



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 10:56 pm GMT

PDB ID : 2KDO  
Title : Structure of the human Shwachman-Bodian-Diamond syndrome protein, SBDS  
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Deposited on : 2009-01-14

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A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

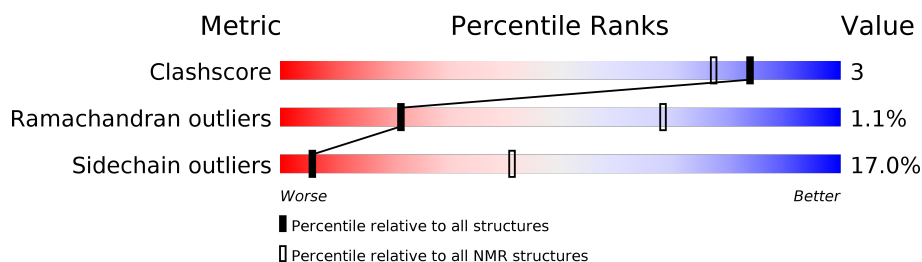
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 81%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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  $\geq 3$ , 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	252	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:9-A:40, A:47-A:97 (83)	0.56	1
2	A:142-A:169 (28)	1.01	11
3	A:174-A:239 (66)	0.41	10

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. No single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 4156 atoms, of which 2127 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribosome maturation protein SBDS.

Mol	Chain	Residues	Atoms						Trace
1	A	252	Total	C	H	N	O	S	0
			4156	1280	2127	356	382	11	

There are 2 discrepancies between the modelled and reference sequences:

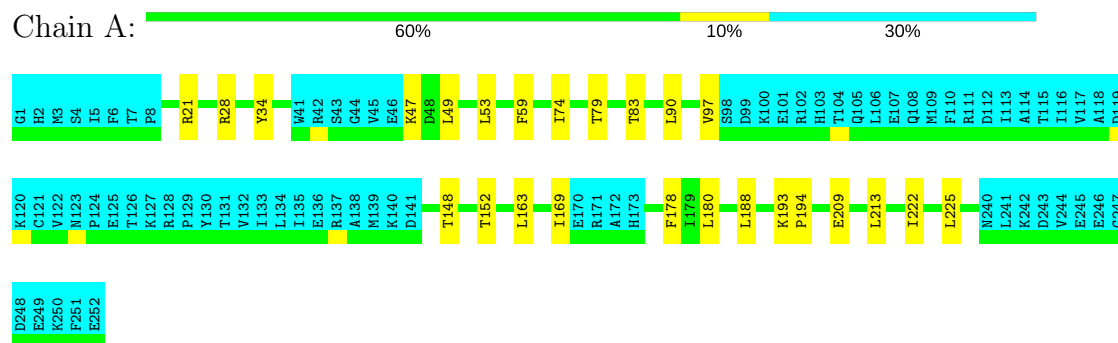
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q9Y3A5
A	2	HIS	-	EXPRESSION TAG	UNP Q9Y3A5

## 4 Residue-property plots

### 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: Ribosome maturation protein SBDS

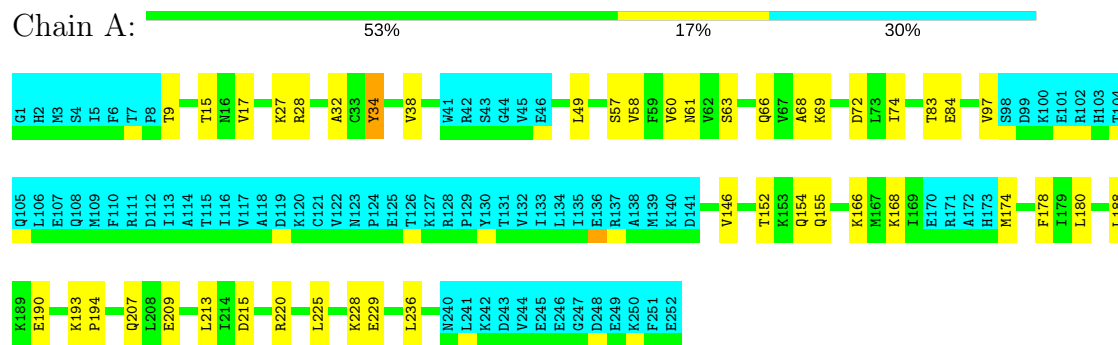


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

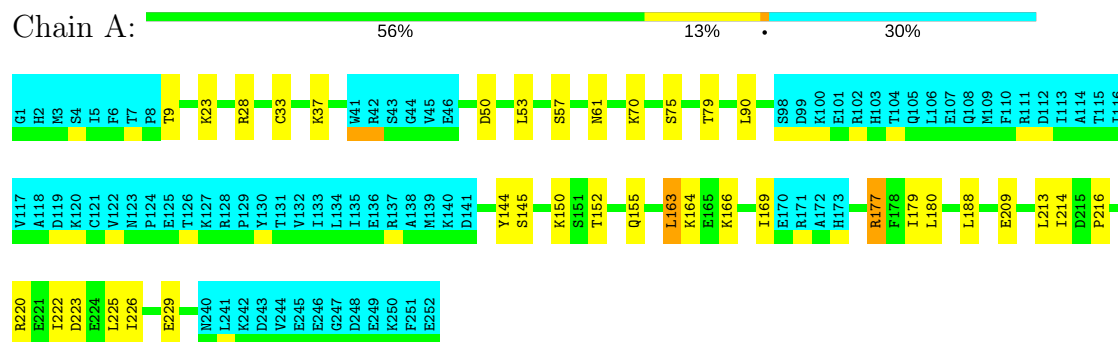
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Ribosome maturation protein SBDS



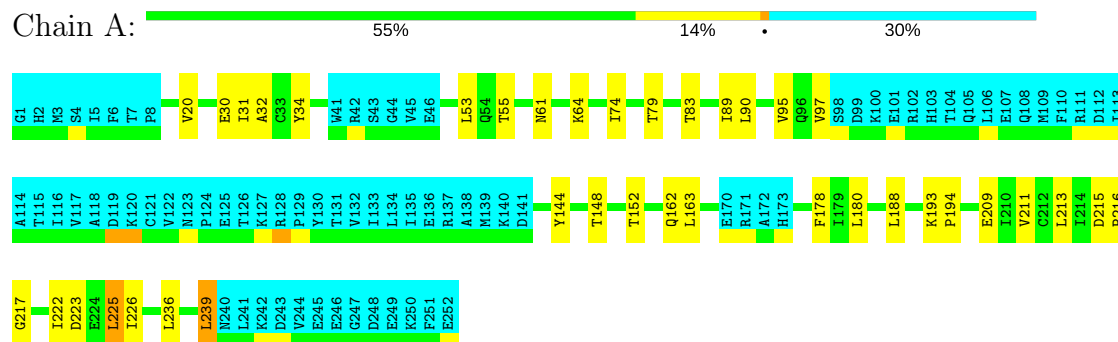
### 4.2.2 Score per residue for model 2

- Molecule 1: Ribosome maturation protein SBDS



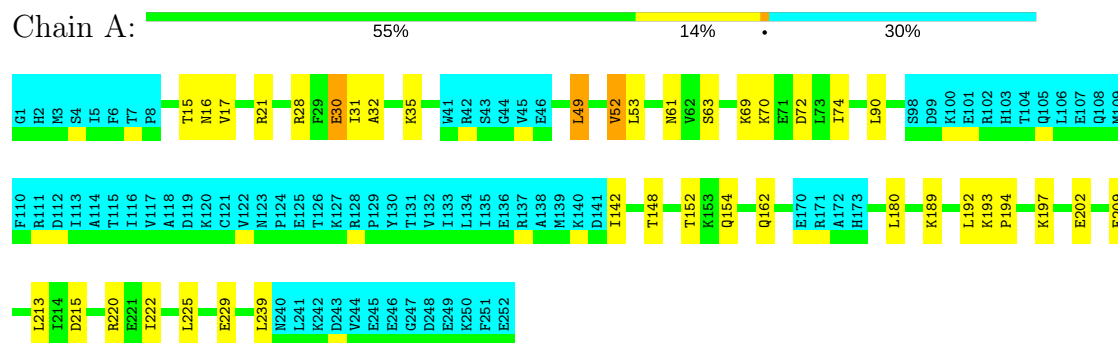
### 4.2.3 Score per residue for model 3

- Molecule 1: Ribosome maturation protein SBDS



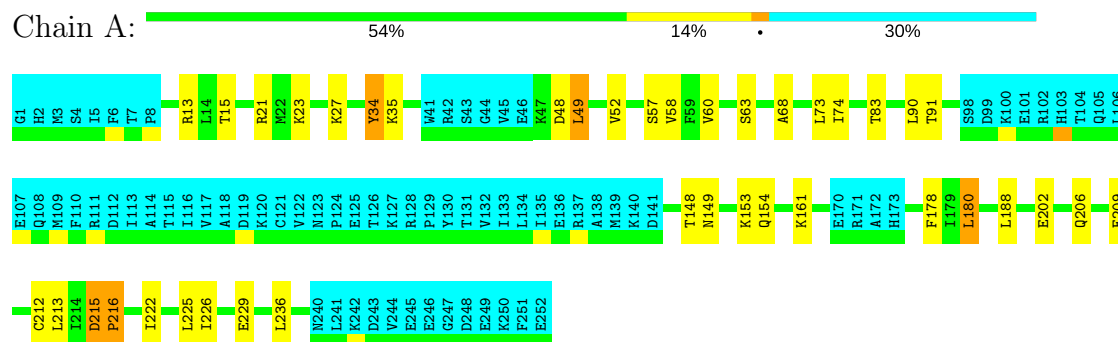
### 4.2.4 Score per residue for model 4

- Molecule 1: Ribosome maturation protein SBDS



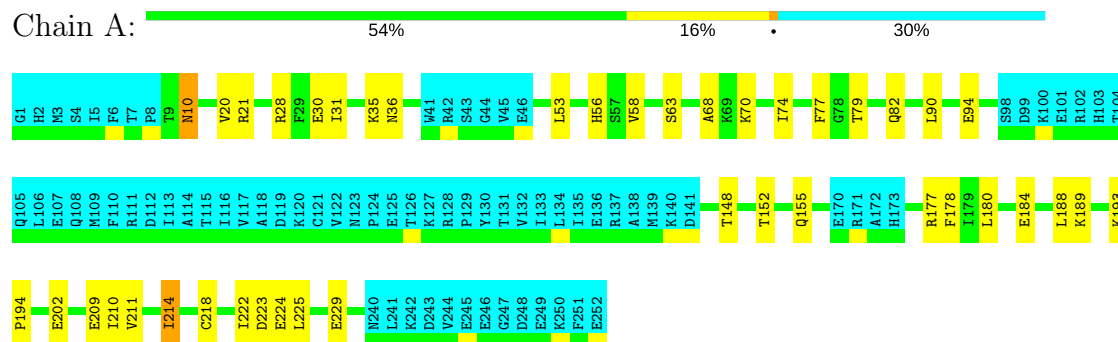
### 4.2.5 Score per residue for model 5

- Molecule 1: Ribosome maturation protein SBDS



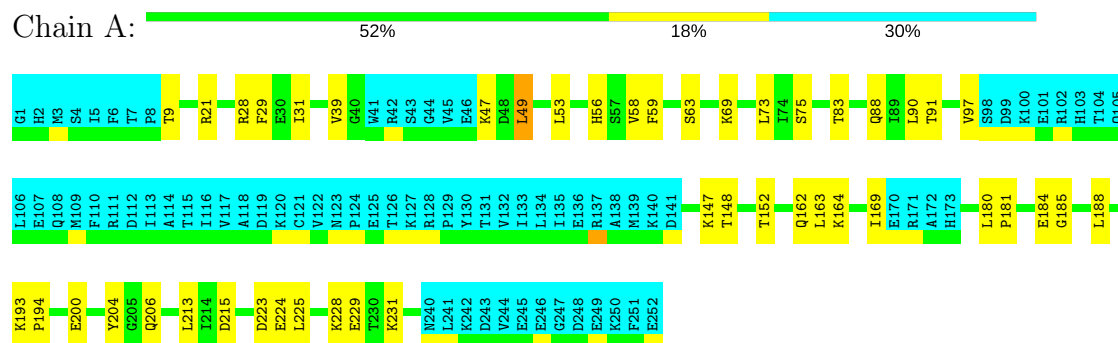
### 4.2.6 Score per residue for model 6

- Molecule 1: Ribosome maturation protein SBDS



### 4.2.7 Score per residue for model 7

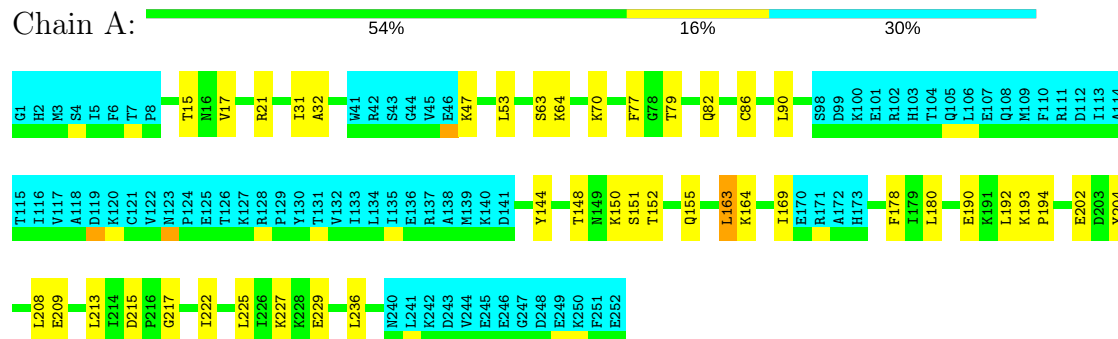
- Molecule 1: Ribosome maturation protein SBDS



#### 4.2.8 Score per residue for model 8

- Molecule 1: Ribosome maturation protein SBDS

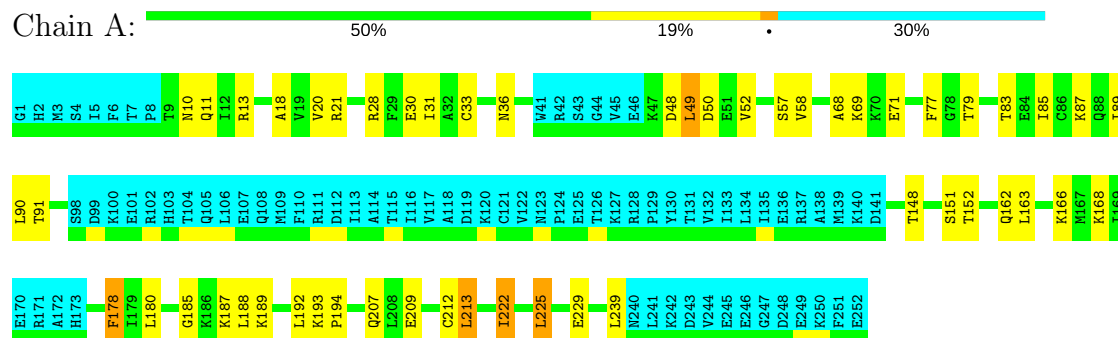
Chain A:



#### 4.2.9 Score per residue for model 9

- Molecule 1: Ribosome maturation protein SBDS

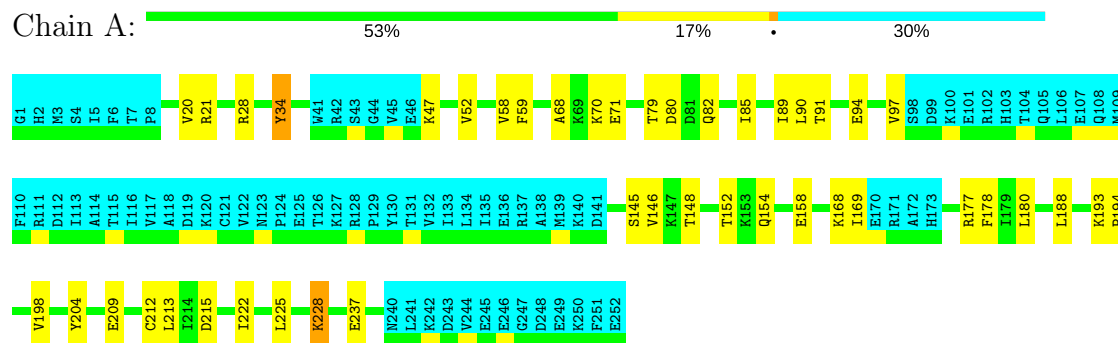
Chain A:



#### 4.2.10 Score per residue for model 10

- Molecule 1: Ribosome maturation protein SBDS

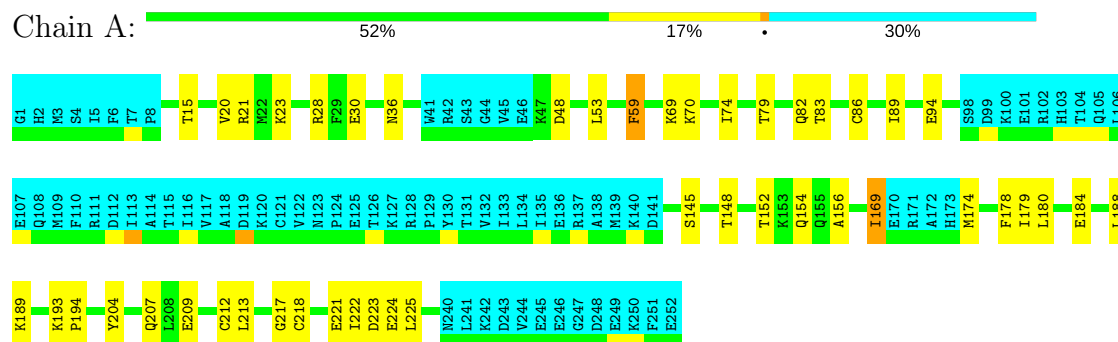
Chain A:





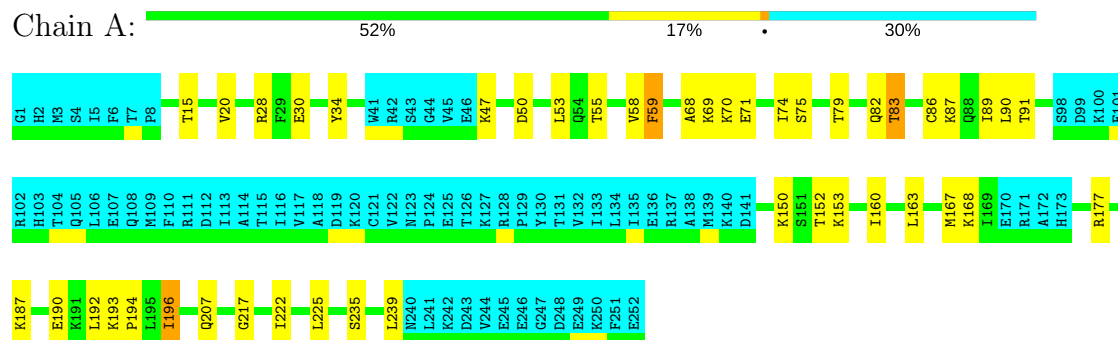
### 4.2.11 Score per residue for model 11

- Molecule 1: Ribosome maturation protein SBDS



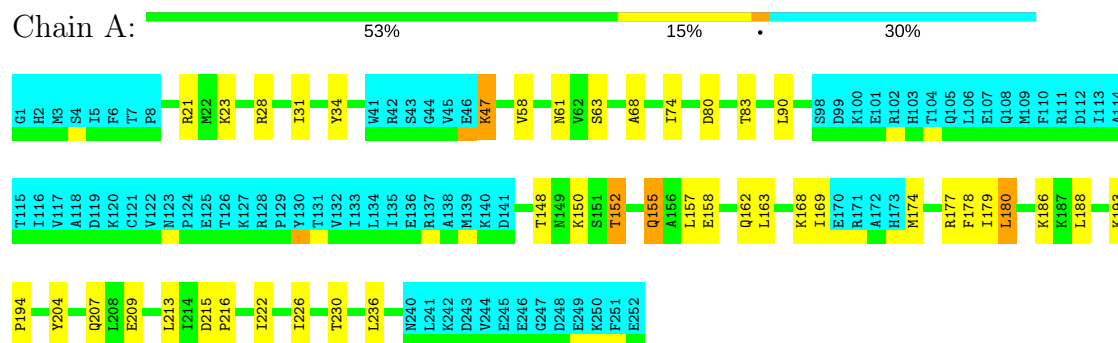
### 4.2.12 Score per residue for model 12

- Molecule 1: Ribosome maturation protein SBDS



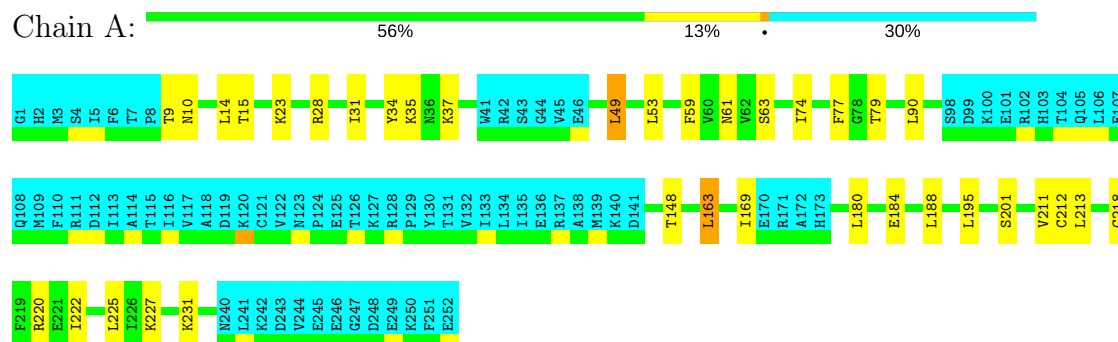
### 4.2.13 Score per residue for model 13

- Molecule 1: Ribosome maturation protein SBDS



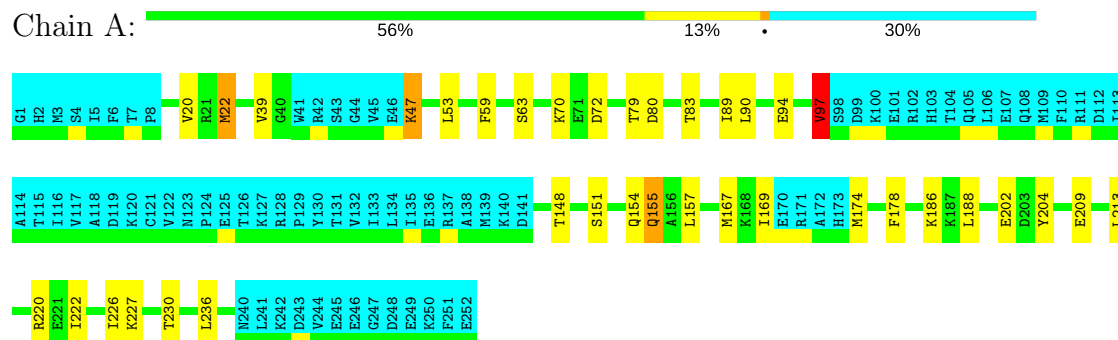
### 4.2.14 Score per residue for model 14

- Molecule 1: Ribosome maturation protein SBDS



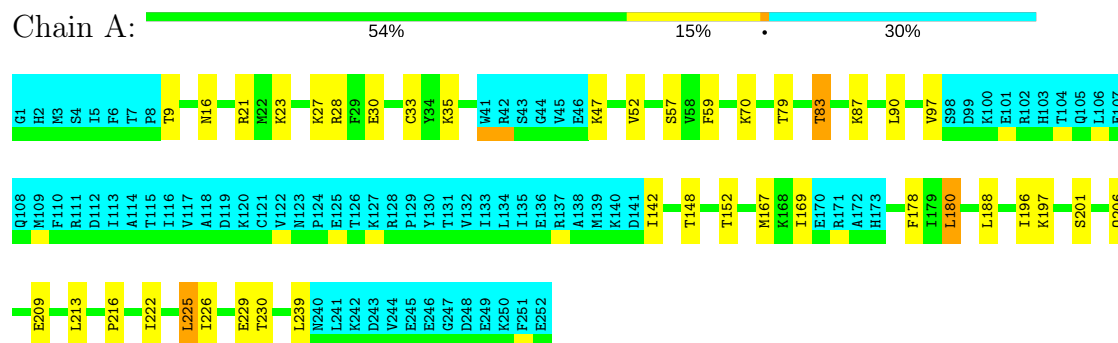
### 4.2.15 Score per residue for model 15

- Molecule 1: Ribosome maturation protein SBDS



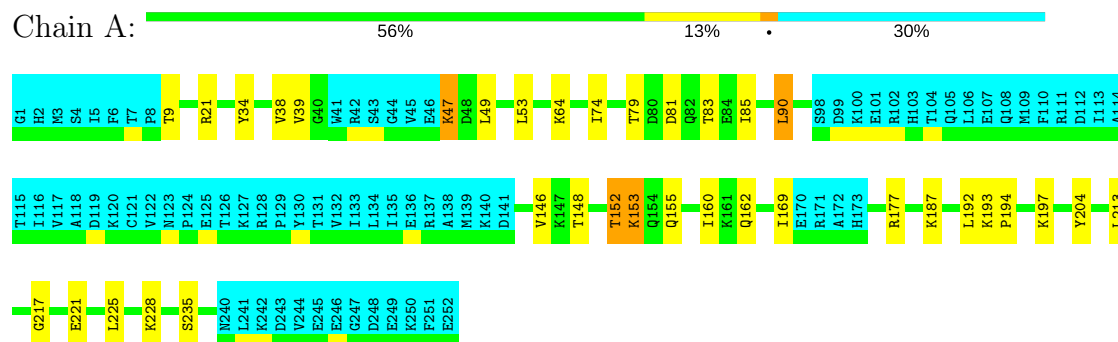
### 4.2.16 Score per residue for model 16

- Molecule 1: Ribosome maturation protein SBDS



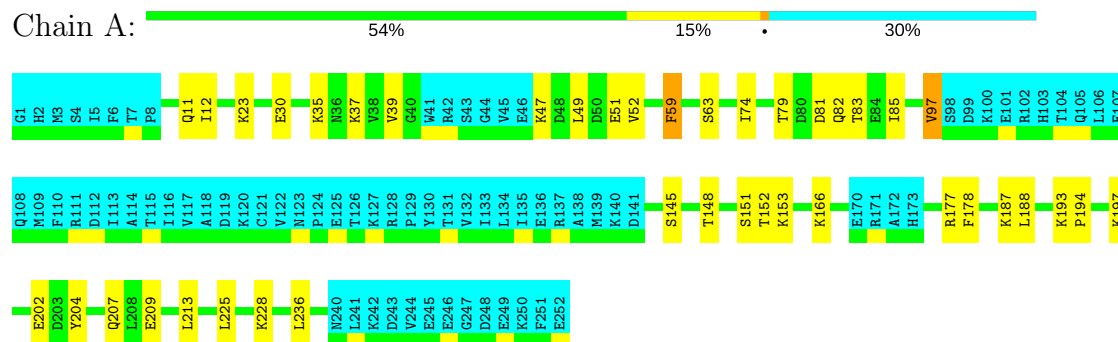
## 4.2.17 Score per residue for model 17

- Molecule 1: Ribosome maturation protein SBDS



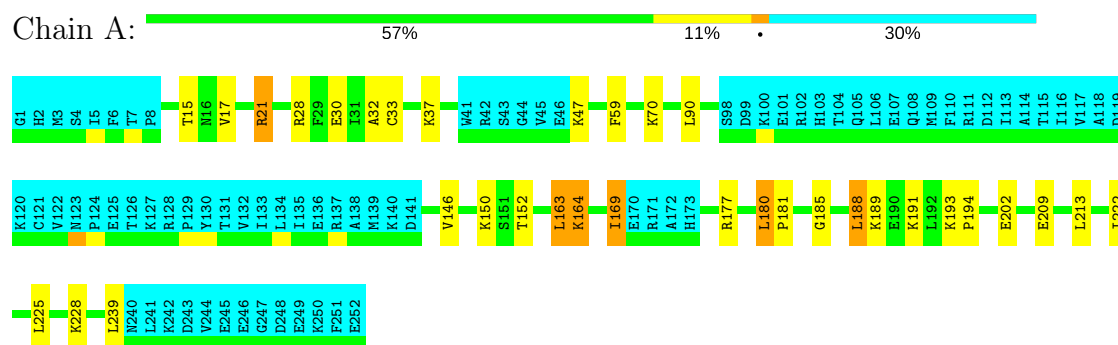
## 4.2.18 Score per residue for model 18

- Molecule 1: Ribosome maturation protein SBDS



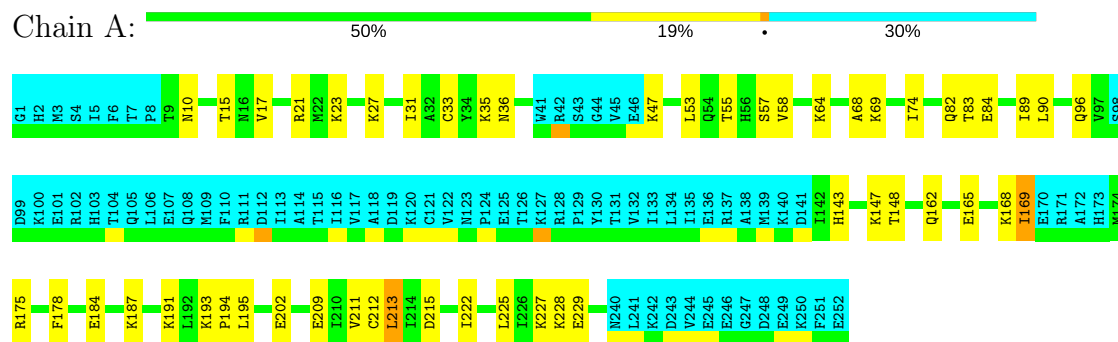
## 4.2.19 Score per residue for model 19

- Molecule 1: Ribosome maturation protein SBDS



## 4.2.20 Score per residue for model 20

- Molecule 1: Ribosome maturation protein SBDS



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing, torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	.
CYANA	geometry optimization	.
DYANA	structure solution	.
DYANA	geometry optimization	.
CYANA	refinement	2.1
CNS	refinement	1.1

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 16119
Number of chemical shift lists	1
Total number of shifts	2498
Number of shifts mapped to atoms	2498
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

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	1412	1522	1520	8±3
All	All	28240	30440	30400	159

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:180:LEU:HD12	1:A:181:PRO:HD2	0.72	1.61	7	1
1:A:49:LEU:H	1:A:49:LEU:HD13	0.61	1.56	7	3
1:A:20:VAL:HG22	1:A:89:ILE:HG22	0.60	1.73	12	6
1:A:17:VAL:HB	1:A:32:ALA:HB1	0.59	1.74	19	4
1:A:222:ILE:O	1:A:225:LEU:HG	0.58	1.97	14	13
1:A:154:GLN:O	1:A:155:GLN:HG2	0.56	2.01	15	1
1:A:83:THR:HA	1:A:86:CYS:SG	0.56	2.41	12	2
1:A:30:GLU:HG2	1:A:59:PHE:CD1	0.55	2.35	12	1
1:A:202:GLU:HA	1:A:209:GLU:O	0.55	2.02	5	6
1:A:193:LYS:N	1:A:194:PRO:HD2	0.55	2.17	20	15
1:A:178:PHE:CZ	1:A:210:ILE:HB	0.55	2.36	6	1
1:A:49:LEU:HB2	1:A:83:THR:HG23	0.55	1.77	17	1
1:A:180:LEU:HD23	1:A:181:PRO:HD2	0.54	1.78	19	1
1:A:20:VAL:HG13	1:A:31:ILE:HG13	0.54	1.80	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:178:PHE:O	1:A:209:GLU:HA	0.54	2.03	20	13
1:A:185:GLY:O	1:A:188:LEU:HG	0.54	2.02	9	2
1:A:17:VAL:HA	1:A:33:CYS:O	0.53	2.03	20	1
1:A:198:VAL:HG12	1:A:212:CYS:HB3	0.53	1.81	10	1
1:A:85:ILE:O	1:A:89:ILE:HG13	0.52	2.05	10	2
1:A:34:TYR:HB2	1:A:52:VAL:HG13	0.52	1.81	5	1
1:A:155:GLN:HA	1:A:158:GLU:OE1	0.52	2.04	13	1
1:A:69:LYS:HB3	1:A:71:GLU:OE2	0.52	2.05	9	1
1:A:31:ILE:HD11	1:A:89:ILE:HD12	0.52	1.82	20	1
1:A:53:LEU:HD21	1:A:86:CYS:SG	0.51	2.46	8	1
1:A:222:ILE:O	1:A:226:ILE:HG12	0.51	2.06	13	6
1:A:60:VAL:HG23	1:A:68:ALA:HB2	0.50	1.84	5	1
1:A:58:VAL:HG13	1:A:68:ALA:HB3	0.49	1.84	10	8
1:A:49:LEU:O	1:A:52:VAL:HG12	0.49	2.07	9	2
1:A:215:ASP:OD2	1:A:216:PRO:HD2	0.49	2.08	5	1
1:A:224:GLU:O	1:A:228:LYS:HE2	0.49	2.07	7	1
1:A:177:ARG:HD2	1:A:209:GLU:OE2	0.49	2.08	19	3
1:A:49:LEU:HA	1:A:52:VAL:HG12	0.49	1.85	4	1
1:A:21:ARG:HD2	1:A:30:GLU:OE1	0.48	2.09	4	1
1:A:177:ARG:HB2	1:A:209:GLU:OE2	0.48	2.09	2	1
1:A:81:ASP:O	1:A:85:ILE:HG12	0.48	2.08	17	2
1:A:163:LEU:HD13	1:A:164:LYS:N	0.47	2.25	19	3
1:A:169:ILE:HD13	1:A:169:ILE:H	0.47	1.68	20	1
1:A:177:ARG:HB3	1:A:211:VAL:HG22	0.47	1.87	6	1
1:A:34:TYR:CD1	1:A:52:VAL:HG23	0.47	2.45	10	1
1:A:87:LYS:O	1:A:91:THR:HG22	0.47	2.10	9	1
1:A:69:LYS:HG2	1:A:72:ASP:OD2	0.47	2.10	4	2
1:A:169:ILE:H	1:A:169:ILE:HD13	0.46	1.70	19	2
1:A:69:LYS:HB3	1:A:71:GLU:OE1	0.46	2.10	12	1
1:A:178:PHE:CE2	1:A:180:LEU:HD22	0.46	2.46	13	3
1:A:211:VAL:HG11	1:A:239:LEU:HD12	0.46	1.87	3	1
1:A:34:TYR:O	1:A:38:VAL:HB	0.46	2.11	1	1
1:A:212:CYS:O	1:A:213:LEU:HD22	0.45	2.11	20	1
1:A:49:LEU:HD21	1:A:83:THR:HG23	0.45	1.88	5	1
1:A:95:VAL:HG13	1:A:97:VAL:HG13	0.45	1.88	3	1
1:A:30:GLU:HB3	1:A:59:PHE:CD1	0.44	2.47	18	2
1:A:70:LYS:HG3	1:A:71:GLU:OE1	0.44	2.12	10	1
1:A:28:ARG:HB2	1:A:60:VAL:O	0.44	2.12	1	1
1:A:227:LYS:HA	1:A:231:LYS:HB3	0.44	1.89	14	1
1:A:39:VAL:HG23	1:A:97:VAL:HG12	0.44	1.90	7	1
1:A:21:ARG:HD3	1:A:30:GLU:OE1	0.44	2.12	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:228:LYS:HE3	1:A:228:LYS:C	0.43	2.33	10	1
1:A:20:VAL:HA	1:A:94:GLU:O	0.43	2.13	11	2
1:A:39:VAL:HB	1:A:97:VAL:HG21	0.43	1.90	15	1
1:A:16:ASN:OD1	1:A:35:LYS:HA	0.43	2.13	4	1
1:A:201:SER:HB2	1:A:211:VAL:HG21	0.43	1.91	14	1
1:A:21:ARG:HD2	1:A:30:GLU:OE2	0.43	2.13	19	1
1:A:29:PHE:HB3	1:A:58:VAL:CG2	0.43	2.44	7	1
1:A:83:THR:O	1:A:87:LYS:HB2	0.42	2.14	12	2
1:A:49:LEU:HD13	1:A:49:LEU:H	0.42	1.74	4	1
1:A:18:ALA:HB3	1:A:33:CYS:O	0.42	2.15	9	1
1:A:22:MET:HB2	1:A:89:ILE:HG23	0.42	1.92	15	1
1:A:152:THR:HG23	1:A:153:LYS:HD2	0.42	1.92	17	1
1:A:187:LYS:O	1:A:191:LYS:HE3	0.42	2.15	20	1
1:A:189:LYS:O	1:A:193:LYS:HB2	0.41	2.15	4	3
1:A:10:ASN:HB3	1:A:13:ARG:CG	0.41	2.45	9	1
1:A:192:LEU:HD11	1:A:212:CYS:SG	0.41	2.56	9	1
1:A:236:LEU:H	1:A:236:LEU:HD23	0.41	1.75	5	1
1:A:69:LYS:O	1:A:73:LEU:HG	0.40	2.16	7	1
1:A:185:GLY:O	1:A:188:LEU:HD23	0.40	2.17	19	1
1:A:32:ALA:HB3	1:A:55:THR:HB	0.40	1.94	3	1
1:A:151:SER:OG	1:A:155:GLN:HA	0.40	2.16	8	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	177/252 (70%)	154±4 (87±3%)	21±4 (12±2%)	2±1 (1±1%)	21	68
All	All	3540/5040 (70%)	3078 (87%)	424 (12%)	38 (1%)	21	68

All 18 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	97	VAL	4

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Mol	Chain	Res	Type	Models (Total)
1	A	216	PRO	4
1	A	35	LYS	4
1	A	61	ASN	3
1	A	10	ASN	3
1	A	146	VAL	3
1	A	196	ILE	2
1	A	39	VAL	2
1	A	47	LYS	2
1	A	154	GLN	2
1	A	152	THR	2
1	A	217	GLY	1
1	A	12	ILE	1
1	A	142	ILE	1
1	A	11	GLN	1
1	A	214	ILE	1
1	A	213	LEU	1
1	A	38	VAL	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	161/229 (70%)	134±3 (83±2%)	27±3 (17±2%)	6	41
All	All	3220/4580 (70%)	2673 (83%)	547 (17%)	6	41

All 120 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	213	LEU	18
1	A	148	THR	16
1	A	90	LEU	16
1	A	152	THR	15
1	A	180	LEU	14
1	A	188	LEU	13
1	A	79	THR	13
1	A	28	ARG	12

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Mol	Chain	Res	Type	Models (Total)
1	A	74	ILE	12
1	A	169	ILE	12
1	A	21	ARG	11
1	A	53	LEU	11
1	A	229	GLU	10
1	A	83	THR	10
1	A	63	SER	10
1	A	59	PHE	9
1	A	70	LYS	9
1	A	47	LYS	9
1	A	163	LEU	9
1	A	15	THR	8
1	A	204	TYR	8
1	A	225	LEU	8
1	A	34	TYR	8
1	A	215	ASP	8
1	A	23	LYS	8
1	A	162	GLN	7
1	A	82	GLN	7
1	A	31	ILE	7
1	A	49	LEU	6
1	A	9	THR	6
1	A	228	LYS	6
1	A	207	GLN	6
1	A	57	SER	6
1	A	239	LEU	6
1	A	155	GLN	6
1	A	236	LEU	6
1	A	223	ASP	5
1	A	220	ARG	5
1	A	168	LYS	5
1	A	184	GLU	5
1	A	150	LYS	5
1	A	192	LEU	4
1	A	77	PHE	4
1	A	153	LYS	4
1	A	27	LYS	4
1	A	37	LYS	4
1	A	64	LYS	4
1	A	187	LYS	4
1	A	166	LYS	4
1	A	30	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	145	SER	4
1	A	177	ARG	4
1	A	197	LYS	4
1	A	174	MET	4
1	A	206	GLN	3
1	A	33	CYS	3
1	A	80	ASP	3
1	A	212	CYS	3
1	A	227	LYS	3
1	A	154	GLN	3
1	A	144	TYR	3
1	A	179	ILE	3
1	A	48	ASP	3
1	A	50	ASP	3
1	A	36	ASN	3
1	A	97	VAL	3
1	A	151	SER	3
1	A	61	ASN	3
1	A	190	GLU	3
1	A	218	CYS	3
1	A	167	MET	3
1	A	230	THR	3
1	A	75	SER	3
1	A	224	GLU	2
1	A	84	GLU	2
1	A	69	LYS	2
1	A	35	LYS	2
1	A	202	GLU	2
1	A	56	HIS	2
1	A	147	LYS	2
1	A	195	LEU	2
1	A	235	SER	2
1	A	94	GLU	2
1	A	52	VAL	2
1	A	164	LYS	2
1	A	91	THR	2
1	A	55	THR	2
1	A	214	ILE	2
1	A	160	ILE	2
1	A	221	GLU	2
1	A	157	LEU	2
1	A	186	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	189	LYS	2
1	A	72	ASP	1
1	A	201	SER	1
1	A	13	ARG	1
1	A	11	GLN	1
1	A	161	LYS	1
1	A	146	VAL	1
1	A	200	GLU	1
1	A	22	MET	1
1	A	96	GLN	1
1	A	73	LEU	1
1	A	208	LEU	1
1	A	222	ILE	1
1	A	88	GLN	1
1	A	14	LEU	1
1	A	237	GLU	1
1	A	158	GLU	1
1	A	196	ILE	1
1	A	178	PHE	1
1	A	211	VAL	1
1	A	165	GLU	1
1	A	142	ILE	1
1	A	51	GLU	1
1	A	16	ASN	1
1	A	231	LYS	1
1	A	175	ARG	1
1	A	191	LYS	1
1	A	66	GLN	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 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 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 81% for the well-defined parts and 76% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 16119

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	2498
Number of shifts mapped to atoms	2498
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	230	$0.90 \pm 0.05$	Should be applied
$^{13}\text{C}_\beta$	217	$1.55 \pm 0.11$	Should be applied
$^{13}\text{C}'$	228	$2.40 \pm 0.10$	Should be applied
$^{15}\text{N}$	212	$-0.13 \pm 0.52$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 1866 atoms were assigned a chemical shift out of a possible 2295. 22 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	822/879 (94%)	327/351 (93%)	337/354 (95%)	158/174 (91%)
Sidechain	1016/1331 (76%)	623/776 (80%)	390/490 (80%)	3/65 (5%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	28/85 (33%)	28/45 (62%)	0/36 (0%)	0/4 (0%)
Overall	1866/2295 (81%)	978/1172 (83%)	727/880 (83%)	161/243 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 2478 atoms were assigned a chemical shift out of a possible 3266. 26 out of 43 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	1110/1248 (89%)	440/498 (88%)	458/504 (91%)	212/246 (86%)
Sidechain	1326/1862 (71%)	815/1088 (75%)	508/681 (75%)	3/93 (3%)
Aromatic	42/156 (27%)	39/82 (48%)	2/63 (3%)	1/11 (9%)
Overall	2478/3266 (76%)	1294/1668 (78%)	968/1248 (78%)	216/350 (62%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	41	TRP	CZ2	7.38	121.76 – 106.66	-70.8
1	A	189	LYS	CE	34.92	46.00 – 37.80	-8.5

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

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:

