



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 5VFK
Title : Solution structure of an archaeal DUF61 family protein SSO0941
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Deposited on : 2017-04-07

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A user guide is available at

<https://www.wwpdb.org/validation/2017/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
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

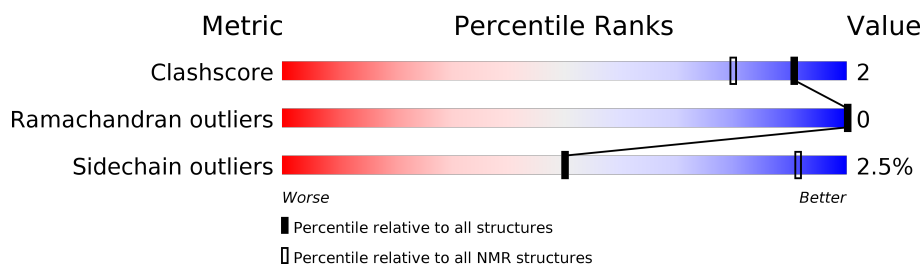
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	146	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 18 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:17-A:73, A:77-A:122 (103)	0.20	18
2	A:130-A:138 (9)	0.15	11

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2448 atoms, of which 1238 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
1	A	146	Total	C	H	N	O	S	0
			2448	787	1238	197	224	2	

There are 8 discrepancies between the modelled and reference sequences:

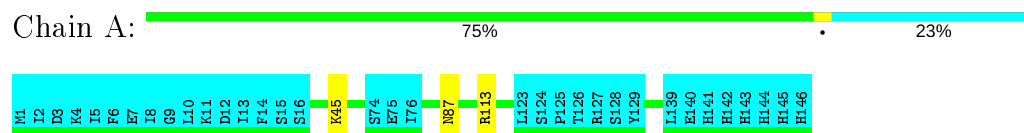
Chain	Residue	Modelled	Actual	Comment	Reference
A	139	LEU	-	expression tag	UNP Q97ZH2
A	140	GLU	-	expression tag	UNP Q97ZH2
A	141	HIS	-	expression tag	UNP Q97ZH2
A	142	HIS	-	expression tag	UNP Q97ZH2
A	143	HIS	-	expression tag	UNP Q97ZH2
A	144	HIS	-	expression tag	UNP Q97ZH2
A	145	HIS	-	expression tag	UNP Q97ZH2
A	146	HIS	-	expression tag	UNP Q97ZH2

4 Residue-property plots [i](#)

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: Uncharacterized protein

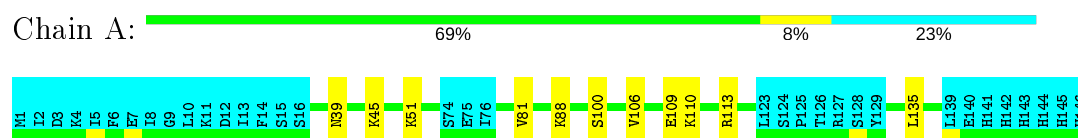


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

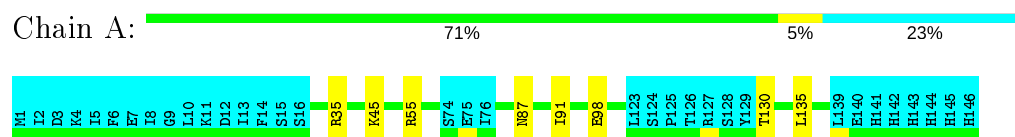
4.2.1 Score per residue for model 1

- Molecule 1: Uncharacterized protein



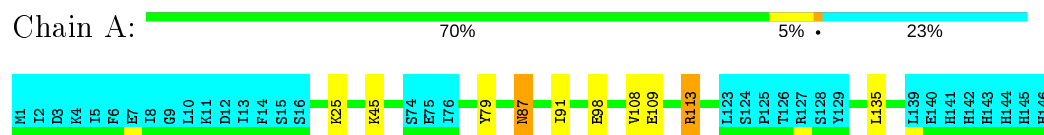
4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized protein



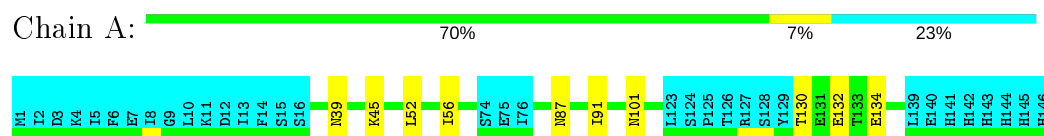
4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein



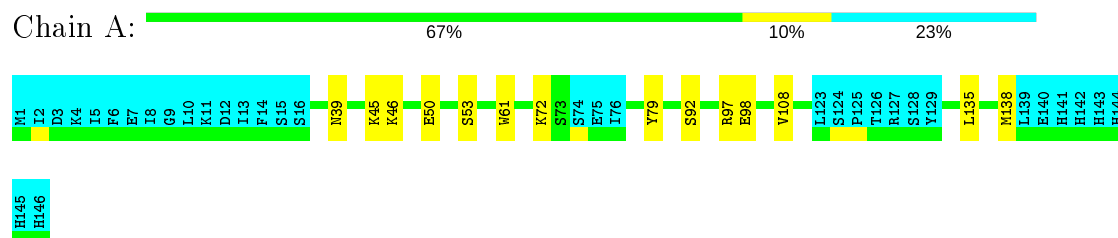
4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein



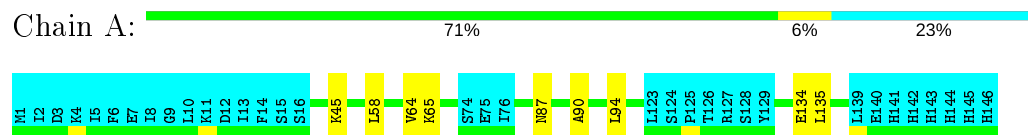
4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein



4.2.6 Score per residue for model 6

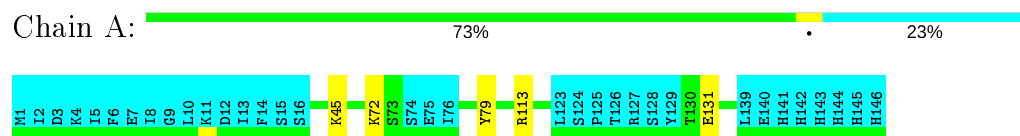
- Molecule 1: Uncharacterized protein



4.2.7 Score per residue for model 7

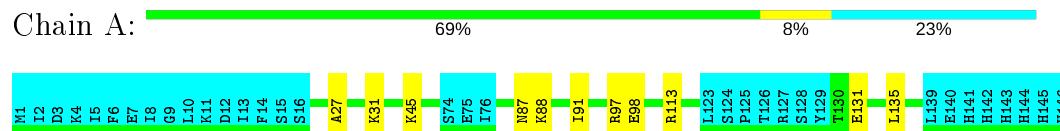
- Molecule 1: Uncharacterized protein





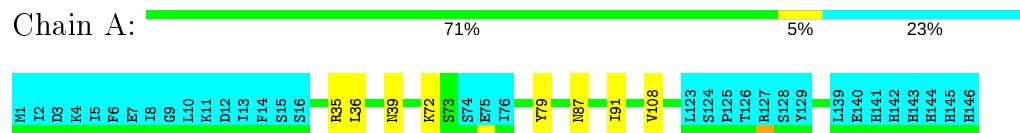
4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein



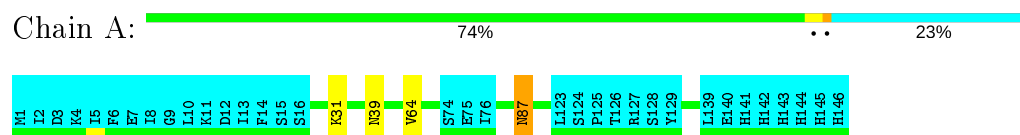
4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein



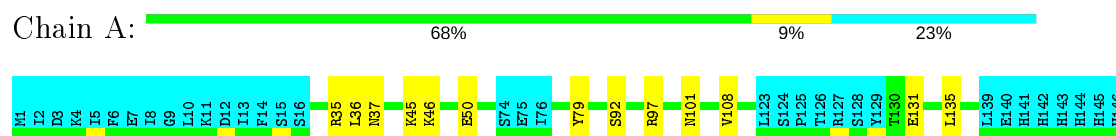
4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein



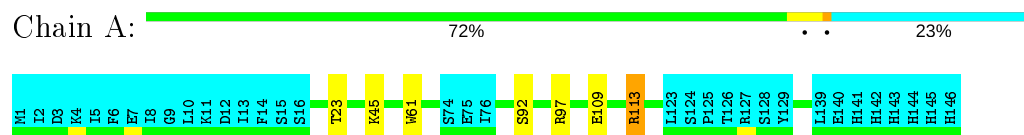
4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein



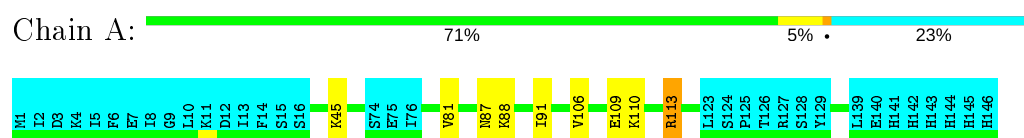
4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized protein



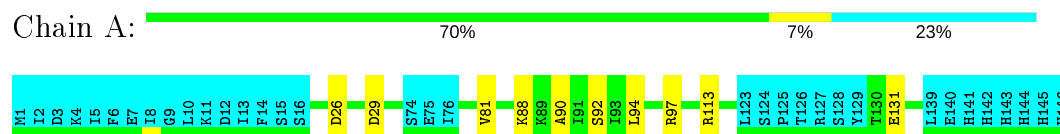
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Uncharacterized protein



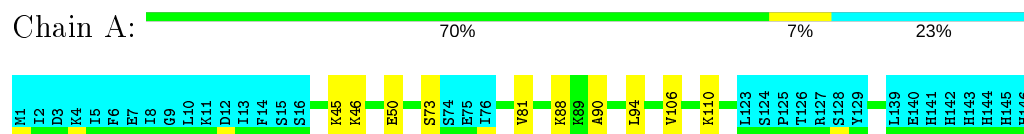
4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein



4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular 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 calculation	
CNS	refinement	
SANE	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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	2024
Number of shifts mapped to atoms	1972
Number of unparsed shifts	0
Number of shifts with mapping errors	52
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

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](#)

There are no covalent bond-length or bond-angle outliers.

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	0.3±0.6
All	All	0	6

There are no bond-length outliers.

There are no bond-angle outliers.

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	113	ARG	Sidechain	3
1	A	35	ARG	Sidechain	1
1	A	55	ARG	Sidechain	1
1	A	97	ARG	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	923	957	956	3±1
All	All	18460	19140	19120	61

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:GLU:O	1:A:113:ARG:HD3	0.57	1.99	11	3
1:A:135:LEU:O	1:A:138:MET:HG2	0.57	2.00	7	2
1:A:92:SER:HA	1:A:97:ARG:O	0.49	2.08	19	4
1:A:106:VAL:O	1:A:110:LYS:HG3	0.49	2.07	1	6
1:A:72:LYS:HD3	1:A:79:TYR:CZ	0.48	2.43	7	2
1:A:87:ASN:O	1:A:91:ILE:HG12	0.47	2.09	13	6
1:A:64:VAL:HA	1:A:87:ASN:ND2	0.47	2.25	15	2
1:A:90:ALA:O	1:A:94:LEU:HG	0.46	2.10	20	4
1:A:109:GLU:HB3	1:A:113:ARG:NH1	0.46	2.26	17	1
1:A:72:LYS:HG2	1:A:79:TYR:CE1	0.46	2.45	5	1
1:A:72:LYS:HG2	1:A:79:TYR:CE2	0.45	2.47	14	1
1:A:46:LYS:O	1:A:50:GLU:HG3	0.45	2.12	5	6
1:A:79:TYR:CG	1:A:108:VAL:HG21	0.44	2.48	14	5
1:A:53:SER:HB2	1:A:61:TRP:CZ2	0.44	2.48	5	1
1:A:79:TYR:CD1	1:A:108:VAL:HG21	0.44	2.48	16	1
1:A:35:ARG:HG2	1:A:36:LEU:O	0.44	2.12	14	2
1:A:81:VAL:O	1:A:88:LYS:HE2	0.43	2.14	18	4
1:A:65:LYS:H	1:A:87:ASN:ND2	0.43	2.12	6	1
1:A:27:ALA:HA	1:A:31:LYS:O	0.43	2.14	13	1
1:A:26:ASP:O	1:A:29:ASP:HB3	0.42	2.14	19	1
1:A:131:GLU:O	1:A:135:LEU:HG	0.42	2.15	13	2
1:A:105:ASN:O	1:A:109:GLU:HG3	0.42	2.14	8	1
1:A:109:GLU:HB3	1:A:113:ARG:NH2	0.42	2.30	1	1
1:A:87:ASN:N	1:A:87:ASN:HD22	0.42	2.13	15	1
1:A:52:LEU:O	1:A:56:ILE:HG22	0.41	2.16	4	1
1:A:23:THR:HB	1:A:61:TRP:O	0.40	2.15	17	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	112/146 (77%)	110±1 (98±1%)	2±1 (2±1%)	0±0 (0±0%)	100	100
All	All	2240/2920 (77%)	2201 (98%)	39 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	105/138 (76%)	102±1 (98±1%)	3±1 (2±1%)	50 91
All	All	2100/2760 (76%)	2048 (98%)	52 (2%)	50 91

All 17 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	45	LYS	17
1	A	39	ASN	6
1	A	98	GLU	5
1	A	113	ARG	3
1	A	87	ASN	3
1	A	131	GLU	3
1	A	134	GLU	2
1	A	130	THR	2
1	A	101	ASN	2
1	A	31	LYS	2
1	A	51	LYS	1
1	A	58	LEU	1
1	A	97	ARG	1
1	A	25	LYS	1
1	A	100	SER	1
1	A	132	GLU	1
1	A	88	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates [i](#)

There are no carbohydrates 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 94% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_0*

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	2024
Number of shifts mapped to atoms	1972
Number of unparsed shifts	0
Number of shifts with mapping errors	52
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Residue not found in structure. All 52 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	206	PHE	HB3	3.028	0.02	2
A	202	ILE	C	175.1	0.3	1
A	202	ILE	CB	38.91	0.3	1
A	205	ILE	H	8.07	0.02	1
A	208	ILE	HB	1.876	0.02	1
A	204	LYS	HB2	1.743	0.02	2
A	204	LYS	C	176.49	0.3	1
A	209	GLY	HA2	3.881	0.02	2
A	207	GLU	CB	30.49	0.3	1
A	203	ASP	HB2	2.632	0.02	2
A	203	ASP	N	125.858	0.2	1
A	202	ILE	CA	60.49	0.3	1
A	205	ILE	HA	4.055	0.02	1
A	206	PHE	HA	4.551	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	208	ILE	C	176.4	0.3	1
A	207	GLU	HA	4.488	0.02	1
A	203	ASP	CA	54.45	0.3	1
A	205	ILE	CA	61.69	0.3	1
A	203	ASP	C	175.62	0.3	1
A	204	LYS	CB	32.93	0.3	1
A	206	PHE	CA	58.03	0.3	1
A	202	ILE	HA	3.902	0.02	1
A	203	ASP	CB	41.57	0.3	1
A	203	ASP	HB3	2.75	0.02	2
A	208	ILE	HA	4.126	0.02	1
A	206	PHE	HB2	3.114	0.02	2
A	205	ILE	HB	1.79	0.02	1
A	204	LYS	N	122.382	0.2	1
A	209	GLY	CA	45.52	0.3	1
A	204	LYS	CA	56.87	0.3	1
A	206	PHE	CB	38.95	0.3	1
A	209	GLY	N	111.37	0.2	1
A	202	ILE	HB	1.973	0.02	1
A	209	GLY	H	8.457	0.02	1
A	208	ILE	CB	38.85	0.3	1
A	207	GLU	H	8.002	0.02	1
A	206	PHE	C	175.3	0.3	1
A	207	GLU	HB2	1.99	0.02	2
A	205	ILE	N	120.472	0.2	1
A	203	ASP	HA	4.712	0.02	1
A	207	GLU	C	176.35	0.3	1
A	209	GLY	HA3	3.881	0.02	2
A	207	GLU	CA	56.43	0.3	1
A	208	ILE	CA	61.68	0.3	1
A	207	GLU	N	121.72	0.2	1
A	205	ILE	CB	38.5	0.3	1
A	209	GLY	C	174.49	0.3	1
A	205	ILE	C	176.07	0.3	1
A	204	LYS	HA	4.249	0.02	1
A	204	LYS	H	8.402	0.02	1
A	203	ASP	H	8.688	0.02	1
A	207	GLU	HB3	1.99	0.02	2

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	154	-0.09 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	148	0.27 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	152	0.04 ± 0.19	None needed (< 0.5 ppm)
^{15}N	144	0.84 ± 0.24	Should be applied

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 94%, i.e. 1384 atoms were assigned a chemical shift out of a possible 1465. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	553/554 (100%)	221/221 (100%)	223/224 (100%)	109/109 (100%)
Sidechain	721/794 (91%)	442/463 (95%)	269/301 (89%)	10/30 (33%)
Aromatic	110/117 (94%)	57/61 (93%)	51/52 (98%)	2/4 (50%)
Overall	1384/1465 (94%)	720/745 (97%)	543/577 (94%)	121/143 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 1765 atoms were assigned a chemical shift out of a possible 1915. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	714/722 (99%)	285/288 (99%)	290/292 (99%)	139/142 (98%)
Sidechain	913/1002 (91%)	561/587 (96%)	341/380 (90%)	11/35 (31%)
Aromatic	138/191 (72%)	71/99 (72%)	65/76 (86%)	2/16 (12%)
Overall	1765/1915 (92%)	917/974 (94%)	696/748 (93%)	152/193 (79%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

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:

