



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 06:47 PM BST

PDB ID : 2AVX  
Title : solution structure of E coli SdiA1-171  
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Deposited on : 2005-08-30

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
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

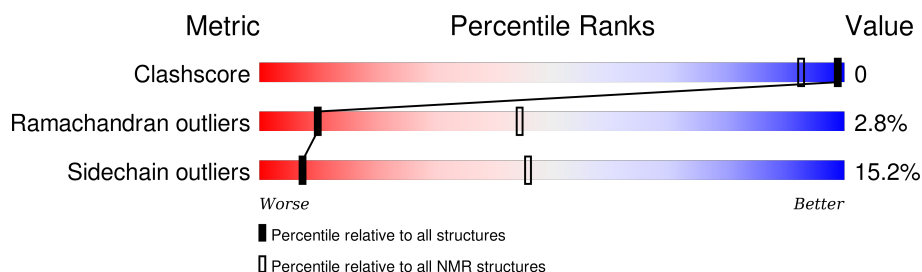
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 74%.

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  $\geq 3$ , 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	171	 81% 13% • 6%

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 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:9-A:169 (161)	0.39	4

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 5 clusters and 3 single-model clusters were found.

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

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

There are 2 unique types of molecules in this entry. The entry contains 2866 atoms, of which 1415 are hydrogens and 0 are deuteriums.

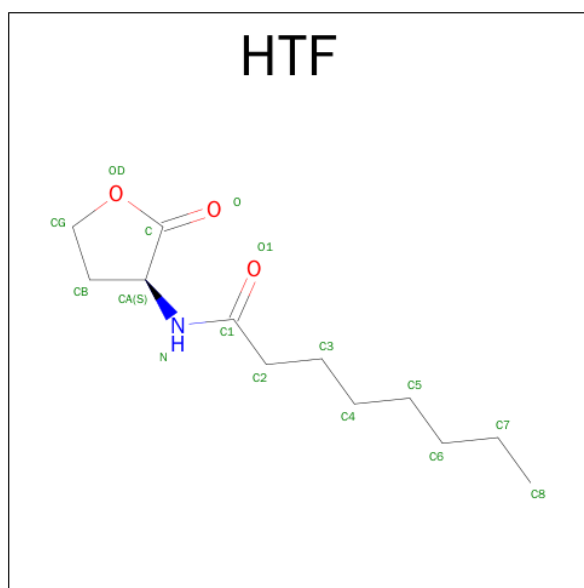
- Molecule 1 is a protein called Regulatory protein sdiA.

Mol	Chain	Residues	Atoms						Trace
1	A	171	Total	C	H	N	O	S	0
			2829	921	1394	245	259	10	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	GLN	engineered	UNP P07026
A	127	GLU	ASN	engineered	UNP P07026

- Molecule 2 is N-(2-OXOTETRAHYDROFURAN-3-YL)OCTANAMIDE (three-letter code: HTF) (formula:  $C_{12}H_{21}NO_3$ ).



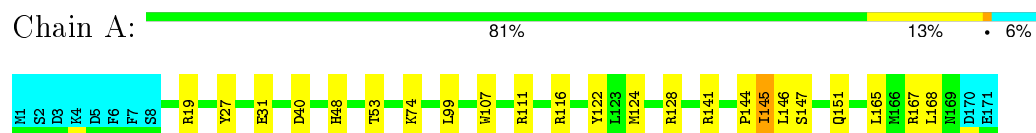
Mol	Chain	Residues	Atoms				
2	A	1	Total	C	H	N	O
			37	12	21	1	3

## 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: Regulatory protein sdiA

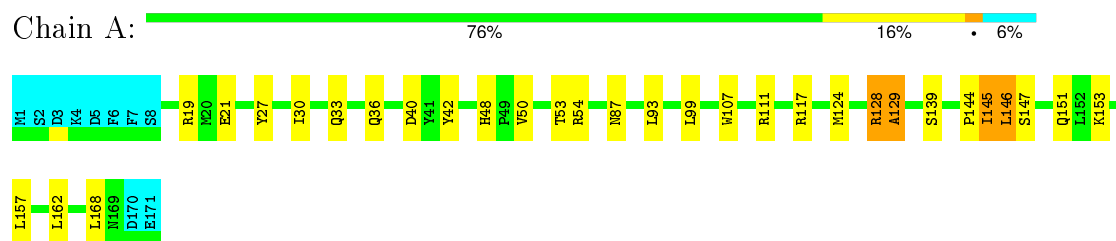


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

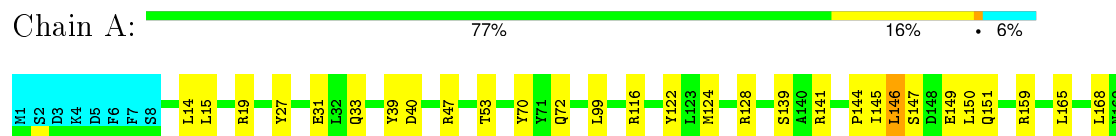
#### 4.2.1 Score per residue for model 1

- Molecule 1: Regulatory protein sdiA



#### 4.2.2 Score per residue for model 2

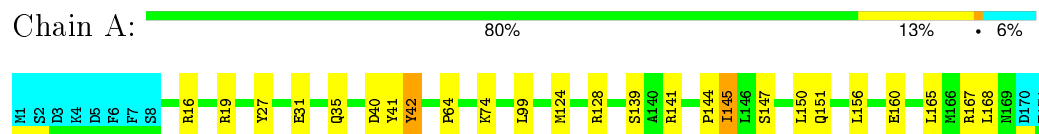
- Molecule 1: Regulatory protein sdiA





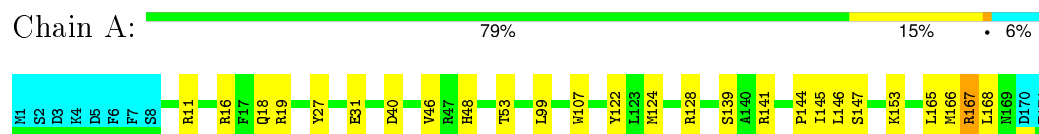
### 4.2.3 Score per residue for model 3

- Molecule 1: Regulatory protein sdiA



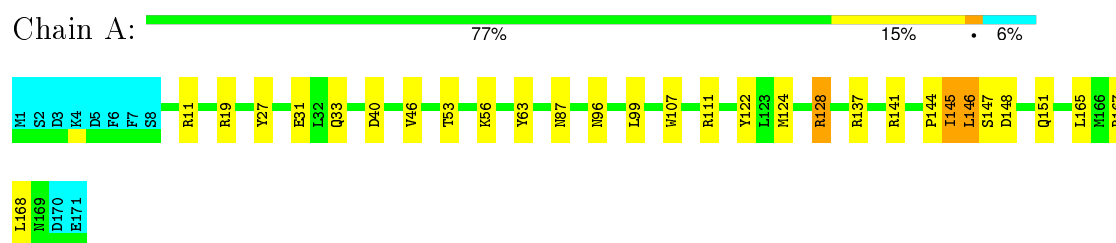
### 4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Regulatory protein sdiA



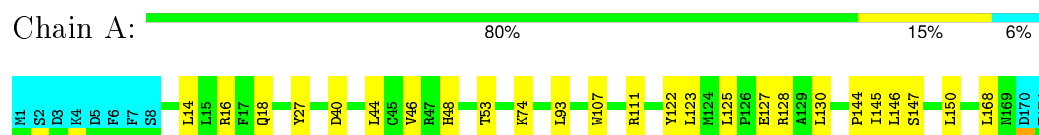
### 4.2.5 Score per residue for model 5

- Molecule 1: Regulatory protein sdiA



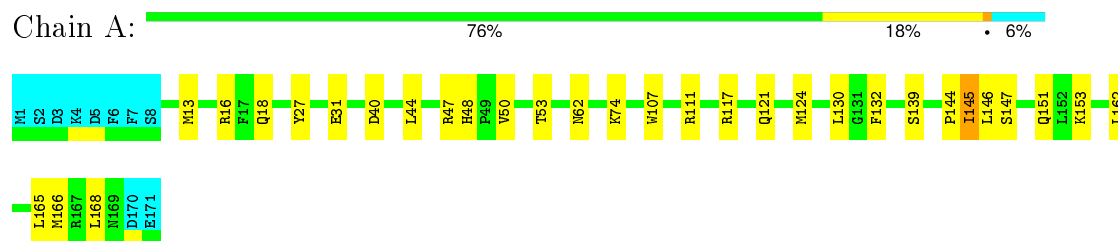
### 4.2.6 Score per residue for model 6

- Molecule 1: Regulatory protein sdiA



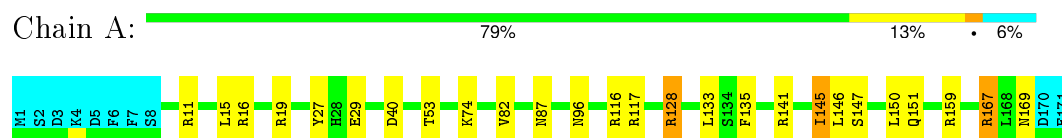
### 4.2.7 Score per residue for model 7

- Molecule 1: Regulatory protein sdiA



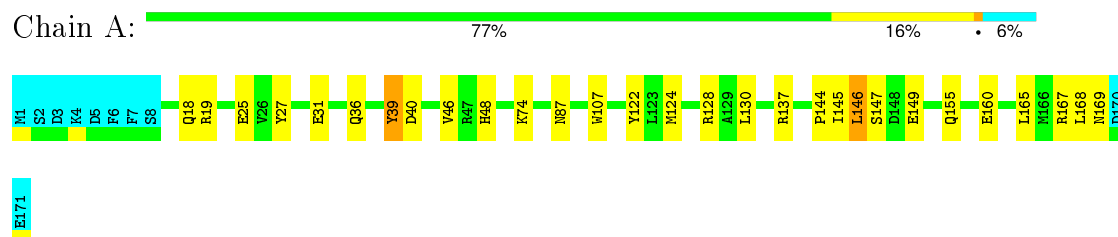
### 4.2.8 Score per residue for model 8

- Molecule 1: Regulatory protein sdiA



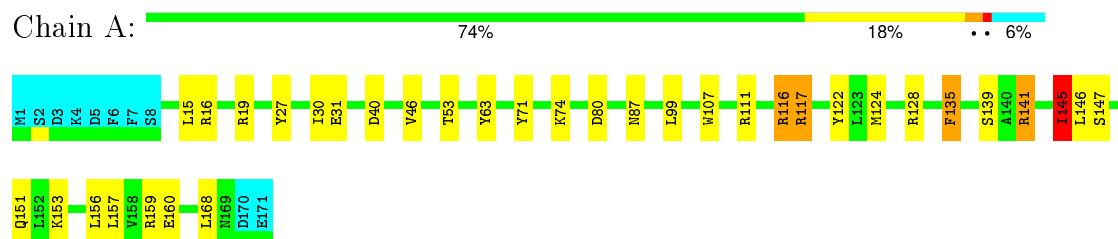
### 4.2.9 Score per residue for model 9

- Molecule 1: Regulatory protein sdiA



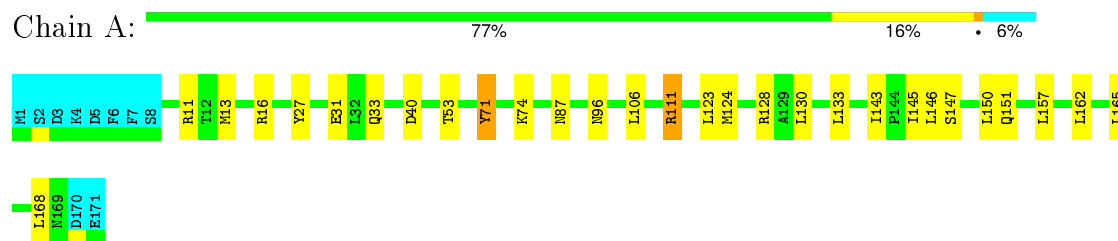
### 4.2.10 Score per residue for model 10

- Molecule 1: Regulatory protein sdiA



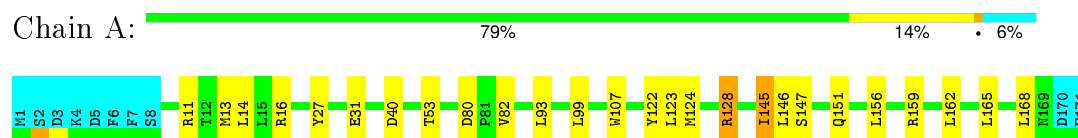
### 4.2.11 Score per residue for model 11

- Molecule 1: Regulatory protein sdiA



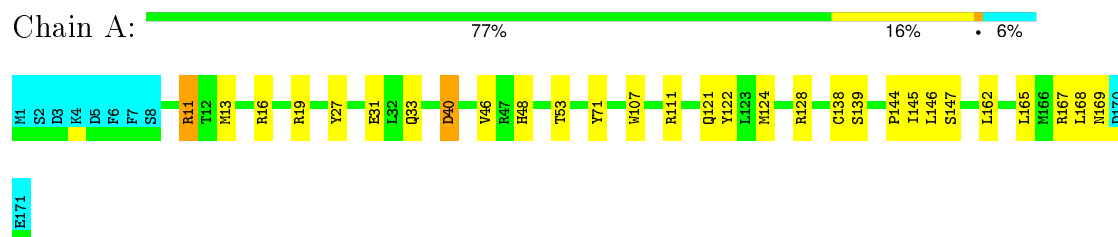
### 4.2.12 Score per residue for model 12

- Molecule 1: Regulatory protein sdiA



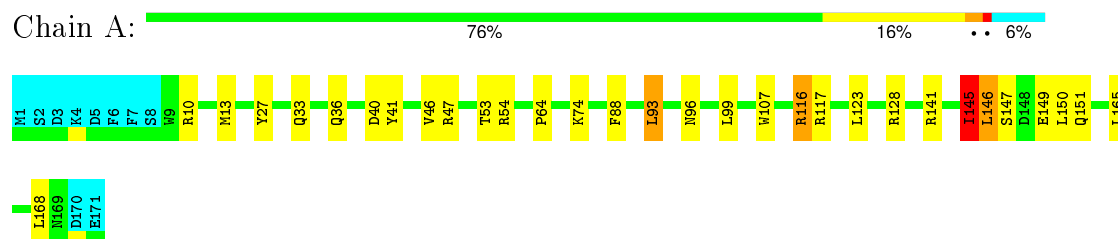
### 4.2.13 Score per residue for model 13

- Molecule 1: Regulatory protein sdiA



### 4.2.14 Score per residue for model 14

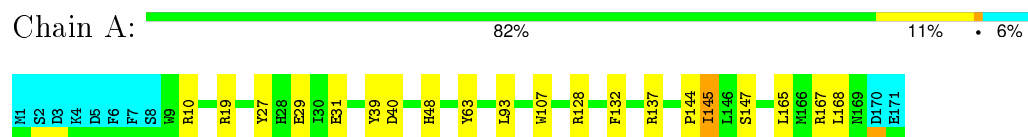
- Molecule 1: Regulatory protein sdiA





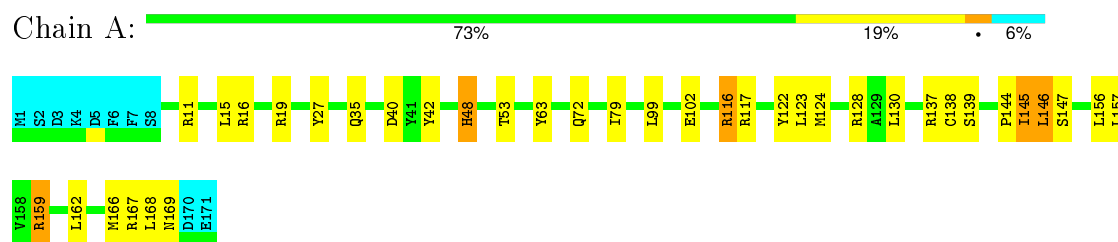
### 4.2.15 Score per residue for model 15

- Molecule 1: Regulatory protein sdiA



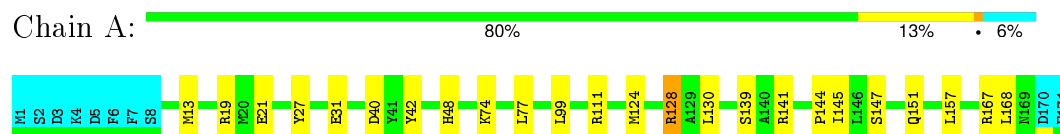
### 4.2.16 Score per residue for model 16

- Molecule 1: Regulatory protein sdiA



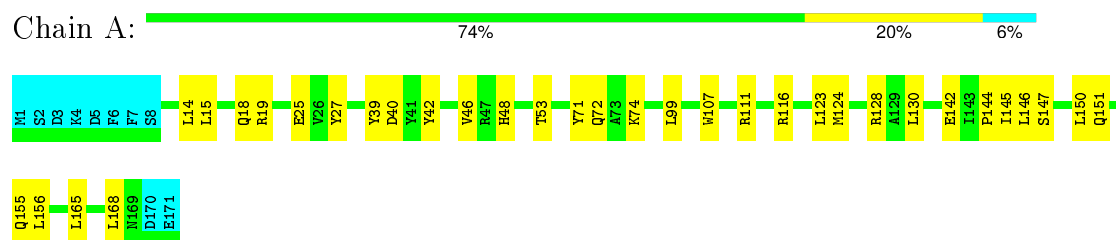
### 4.2.17 Score per residue for model 17

- Molecule 1: Regulatory protein sdiA



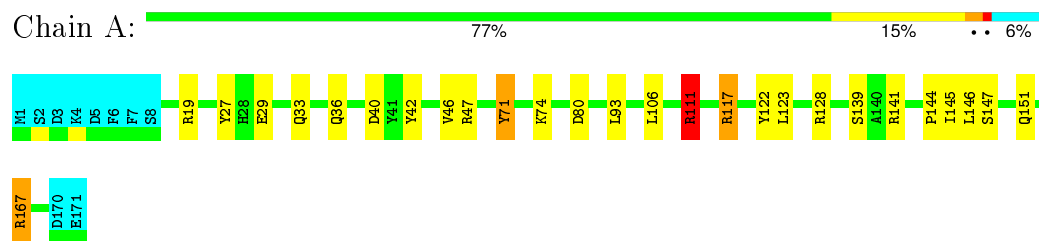
### 4.2.18 Score per residue for model 18

- Molecule 1: Regulatory protein sdiA



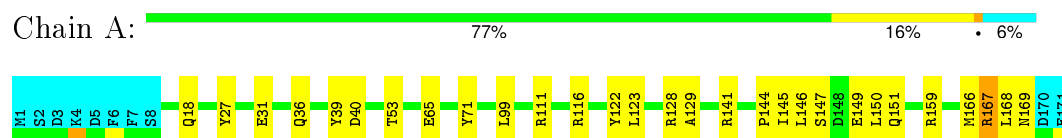
### 4.2.19 Score per residue for model 19

- Molecule 1: Regulatory protein sdiA



### 4.2.20 Score per residue for model 20

- Molecule 1: Regulatory protein sdiA



## 5 Refinement protocol and experimental data overview

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: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	1.5
AMBER	refinement	8.0

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 6454
Number of chemical shift lists	1
Total number of shifts	1867
Number of shifts mapped to atoms	1867
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

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

## 6 Model quality i

### 6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: HTF

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	0.73±0.01	0±0/1388 (0.0±0.0%)	1.10±0.02	3±2/1884 (0.2±0.1%)
All	All	0.73	0/27760 (0.0%)	1.10	68/37680 (0.2%)

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	0.8±1.1
All	All	0	16

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	159	ARG	NE-CZ-NH1	8.09	124.35	120.30	16	3
1	A	137	ARG	NE-CZ-NH2	-7.92	116.34	120.30	5	1
1	A	10	ARG	NE-CZ-NH2	-6.92	116.84	120.30	15	1
1	A	10	ARG	NE-CZ-NH1	6.91	123.76	120.30	15	1
1	A	137	ARG	NE-CZ-NH1	6.53	123.56	120.30	5	2
1	A	167	ARG	NE-CZ-NH1	6.36	123.48	120.30	20	4
1	A	11	ARG	NE-CZ-NH1	6.35	123.47	120.30	16	2
1	A	116	ARG	NE-CZ-NH1	6.34	123.47	120.30	8	5
1	A	159	ARG	CD-NE-CZ	6.20	132.28	123.60	16	1
1	A	111	ARG	NE-CZ-NH1	6.12	123.36	120.30	11	7
1	A	63	TYR	CB-CG-CD2	-6.02	117.39	121.00	15	3
1	A	19	ARG	NE-CZ-NH1	6.00	123.30	120.30	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	117	ARG	NE-CZ-NH1	5.96	123.28	120.30	19	5
1	A	16	ARG	NE-CZ-NH1	5.91	123.25	120.30	7	10
1	A	47	ARG	NE-CZ-NH1	5.79	123.19	120.30	19	2
1	A	16	ARG	NE-CZ-NH2	-5.74	117.43	120.30	13	2
1	A	141	ARG	NE-CZ-NH1	5.56	123.08	120.30	5	2
1	A	39	TYR	CB-CG-CD2	-5.53	117.68	121.00	15	3
1	A	145	ILE	C-N-CA	5.46	135.34	121.70	10	2
1	A	128	ARG	NE-CZ-NH1	5.41	123.01	120.30	17	3
1	A	146	LEU	C-N-CA	5.34	135.04	121.70	16	3
1	A	135	PHE	CB-CG-CD2	-5.27	117.11	120.80	10	1
1	A	70	TYR	CB-CG-CD2	-5.18	117.89	121.00	2	1
1	A	111	ARG	NE-CZ-NH2	-5.18	117.71	120.30	17	1
1	A	137	ARG	CD-NE-CZ	5.11	130.76	123.60	5	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	71	TYR	Sidechain	4
1	A	42	TYR	Sidechain	4
1	A	128	ARG	Sidechain	2
1	A	146	LEU	Peptide	1
1	A	167	ARG	Sidechain	1
1	A	39	TYR	Sidechain	1
1	A	111	ARG	Sidechain	1
1	A	129	ALA	Peptide	1
1	A	63	TYR	Sidechain	1

## 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	1350	1324	1324	0±1
All	All	27320	26900	26900	8

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:ASP:OD1	1:A:82:VAL:HG22	0.45	2.11	12	1
1:A:48:HIS:H	1:A:48:HIS:CD2	0.44	2.31	16	1
1:A:48:HIS:CD2	1:A:50:VAL:HG22	0.43	2.48	7	1
1:A:50:VAL:HB	1:A:53:THR:HG22	0.42	1.90	1	1
1:A:30:ILE:HG22	1:A:157:LEU:HD22	0.41	1.93	10	1
1:A:41:TYR:CE2	1:A:64:PRO:HD3	0.41	2.51	14	2
1:A:88:PHE:CD2	1:A:93:LEU:HD23	0.40	2.52	14	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	161/171 (94%)	151±2 (94±1%)	6±2 (4±1%)	5±1 (3±1%)	10	44
All	All	3220/3420 (94%)	3013 (94%)	116 (4%)	91 (3%)	10	44

All 7 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	40	ASP	20
1	A	147	SER	20
1	A	144	PRO	15
1	A	128	ARG	14
1	A	145	ILE	10
1	A	146	LEU	10
1	A	129	ALA	2

### 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	144/154 (94%)	122±4 (85±3%)	22±4 (15±3%)	7	46
All	All	2880/3080 (94%)	2441 (85%)	439 (15%)	7	46

All 80 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	27	TYR	20
1	A	145	ILE	20
1	A	168	LEU	18
1	A	124	MET	14
1	A	53	THR	14
1	A	151	GLN	14
1	A	31	GLU	13
1	A	165	LEU	13
1	A	19	ARG	12
1	A	107	TRP	12
1	A	99	LEU	12
1	A	122	TYR	11
1	A	74	LYS	11
1	A	167	ARG	10
1	A	139	SER	10
1	A	46	VAL	9
1	A	146	LEU	9
1	A	141	ARG	9
1	A	48	HIS	9
1	A	150	LEU	8
1	A	123	LEU	8
1	A	130	LEU	7
1	A	33	GLN	7
1	A	162	LEU	7
1	A	18	GLN	6
1	A	13	MET	6
1	A	11	ARG	6
1	A	87	ASN	6
1	A	111	ARG	6
1	A	93	LEU	6
1	A	36	GLN	5
1	A	166	MET	5
1	A	116	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	15	LEU	5
1	A	156	LEU	5
1	A	128	ARG	5
1	A	169	ASN	5
1	A	159	ARG	4
1	A	117	ARG	4
1	A	157	LEU	4
1	A	149	GLU	4
1	A	153	LYS	4
1	A	14	LEU	4
1	A	71	TYR	4
1	A	96	ASN	4
1	A	160	GLU	3
1	A	42	TYR	3
1	A	29	GLU	3
1	A	72	GLN	3
1	A	121	GLN	2
1	A	47	ARG	2
1	A	35	GLN	2
1	A	133	LEU	2
1	A	155	GLN	2
1	A	39	TYR	2
1	A	80	ASP	2
1	A	137	ARG	2
1	A	138	CYS	2
1	A	44	LEU	2
1	A	54	ARG	2
1	A	135	PHE	2
1	A	106	LEU	2
1	A	132	PHE	2
1	A	21	GLU	2
1	A	25	GLU	2
1	A	79	ILE	1
1	A	82	VAL	1
1	A	143	ILE	1
1	A	148	ASP	1
1	A	127	GLU	1
1	A	40	ASP	1
1	A	30	ILE	1
1	A	56	LYS	1
1	A	125	LEU	1
1	A	65	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	102	GLU	1
1	A	77	LEU	1
1	A	142	GLU	1
1	A	10	ARG	1
1	A	62	ASN	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	HTF	A	172	-	16,16,16	0.71±0.03	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	HTF	A	172	-	14,19,19	1.38±0.14	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HTF	A	172	-	-	0±0,11,21,21	0±0,1,1,1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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](#)

The completeness of assignment taking into account all chemical shift lists is 74% for the well-defined parts and 74% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 6454

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 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	1867
Number of shifts mapped to atoms	1867
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	166	$-0.00 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	156	$0.16 \pm 0.16$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	—
$^{15}\text{N}$	154	$0.82 \pm 0.34$	Should be applied

#### 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 74%, i.e. 1583 atoms were assigned a chemical shift out of a possible 2140. 11 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	607/787 (77%)	304/313 (97%)	157/322 (49%)	146/152 (96%)
Sidechain	805/1133 (71%)	500/671 (75%)	305/401 (76%)	0/61 (0%)

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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	171/220 (78%)	89/116 (77%)	78/96 (81%)	4/8 (50%)
Overall	1583/2140 (74%)	893/1100 (81%)	540/819 (66%)	150/221 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 1672 atoms were assigned a chemical shift out of a possible 2260. 11 out of 31 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	641/837 (77%)	321/333 (96%)	166/342 (49%)	154/162 (95%)
Sidechain	844/1185 (71%)	526/702 (75%)	318/421 (76%)	0/62 (0%)
Aromatic	187/238 (79%)	97/126 (77%)	86/104 (83%)	4/8 (50%)
Overall	1672/2260 (74%)	944/1161 (81%)	570/867 (66%)	158/232 (68%)

#### 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	74	LYS	HB3	-0.30	3.10 – 0.40	-7.6
1	A	160	GLU	HB3	0.65	3.10 – 0.90	-6.1
1	A	110	ALA	HA	1.98	6.46 – 2.06	-5.2

#### 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:

