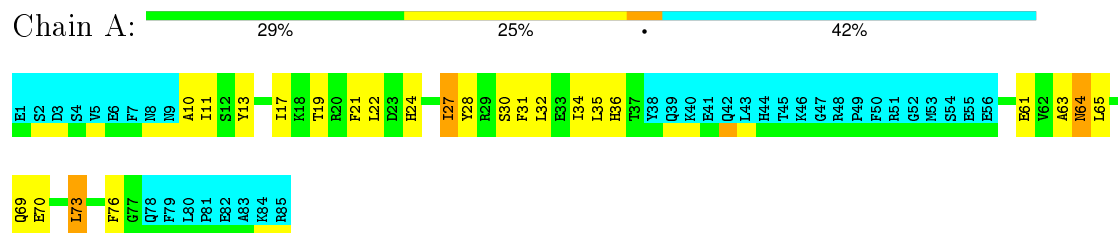


- Molecule 2: MAD PROTEIN (MAX DIMERIZER)

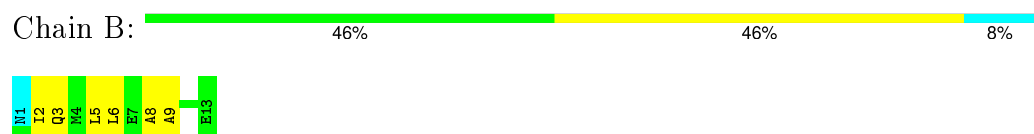


4.2.13 Score per residue for model 13

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B

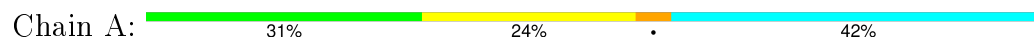


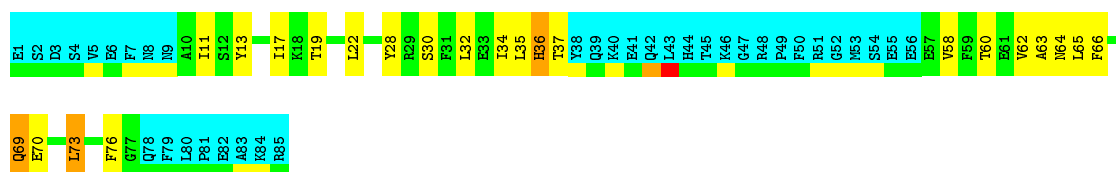
- Molecule 2: MAD PROTEIN (MAX DIMERIZER)



4.2.14 Score per residue for model 14

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B



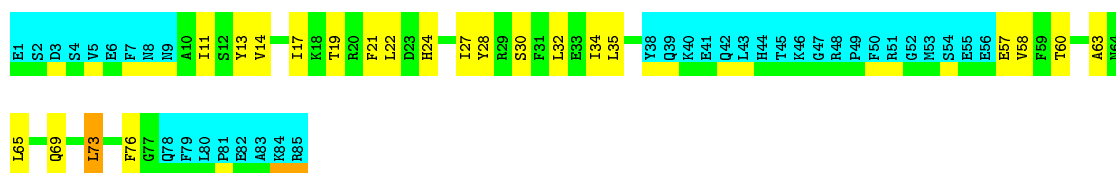
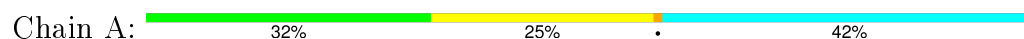


- Molecule 2: MAD PROTEIN (MAX DIMERIZER)



4.2.15 Score per residue for model 15

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B

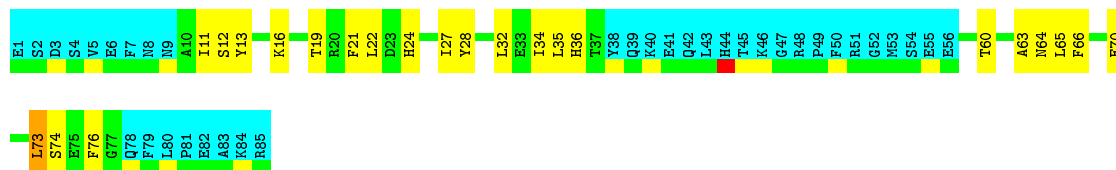
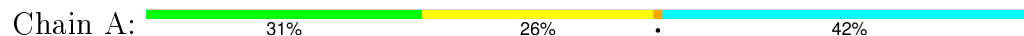


- Molecule 2: MAD PROTEIN (MAX DIMERIZER)



4.2.16 Score per residue for model 16

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B



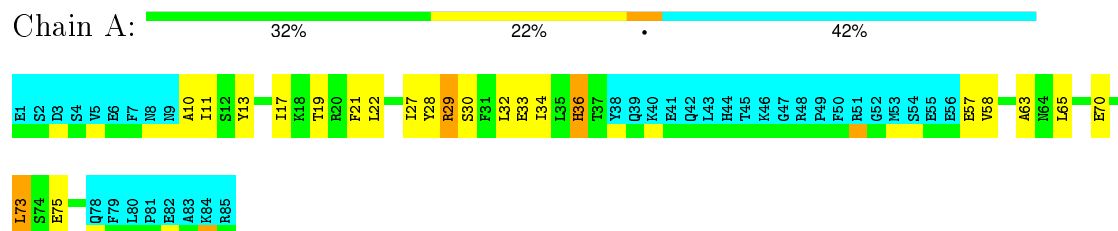
- Molecule 2: MAD PROTEIN (MAX DIMERIZER)





4.2.17 Score per residue for model 17

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B

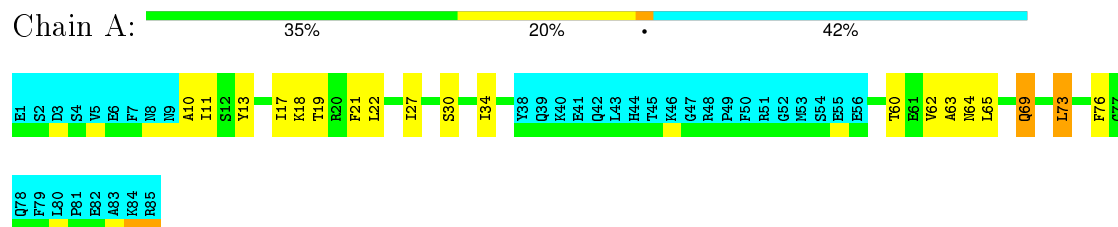


- Molecule 2: MAD PROTEIN (MAX DIMERIZER)



4.2.18 Score per residue for model 18

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B

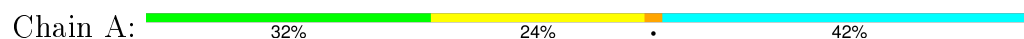


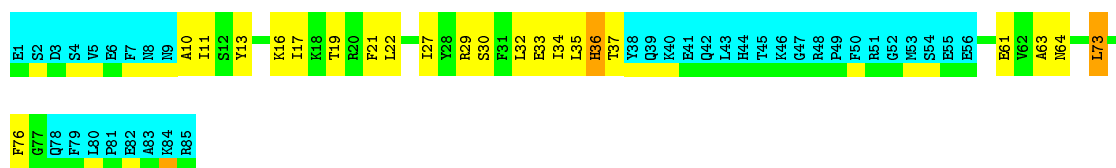
- Molecule 2: MAD PROTEIN (MAX DIMERIZER)



4.2.19 Score per residue for model 19 (medoid)

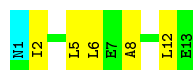
- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B





- Molecule 2: MAD PROTEIN (MAX DIMERIZER)

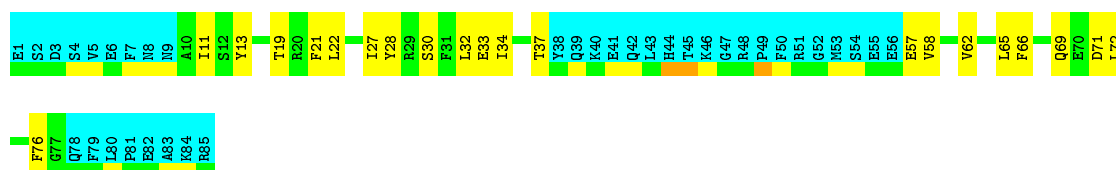
Chain B: 54% 38% 8%



4.2.20 Score per residue for model 20

- Molecule 1: PAIRED AMPHIPATHIC HELIX PROTEIN SIN3B

Chain A: 33% 25% 42%



- Molecule 2: MAD PROTEIN (MAX DIMERIZER)

Chain B: 69% 15% 8% 8%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING, ITERATIVE NOE-ASSIGNMENT*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *30 STRUCTURES WITH NO RESTRAINT VIOLATIONS, 20 LOWEST ENERGY STRUCTURES FINALLY SELECTED*.

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

Software name	Classification	Version
CNS 1.0	refinement	
CNS; ARIA	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)	BMRB entry 5457, BMRB entry 4841
Number of chemical shift lists	3
Total number of shifts	1538
Number of shifts mapped to atoms	1257
Number of unparsed shifts	0
Number of shifts with mapping errors	281
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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 ⓘ

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	410	404	402	16±3
2	B	98	96	96	4±2
All	All	10160	10000	9960	326

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:ALA:HA	1:A:73:LEU:HD21	0.81	1.53	3	16
1:A:11:ILE:HG23	2:B:12:LEU:HD11	0.70	1.63	19	1
1:A:35:LEU:HB2	2:B:6:LEU:HD13	0.65	1.68	10	9
1:A:35:LEU:HD22	2:B:2:ILE:HG23	0.63	1.68	4	15
1:A:66:PHE:HB2	1:A:73:LEU:HD23	0.63	1.70	7	3
1:A:34:ILE:HD11	1:A:65:LEU:HD12	0.63	1.70	16	6
1:A:61:GLU:HA	1:A:64:ASN:ND2	0.61	2.09	19	3
1:A:10:ALA:HB1	2:B:5:LEU:HD23	0.61	1.71	18	7
1:A:21:PHE:HB3	1:A:24:HIS:HB2	0.60	1.73	13	4
1:A:29:ARG:HH21	1:A:32:LEU:HD12	0.59	1.57	19	1
1:A:11:ILE:HD13	2:B:8:ALA:HB1	0.58	1.75	10	12
1:A:34:ILE:HG22	1:A:58:VAL:HG13	0.56	1.77	10	8
1:A:30:SER:HB3	1:A:65:LEU:HD11	0.56	1.77	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:TYR:CZ	1:A:17:ILE:HD11	0.55	2.36	10	8
1:A:21:PHE:CD2	1:A:27:ILE:HG13	0.55	2.37	15	13
1:A:30:SER:O	1:A:34:ILE:HG13	0.55	2.01	20	16
1:A:29:ARG:HE	1:A:29:ARG:HA	0.54	1.62	19	1
1:A:71:ASP:OD1	1:A:72:LEU:HG	0.54	2.02	20	3
1:A:13:TYR:HD2	2:B:5:LEU:HD11	0.54	1.63	5	3
1:A:19:THR:O	1:A:22:LEU:HG	0.54	2.03	13	19
1:A:13:TYR:OH	1:A:76:PHE:HB2	0.53	2.04	19	18
1:A:11:ILE:HD13	2:B:8:ALA:CB	0.53	2.34	2	15
1:A:30:SER:HB2	1:A:65:LEU:HD11	0.53	1.80	11	5
1:A:70:GLU:HA	1:A:73:LEU:HB2	0.52	1.82	1	10
1:A:30:SER:CB	1:A:65:LEU:HD11	0.52	2.35	4	9
1:A:29:ARG:NH2	1:A:32:LEU:HD12	0.52	2.19	1	1
1:A:24:HIS:HB3	1:A:27:ILE:CG1	0.52	2.34	12	4
1:A:28:TYR:CE2	1:A:32:LEU:HD11	0.51	2.41	20	8
1:A:28:TYR:O	1:A:32:LEU:HG	0.50	2.05	13	10
2:B:3:GLN:HG3	2:B:4:MET:N	0.50	2.21	18	1
1:A:32:LEU:HD22	2:B:9:ALA:HB2	0.48	1.85	13	2
1:A:27:ILE:HG23	1:A:65:LEU:HD22	0.48	1.83	18	2
1:A:18:LYS:NZ	1:A:18:LYS:HB2	0.48	2.23	18	1
1:A:17:ILE:HG12	1:A:72:LEU:HD13	0.48	1.85	4	1
1:A:30:SER:OG	1:A:65:LEU:HD11	0.47	2.09	8	2
1:A:30:SER:O	1:A:33:GLU:HG2	0.47	2.10	20	1
1:A:60:THR:HG22	1:A:64:ASN:HD21	0.47	1.69	16	7
1:A:12:SER:O	1:A:16:LYS:HG3	0.47	2.10	2	2
1:A:13:TYR:O	1:A:17:ILE:HG13	0.47	2.10	15	13
1:A:69:GLN:N	1:A:69:GLN:OE1	0.46	2.48	8	3
1:A:69:GLN:OE1	1:A:69:GLN:N	0.46	2.48	2	2
1:A:34:ILE:CD1	1:A:65:LEU:HD12	0.46	2.41	16	3
1:A:29:ARG:O	1:A:33:GLU:HG2	0.46	2.11	19	2
1:A:32:LEU:HD22	2:B:9:ALA:CB	0.46	2.41	13	3
1:A:21:PHE:CE2	1:A:27:ILE:HG21	0.46	2.46	16	2
1:A:60:THR:HG22	1:A:64:ASN:ND2	0.45	2.26	12	8
1:A:66:PHE:HB2	1:A:73:LEU:CD2	0.45	2.42	12	5
2:B:12:LEU:HD12	2:B:12:LEU:N	0.45	2.26	19	1
1:A:14:VAL:HG11	2:B:9:ALA:HA	0.44	1.90	15	1
1:A:10:ALA:CB	2:B:5:LEU:HD23	0.44	2.42	9	1
1:A:25:PRO:O	1:A:29:ARG:HD3	0.44	2.13	9	1
1:A:16:LYS:HA	1:A:19:THR:HG22	0.43	1.90	16	9
1:A:66:PHE:N	1:A:66:PHE:CD1	0.43	2.86	16	3
1:A:29:ARG:HD2	1:A:29:ARG:N	0.43	2.28	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:PHE:HA	1:A:34:ILE:HD12	0.43	1.91	13	2
1:A:32:LEU:O	1:A:36:HIS:HB2	0.43	2.13	17	1
1:A:69:GLN:C	1:A:71:ASP:H	0.42	2.18	12	1
1:A:18:LYS:HZ3	2:B:12:LEU:HD13	0.42	1.74	3	1
1:A:58:VAL:HG12	1:A:76:PHE:HZ	0.41	1.75	11	1
1:A:58:VAL:O	1:A:62:VAL:HG23	0.41	2.16	14	3
1:A:66:PHE:CD1	1:A:66:PHE:N	0.41	2.89	8	1
1:A:57:GLU:O	1:A:60:THR:HB	0.41	2.15	15	1
1:A:19:THR:HA	1:A:22:LEU:HG	0.41	1.92	6	1
1:A:34:ILE:HG21	1:A:62:VAL:HG23	0.40	1.93	18	2
1:A:29:ARG:HA	1:A:29:ARG:NE	0.40	2.31	19	1
1:A:35:LEU:CB	2:B:6:LEU:HD13	0.40	2.44	10	1
1:A:16:LYS:NZ	1:A:16:LYS:HB2	0.40	2.32	4	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	49/85 (58%)	44±1 (90±2%)	5±1 (10±2%)	0±0 (0±1%)	56	85
2	B	11/13 (85%)	11±1 (97±5%)	0±0 (1±3%)	0±0 (1±3%)	19	64
All	All	1200/1960 (61%)	1094 (91%)	101 (8%)	5 (0%)	43	81

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	2	ILE	3
1	A	70	GLU	1
1	A	66	PHE	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	45/78 (58%)	43±1 (95±2%)	2±1 (5±2%)	38	81
2	B	10/11 (91%)	9±1 (93±6%)	1±1 (7±6%)	23	69
All	All	1100/1780 (62%)	1045 (95%)	55 (5%)	35	79

All 11 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	73	LEU	16
2	B	3	GLN	12
1	A	69	GLN	9
1	A	36	HIS	7
1	A	27	ILE	3
1	A	29	ARG	3
2	B	5	LEU	1
1	A	64	ASN	1
1	A	24	HIS	1
2	B	13	GLU	1
1	A	33	GLU	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

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

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4841

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	1271
Number of shifts mapped to atoms	1061
Number of unparsed shifts	0
Number of shifts with mapping errors	210
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Residue not found in structure. All 210 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	101	LYS	HE3	2.981	0.03	1
A	100	GLN	HB2	1.951	0.03	2
A	102	ASN	N	120.559	0.1	1
A	92	GLY	CA	45.444	0.1	1
A	96	MET	C	176.199	0.1	1
A	96	MET	N	120.994	0.1	1
A	93	SER	HB3	3.874	0.03	1
A	94	ALA	HB2	1.386	0.03	1
A	99	GLY	C	174.158	0.1	1
A	86	SER	HB2	3.778	0.03	1
A	105	LYS	HA	4.153	0.03	1
A	100	GLN	CA	55.898	0.1	1
A	89	THR	HB	4.256	0.03	1
A	89	THR	N	114.066	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	96	MET	CB	32.765	0.1	1
A	87	LEU	H	7.876	0.03	1
A	86	SER	N	115.045	0.1	1
A	100	GLN	CB	29.485	0.1	1
A	103	GLU	N	121.429	0.1	1
A	104	GLU	HB2	2.011	0.03	1
A	91	ASN	HD22	7.625	0.03	2
A	88	PHE	HB2	2.94	0.03	2
A	104	GLU	HA	4.25	0.03	1
A	88	PHE	CD1	132.438	0.1	1
A	92	GLY	H	8.494	0.03	1
A	95	GLU	CA	56.71	0.1	1
A	101	LYS	C	176.283	0.1	1
A	101	LYS	CA	56.427	0.1	1
A	103	GLU	HB3	2.075	0.03	2
A	98	SER	C	175.247	0.1	1
A	98	SER	HB2	3.917	0.03	1
A	89	THR	CB	69.906	0.1	1
A	102	ASN	HD22	7.625	0.03	2
A	101	LYS	HD3	1.668	0.03	1
A	101	LYS	CG	24.838	0.1	1
A	105	LYS	HG2	1.421	0.03	1
A	89	THR	HA	4.325	0.03	1
A	98	SER	H	8.337	0.03	1
A	99	GLY	H	8.463	0.03	1
A	101	LYS	HD2	1.668	0.03	1
A	100	GLN	HA	4.306	0.03	1
A	102	ASN	HA	4.706	0.03	1
A	87	LEU	CB	42.054	0.1	1
A	91	ASN	H	8.386	0.03	1
A	89	THR	HG21	1.169	0.03	1
A	105	LYS	CG	24.732	0.1	1
A	86	SER	HB3	3.778	0.03	1
A	105	LYS	CD	29.115	0.1	1
A	86	SER	C	174.974	0.1	1
A	89	THR	C	175.121	0.1	1
A	92	GLY	HA3	3.963	0.03	1
A	105	LYS	CE	42.112	0.1	1
A	98	SER	CA	58.895	0.1	1
A	103	GLU	C	176.209	0.1	1
A	105	LYS	HE3	2.982	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	91	ASN	CA	53.327	0.1	1
A	91	ASN	N	118.708	0.1	1
A	86	SER	CB	63.284	0.1	1
A	87	LEU	N	122.454	0.1	1
A	99	GLY	HA3	3.95	0.03	1
A	97	ASN	HB2	2.78	0.03	1
A	100	GLN	C	176.01	0.1	1
A	93	SER	CA	58.532	0.1	1
A	104	GLU	CA	56.571	0.1	1
A	89	THR	CG2	21.466	0.1	1
A	97	ASN	N	119.689	0.1	1
A	102	ASN	CA	53.452	0.1	1
A	104	GLU	C	175.487	0.1	1
A	93	SER	H	8.191	0.03	1
A	92	GLY	N	109.669	0.1	1
A	103	GLU	CA	56.383	0.1	1
A	87	LEU	C	177.298	0.1	1
A	102	ASN	C	175.121	0.1	1
A	98	SER	CB	63.768	0.1	1
A	100	GLN	HE22	7.548	0.03	2
A	105	LYS	HB3	1.825	0.03	2
A	95	GLU	C	176.858	0.1	1
A	102	ASN	HB2	2.796	0.03	1
A	100	GLN	HB3	2.078	0.03	2
A	87	LEU	HG	1.489	0.03	1
A	101	LYS	N	122.891	0.1	1
A	91	ASN	HA	4.77	0.03	1
A	95	GLU	HA	4.224	0.03	1
A	100	GLN	CG	33.785	0.1	1
A	86	SER	CA	59.23	0.1	1
A	105	LYS	HD3	1.668	0.03	1
A	87	LEU	HD23	0.737	0.03	1
A	87	LEU	HD13	0.803	0.03	1
A	93	SER	N	115.747	0.1	1
A	99	GLY	HA2	3.95	0.03	1
A	97	ASN	C	175.435	0.1	1
A	97	ASN	CA	53.368	0.1	1
A	88	PHE	N	118.696	0.1	1
A	93	SER	CB	63.906	0.1	1
A	94	ALA	CB	19.131	0.1	1
A	90	GLY	N	110.382	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	104	GLU	CB	30.195	0.1	1
A	105	LYS	HD2	1.668	0.03	1
A	87	LEU	CD1	25.047	0.1	1
A	94	ALA	C	177.988	0.1	1
A	90	GLY	C	174.033	0.1	1
A	101	LYS	CD	29.217	0.1	1
A	94	ALA	CA	52.957	0.1	1
A	94	ALA	HB3	1.386	0.03	1
A	90	GLY	HA2	3.918	0.03	1
A	91	ASN	HD21	6.943	0.03	2
A	100	GLN	HE21	6.846	0.03	2
A	94	ALA	HB1	1.386	0.03	1
A	105	LYS	HG3	1.421	0.03	1
A	103	GLU	HB2	1.932	0.03	2
A	95	GLU	CB	29.87	0.1	1
A	100	GLN	HG3	2.33	0.03	1
A	102	ASN	HD21	6.943	0.03	2
A	97	ASN	HD21	6.943	0.03	2
A	87	LEU	CA	55.681	0.1	1
A	95	GLU	H	8.326	0.03	1
A	101	LYS	CE	42.163	0.1	1
A	97	ASN	HD22	7.625	0.03	2
A	96	MET	HA	4.439	0.03	1
A	94	ALA	N	125.832	0.1	1
A	87	LEU	HA	4.152	0.03	1
A	104	GLU	H	8.399	0.03	1
A	101	LYS	HA	4.319	0.03	1
A	100	GLN	N	119.903	0.1	1
A	87	LEU	HD12	0.803	0.03	1
A	91	ASN	HB2	2.78	0.03	1
A	103	GLU	H	8.462	0.03	1
A	95	GLU	N	119.467	0.1	1
A	88	PHE	HA	4.644	0.03	1
A	90	GLY	H	7.926	0.03	1
A	96	MET	CG	31.997	0.1	1
A	98	SER	HA	4.366	0.03	1
A	89	THR	HG22	1.169	0.03	1
A	97	ASN	HA	4.78	0.03	1
A	88	PHE	C	176.052	0.1	1
A	100	GLN	NE2	112.59	0.1	1
A	97	ASN	HB3	2.78	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	96	MET	HE3	2.08	0.03	1
A	101	LYS	HG3	1.438	0.03	1
A	87	LEU	CD2	23.269	0.1	1
A	96	MET	HB2	2.014	0.03	2
A	88	PHE	H	7.895	0.03	1
A	101	LYS	HB3	1.746	0.03	1
A	89	THR	CA	61.846	0.1	1
A	87	LEU	HD22	0.737	0.03	1
A	105	LYS	CB	33.769	0.1	1
A	105	LYS	N	127.687	0.1	1
A	96	MET	CA	55.75	0.1	1
A	104	GLU	N	122.692	0.1	1
A	87	LEU	CG	26.862	0.1	1
A	88	PHE	HD2	7.2	0.03	1
A	91	ASN	ND2	113.102	0.1	1
A	101	LYS	HB2	1.746	0.03	1
A	87	LEU	HD11	0.803	0.03	1
A	97	ASN	CB	38.899	0.1	1
A	91	ASN	HB3	2.78	0.03	1
A	98	SER	N	116.34	0.1	1
A	101	LYS	CB	32.977	0.1	1
A	93	SER	HA	4.419	0.03	1
A	88	PHE	HB3	3.15	0.03	2
A	91	ASN	CB	39.107	0.1	1
A	95	GLU	HB3	2.04	0.03	2
A	101	LYS	HG2	1.438	0.03	1
A	102	ASN	ND2	113.102	0.1	1
A	105	LYS	CA	57.483	0.1	1
A	100	GLN	H	8.16	0.03	1
A	88	PHE	CB	39.432	0.1	1
A	98	SER	HB3	3.917	0.03	1
A	96	MET	HE2	2.08	0.03	1
A	105	LYS	H	7.949	0.03	1
A	101	LYS	HE2	2.981	0.03	1
A	102	ASN	HB3	2.796	0.03	1
A	94	ALA	H	8.406	0.03	1
A	96	MET	CE	16.947	0.1	1
A	90	GLY	HA3	3.918	0.03	1
A	102	ASN	CB	38.968	0.1	1
A	96	MET	H	8.287	0.03	1
A	90	GLY	CA	45.444	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	97	ASN	ND2	113.102	0.1	1
A	100	GLN	HG2	2.33	0.03	1
A	104	GLU	HB3	2.011	0.03	1
A	92	GLY	HA2	3.963	0.03	1
A	96	MET	HG2	2.519	0.03	2
A	101	LYS	H	8.426	0.03	1
A	105	LYS	HE2	2.982	0.03	1
A	88	PHE	HD1	7.2	0.03	1
A	103	GLU	CB	30.403	0.1	1
A	86	SER	H	8.167	0.03	1
A	93	SER	HB2	3.874	0.03	1
A	86	SER	HA	4.279	0.03	1
A	95	GLU	HB2	1.946	0.03	2
A	96	MET	HG3	2.595	0.03	2
A	97	ASN	H	8.454	0.03	1
A	91	ASN	C	175.969	0.1	1
A	99	GLY	CA	45.444	0.1	1
A	87	LEU	HD21	0.737	0.03	1
A	94	ALA	HA	4.302	0.03	1
A	87	LEU	HB3	1.39	0.03	2
A	96	MET	HE1	2.08	0.03	1
A	87	LEU	HB2	1.185	0.03	2
A	93	SER	C	174.66	0.1	1
A	103	GLU	HA	4.259	0.03	1
A	102	ASN	H	8.545	0.03	1
A	92	GLY	C	174.378	0.1	1
A	88	PHE	CA	57.636	0.1	1
A	96	MET	HB3	2.081	0.03	2
A	105	LYS	HB2	1.707	0.03	2
A	89	THR	HG23	1.169	0.03	1
A	99	GLY	N	110.656	0.1	1
A	89	THR	H	7.96	0.03	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, <i>ppm</i>	Suggested action
$^{13}\text{C}_\alpha$	105	-0.51 ± 0.09	Should be applied
$^{13}\text{C}_\beta$	98	0.42 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	101	-0.46 ± 0.10	None needed (< 0.5 ppm)

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Nucleus	# values	Correction \pm precision, ppm	Suggested action
^{15}N	102	-0.36 \pm 0.37	None needed (< 0.5 ppm)

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 71%, i.e. 557 atoms were assigned a chemical shift out of a possible 790. 9 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	242/303 (80%)	97/121 (80%)	97/122 (80%)	48/60 (80%)
Sidechain	272/402 (68%)	166/233 (71%)	103/154 (67%)	3/15 (20%)
Aromatic	43/85 (51%)	28/45 (62%)	15/36 (42%)	0/4 (0%)
Overall	557/790 (71%)	291/399 (73%)	215/312 (69%)	51/79 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 969 atoms were assigned a chemical shift out of a possible 1284. 12 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	416/484 (86%)	167/193 (87%)	167/196 (85%)	82/95 (86%)
Sidechain	485/672 (72%)	304/395 (77%)	173/244 (71%)	8/33 (24%)
Aromatic	68/128 (53%)	43/68 (63%)	25/54 (46%)	0/6 (0%)
Overall	969/1284 (75%)	514/656 (78%)	365/494 (74%)	90/134 (67%)

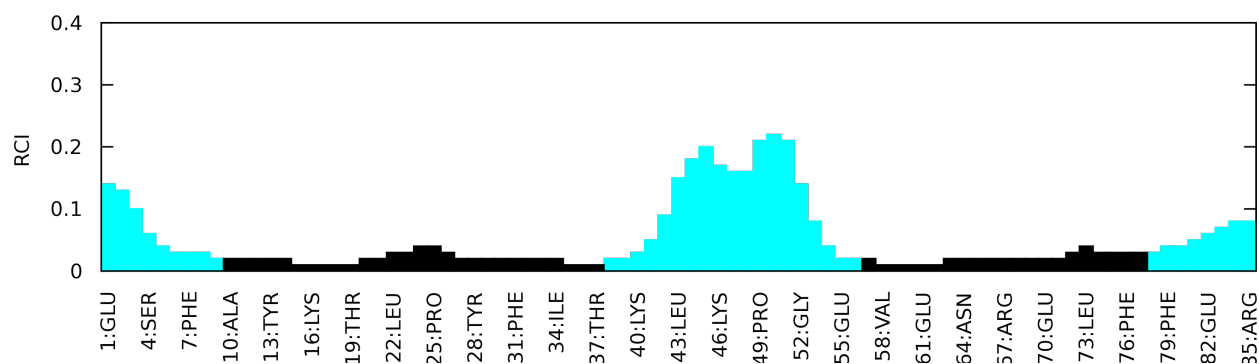
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: BMRB entry 5457

Chemical shift list name: *assigned_chem_shift_list_1*

7.2.1 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	169
Number of shifts mapped to atoms	98
Number of unparsed shifts	0
Number of shifts with mapping errors	71
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Residue not found in structure. All 71 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	19	GLU	HB3	2.082	0.01	1
B	18	ARG	HG2	1.448	0.01	2
B	22	ALA	HB1	1.404	0.01	1
B	18	ARG	HD3	3.033	0.01	2
B	2	ARG	HE	7.329	0.01	1
B	2	ARG	HG3	1.628	0.01	1
B	2	ARG	HD2	3.197	0.01	1
B	20	ARG	HD2	3.195	0.01	1
B	23	GLU	HB2	1.946	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	3	MET	HG3	2.439	0.01	2
B	20	ARG	HG2	1.689	0.01	2
B	3	MET	H	8.495	0.01	1
B	20	ARG	HG3	1.741	0.01	2
B	17	ARG	H	8.09	0.01	1
B	17	ARG	HD2	3.135	0.01	2
B	20	ARG	HB3	1.9	0.01	1
B	22	ALA	HB2	1.404	0.01	1
B	21	GLU	HB2	2.01	0.01	1
B	2	ARG	HB2	1.73	0.01	2
B	18	ARG	HE	7.238	0.01	1
B	20	ARG	HA	4.189	0.01	1
B	18	ARG	HA	3.966	0.01	1
B	17	ARG	HE	7.45	0.01	1
B	19	GLU	H	7.885	0.01	1
B	22	ALA	H	7.81	0.01	1
B	18	ARG	HG3	1.482	0.01	2
B	2	ARG	HA	4.373	0.01	1
B	18	ARG	HD2	2.949	0.01	2
B	24	HIS	H	8.181	0.01	1
B	19	GLU	HG3	2.363	0.01	2
B	18	ARG	HB2	1.64	0.01	2
B	3	MET	HG2	2.322	0.01	2
B	23	GLU	H	7.972	0.01	1
B	17	ARG	HD3	3.202	0.01	2
B	18	ARG	H	8.003	0.01	1
B	22	ALA	HB3	1.404	0.01	1
B	21	GLU	HG2	2.251	0.01	2
B	21	GLU	HA	4.095	0.01	1
B	23	GLU	HG2	2.261	0.01	2
B	23	GLU	HA	4.118	0.01	1
B	20	ARG	HD3	3.195	0.01	1
B	21	GLU	H	8.056	0.01	1
B	22	ALA	HA	4.198	0.01	1
B	18	ARG	HB3	1.774	0.01	2
B	17	ARG	HA	3.954	0.01	1
B	24	HIS	HD2	7.215	0.01	3
B	3	MET	HB2	1.754	0.01	2
B	24	HIS	HA	4.629	0.01	1
B	20	ARG	H	7.929	0.01	1
B	19	GLU	HB2	2.082	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	2	ARG	HG2	1.628	0.01	1
B	21	GLU	HB3	2.01	0.01	1
B	24	HIS	HB3	3.271	0.01	2
B	3	MET	HB3	1.803	0.01	2
B	2	ARG	HD3	3.197	0.01	1
B	19	GLU	HA	4.066	0.01	1
B	19	GLU	HG2	2.222	0.01	2
B	17	ARG	HG2	1.528	0.01	2
B	24	HIS	HE1	7.47	0.01	3
B	17	ARG	HG3	1.755	0.01	2
B	20	ARG	HB2	1.9	0.01	1
B	23	GLU	HB3	1.946	0.01	1
B	21	GLU	HG3	2.39	0.01	2
B	23	GLU	HG3	2.139	0.01	2
B	24	HIS	HB2	3.132	0.01	2
B	3	MET	HA	4.497	0.01	1
B	2	ARG	HB3	1.8	0.01	2
B	17	ARG	HB3	1.852	0.01	2
B	2	ARG	H	8.498	0.01	1
B	17	ARG	HB2	1.81	0.01	2
B	20	ARG	HE	7.439	0.01	1

7.2.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.2.3 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 9%, i.e. 72 atoms were assigned a chemical shift out of a possible 790. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	24/303 (8%)	24/121 (20%)	0/122 (0%)	0/60 (0%)
Sidechain	44/402 (11%)	44/233 (19%)	0/154 (0%)	0/15 (0%)
Aromatic	4/85 (5%)	4/45 (9%)	0/36 (0%)	0/4 (0%)
Overall	72/790 (9%)	72/399 (18%)	0/312 (0%)	0/79 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 6%, i.e. 78 atoms were assigned a chemical shift out of a possible 1284.

0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	26/484 (5%)	26/193 (13%)	0/196 (0%)	0/95 (0%)
Sidechain	48/672 (7%)	48/395 (12%)	0/244 (0%)	0/33 (0%)
Aromatic	4/128 (3%)	4/68 (6%)	0/54 (0%)	0/6 (0%)
Overall	78/1284 (6%)	78/656 (12%)	0/494 (0%)	0/134 (0%)

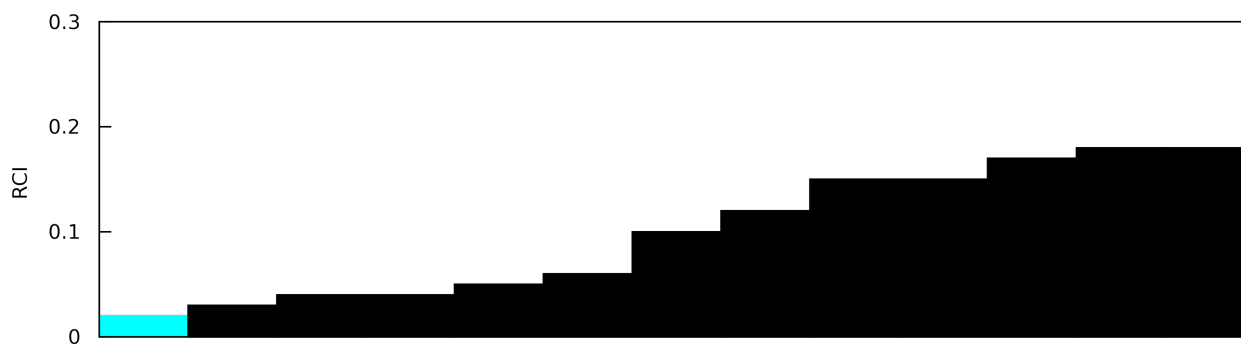
7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain B:



7.3 Chemical shift list 3

File name: BMRB entry 4841

Chemical shift list name: *assigned_chem_shift_list_2*

7.3.1 Bookkeeping [i](#)

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

Total number of shifts	98
Number of shifts mapped to atoms	98
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.3.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.3.3 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 9%, i.e. 72 atoms were assigned a chemical shift out of a possible 790. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

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7.3.4 Statistically unusual chemical shifts [i](#)

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from

the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain B:

