



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2MAX / pdb_00002max
BMRB ID : 19380
Title : NMR structure of the RNA polymerase alpha subunit C-terminal domain from
Helicobacter pylori
Authors : Borin, B.N.; Krezel, A.M.
Deposited on : 2013-07-21

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<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) 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
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

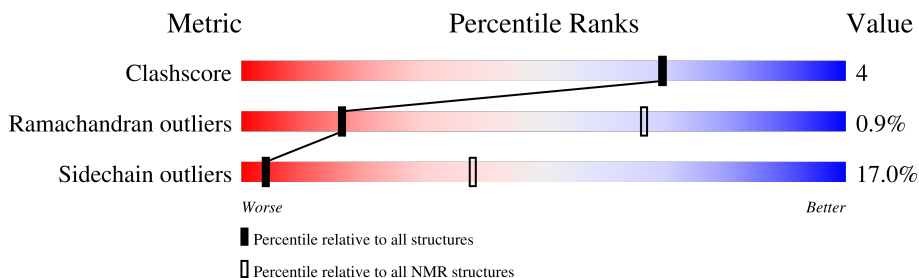
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	126	

2 Ensemble composition and analysis

This entry contains 15 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:255-A:318, A:324-A:337 (78)	0.39	1

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1778 atoms, of which 887 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	114	1778	552	887	150	184	5	0

There are 12 discrepancies between the modelled and reference sequences:

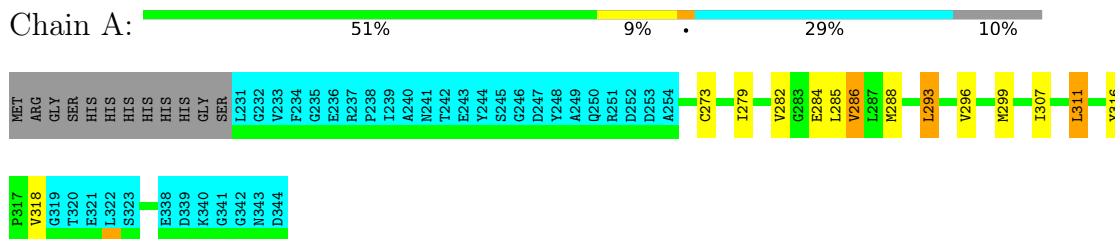
Chain	Residue	Modelled	Actual	Comment	Reference
A	219	MET	-	expression tag	UNP Q9ZJT5
A	220	ARG	-	expression tag	UNP Q9ZJT5
A	221	GLY	-	expression tag	UNP Q9ZJT5
A	222	SER	-	expression tag	UNP Q9ZJT5
A	223	HIS	-	expression tag	UNP Q9ZJT5
A	224	HIS	-	expression tag	UNP Q9ZJT5
A	225	HIS	-	expression tag	UNP Q9ZJT5
A	226	HIS	-	expression tag	UNP Q9ZJT5
A	227	HIS	-	expression tag	UNP Q9ZJT5
A	228	HIS	-	expression tag	UNP Q9ZJT5
A	229	GLY	-	expression tag	UNP Q9ZJT5
A	230	SER	-	expression tag	UNP Q9ZJT5

4 Residue-property plots [i](#)

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: DNA-directed RNA polymerase subunit alpha

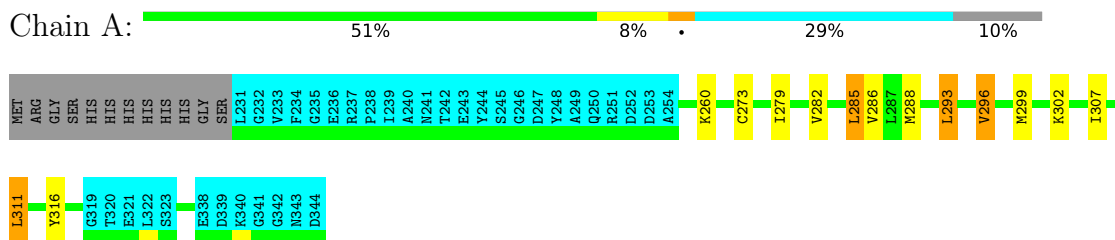


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

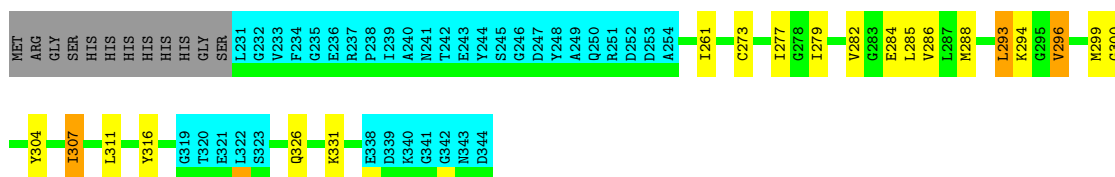
- Molecule 1: DNA-directed RNA polymerase subunit alpha



4.2.2 Score per residue for model 2

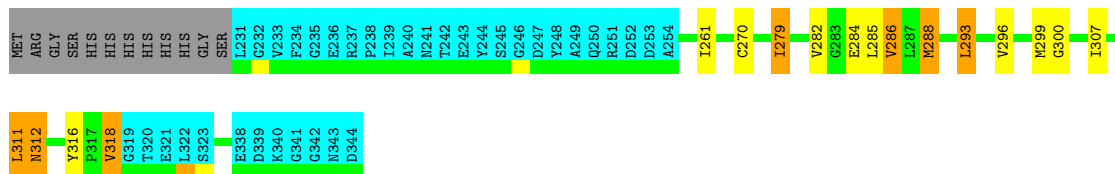
- Molecule 1: DNA-directed RNA polymerase subunit alpha





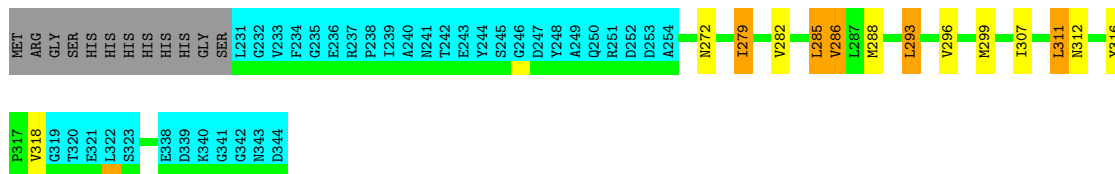
4.2.3 Score per residue for model 3

- Molecule 1: DNA-directed RNA polymerase subunit alpha



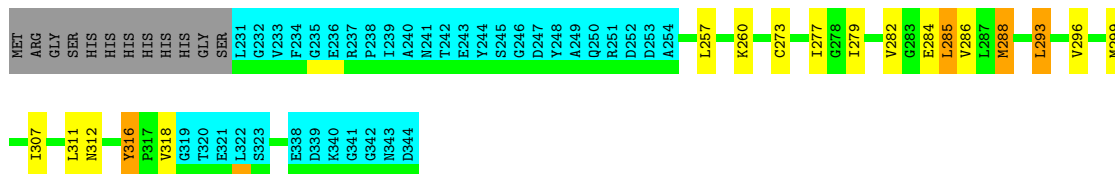
4.2.4 Score per residue for model 4

- Molecule 1: DNA-directed RNA polymerase subunit alpha



4.2.5 Score per residue for model 5

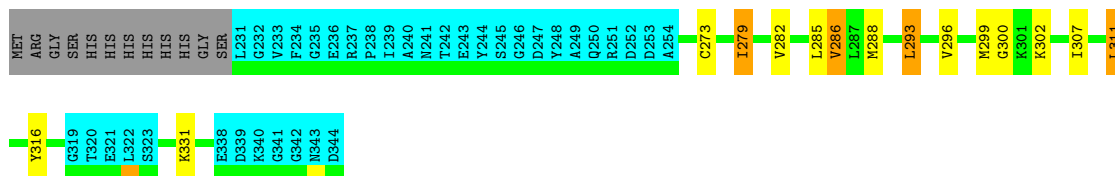
- Molecule 1: DNA-directed RNA polymerase subunit alpha



4.2.6 Score per residue for model 6

- Molecule 1: DNA-directed RNA polymerase subunit alpha

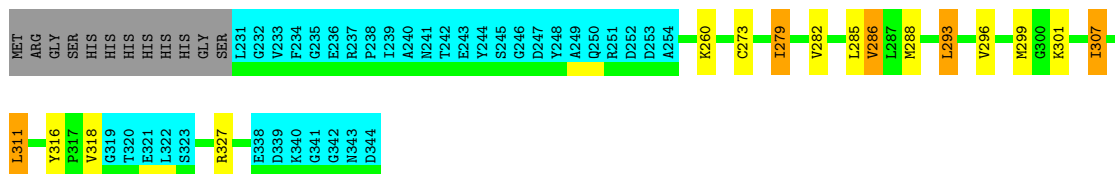
Chain A: 



4.2.7 Score per residue for model 7

- Molecule 1: DNA-directed RNA polymerase subunit alpha

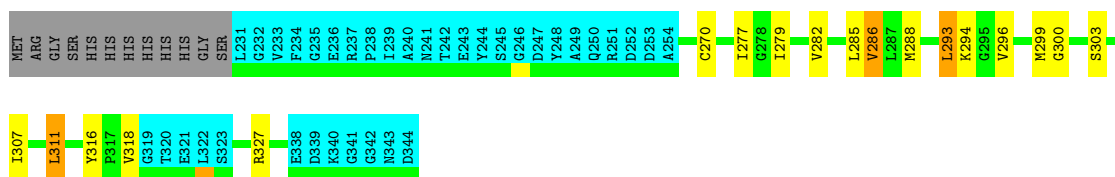
Chain A: 



4.2.8 Score per residue for model 8

- Molecule 1: DNA-directed RNA polymerase subunit alpha

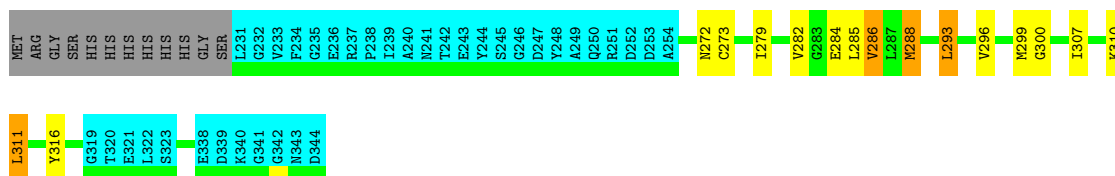
Chain A: 



4.2.9 Score per residue for model 9

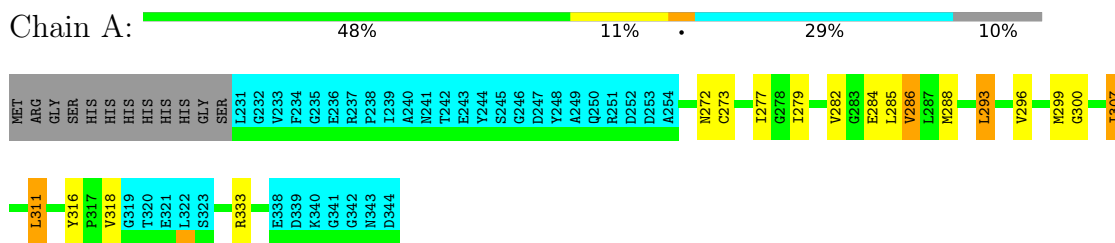
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A: 



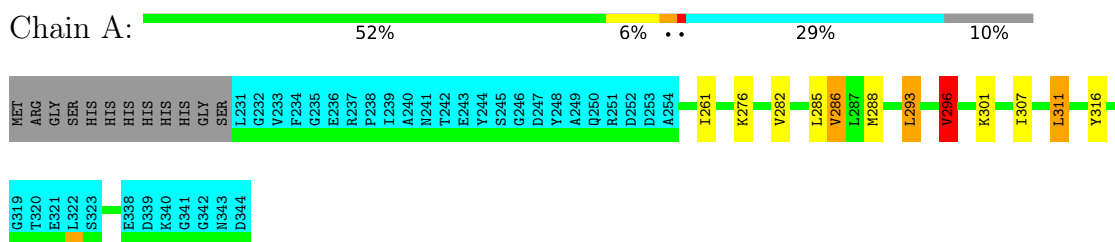
4.2.10 Score per residue for model 10

- Molecule 1: DNA-directed RNA polymerase subunit alpha



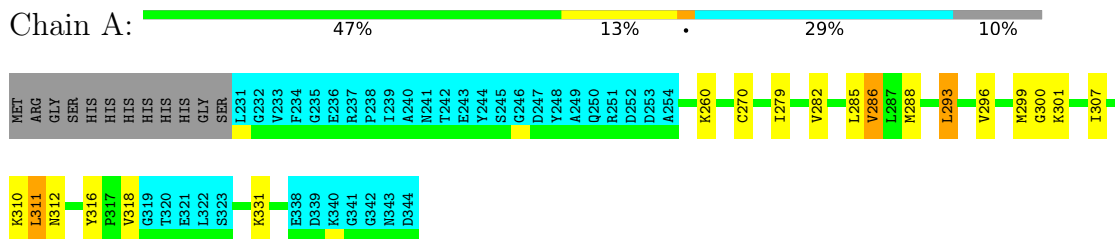
4.2.11 Score per residue for model 11

- Molecule 1: DNA-directed RNA polymerase subunit alpha



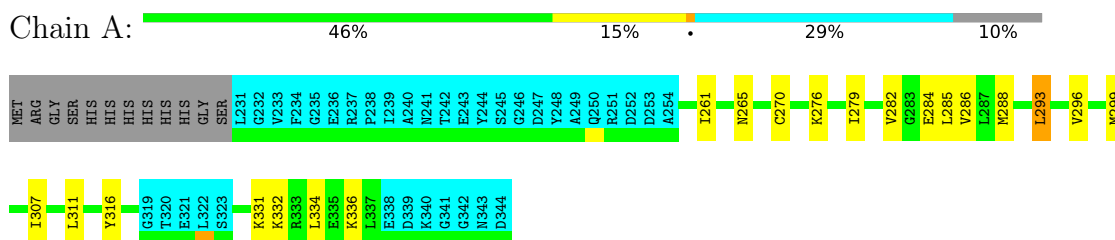
4.2.12 Score per residue for model 12

- Molecule 1: DNA-directed RNA polymerase subunit alpha



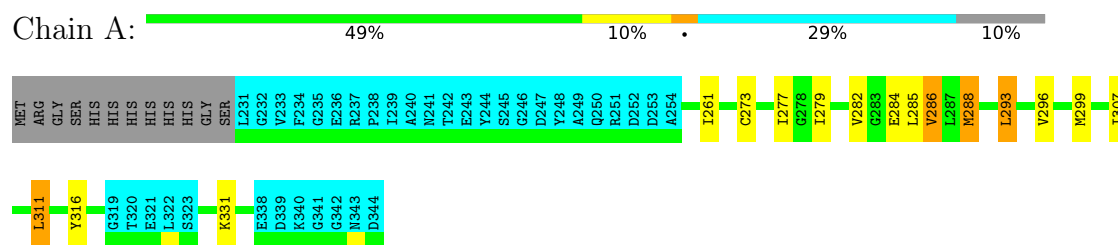
4.2.13 Score per residue for model 13

- Molecule 1: DNA-directed RNA polymerase subunit alpha



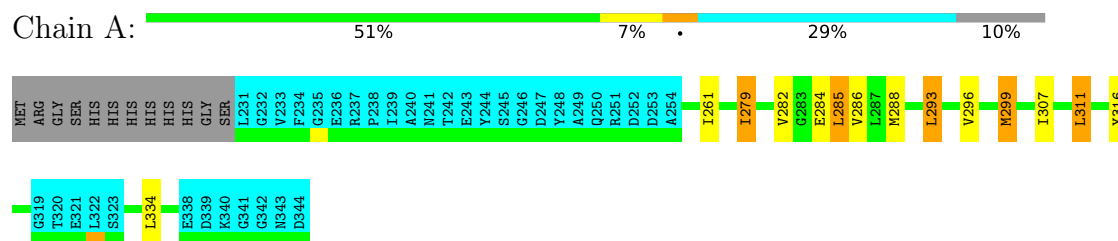
4.2.14 Score per residue for model 14

- Molecule 1: DNA-directed RNA polymerase subunit alpha



4.2.15 Score per residue for model 15

- Molecule 1: DNA-directed RNA polymerase subunit alpha



5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 15 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	
TALOS	geometry optimization	
Amber	refinement	
ProcheckNMR	geometry optimization	
CYANA	refinement	

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	1188
Number of shifts mapped to atoms	1188
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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	0.82±0.01	0±0/626 (0.0± 0.0%)	1.46±0.03	3±1/832 (0.3± 0.1%)
All	All	0.82	0/9390 (0.0%)	1.46	38/12480 (0.3%)

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	0.1±0.2
All	All	0	1

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	282	VAL	CA-C-N	7.08	127.99	119.99	5	15
1	A	282	VAL	C-N-CA	7.08	127.99	119.99	5	15
1	A	296	VAL	CA-CB-CG2	5.62	119.95	110.40	11	1
1	A	318	VAL	N-CA-C	5.37	116.33	109.30	8	1
1	A	312	ASN	CA-CB-CG	5.31	117.91	112.60	3	1
1	A	307	ILE	CA-CB-CG2	5.22	119.38	110.50	7	3
1	A	318	VAL	CA-CB-CG1	5.16	119.18	110.40	3	2

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	304	TYR	Sidechain	1

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	620	651	651	5±1
All	All	9300	9765	9765	69

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:288:MET:HE1	1:A:296:VAL:CG1	0.69	2.18	11	15
1:A:286:VAL:HG23	1:A:316:TYR:CE2	0.68	2.24	5	1
1:A:257:LEU:HD13	1:A:286:VAL:HG11	0.67	1.65	5	1
1:A:285:LEU:CD2	1:A:318:VAL:HG21	0.63	2.24	5	2
1:A:285:LEU:HD13	1:A:311:LEU:HD23	0.60	1.71	15	2
1:A:288:MET:HE2	1:A:293:LEU:HA	0.59	1.74	15	15
1:A:288:MET:HE1	1:A:296:VAL:HG12	0.55	1.77	11	4
1:A:296:VAL:HG21	1:A:299:MET:HE2	0.51	1.80	15	1
1:A:286:VAL:HG23	1:A:311:LEU:HD21	0.51	1.81	7	10
1:A:284:GLU:CG	1:A:334:LEU:HD21	0.48	2.38	15	2
1:A:273:CYS:SG	1:A:296:VAL:HG21	0.48	2.48	6	8
1:A:296:VAL:CG2	1:A:299:MET:HE2	0.46	2.41	15	1
1:A:279:ILE:HD13	1:A:288:MET:SD	0.46	2.51	12	7

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	78/126 (62%)	71±1 (91±2%)	6±1 (8±2%)	1±1 (1±1%)	16	66
All	All	1170/1890 (62%)	1070 (91%)	89 (8%)	11 (1%)	16	66

All 2 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	300	GLY	7
1	A	288	MET	4

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	70/107 (65%)	58±2 (83±2%)	12±2 (17±2%)	4	38
All	All	1050/1605 (65%)	872 (83%)	178 (17%)	4	38

All 30 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	285	LEU	15
1	A	293	LEU	15
1	A	307	ILE	15
1	A	311	LEU	15
1	A	316	TYR	15
1	A	286	VAL	14
1	A	299	MET	14
1	A	279	ILE	12
1	A	261	ILE	6
1	A	284	GLU	6
1	A	277	ILE	5
1	A	331	LYS	5
1	A	260	LYS	4
1	A	270	CYS	4
1	A	312	ASN	4
1	A	318	VAL	4
1	A	296	VAL	3
1	A	272	ASN	3
1	A	301	LYS	3
1	A	302	LYS	2
1	A	294	LYS	2
1	A	327	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	310	LYS	2
1	A	276	LYS	2
1	A	326	GLN	1
1	A	303	SER	1
1	A	333	ARG	1
1	A	265	ASN	1
1	A	332	LYS	1
1	A	336	LYS	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 i

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 78% 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 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	1188
Number of shifts mapped to atoms	1188
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing i

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	109	-0.47 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	98	0.08 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	107	-1.08 ± 0.19	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 83%, i.e. 909 atoms were assigned a chemical shift out of a possible 1093. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	309/391 (79%)	158/159 (99%)	76/156 (49%)	75/76 (99%)
Sidechain	584/665 (88%)	397/428 (93%)	182/211 (86%)	5/26 (19%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	16/37 (43%)	16/17 (94%)	0/20 (0%)	0/0 (—%)
Overall	909/1093 (83%)	571/604 (95%)	258/387 (67%)	80/102 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1188 atoms were assigned a chemical shift out of a possible 1523. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	439/575 (76%)	223/236 (94%)	109/228 (48%)	107/111 (96%)
Sidechain	727/883 (82%)	491/565 (87%)	231/282 (82%)	5/36 (14%)
Aromatic	22/65 (34%)	22/30 (73%)	0/35 (0%)	0/0 (—%)
Overall	1188/1523 (78%)	736/831 (89%)	340/545 (62%)	112/147 (76%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

