Full wwPDB NMR Structure Validation Report (i)

Mar 10, 2026 – 08:30 AM UTC

PDB ID	:	2JWT / pdb_00002jwt
BMRB ID	:	15536
Title	:	Solution structure of Engrailed homeodomain WT
Authors	:	Religa, T.L.
Deposited on	:	2007-10-24

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

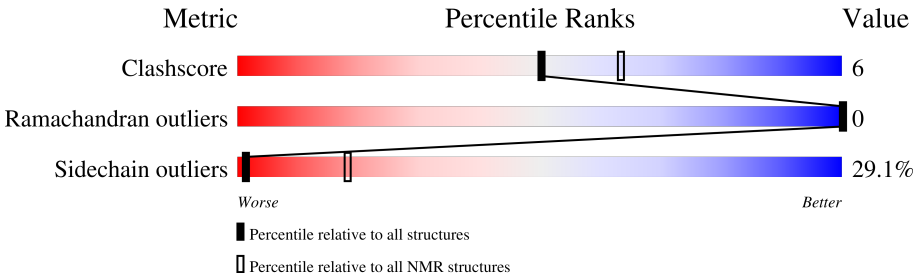
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment 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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	61	44% 30% 26%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 3 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:53 (45)	0.33	3

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 4 single-model clusters were found.

Cluster number	Models
1	2, 3, 6, 9, 12, 16, 18, 21, 23
2	8, 10, 19, 24
3	4, 5, 13
4	1, 17, 20
5	22, 25
Single-model clusters	7; 11; 14; 15

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1068 atoms, of which 543 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Segmentation polarity homeobox protein engrailed.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	61	1068	324	543	105	95	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P02836

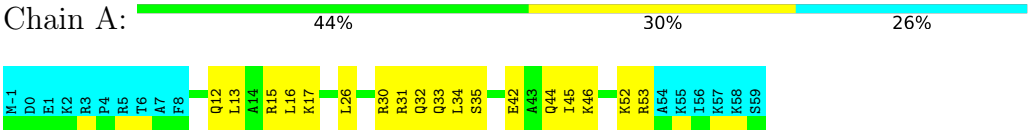
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Segmentation polarity homeobox protein engrailed

Chain A:



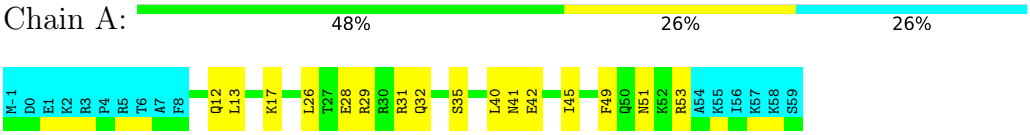
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Segmentation polarity homeobox protein engrailed

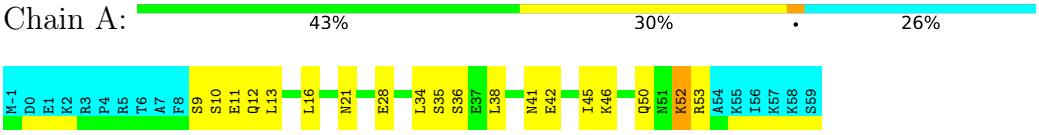
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Segmentation polarity homeobox protein engrailed

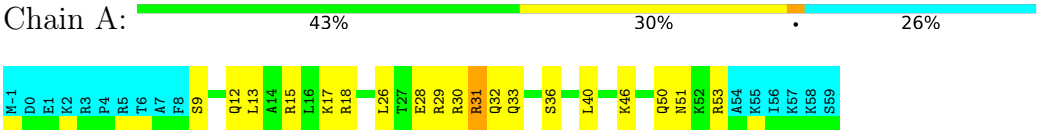
Chain A:



4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: Segmentation polarity homeobox protein engrailed

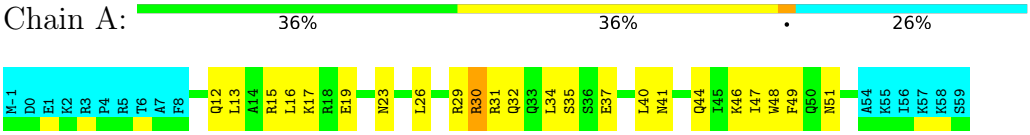
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Segmentation polarity homeobox protein engrailed

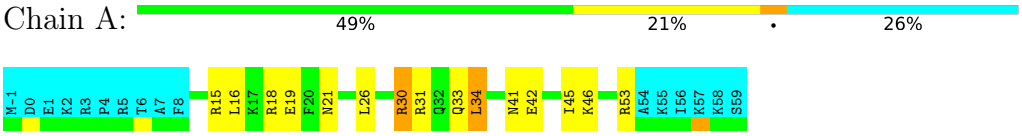
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Segmentation polarity homeobox protein engrailed

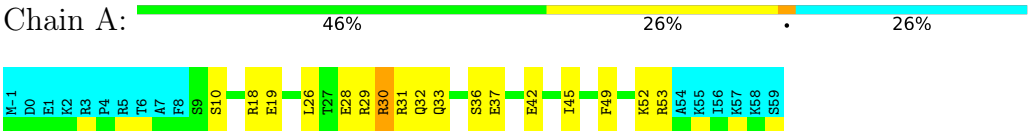
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Segmentation polarity homeobox protein engrailed

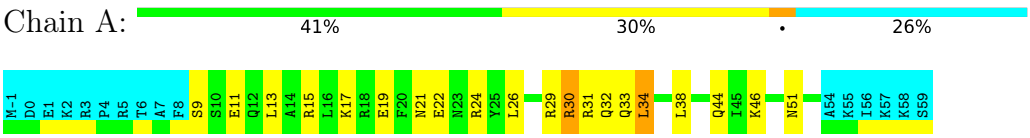
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Segmentation polarity homeobox protein engrailed

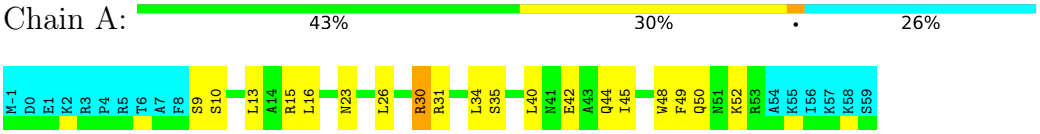
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Segmentation polarity homeobox protein engrailed

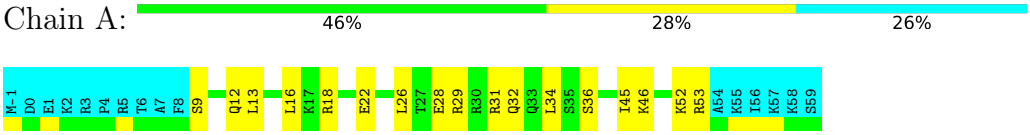
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Segmentation polarity homeobox protein engrailed

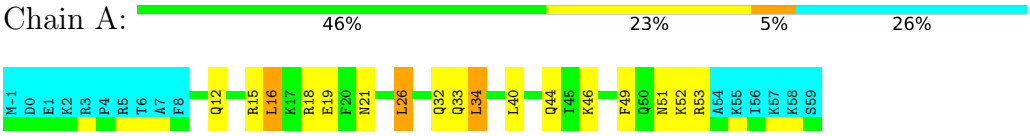
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Segmentation polarity homeobox protein engrailed

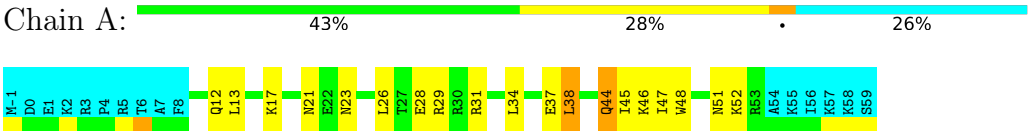
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Segmentation polarity homeobox protein engrailed

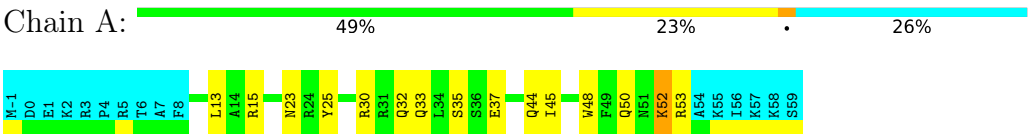
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Segmentation polarity homeobox protein engrailed

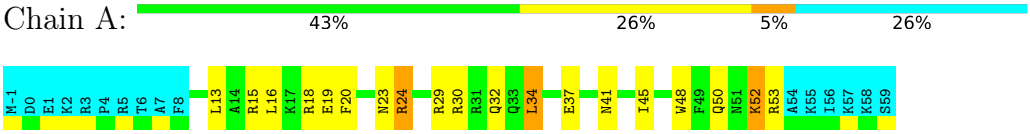
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Segmentation polarity homeobox protein engrailed

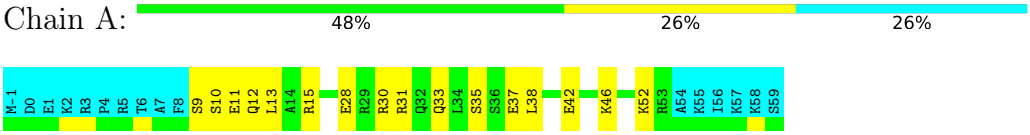
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Segmentation polarity homeobox protein engrailed

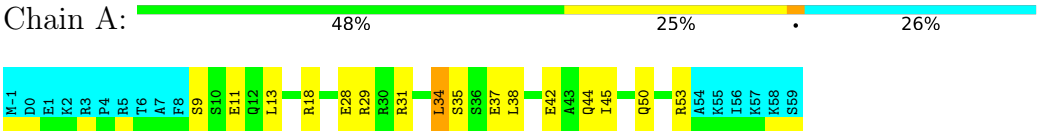
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Segmentation polarity homeobox protein engrailed

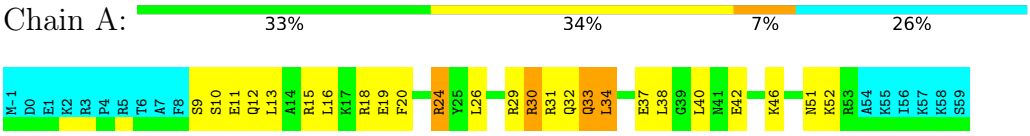
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Segmentation polarity homeobox protein engrailed

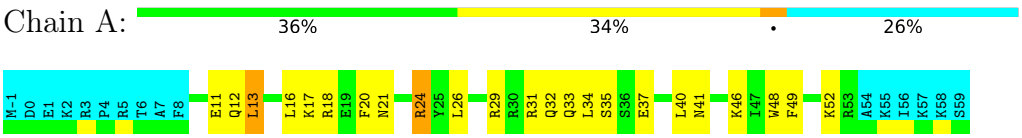
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Segmentation polarity homeobox protein engrailed

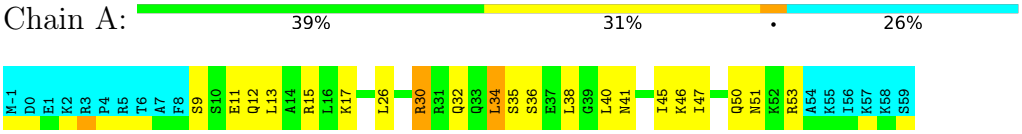
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Segmentation polarity homeobox protein engrailed

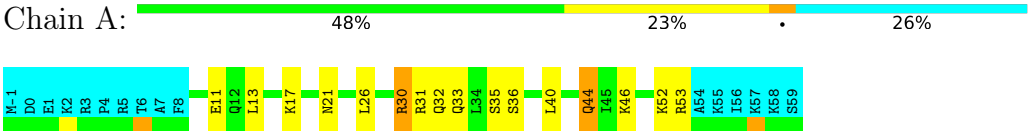
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Segmentation polarity homeobox protein engrailed

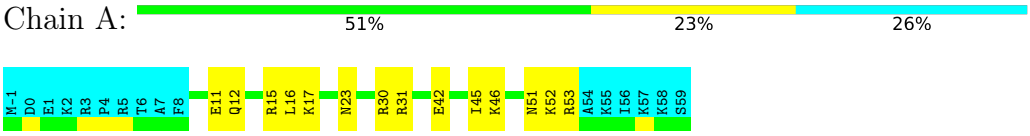
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Segmentation polarity homeobox protein engrailed

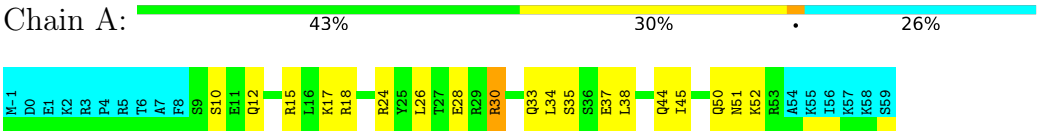
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: Segmentation polarity homeobox protein engrailed

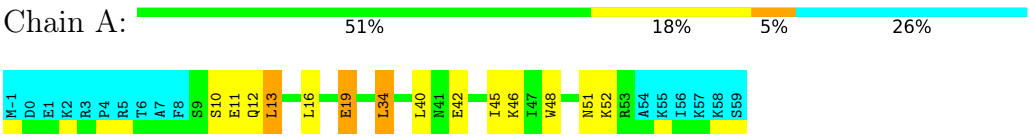
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: Segmentation polarity homeobox protein engrailed

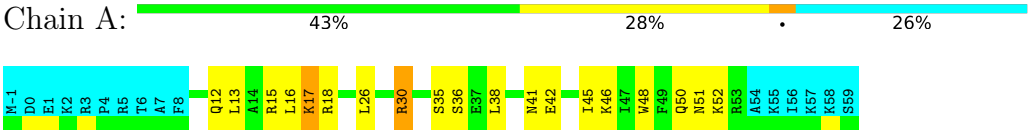
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: Segmentation polarity homeobox protein engrailed

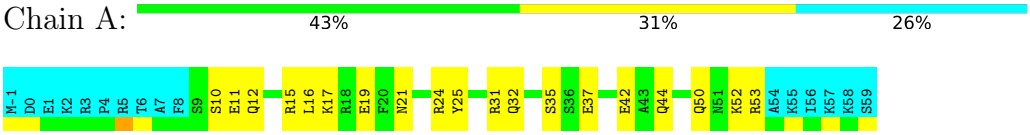
Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: Segmentation polarity homeobox protein engrailed

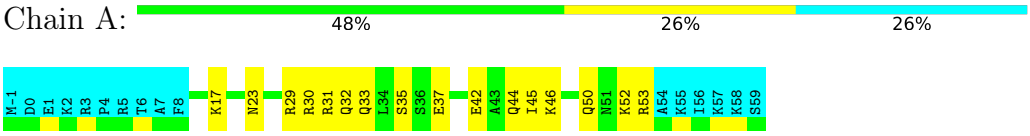
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: Segmentation polarity homeobox protein engrailed

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing.*

Of the 50 calculated structures, 25 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
CNS	refinement	
NMRPipe	structure solution	
Sparky	structure solution	
CNS	structure solution	
TENSOR	structure solution	2

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	733
Number of shifts mapped to atoms	733
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

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	392	395	395	4±2
All	All	9800	9875	9875	111

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:GLU:HA	1:A:45:ILE:HD12	0.71	1.62	5	8
1:A:30:ARG:O	1:A:34:LEU:HD12	0.70	1.86	7	3
1:A:12:GLN:O	1:A:16:LEU:HD12	0.69	1.86	22	10
1:A:9:SER:O	1:A:13:LEU:HD23	0.66	1.90	9	9
1:A:16:LEU:HD23	1:A:34:LEU:HD22	0.62	1.72	5	1
1:A:35:SER:HA	1:A:45:ILE:HD11	0.60	1.72	8	6
1:A:26:LEU:HD22	1:A:30:ARG:HB3	0.59	1.74	8	9
1:A:19:GLU:OE1	1:A:34:LEU:HD11	0.59	1.96	22	1
1:A:34:LEU:HD23	1:A:38:LEU:HD12	0.58	1.76	16	1
1:A:13:LEU:HD22	1:A:48:TRP:NE1	0.56	2.15	12	4
1:A:12:GLN:HG2	1:A:38:LEU:HD22	0.56	1.76	21	1
1:A:34:LEU:HD22	1:A:38:LEU:HD11	0.55	1.77	2	1
1:A:12:GLN:HA	1:A:38:LEU:HD21	0.54	1.77	11	1
1:A:13:LEU:HD21	1:A:48:TRP:HE1	0.54	1.63	22	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LEU:HD21	1:A:45:ILE:HG23	0.53	1.79	13	1
1:A:19:GLU:OE2	1:A:34:LEU:HD11	0.51	2.06	13	1
1:A:12:GLN:CD	1:A:40:LEU:HD11	0.49	2.32	4	4
1:A:47:ILE:HG22	1:A:51:ASN:OD1	0.49	2.07	18	3
1:A:34:LEU:HD23	1:A:38:LEU:HD11	0.49	1.85	7	1
1:A:26:LEU:HD11	1:A:49:PHE:CD2	0.48	2.43	10	1
1:A:35:SER:CA	1:A:45:ILE:HD11	0.48	2.38	8	4
1:A:12:GLN:HB3	1:A:38:LEU:HD13	0.47	1.86	14	1
1:A:13:LEU:HD21	1:A:48:TRP:NE1	0.47	2.23	22	2
1:A:20:PHE:CZ	1:A:24:ARG:CG	0.47	2.98	17	2
1:A:26:LEU:HG	1:A:49:PHE:CD2	0.47	2.45	4	2
1:A:26:LEU:HD11	1:A:45:ILE:HG22	0.46	1.87	9	3
1:A:34:LEU:O	1:A:38:LEU:HB2	0.45	2.12	15	2
1:A:12:GLN:HA	1:A:38:LEU:HD22	0.45	1.88	18	2
1:A:16:LEU:CD2	1:A:34:LEU:HD22	0.45	2.42	10	1
1:A:16:LEU:HD23	1:A:34:LEU:HD23	0.44	1.89	4	1
1:A:13:LEU:O	1:A:17:LYS:HB2	0.44	2.13	23	1
1:A:16:LEU:CD2	1:A:34:LEU:HD21	0.44	2.43	16	1
1:A:25:TYR:N	1:A:25:TYR:CD1	0.43	2.86	12	1
1:A:34:LEU:CD2	1:A:38:LEU:HD12	0.43	2.43	16	1
1:A:48:TRP:CE2	1:A:52:LYS:HE2	0.43	2.48	13	1
1:A:32:GLN:HG3	1:A:33:GLN:N	0.42	2.28	3	1
1:A:34:LEU:HD22	1:A:38:LEU:CD1	0.42	2.45	2	1
1:A:13:LEU:CD2	1:A:48:TRP:CZ2	0.42	3.02	17	1
1:A:34:LEU:CD2	1:A:38:LEU:HD11	0.41	2.44	2	1
1:A:16:LEU:HB3	1:A:48:TRP:CZ2	0.41	2.50	8	1
1:A:26:LEU:HD11	1:A:49:PHE:CD1	0.41	2.51	8	2
1:A:41:ASN:O	1:A:45:ILE:HD12	0.41	2.14	18	1
1:A:20:PHE:CZ	1:A:24:ARG:HG3	0.41	2.50	16	1
1:A:26:LEU:CD1	1:A:49:PHE:CD2	0.41	3.04	1	1
1:A:29:ARG:O	1:A:33:GLN:HB2	0.41	2.15	16	1
1:A:35:SER:HB2	1:A:40:LEU:O	0.41	2.16	17	2
1:A:12:GLN:C	1:A:16:LEU:HD12	0.41	2.41	23	1
1:A:20:PHE:CE2	1:A:24:ARG:HB2	0.41	2.51	13	1
1:A:29:ARG:O	1:A:32:GLN:HG3	0.40	2.15	7	1
1:A:48:TRP:CZ2	1:A:52:LYS:HE3	0.40	2.51	13	1
1:A:26:LEU:HD13	1:A:31:ARG:HG3	0.40	1.92	3	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	45/61 (74%)	44±1 (98±2%)	1±1 (2±2%)	0±0 (0±0%)	100	100
All	All	1125/1525 (74%)	1108 (98%)	17 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	42/56 (75%)	30±2 (71±5%)	12±2 (29±5%)	1	18
All	All	1050/1400 (75%)	744 (71%)	306 (29%)	1	18

All 34 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	52	LYS	18
1	A	31	ARG	17
1	A	46	LYS	17
1	A	53	ARG	15
1	A	15	ARG	15
1	A	30	ARG	15
1	A	17	LYS	13
1	A	32	GLN	13
1	A	37	GLU	12
1	A	34	LEU	12
1	A	11	GLU	11
1	A	50	GLN	11
1	A	18	ARG	11

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Mol	Chain	Res	Type	Models (Total)
1	A	33	GLN	11
1	A	29	ARG	10
1	A	28	GLU	9
1	A	51	ASN	9
1	A	44	GLN	9
1	A	10	SER	8
1	A	21	ASN	8
1	A	19	GLU	8
1	A	35	SER	7
1	A	41	ASN	7
1	A	36	SER	7
1	A	23	ASN	7
1	A	24	ARG	6
1	A	13	LEU	5
1	A	42	GLU	5
1	A	40	LEU	4
1	A	22	GLU	2
1	A	16	LEU	1
1	A	26	LEU	1
1	A	38	LEU	1
1	A	25	TYR	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 oligosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

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	733
Number of shifts mapped to atoms	733
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	56	-0.35 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	58	0.23 ± 0.15	None needed (< 0.5 ppm)
$^{13}C'$	57	-0.79 ± 0.18	Should be applied
^{15}N	59	-0.39 ± 0.47	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 80%, i.e. 554 atoms were assigned a chemical shift out of a possible 694. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	224/226 (99%)	90/91 (99%)	89/90 (99%)	45/45 (100%)
Sidechain	309/427 (72%)	236/269 (88%)	64/125 (51%)	9/33 (27%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	21/41 (51%)	20/20 (100%)	0/20 (0%)	1/1 (100%)
Overall	554/694 (80%)	346/380 (91%)	153/235 (65%)	55/79 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 733 atoms were assigned a chemical shift out of a possible 933. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	292/304 (96%)	120/122 (98%)	113/122 (93%)	59/60 (98%)
Sidechain	415/578 (72%)	320/365 (88%)	86/170 (51%)	9/43 (21%)
Aromatic	26/51 (51%)	25/25 (100%)	0/25 (0%)	1/1 (100%)
Overall	733/933 (79%)	465/512 (91%)	199/317 (63%)	69/104 (66%)

7.1.4 Statistically unusual chemical shifts (i)

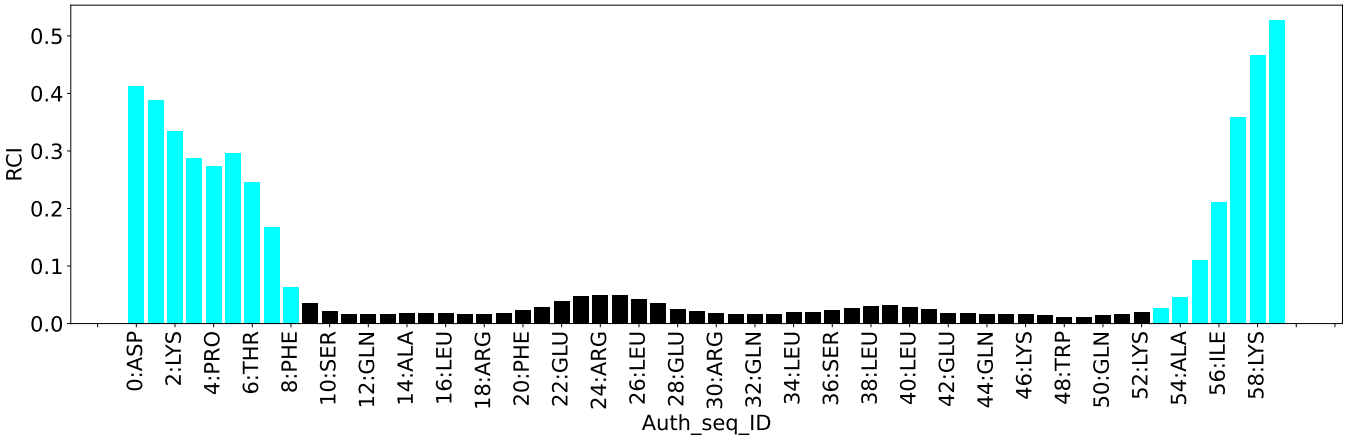
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	52	LYS	HG3	-0.48	0.04 – 2.67	-7.0
1	A	52	LYS	HG2	-0.35	0.13 – 2.61	-7.0
1	A	52	LYS	HD2	0.37	0.58 – 2.64	-6.0
1	A	52	LYS	HB3	0.28	0.46 – 3.04	-5.7
1	A	52	LYS	HB2	0.55	0.58 – 2.97	-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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
0:ASP
2:LYS
4:PRO
6:THR
8:PHE
10:SER
12:GLN
14:ALA
16:LEU
18:ARG
20:PHE
22:GLU
24:ARG
26:LEU
28:GLU
30:ARG
32:GLN
34:LEU
36:SER
38:LEU
40:LEU
42:GLU
44:GLN
46:LYS
48:TRP
50:GLN
52:LYS
54:ALA
56:ILE
58:LYS
Auth_seq_ID

8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	723
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	260
Medium range (|i-j|>1 and |i-j|<5)	205
Long range (|i-j|≥5)	198
Inter-chain	0
Hydrogen bond restraints	60
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	11.9
Number of long range restraints per residue[1]	3.3

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å
are not included in the calculation.There are no distance violations

8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

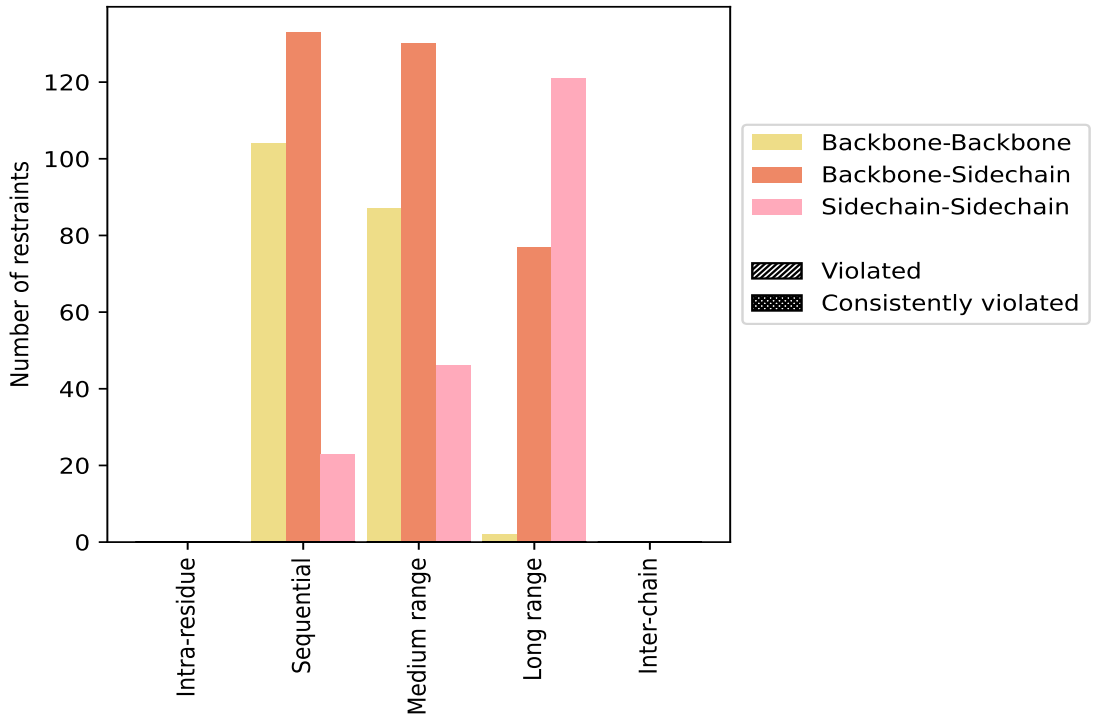
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	260	36.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	104	14.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	133	18.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	23	3.2	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	205	28.4	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	87	12.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	72	10.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	46	6.4	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	198	27.4	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	2	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	75	10.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	121	16.7	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	60	8.3	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	723	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	193	26.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	340	47.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	190	26.3	0	0.0	0.0	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model

No violations found

9.3 Distance violation statistics for the ensemble

No violations found

9.4 Most violated distance restraints in the ensemble

No violations found

9.5 All violated distance restraints

No violations found

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found