



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:17 PM BST

PDB ID : 1D8B
Title : NMR STRUCTURE OF THE HRDC DOMAIN FROM SACCHAROMYCES
CEREVISIAE RECQ HELICASE
Authors : Liu, Z.; Macias, M.J.; Bottomley, M.J.; Stier, G.; Linge, J.P.; Nilges, M.; Bork,
P.; Sattler, M.
Deposited on : 1999-10-21

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

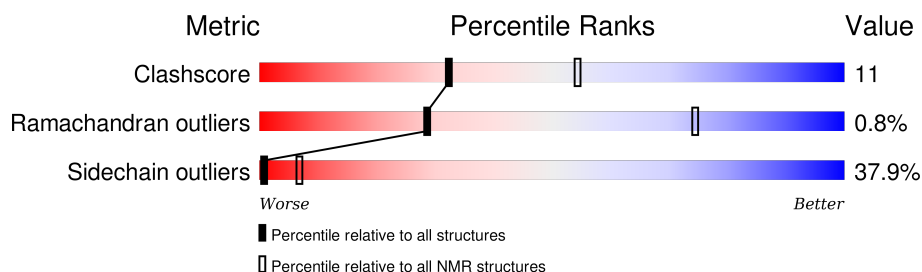
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 77%.

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	81	

2 Ensemble composition and analysis ⓘ

This entry contains 15 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:14-A:87 (74)	0.40	7

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

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

The models can be grouped into 5 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1336 atoms, of which 680 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SGS1 RECQ HELICASE.

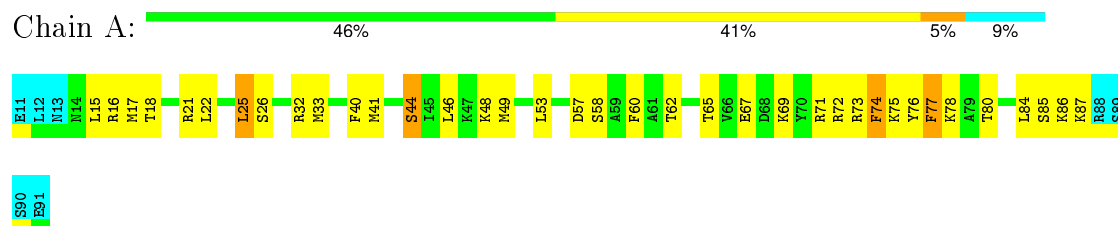
Mol	Chain	Residues	Atoms						Trace
1	A	81	Total	C	H	N	O	S	0
			1336	414	680	118	119	5	

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: SGS1 RECQ HELICASE

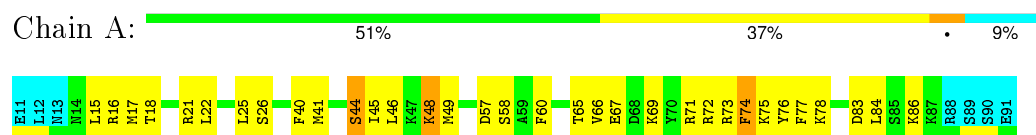


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

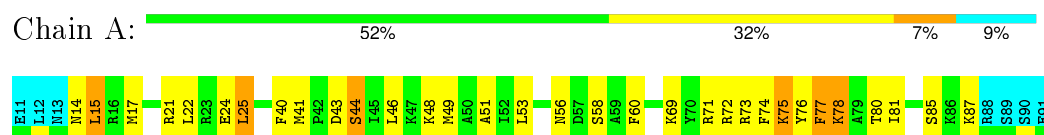
4.2.1 Score per residue for model 1

- Molecule 1: SGS1 RECQ HELICASE



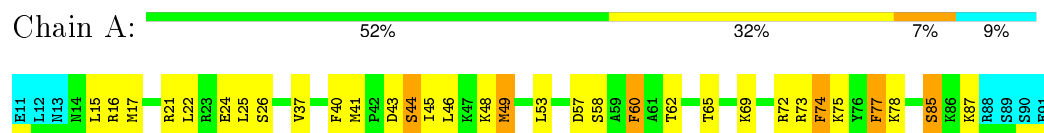
4.2.2 Score per residue for model 2

- Molecule 1: SGS1 RECQ HELICASE



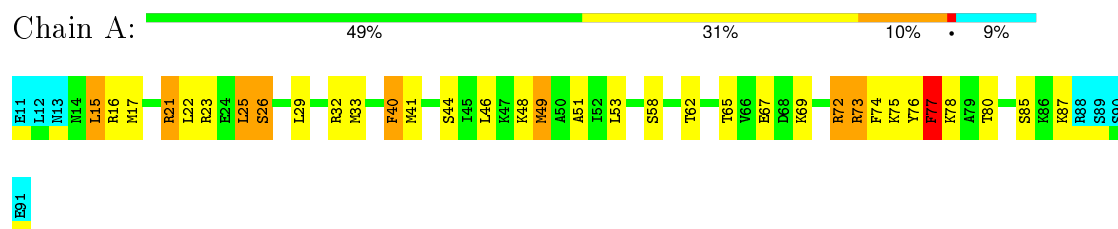
4.2.3 Score per residue for model 3

- Molecule 1: SGS1 RECQ HELICASE



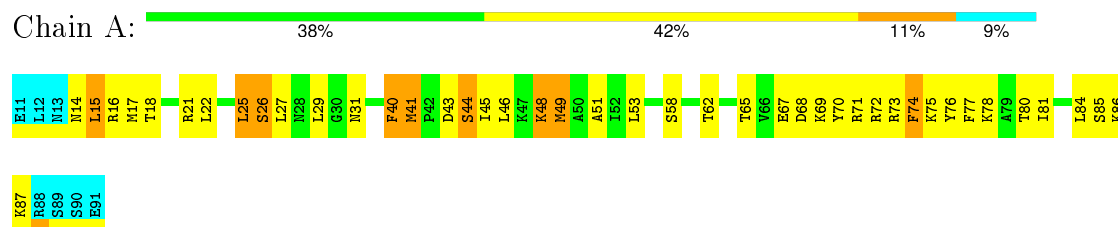
4.2.4 Score per residue for model 4

- Molecule 1: SGS1 RECQ HELICASE



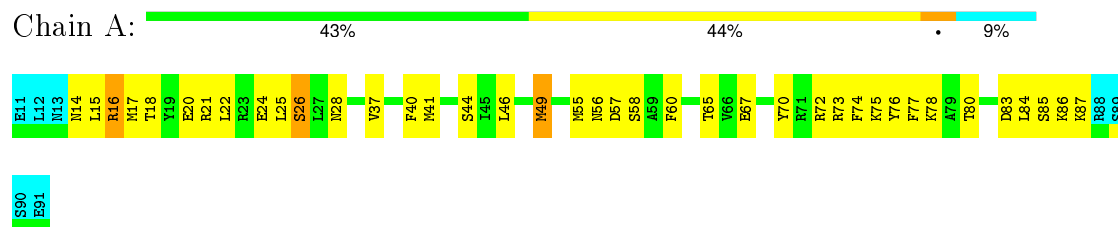
4.2.5 Score per residue for model 5

- Molecule 1: SGS1 RECQ HELICASE



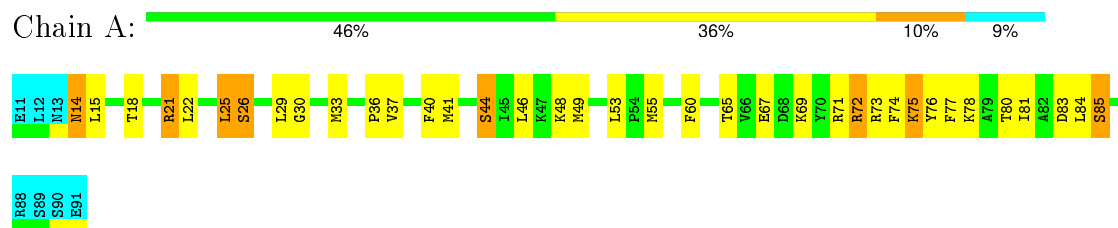
4.2.6 Score per residue for model 6

- Molecule 1: SGS1 RECQ HELICASE



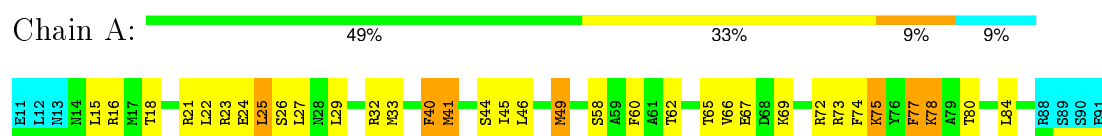
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: SGS1 RECQ HELICASE



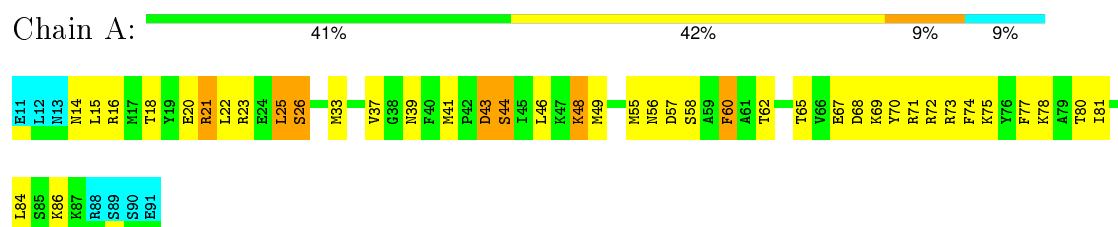
4.2.8 Score per residue for model 8

- Molecule 1: SGS1 RECQ HELICASE



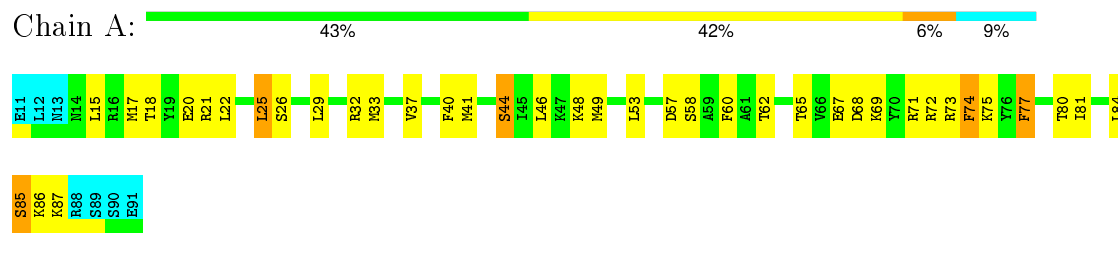
4.2.9 Score per residue for model 9

- Molecule 1: SGS1 RECQ HELICASE



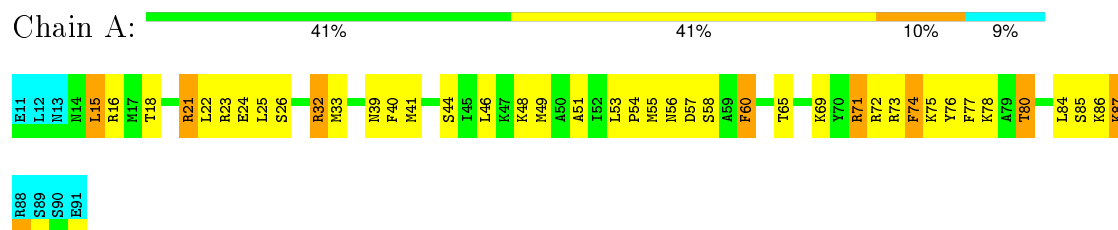
4.2.10 Score per residue for model 10

- Molecule 1: SGS1 RECQ HELICASE



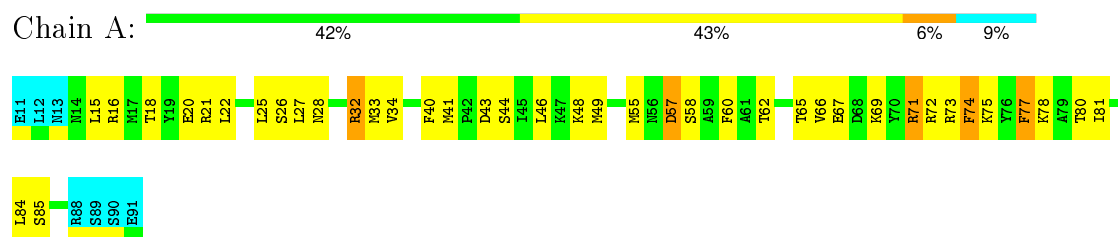
4.2.11 Score per residue for model 11

- Molecule 1: SGS1 RECQ HELICASE



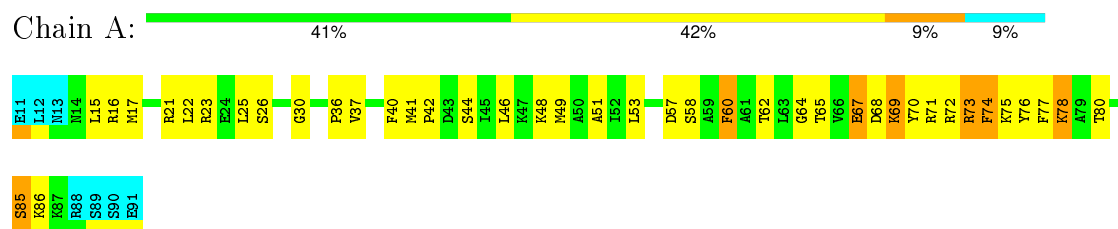
4.2.12 Score per residue for model 12

- Molecule 1: SGS1 RECQ HELICASE



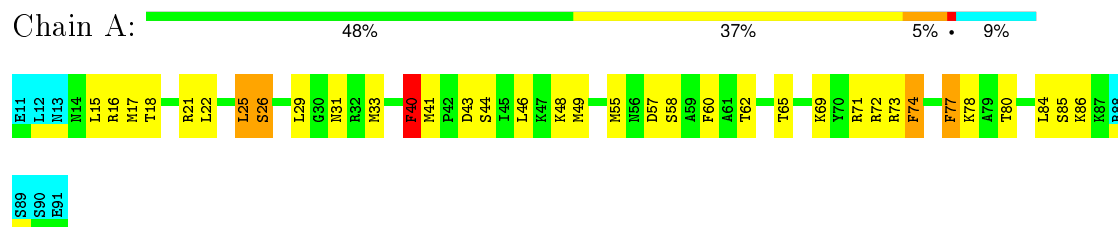
4.2.13 Score per residue for model 13

- Molecule 1: SGS1 RECQ HELICASE



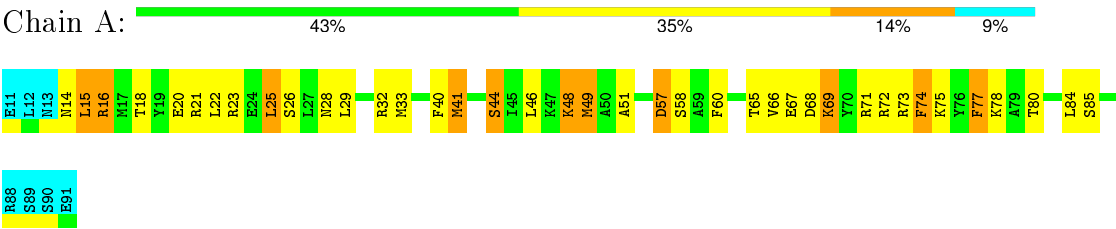
4.2.14 Score per residue for model 14

- Molecule 1: SGS1 RECQ HELICASE



4.2.15 Score per residue for model 15

● Molecule 1: SGS1 RECQ HELICASE



5 Refinement protocol and experimental data overview

The models were refined using the following method: *ARIA (AMBIGUOUS RESTRAINTS IN ITERATIVE ASSIGNMENTS) AMBIGUOUS DISTANCE RESTRAINTS SIMULATED ANNEALING WITH TORSION ANGLE DYNAMICS*.

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *STRUCTURES WITH ACCEPTABLE COVALENT GEOMETRY, STRUCTURES WITH FAVORABLE NON- BOND ENERGY*.

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

Software name	Classification	Version
ARIA	structure solution	0.9
CNS	structure solution	0.9
CNS	refinement	0.9

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 4445
Number of chemical shift lists	2
Total number of shifts	1534
Number of shifts mapped to atoms	1507
Number of unparsed shifts	0
Number of shifts with mapping errors	27
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

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](#)

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	0.39±0.05	0±0/609 (0.0±0.1%)	0.45±0.01	0±0/817 (0.0±0.0%)
All	All	0.40	3/9135 (0.0%)	0.45	0/12255 (0.0%)

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	40	PHE	CE1-CZ	6.60	1.49	1.37	14	1
1	A	77	PHE	CE1-CZ	5.24	1.47	1.37	4	1
1	A	74	PHE	CE2-CZ	5.08	1.47	1.37	5	1

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	598	628	628	14±3
All	All	8970	9420	9420	206

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:LEU:HB3	1:A:46:LEU:HD22	0.80	1.49	2	14
1:A:83:ASP:HA	1:A:86:LYS:HD3	0.80	1.51	6	1
1:A:18:THR:HG23	1:A:84:LEU:HD13	0.79	1.54	1	8
1:A:46:LEU:HA	1:A:49:MET:SD	0.76	2.21	6	4
1:A:57:ASP:HA	1:A:60:PHE:HD2	0.70	1.45	12	1
1:A:15:LEU:HD11	1:A:51:ALA:HA	0.68	1.64	5	5
1:A:41:MET:HB2	1:A:77:PHE:HE2	0.68	1.49	3	13
1:A:53:LEU:HD13	1:A:85:SER:HA	0.63	1.71	13	8
1:A:45:ILE:HD12	1:A:66:VAL:HG12	0.61	1.71	1	1
1:A:72:ARG:O	1:A:75:LYS:HG2	0.60	1.97	4	7
1:A:26:SER:HA	1:A:40:PHE:CD2	0.59	2.33	6	10
1:A:57:ASP:HA	1:A:60:PHE:CD2	0.59	2.32	12	2
1:A:71:ARG:HA	1:A:74:PHE:HD2	0.58	1.58	14	5
1:A:26:SER:HA	1:A:40:PHE:HD2	0.58	1.58	4	7
1:A:73:ARG:HA	1:A:76:TYR:CD2	0.57	2.35	4	4
1:A:22:LEU:HD23	1:A:77:PHE:CE1	0.57	2.34	1	12
1:A:71:ARG:HA	1:A:74:PHE:HB2	0.57	1.75	13	2
1:A:75:LYS:HA	1:A:78:LYS:HD3	0.57	1.77	8	2
1:A:18:THR:HA	1:A:84:LEU:HD22	0.55	1.78	14	7
1:A:71:ARG:O	1:A:74:PHE:HB2	0.54	2.03	14	4
1:A:42:PRO:HG2	1:A:70:TYR:HE2	0.54	1.60	13	1
1:A:41:MET:HB3	1:A:46:LEU:HD21	0.54	1.80	2	12
1:A:32:ARG:HG2	1:A:32:ARG:O	0.53	2.04	11	1
1:A:68:ASP:O	1:A:72:ARG:HG2	0.53	2.04	10	1
1:A:44:SER:O	1:A:48:LYS:HG2	0.52	2.04	7	9
1:A:22:LEU:HD22	1:A:49:MET:SD	0.52	2.44	4	3
1:A:49:MET:HE3	1:A:74:PHE:HE1	0.52	1.65	3	1
1:A:57:ASP:O	1:A:60:PHE:HB2	0.51	2.06	9	2
1:A:40:PHE:HZ	1:A:76:TYR:HB2	0.51	1.65	11	3
1:A:25:LEU:HD22	1:A:29:LEU:HG	0.50	1.82	8	3
1:A:60:PHE:HE2	1:A:78:LYS:HE3	0.50	1.66	13	2
1:A:81:ILE:O	1:A:85:SER:HB2	0.50	2.07	10	1
1:A:30:GLY:O	1:A:36:PRO:HA	0.50	2.06	7	2
1:A:22:LEU:O	1:A:26:SER:HB2	0.48	2.08	9	1
1:A:87:LYS:HE3	1:A:87:LYS:HA	0.47	1.85	11	1
1:A:40:PHE:HZ	1:A:76:TYR:CB	0.46	2.24	11	1
1:A:57:ASP:HA	1:A:60:PHE:HB2	0.46	1.87	11	2
1:A:77:PHE:O	1:A:81:ILE:HG13	0.46	2.10	10	6
1:A:67:GLU:HB2	1:A:70:TYR:CD1	0.46	2.45	13	2
1:A:25:LEU:HB3	1:A:77:PHE:HE1	0.45	1.71	4	5
1:A:60:PHE:CE2	1:A:78:LYS:HE3	0.45	2.47	13	1
1:A:41:MET:SD	1:A:42:PRO:HD2	0.45	2.52	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ILE:O	1:A:49:MET:HB3	0.45	2.12	5	3
1:A:21:ARG:HG2	1:A:80:THR:HG22	0.43	1.89	11	1
1:A:21:ARG:O	1:A:25:LEU:HB2	0.43	2.13	9	3
1:A:67:GLU:HB3	1:A:69:LYS:HD3	0.43	1.89	13	1
1:A:55:MET:SD	1:A:85:SER:HB3	0.43	2.54	6	1
1:A:18:THR:HG23	1:A:84:LEU:HB3	0.43	1.89	11	1
1:A:25:LEU:HD13	1:A:29:LEU:CD1	0.42	2.44	4	2
1:A:54:PRO:HG2	1:A:60:PHE:CD1	0.42	2.49	11	1
1:A:32:ARG:O	1:A:32:ARG:HG3	0.42	2.15	12	1
1:A:67:GLU:H	1:A:70:TYR:HD2	0.42	1.55	6	1
1:A:41:MET:HB2	1:A:77:PHE:CE2	0.42	2.40	3	1
1:A:25:LEU:HD13	1:A:29:LEU:HD11	0.42	1.89	5	1
1:A:67:GLU:HG3	1:A:69:LYS:HD2	0.42	1.92	15	1
1:A:67:GLU:HB2	1:A:70:TYR:CD2	0.42	2.50	5	1
1:A:26:SER:OG	1:A:77:PHE:HZ	0.41	1.97	1	1
1:A:43:ASP:HA	1:A:46:LEU:HD12	0.41	1.90	9	1
1:A:29:LEU:HD13	1:A:76:TYR:HB3	0.41	1.91	7	1
1:A:16:ARG:NH1	1:A:20:GLU:HB2	0.41	2.30	6	1
1:A:60:PHE:CE1	1:A:74:PHE:CZ	0.41	3.09	12	1
1:A:21:ARG:HG2	1:A:80:THR:CG2	0.41	2.46	11	1
1:A:20:GLU:HA	1:A:20:GLU:OE1	0.41	2.15	12	1
1:A:15:LEU:HD21	1:A:51:ALA:HA	0.41	1.92	4	1
1:A:49:MET:HE1	1:A:77:PHE:CD2	0.40	2.51	15	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	74/81 (91%)	70±1 (94±2%)	4±1 (5±1%)	1±1 (1±1%)	29	74
All	All	1110/1215 (91%)	1048 (94%)	53 (5%)	9 (1%)	29	74

All 4 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	PHE	6
1	A	64	GLY	1
1	A	72	ARG	1
1	A	34	VAL	1

6.3.2 Protein sidechains ⓘ

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	65/72 (90%)	40±3 (62±5%)	25±3 (38±5%)	1	7
All	All	975/1080 (90%)	605 (62%)	370 (38%)	1	7

All 45 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	49	MET	15
1	A	74	PHE	15
1	A	25	LEU	15
1	A	21	ARG	15
1	A	15	LEU	14
1	A	44	SER	14
1	A	65	THR	14
1	A	58	SER	14
1	A	69	LYS	14
1	A	73	ARG	13
1	A	80	THR	13
1	A	78	LYS	13
1	A	16	ARG	12
1	A	60	PHE	10
1	A	33	MET	9
1	A	72	ARG	9
1	A	26	SER	9
1	A	17	MET	9
1	A	62	THR	9
1	A	75	LYS	8
1	A	77	PHE	8
1	A	48	LYS	8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	87	LYS	7
1	A	85	SER	7
1	A	67	GLU	7
1	A	86	LYS	7
1	A	57	ASP	7
1	A	37	VAL	6
1	A	32	ARG	6
1	A	43	ASP	6
1	A	23	ARG	6
1	A	71	ARG	6
1	A	14	ASN	6
1	A	24	GLU	5
1	A	55	MET	5
1	A	68	ASP	4
1	A	56	ASN	4
1	A	28	ASN	3
1	A	27	LEU	3
1	A	66	VAL	3
1	A	41	MET	3
1	A	20	GLU	3
1	A	83	ASP	2
1	A	31	ASN	2
1	A	39	ASN	2

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 [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

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4445

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	940
Number of shifts mapped to atoms	920
Number of unparsed shifts	0
Number of shifts with mapping errors	20
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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

- Residue not found in structure. All 20 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	9	PRO	CD	48.498	0.4	1
A	10	MET	CB	30.515	0.4	1
A	10	MET	N	119.917	0.1	1
A	9	PRO	HA	4.316	0.04	1
A	10	MET	H	8.874	0.04	1
A	9	PRO	CA	61.798	0.4	1
A	9	PRO	CG	25.287	0.4	1
A	10	MET	CA	53.674	0.4	1
A	10	MET	HB3	1.97	0.04	1
A	9	PRO	HG2	1.932	0.04	1
A	10	MET	HB2	2.051	0.04	1
A	10	MET	HG2	2.571	0.04	1
A	9	PRO	HD3	3.37	0.04	1
A	10	MET	CG	29.646	0.4	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	10	MET	HG3	2.501	0.04	1
A	9	PRO	HD2	3.598	0.04	1
A	9	PRO	HB3	1.848	0.04	1
A	9	PRO	CB	29.646	0.4	1
A	10	MET	HA	4.394	0.04	1
A	9	PRO	HB2	2.279	0.04	1

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
$^{13}\text{C}_\alpha$	83	1.95 ± 0.14	Should be applied
$^{13}\text{C}_\beta$	80	2.41 ± 0.06	Should be applied
$^{13}\text{C}'$	0	—	—
^{15}N	77	0.60 ± 0.45	None needed (imprecise)

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 77%, i.e. 751 atoms were assigned a chemical shift out of a possible 974. 11 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	286/362 (79%)	143/144 (99%)	74/148 (50%)	69/70 (99%)
Sidechain	433/552 (78%)	262/327 (80%)	166/192 (86%)	5/33 (15%)
Aromatic	32/60 (53%)	19/32 (59%)	13/28 (46%)	0/0 (—%)
Overall	751/974 (77%)	424/503 (84%)	253/368 (69%)	74/103 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 813 atoms were assigned a chemical shift out of a possible 1063. 12 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	314/397 (79%)	157/158 (99%)	81/162 (50%)	76/77 (99%)
Sidechain	467/606 (77%)	281/359 (78%)	180/210 (86%)	6/37 (16%)
Aromatic	32/60 (53%)	19/32 (59%)	13/28 (46%)	0/0 (—%)
Overall	813/1063 (76%)	457/549 (83%)	274/400 (68%)	82/114 (72%)

7.1.4 Statistically unusual chemical shifts [i](#)

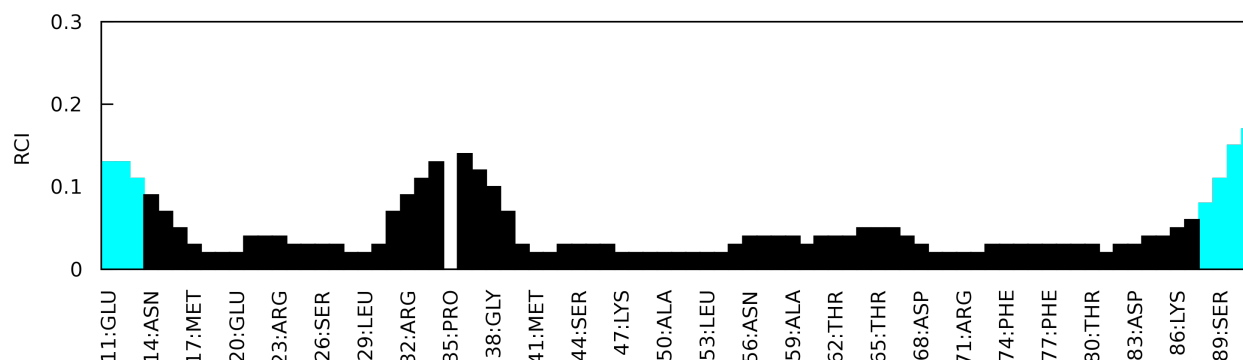
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
1	A	73	ARG	HD3	1.22	4.36 – 1.86	-7.6
1	A	29	LEU	HB3	-0.29	3.34 – -0.26	-5.1

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 4445

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	594
Number of shifts mapped to atoms	587
Number of unparsed shifts	0

Number of shifts with mapping errors	7
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- Residue not found in structure. All 7 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	10	MET	HB3	1.97	0.04	1
A	9	PRO	HA	4.299	0.04	1
A	10	MET	H	8.874	0.04	1
A	10	MET	HB2	2.051	0.04	1
A	10	MET	HG2	2.589	0.04	1
A	10	MET	HG3	2.5	0.04	1
A	10	MET	HA	4.39	0.04	1

7.2.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	—
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	0	—	—
^{15}N	75	0.46 ± 0.45	None needed (< 0.5 ppm)

7.2.3 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 47%, i.e. 454 atoms were assigned a chemical shift out of a possible 974. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	207/362 (57%)	139/144 (97%)	0/148 (0%)	68/70 (97%)
Sidechain	228/552 (41%)	228/327 (70%)	0/192 (0%)	0/33 (0%)
Aromatic	19/60 (32%)	19/32 (59%)	0/28 (0%)	0/0 (—%)
Overall	454/974 (47%)	386/503 (77%)	0/368 (0%)	68/103 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure.

The overall completeness is 46%, i.e. 492 atoms were assigned a chemical shift out of a possible 1063. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	228/397 (57%)	153/158 (97%)	0/162 (0%)	75/77 (97%)
Sidechain	245/606 (40%)	245/359 (68%)	0/210 (0%)	0/37 (0%)
Aromatic	19/60 (32%)	19/32 (59%)	0/28 (0%)	0/0 (—%)
Overall	492/1063 (46%)	417/549 (76%)	0/400 (0%)	75/114 (66%)

7.2.4 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	29	LEU	HB3	-0.29	3.34 – -0.26	-5.1

7.2.5 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:

