



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:18 PM BST

PDB ID : 1K8B
Title : NMR Structure Analysis of the N-terminal Domain of Archaeal Translation Initiation Factor 2 Subunit beta
Authors : Cho, S.; Hoffman, D.W.
Deposited on : 2001-10-23

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

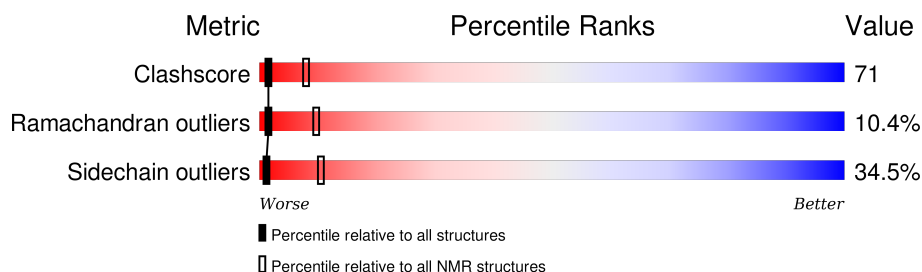
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 51%.

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	52	

2 Ensemble composition and analysis ⓘ

This entry contains 10 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:40-A:88 (49)	0.22	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 1 clusters and 6 single-model clusters were found.

Cluster number	Models
1	1, 4, 7, 10
Single-model clusters	2; 3; 5; 6; 8; 9

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 863 atoms, of which 439 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROBABLE TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT.

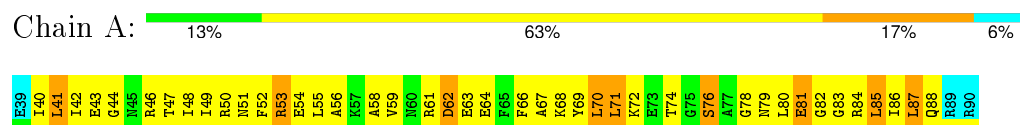
Mol	Chain	Residues	Atoms					Trace
1	A	52	Total	C	H	N	O	0
			863	266	439	81	77	

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: PROBABLE TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT

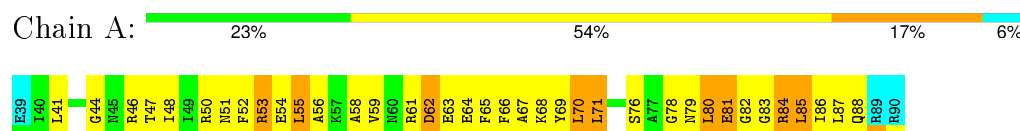


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

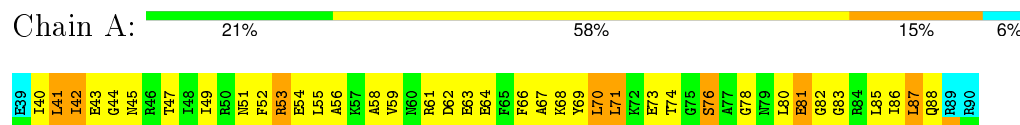
4.2.1 Score per residue for model 1

- Molecule 1: PROBABLE TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT



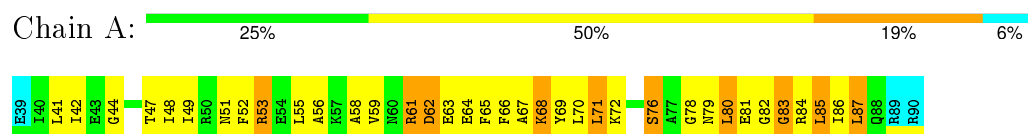
4.2.2 Score per residue for model 2

- Molecule 1: PROBABLE TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT



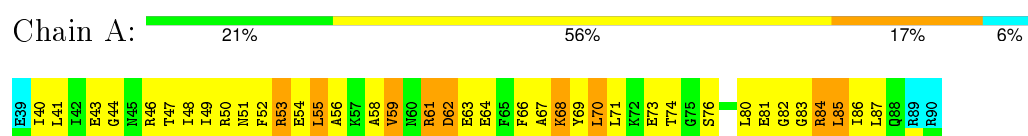
4.2.3 Score per residue for model 3

- Molecule 1: PROBABLE TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT



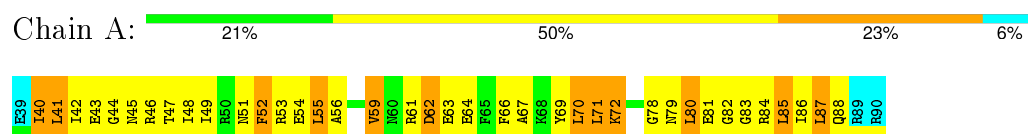
4.2.4 Score per residue for model 4

- Molecule 1: PROBABLE TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT



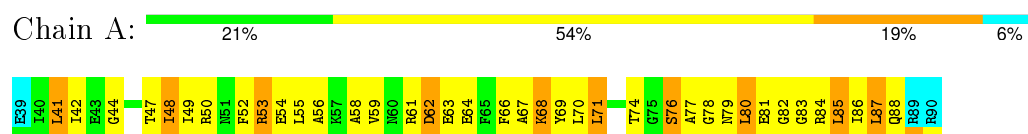
4.2.5 Score per residue for model 5

- Molecule 1: PROBABLE TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT



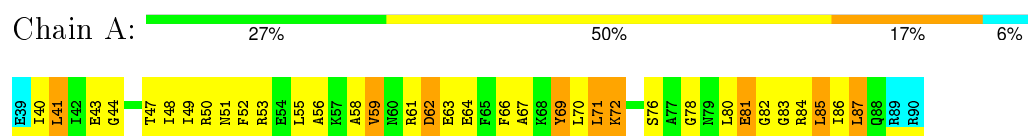
4.2.6 Score per residue for model 6

- Molecule 1: PROBABLE TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT



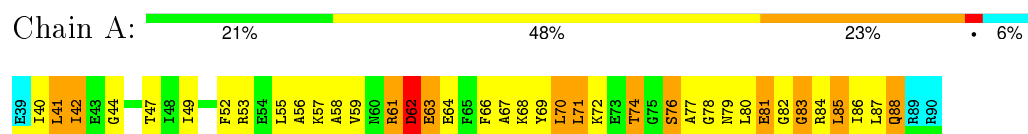
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: PROBABLE TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT



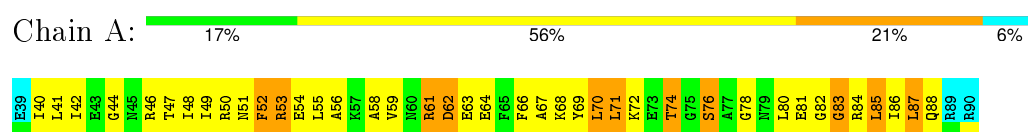
4.2.8 Score per residue for model 8

- Molecule 1: PROBABLE TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT



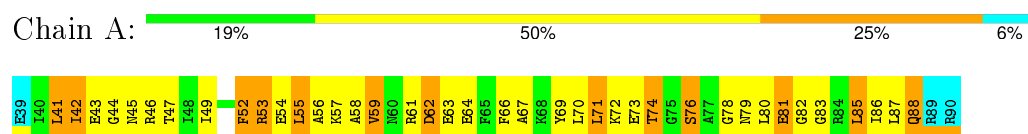
4.2.9 Score per residue for model 9

- Molecule 1: PROBABLE TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT



4.2.10 Score per residue for model 10

- Molecule 1: PROBABLE TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT



5 Refinement protocol and experimental data overview

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

Of the 170 calculated structures, 10 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	1.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 5294
Number of chemical shift lists	1
Total number of shifts	769
Number of shifts mapped to atoms	378
Number of unparsed shifts	0
Number of shifts with mapping errors	391
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	51%

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.

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 [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	393	407	407	56±8
All	All	3930	4070	4070	565

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 71.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LEU:HD22	1:A:85:LEU:HD11	1.13	1.17	3	2
1:A:70:LEU:HD12	1:A:87:LEU:HD13	1.05	1.16	4	1
1:A:70:LEU:HD12	1:A:85:LEU:HD11	0.99	1.05	5	2
1:A:85:LEU:HD22	1:A:86:ILE:N	0.93	1.79	8	2
1:A:67:ALA:HB2	1:A:80:LEU:HD12	0.91	1.39	8	2
1:A:70:LEU:HD23	1:A:87:LEU:HB3	0.87	1.47	3	1
1:A:70:LEU:CD1	1:A:85:LEU:HD11	0.86	1.97	5	2
1:A:70:LEU:HD13	1:A:87:LEU:CB	0.85	2.01	7	2
1:A:67:ALA:HB3	1:A:80:LEU:HB3	0.85	1.47	1	6
1:A:70:LEU:HD12	1:A:87:LEU:CD1	0.84	2.03	4	1
1:A:51:ASN:CB	1:A:85:LEU:HD23	0.84	2.03	1	5
1:A:70:LEU:CD2	1:A:85:LEU:HD11	0.82	2.03	3	2
1:A:70:LEU:HD12	1:A:71:LEU:N	0.81	1.90	7	1
1:A:41:LEU:O	1:A:47:THR:HG23	0.80	1.75	10	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:PHE:CE2	1:A:85:LEU:HD22	0.80	2.10	7	6
1:A:63:GLU:O	1:A:80:LEU:HD13	0.80	1.76	5	3
1:A:71:LEU:HD23	1:A:72:LYS:N	0.80	1.91	3	1
1:A:66:PHE:CE2	1:A:85:LEU:HD13	0.80	2.12	3	3
1:A:67:ALA:CB	1:A:80:LEU:HD12	0.79	2.08	8	1
1:A:70:LEU:HD12	1:A:85:LEU:CD1	0.78	2.00	5	1
1:A:47:THR:O	1:A:86:ILE:HG23	0.78	1.78	10	10
1:A:67:ALA:CB	1:A:85:LEU:HD23	0.78	2.08	8	1
1:A:59:VAL:HA	1:A:63:GLU:H	0.77	1.39	4	10
1:A:70:LEU:HD13	1:A:87:LEU:HB3	0.77	1.57	7	2
1:A:70:LEU:HD22	1:A:85:LEU:CD1	0.76	2.05	3	1
1:A:56:ALA:O	1:A:59:VAL:HG13	0.75	1.82	4	10
1:A:85:LEU:O	1:A:85:LEU:HD13	0.74	1.82	10	1
1:A:55:LEU:O	1:A:58:ALA:HB3	0.74	1.83	8	9
1:A:55:LEU:HD21	1:A:63:GLU:HB2	0.73	1.59	8	1
1:A:64:GLU:CB	1:A:80:LEU:HD13	0.73	2.13	10	4
1:A:67:ALA:HA	1:A:85:LEU:HD23	0.73	1.61	10	2
1:A:87:LEU:HD22	1:A:87:LEU:O	0.73	1.83	3	2
1:A:52:PHE:HA	1:A:83:GLY:O	0.72	1.85	9	5
1:A:80:LEU:HD13	1:A:81:GLU:N	0.72	1.99	9	1
1:A:59:VAL:HA	1:A:63:GLU:N	0.72	1.98	8	10
1:A:51:ASN:HB2	1:A:85:LEU:HD23	0.72	1.61	4	5
1:A:87:LEU:O	1:A:87:LEU:HD22	0.72	1.85	9	3
1:A:80:LEU:HD22	1:A:84:ARG:O	0.71	1.85	9	1
1:A:42:ILE:HG22	1:A:47:THR:OG1	0.71	1.86	9	4
1:A:40:ILE:CG1	1:A:49:ILE:HD12	0.71	2.15	4	1
1:A:64:GLU:HA	1:A:80:LEU:HD13	0.71	1.61	3	5
1:A:66:PHE:O	1:A:69:TYR:HB2	0.69	1.87	1	10
1:A:48:ILE:HG23	1:A:86:ILE:CG1	0.69	2.18	5	3
1:A:67:ALA:HB1	1:A:85:LEU:HD23	0.68	1.64	8	1
1:A:70:LEU:HD12	1:A:87:LEU:HG	0.68	1.65	1	1
1:A:70:LEU:HD13	1:A:87:LEU:HB2	0.68	1.66	5	1
1:A:40:ILE:HG22	1:A:49:ILE:HG12	0.68	1.64	2	2
1:A:64:GLU:O	1:A:80:LEU:HD22	0.67	1.90	2	3
1:A:66:PHE:O	1:A:69:TYR:N	0.67	2.28	6	10
1:A:48:ILE:HG23	1:A:86:ILE:HG12	0.66	1.66	3	4
1:A:81:GLU:O	1:A:83:GLY:N	0.66	2.29	3	10
1:A:70:LEU:HD22	1:A:87:LEU:CD1	0.66	2.20	5	1
1:A:66:PHE:CD2	1:A:85:LEU:HD22	0.66	2.26	7	2
1:A:67:ALA:CA	1:A:85:LEU:HD23	0.66	2.21	8	2
1:A:70:LEU:HD12	1:A:87:LEU:CB	0.65	2.21	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LEU:CD1	1:A:87:LEU:HD13	0.65	2.08	4	1
1:A:70:LEU:CD1	1:A:85:LEU:HD21	0.65	2.21	10	1
1:A:52:PHE:CB	1:A:83:GLY:O	0.64	2.45	6	7
1:A:64:GLU:HA	1:A:80:LEU:HD22	0.64	1.68	6	2
1:A:85:LEU:HD13	1:A:85:LEU:O	0.64	1.93	8	1
1:A:49:ILE:HD11	1:A:87:LEU:CD2	0.64	2.22	10	1
1:A:85:LEU:C	1:A:85:LEU:HD22	0.64	2.13	10	2
1:A:55:LEU:HD22	1:A:83:GLY:C	0.63	2.13	10	2
1:A:55:LEU:HD11	1:A:80:LEU:HD11	0.63	1.69	8	1
1:A:42:ILE:HG23	1:A:47:THR:OG1	0.63	1.92	3	2
1:A:59:VAL:CB	1:A:63:GLU:HB3	0.63	2.23	8	7
1:A:70:LEU:CG	1:A:85:LEU:HD11	0.63	2.23	4	2
1:A:51:ASN:HB3	1:A:85:LEU:HD21	0.62	1.69	2	2
1:A:40:ILE:HG12	1:A:49:ILE:HD12	0.62	1.70	4	1
1:A:70:LEU:HD13	1:A:85:LEU:HD21	0.62	1.70	10	1
1:A:70:LEU:HD22	1:A:87:LEU:HD13	0.61	1.70	5	1
1:A:70:LEU:HD12	1:A:71:LEU:H	0.61	1.53	7	1
1:A:51:ASN:CB	1:A:85:LEU:HD21	0.61	2.26	2	1
1:A:70:LEU:HD12	1:A:87:LEU:CG	0.61	2.25	1	1
1:A:55:LEU:HD22	1:A:83:GLY:O	0.61	1.95	8	1
1:A:55:LEU:HD13	1:A:83:GLY:O	0.60	1.95	8	1
1:A:40:ILE:HD11	1:A:47:THR:HG21	0.60	1.73	5	1
1:A:40:ILE:CG2	1:A:49:ILE:HD12	0.59	2.27	9	1
1:A:41:LEU:C	1:A:47:THR:HG23	0.59	2.18	4	5
1:A:55:LEU:HD21	1:A:80:LEU:CD2	0.59	2.27	9	1
1:A:55:LEU:HD11	1:A:63:GLU:HB2	0.59	1.72	9	1
1:A:70:LEU:HD23	1:A:85:LEU:HD13	0.59	1.74	2	1
1:A:87:LEU:HD22	1:A:87:LEU:C	0.59	2.18	2	4
1:A:87:LEU:C	1:A:87:LEU:HD22	0.59	2.18	6	1
1:A:55:LEU:HD21	1:A:80:LEU:HD21	0.59	1.75	9	1
1:A:59:VAL:CA	1:A:63:GLU:HB3	0.58	2.28	3	10
1:A:80:LEU:HG	1:A:84:ARG:O	0.58	1.99	8	1
1:A:67:ALA:O	1:A:70:LEU:HG	0.58	1.97	7	1
1:A:71:LEU:HD13	1:A:71:LEU:C	0.58	2.18	8	2
1:A:71:LEU:HD23	1:A:77:ALA:N	0.57	2.13	6	1
1:A:71:LEU:HD22	1:A:78:GLY:H	0.57	1.59	5	4
1:A:64:GLU:CA	1:A:80:LEU:HD22	0.57	2.29	5	1
1:A:51:ASN:HB3	1:A:85:LEU:HD23	0.56	1.72	1	2
1:A:48:ILE:HG23	1:A:86:ILE:HG13	0.56	1.77	5	1
1:A:66:PHE:CE2	1:A:70:LEU:HD23	0.56	2.35	7	1
1:A:71:LEU:HD23	1:A:77:ALA:CA	0.56	2.31	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:PHE:CE1	1:A:83:GLY:HA3	0.56	2.35	8	3
1:A:71:LEU:HD22	1:A:78:GLY:N	0.56	2.15	7	5
1:A:49:ILE:CD1	1:A:87:LEU:HD22	0.56	2.30	8	1
1:A:49:ILE:CD1	1:A:87:LEU:HD23	0.55	2.31	10	1
1:A:59:VAL:HG12	1:A:63:GLU:HB3	0.55	1.76	1	7
1:A:52:PHE:CG	1:A:83:GLY:O	0.55	2.60	6	7
1:A:64:GLU:HB3	1:A:80:LEU:HD13	0.55	1.78	7	2
1:A:52:PHE:HB2	1:A:83:GLY:O	0.55	2.02	6	3
1:A:40:ILE:HG22	1:A:49:ILE:HB	0.55	1.77	9	1
1:A:70:LEU:HD13	1:A:87:LEU:CA	0.55	2.32	7	1
1:A:67:ALA:HB2	1:A:80:LEU:HD23	0.55	1.79	9	1
1:A:55:LEU:HD13	1:A:63:GLU:HB2	0.54	1.80	1	2
1:A:70:LEU:HD12	1:A:87:LEU:HB2	0.54	1.78	9	2
1:A:49:ILE:CG2	1:A:85:LEU:HG	0.54	2.32	9	4
1:A:56:ALA:HA	1:A:59:VAL:HG13	0.54	1.79	8	6
1:A:87:LEU:H	1:A:87:LEU:HD23	0.54	1.61	8	1
1:A:66:PHE:HE2	1:A:85:LEU:HD22	0.54	1.63	4	5
1:A:51:ASN:HB3	1:A:85:LEU:CD2	0.54	2.32	2	1
1:A:49:ILE:HD11	1:A:87:LEU:HD23	0.53	1.79	10	1
1:A:59:VAL:HB	1:A:63:GLU:CG	0.53	2.33	4	6
1:A:70:LEU:HG	1:A:85:LEU:HD11	0.53	1.79	4	3
1:A:66:PHE:O	1:A:67:ALA:C	0.53	2.47	3	10
1:A:87:LEU:C	1:A:87:LEU:HD13	0.53	2.24	1	1
1:A:70:LEU:O	1:A:74:THR:HG23	0.53	2.04	2	1
1:A:49:ILE:HB	1:A:85:LEU:HD13	0.52	1.79	10	2
1:A:55:LEU:HD22	1:A:83:GLY:CA	0.52	2.34	8	1
1:A:70:LEU:HD22	1:A:87:LEU:CB	0.52	2.33	10	1
1:A:67:ALA:HB2	1:A:80:LEU:CD1	0.52	2.25	8	1
1:A:49:ILE:HB	1:A:85:LEU:HD12	0.52	1.82	6	2
1:A:79:ASN:O	1:A:86:ILE:HB	0.52	2.05	5	4
1:A:48:ILE:HD12	1:A:48:ILE:N	0.51	2.21	7	1
1:A:70:LEU:HD22	1:A:87:LEU:HB3	0.51	1.82	6	2
1:A:87:LEU:H	1:A:87:LEU:HD13	0.51	1.64	3	3
1:A:79:ASN:O	1:A:86:ILE:HD12	0.51	2.05	3	1
1:A:67:ALA:HB3	1:A:80:LEU:HB2	0.51	1.82	5	3
1:A:64:GLU:HB2	1:A:80:LEU:HD13	0.50	1.83	10	1
1:A:67:ALA:HB3	1:A:80:LEU:CB	0.50	2.31	1	2
1:A:64:GLU:HG3	1:A:80:LEU:HD21	0.50	1.82	3	1
1:A:59:VAL:HB	1:A:63:GLU:HB3	0.50	1.84	8	2
1:A:66:PHE:HE2	1:A:70:LEU:HD23	0.50	1.67	7	1
1:A:59:VAL:CG1	1:A:63:GLU:HB3	0.50	2.37	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:ALA:HA	1:A:59:VAL:CG1	0.49	2.36	8	3
1:A:55:LEU:O	1:A:55:LEU:HD13	0.49	2.07	9	1
1:A:55:LEU:C	1:A:55:LEU:HD23	0.49	2.28	8	1
1:A:66:PHE:C	1:A:66:PHE:CD2	0.48	2.83	5	4
1:A:81:GLU:OE1	1:A:86:ILE:HD11	0.48	2.09	2	1
1:A:64:GLU:CA	1:A:80:LEU:HD13	0.48	2.39	6	4
1:A:87:LEU:HD22	1:A:88:GLN:N	0.48	2.23	1	1
1:A:70:LEU:O	1:A:74:THR:HG22	0.48	2.08	9	1
1:A:55:LEU:O	1:A:58:ALA:CB	0.48	2.61	8	1
1:A:71:LEU:HD12	1:A:78:GLY:H	0.48	1.68	3	1
1:A:66:PHE:CD2	1:A:67:ALA:N	0.48	2.82	2	6
1:A:80:LEU:HD13	1:A:80:LEU:C	0.48	2.29	9	1
1:A:64:GLU:N	1:A:80:LEU:HD22	0.48	2.24	5	1
1:A:71:LEU:HD21	1:A:77:ALA:N	0.48	2.23	8	1
1:A:59:VAL:HA	1:A:63:GLU:CB	0.47	2.39	1	8
1:A:85:LEU:C	1:A:85:LEU:HD13	0.47	2.29	10	2
1:A:71:LEU:HG	1:A:72:LYS:N	0.47	2.24	5	1
1:A:42:ILE:HD13	1:A:42:ILE:C	0.47	2.29	2	1
1:A:55:LEU:C	1:A:55:LEU:HD13	0.47	2.30	7	2
1:A:66:PHE:CD2	1:A:66:PHE:C	0.47	2.84	1	1
1:A:63:GLU:HG3	1:A:64:GLU:N	0.47	2.23	3	6
1:A:58:ALA:O	1:A:61:ARG:N	0.47	2.48	8	4
1:A:76:SER:CB	1:A:88:GLN:O	0.47	2.63	9	2
1:A:63:GLU:O	1:A:80:LEU:CD1	0.47	2.58	8	1
1:A:67:ALA:O	1:A:70:LEU:HB2	0.47	2.10	6	1
1:A:49:ILE:HD11	1:A:87:LEU:CG	0.46	2.39	10	1
1:A:64:GLU:HG2	1:A:80:LEU:HD13	0.46	1.86	2	1
1:A:52:PHE:CD1	1:A:83:GLY:HA3	0.46	2.46	8	1
1:A:70:LEU:HD13	1:A:86:ILE:C	0.46	2.31	6	1
1:A:52:PHE:CE1	1:A:83:GLY:HA2	0.46	2.45	10	7
1:A:55:LEU:HD12	1:A:85:LEU:HB3	0.46	1.87	2	1
1:A:68:LYS:O	1:A:71:LEU:HB3	0.46	2.11	3	2
1:A:70:LEU:HD11	1:A:86:ILE:O	0.46	2.11	7	1
1:A:61:ARG:O	1:A:62:ASP:HB2	0.46	2.11	8	1
1:A:71:LEU:HD13	1:A:72:LYS:N	0.46	2.26	8	1
1:A:55:LEU:CD1	1:A:85:LEU:CB	0.45	2.94	5	1
1:A:55:LEU:HD22	1:A:84:ARG:N	0.45	2.26	5	1
1:A:71:LEU:HD23	1:A:71:LEU:O	0.45	2.11	4	1
1:A:70:LEU:HB3	1:A:87:LEU:CB	0.45	2.41	6	1
1:A:70:LEU:HD13	1:A:85:LEU:CD1	0.45	2.41	8	1
1:A:84:ARG:HE	1:A:86:ILE:HD11	0.45	1.71	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ILE:H	1:A:42:ILE:HD13	0.45	1.72	8	1
1:A:71:LEU:HD23	1:A:71:LEU:C	0.45	2.32	3	1
1:A:49:ILE:HB	1:A:85:LEU:CD1	0.45	2.41	10	2
1:A:64:GLU:O	1:A:80:LEU:HD13	0.45	2.11	1	1
1:A:85:LEU:O	1:A:85:LEU:HG	0.45	2.12	9	1
1:A:66:PHE:HE2	1:A:85:LEU:HD13	0.45	1.67	3	1
1:A:40:ILE:HD13	1:A:40:ILE:C	0.45	2.32	5	1
1:A:87:LEU:HD13	1:A:87:LEU:H	0.45	1.72	7	2
1:A:49:ILE:HD12	1:A:85:LEU:CD1	0.45	2.42	8	1
1:A:49:ILE:CG2	1:A:85:LEU:O	0.44	2.65	3	2
1:A:71:LEU:CB	1:A:78:GLY:HA3	0.44	2.43	1	2
1:A:63:GLU:CD	1:A:64:GLU:N	0.44	2.70	10	2
1:A:59:VAL:N	1:A:63:GLU:HB3	0.44	2.26	1	1
1:A:64:GLU:C	1:A:80:LEU:HD13	0.44	2.32	1	1
1:A:61:ARG:O	1:A:62:ASP:CB	0.44	2.64	9	8
1:A:48:ILE:HG22	1:A:86:ILE:HG12	0.44	1.90	6	2
1:A:66:PHE:HE2	1:A:85:LEU:HG	0.44	1.72	10	1
1:A:55:LEU:O	1:A:55:LEU:HD23	0.44	2.12	8	1
1:A:49:ILE:HD11	1:A:87:LEU:HG	0.44	1.87	10	1
1:A:70:LEU:HD23	1:A:87:LEU:HD13	0.44	1.88	8	1
1:A:64:GLU:C	1:A:80:LEU:HD22	0.44	2.32	2	1
1:A:69:TYR:O	1:A:72:LYS:N	0.44	2.51	7	2
1:A:52:PHE:CA	1:A:83:GLY:O	0.44	2.66	2	2
1:A:40:ILE:HG22	1:A:47:THR:CG2	0.44	2.42	4	1
1:A:40:ILE:HG22	1:A:49:ILE:CG1	0.44	2.42	8	1
1:A:52:PHE:CD1	1:A:83:GLY:O	0.44	2.71	2	4
1:A:85:LEU:HD12	1:A:85:LEU:O	0.43	2.12	6	1
1:A:66:PHE:CD1	1:A:69:TYR:HB2	0.43	2.48	3	1
1:A:47:THR:O	1:A:86:ILE:CG2	0.43	2.65	7	5
1:A:63:GLU:HG2	1:A:64:GLU:N	0.43	2.27	8	1
1:A:85:LEU:O	1:A:85:LEU:HD12	0.43	2.12	7	1
1:A:49:ILE:N	1:A:49:ILE:HD12	0.43	2.28	10	1
1:A:87:LEU:HD23	1:A:87:LEU:O	0.43	2.13	5	1
1:A:63:GLU:OE1	1:A:63:GLU:N	0.43	2.52	8	1
1:A:87:LEU:H	1:A:87:LEU:CD1	0.43	2.26	3	1
1:A:56:ALA:O	1:A:59:VAL:CG1	0.43	2.62	4	1
1:A:70:LEU:CD2	1:A:87:LEU:HD13	0.43	2.44	8	1
1:A:55:LEU:HD22	1:A:83:GLY:HA2	0.43	1.89	8	1
1:A:40:ILE:CD1	1:A:47:THR:HG21	0.43	2.41	5	1
1:A:71:LEU:HD22	1:A:71:LEU:O	0.43	2.13	6	1
1:A:74:THR:HG21	1:A:87:LEU:HD12	0.43	1.89	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LEU:HB2	1:A:85:LEU:CD1	0.43	2.43	4	1
1:A:55:LEU:O	1:A:59:VAL:HG12	0.43	2.14	5	1
1:A:42:ILE:HD13	1:A:42:ILE:H	0.42	1.75	10	1
1:A:49:ILE:CD1	1:A:87:LEU:HD12	0.42	2.44	7	1
1:A:67:ALA:O	1:A:68:LYS:C	0.42	2.58	6	2
1:A:49:ILE:HD11	1:A:87:LEU:HD22	0.42	1.90	8	1
1:A:74:THR:OG1	1:A:87:LEU:HD11	0.42	2.15	4	1
1:A:49:ILE:HD12	1:A:85:LEU:HD11	0.42	1.90	8	1
1:A:64:GLU:HB2	1:A:80:LEU:HD22	0.42	1.91	7	1
1:A:48:ILE:HA	1:A:86:ILE:HG23	0.42	1.91	3	1
1:A:59:VAL:HA	1:A:63:GLU:HB3	0.42	1.91	8	2
1:A:70:LEU:HD12	1:A:87:LEU:HB3	0.42	1.90	2	1
1:A:40:ILE:HG22	1:A:49:ILE:CD1	0.42	2.45	8	1
1:A:66:PHE:HZ	1:A:70:LEU:HD12	0.42	1.74	8	1
1:A:70:LEU:CG	1:A:87:LEU:HB3	0.42	2.45	2	1
1:A:52:PHE:HA	1:A:55:LEU:HB2	0.41	1.92	1	1
1:A:71:LEU:HB2	1:A:78:GLY:N	0.41	2.30	6	2
1:A:71:LEU:HG	1:A:78:GLY:N	0.41	2.30	8	1
1:A:55:LEU:CD2	1:A:80:LEU:HD21	0.41	2.43	9	1
1:A:71:LEU:HD12	1:A:78:GLY:N	0.41	2.30	3	1
1:A:59:VAL:HB	1:A:63:GLU:HG2	0.41	1.91	10	1
1:A:52:PHE:CD1	1:A:83:GLY:HA2	0.41	2.51	4	4
1:A:70:LEU:HD23	1:A:87:LEU:CB	0.41	2.33	3	1
1:A:66:PHE:CZ	1:A:70:LEU:HG	0.41	2.51	6	1
1:A:59:VAL:HA	1:A:63:GLU:CA	0.41	2.45	8	1
1:A:52:PHE:CD1	1:A:52:PHE:O	0.41	2.73	8	2
1:A:87:LEU:C	1:A:87:LEU:CD2	0.41	2.89	6	1
1:A:80:LEU:HD12	1:A:80:LEU:O	0.41	2.15	10	1
1:A:81:GLU:CB	1:A:84:ARG:CG	0.40	2.99	4	1
1:A:56:ALA:CA	1:A:59:VAL:HG13	0.40	2.45	2	1
1:A:68:LYS:O	1:A:71:LEU:N	0.40	2.54	4	1
1:A:71:LEU:C	1:A:71:LEU:HD12	0.40	2.37	9	1
1:A:66:PHE:CE2	1:A:85:LEU:HG	0.40	2.51	8	1
1:A:63:GLU:CG	1:A:64:GLU:N	0.40	2.85	8	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	49/52 (94%)	39±1 (79±2%)	5±1 (11±2%)	5±1 (10±2%)	1	10
All	All	490/520 (94%)	385 (79%)	54 (11%)	51 (10%)	1	10

All 6 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	62	ASP	10
1	A	44	GLY	10
1	A	82	GLY	10
1	A	53	ARG	9
1	A	76	SER	9
1	A	83	GLY	3

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	40/43 (93%)	26±2 (66±6%)	14±2 (34±6%)	1	10
All	All	400/430 (93%)	262 (66%)	138 (34%)	1	10

All 33 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	71	LEU	9
1	A	85	LEU	9
1	A	53	ARG	8
1	A	54	GLU	7
1	A	87	LEU	6
1	A	70	LEU	6
1	A	68	LYS	6
1	A	41	LEU	6
1	A	50	ARG	5
1	A	88	GLN	5

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Mol	Chain	Res	Type	Models (Total)
1	A	61	ARG	5
1	A	84	ARG	5
1	A	46	ARG	5
1	A	81	GLU	5
1	A	43	GLU	5
1	A	59	VAL	4
1	A	80	LEU	4
1	A	72	LYS	4
1	A	55	LEU	4
1	A	45	ASN	3
1	A	42	ILE	3
1	A	73	GLU	3
1	A	76	SER	3
1	A	74	THR	3
1	A	52	PHE	3
1	A	65	PHE	2
1	A	79	ASN	2
1	A	40	ILE	2
1	A	57	LYS	2
1	A	69	TYR	1
1	A	48	ILE	1
1	A	62	ASP	1
1	A	63	GLU	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 ⓘ

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 51% for the well-defined parts and 50% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5294

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	769
Number of shifts mapped to atoms	378
Number of unparsed shifts	0
Number of shifts with mapping errors	391
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 391 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	115	LYS	H	7.99	-1.0	1
A	131	CYS	HB3	3.27	-1.0	2
A	123	GLU	HA	4.45	-1.0	1
A	135	GLY	CA	46.08	-1.0	1
A	97	LYS	N	117.4	-1.0	1
A	131	CYS	HA	4.44	-1.0	1
A	96	LEU	CA	58.35	-1.0	1
A	30	LYS	HA	3.73	-1.0	1
A	97	LYS	HA	3.8	-1.0	1
A	125	ARG	HA	4.3	-1.0	1
A	107	TYR	HB2	2.7	-1.0	2
A	23	ILE	HA	4.14	-1.0	1
A	91	ILE	HG22	0.75	-1.0	1
A	110	CYS	CA	60.65	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	127	HIS	CA	56.1	-1.0	1
A	134	CYS	H	9.7	-1.0	1
A	121	ILE	H	9.38	-1.0	1
A	126	VAL	HG23	1.65	-1.0	2
A	128	LEU	HA	4.96	-1.0	1
A	95	LEU	HD21	0.95	-1.0	2
A	103	PHE	HB3	3.35	-1.0	2
A	28	PHE	C	173.79	-1.0	1
A	127	HIS	HE1	7.65	-1.0	4
A	23	ILE	N	124.7	-1.0	1
A	114	GLY	HA2	3.92	-1.0	2
A	38	ILE	C	174.39	-1.0	1
A	122	LYS	N	124.05	-1.0	1
A	129	LEU	N	123.11	-1.0	1
A	111	ARG	N	130.72	-1.0	1
A	131	CYS	N	128.79	-1.0	1
A	113	CYS	C	176.17	-1.0	1
A	140	ILE	H	8.11	-1.0	1
A	134	CYS	C	176.42	-1.0	1
A	27	VAL	N	121.82	-1.0	1
A	138	ARG	H	8.42	-1.0	1
A	108	VAL	HG13	0.54	-1.0	2
A	99	ARG	H	8.08	-1.0	1
A	38	ILE	HA	3.96	-1.0	1
A	112	GLU	N	120.72	-1.0	1
A	104	LEU	CA	57.9	-1.0	1
A	126	VAL	HA	4.29	-1.0	1
A	31	ASP	HA	4.5	-1.0	1
A	134	CYS	CA	58.83	-1.0	1
A	38	ILE	H	7.44	-1.0	1
A	128	LEU	H	9.13	-1.0	1
A	108	VAL	HG23	0.78	-1.0	2
A	111	ARG	HB2	1.69	-1.0	2
A	132	MET	C	174.21	-1.0	1
A	31	ASP	HB3	2.62	-1.0	2
A	121	ILE	HG21	0.81	-1.0	4
A	26	TYR	HB2	2.9	-1.0	2
A	33	PHE	HB3	3.15	-1.0	2
A	125	ARG	H	8.83	-1.0	1
A	98	SER	C	179.0	-1.0	1
A	108	VAL	N	117.68	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	98	SER	HB2	4.32	-1.0	2
A	138	ARG	HA	5.03	-1.0	1
A	127	HIS	HB3	2.98	-1.0	2
A	117	ASP	H	6.74	-1.0	1
A	127	HIS	HB2	2.72	-1.0	2
A	91	ILE	HB	1.5	-1.0	1
A	26	TYR	C	175.07	-1.0	1
A	131	CYS	HB2	2.73	-1.0	2
A	126	VAL	HG11	1.83	-1.0	2
A	107	TYR	HB3	3.18	-1.0	2
A	107	TYR	CA	58.59	-1.0	1
A	133	ALA	H	9.33	-1.0	1
A	119	LYS	HA	4.75	-1.0	1
A	128	LEU	HD13	0.72	-1.0	2
A	107	TYR	N	110.21	-1.0	1
A	103	PHE	C	176.8	-1.0	1
A	128	LEU	HD12	0.72	-1.0	2
A	91	ILE	HG23	0.75	-1.0	1
A	122	LYS	H	8.38	-1.0	1
A	126	VAL	HG22	1.65	-1.0	2
A	133	ALA	HA	4.44	-1.0	1
A	112	GLU	CA	57.87	-1.0	1
A	112	GLU	H	9.14	-1.0	1
A	21	SER	H	8.28	-1.0	1
A	135	GLY	HA3	3.82	-1.0	2
A	111	ARG	H	9.07	-1.0	1
A	95	LEU	HD12	0.91	-1.0	2
A	23	ILE	HG23	0.95	-1.0	4
A	120	ILE	HA	4.87	-1.0	1
A	131	CYS	C	177.17	-1.0	1
A	108	VAL	HA	3.89	-1.0	1
A	128	LEU	HD21	0.76	-1.0	2
A	30	LYS	C	177.14	-1.0	1
A	109	ILE	CA	61.0	-1.0	1
A	91	ILE	H	7.95	-1.0	1
A	135	GLY	C	173.44	-1.0	1
A	123	GLU	H	8.5	-1.0	1
A	95	LEU	HB2	1.82	-1.0	2
A	127	HIS	HD1	6.68	-1.0	4
A	131	CYS	CA	59.6	-1.0	1
A	98	SER	CA	62.88	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	92	SER	H	8.24	-1.0	1
A	30	LYS	CA	60.39	-1.0	1
A	98	SER	H	7.91	-1.0	1
A	38	ILE	N	110.8	-1.0	1
A	137	ILE	HG23	0.82	-1.0	4
A	103	PHE	H	8.2	-1.0	1
A	91	ILE	HD13	0.96	-1.0	1
A	123	GLU	HG2	1.65	-1.0	2
A	118	THR	HG21	1.01	-1.0	1
A	23	ILE	H	7.19	-1.0	1
A	104	LEU	N	117.62	-1.0	1
A	120	ILE	H	8.58	-1.0	1
A	117	ASP	HB2	2.36	-1.0	2
A	91	ILE	C	174.45	-1.0	1
A	130	LYS	HB2	1.7	-1.0	2
A	91	ILE	HD11	0.96	-1.0	1
A	129	LEU	H	9.14	-1.0	1
A	111	ARG	HA	3.98	-1.0	1
A	106	GLU	C	177.22	-1.0	1
A	134	CYS	HB2	2.57	-1.0	2
A	93	PRO	HA	4.05	-1.0	1
A	108	VAL	HG22	0.78	-1.0	2
A	135	GLY	H	7.3	-1.0	1
A	111	ARG	HB3	1.87	-1.0	2
A	109	ILE	HG22	0.55	-1.0	4
A	115	LYS	HA	4.35	-1.0	2
A	33	PHE	HB2	3.43	-1.0	2
A	137	ILE	N	119.35	-1.0	1
A	94	GLU	HA	3.95	-1.0	1
A	109	ILE	N	119.9	-1.0	1
A	95	LEU	HG	1.74	-1.0	1
A	26	TYR	HA	4.43	-1.0	1
A	33	PHE	C	177.01	-1.0	1
A	105	ARG	H	8.08	-1.0	1
A	21	SER	N	116.38	-1.0	1
A	126	VAL	HG12	1.83	-1.0	2
A	29	GLN	HB2	1.74	-1.0	2
A	136	ALA	H	8.86	-1.0	1
A	125	ARG	N	124.55	-1.0	1
A	113	CYS	N	118.89	-1.0	1
A	124	GLY	CA	46.8	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	138	ARG	N	123.15	-1.0	1
A	114	GLY	N	109.64	-1.0	1
A	92	SER	N	120.2	-1.0	1
A	137	ILE	HG22	0.82	-1.0	4
A	31	ASP	H	7.87	-1.0	1
A	27	VAL	C	176.44	-1.0	1
A	135	GLY	HA2	4.3	-1.0	2
A	133	ALA	HB3	1.47	-1.0	1
A	29	GLN	CA	55.41	-1.0	1
A	129	LEU	HB2	1.77	-1.0	2
A	101	ASN	N	119.0	-1.0	1
A	23	ILE	HG22	0.95	-1.0	4
A	109	ILE	HA	3.51	-1.0	1
A	113	CYS	HB3	2.69	-1.0	2
A	133	ALA	N	126.58	-1.0	1
A	133	ALA	HB1	1.47	-1.0	1
A	138	ARG	CA	55.73	-1.0	1
A	96	LEU	H	7.82	-1.0	1
A	128	LEU	CA	53.3	-1.0	1
A	100	ILE	H	8.42	-1.0	1
A	95	LEU	HD13	0.91	-1.0	2
A	25	ASP	N	119.93	-1.0	1
A	104	LEU	H	8.39	-1.0	1
A	128	LEU	N	121.33	-1.0	1
A	107	TYR	H	7.93	-1.0	1
A	27	VAL	HG21	0.74	-1.0	1
A	137	ILE	HA	5.41	-1.0	1
A	124	GLY	HA2	3.99	-1.0	2
A	126	VAL	CA	61.92	-1.0	1
A	28	PHE	HB3	3.08	-1.0	2
A	118	THR	HA	5.35	-1.0	1
A	110	CYS	H	8.45	-1.0	1
A	38	ILE	CA	62.0	-1.0	1
A	29	GLN	H	8.04	-1.0	1
A	137	ILE	HB	1.58	-1.0	1
A	97	LYS	HB2	1.88	-1.0	2
A	126	VAL	N	119.5	-1.0	1
A	123	GLU	HG3	1.83	-1.0	2
A	94	GLU	HG2	2.3	-1.0	2
A	122	LYS	HB3	1.56	-1.0	2
A	126	VAL	C	173.44	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	112	GLU	HA	4.34	-1.0	1
A	134	CYS	HB3	3.27	-1.0	2
A	28	PHE	H	8.01	-1.0	1
A	104	LEU	C	178.98	-1.0	1
A	122	LYS	CA	55.37	-1.0	1
A	95	LEU	HD23	0.95	-1.0	2
A	103	PHE	N	122.47	-1.0	1
A	140	ILE	CA	59.3	-1.0	1
A	97	LYS	H	8.55	-1.0	1
A	122	LYS	C	175.04	-1.0	1
A	33	PHE	N	124.7	-1.0	1
A	29	GLN	C	177.75	-1.0	1
A	128	LEU	C	173.79	-1.0	1
A	104	LEU	HA	4.45	-1.0	1
A	27	VAL	HB	1.85	-1.0	1
A	27	VAL	HG11	0.7	-1.0	1
A	113	CYS	H	8.8	-1.0	1
A	121	ILE	N	126.96	-1.0	1
A	124	GLY	HA3	3.54	-1.0	2
A	22	GLN	C	174.6	-1.0	1
A	21	SER	CA	58.49	-1.0	1
A	124	GLY	H	8.76	-1.0	1
A	29	GLN	HA	4.28	-1.0	1
A	126	VAL	HG13	1.83	-1.0	2
A	110	CYS	HA	3.88	-1.0	1
A	135	GLY	N	112.42	-1.0	1
A	30	LYS	N	117.56	-1.0	1
A	125	ARG	CA	56.51	-1.0	1
A	23	ILE	HB	1.85	-1.0	2
A	127	HIS	N	123.15	-1.0	1
A	91	ILE	HG21	0.75	-1.0	1
A	110	CYS	N	131.24	-1.0	1
A	114	GLY	CA	45.34	-1.0	1
A	134	CYS	HA	5.01	-1.0	1
A	25	ASP	C	175.02	-1.0	1
A	29	GLN	N	124.69	-1.0	1
A	117	ASP	CA	53.35	-1.0	1
A	98	SER	N	115.8	-1.0	1
A	113	CYS	HB2	3.15	-1.0	2
A	25	ASP	CA	54.83	-1.0	1
A	23	ILE	CA	63.07	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	126	VAL	H	7.75	-1.0	1
A	103	PHE	HA	3.61	-1.0	1
A	27	VAL	HG22	0.74	-1.0	1
A	129	LEU	CA	53.82	-1.0	1
A	28	PHE	HB2	2.98	-1.0	2
A	136	ALA	HB1	1.39	-1.0	1
A	136	ALA	HB3	1.39	-1.0	1
A	91	ILE	HD12	0.96	-1.0	1
A	27	VAL	CA	62.96	-1.0	1
A	132	MET	H	9.37	-1.0	1
A	101	ASN	H	8.19	-1.0	1
A	130	LYS	HA	4.94	-1.0	1
A	136	ALA	HA	4.2	-1.0	1
A	33	PHE	H	7.19	-1.0	1
A	118	THR	HG23	1.01	-1.0	1
A	108	VAL	H	7.44	-1.0	1
A	123	GLU	N	127.96	-1.0	1
A	91	ILE	N	128.51	-1.0	1
A	130	LYS	N	129.34	-1.0	1
A	105	ARG	CA	56.8	-1.0	1
A	123	GLU	HB3	2.06	-1.0	2
A	33	PHE	HA	4.2	-1.0	1
A	131	CYS	H	9.02	-1.0	1
A	98	SER	HA	4.13	-1.0	1
A	123	GLU	HB2	2.01	-1.0	2
A	134	CYS	N	120.83	-1.0	1
A	119	LYS	HB2	1.61	-1.0	2
A	95	LEU	HD22	0.95	-1.0	2
A	123	GLU	C	175.46	-1.0	1
A	100	ILE	N	121.42	-1.0	1
A	122	LYS	HB2	1.29	-1.0	2
A	126	VAL	HB	2.21	-1.0	1
A	121	ILE	CA	59.39	-1.0	1
A	27	VAL	HA	3.88	-1.0	1
A	119	LYS	HG2	1.36	-1.0	2
A	95	LEU	C	178.64	-1.0	1
A	107	TYR	HD1	6.54	-1.0	3
A	91	ILE	HA	4.21	-1.0	1
A	96	LEU	C	178.23	-1.0	1
A	28	PHE	N	122.87	-1.0	1
A	118	THR	N	110.48	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	129	LEU	C	174.7	-1.0	1
A	122	LYS	HA	4.6	-1.0	1
A	121	ILE	HA	4.56	-1.0	1
A	25	ASP	HB3	3.75	-1.0	2
A	125	ARG	HB2	1.76	-1.0	2
A	26	TYR	N	119.05	-1.0	1
A	110	CYS	HB2	3.13	-1.0	2
A	128	LEU	HD11	0.72	-1.0	2
A	25	ASP	HA	4.65	-1.0	1
A	126	VAL	HG21	1.65	-1.0	2
A	107	TYR	C	175.04	-1.0	1
A	108	VAL	HG21	0.78	-1.0	2
A	132	MET	HA	4.4	-1.0	1
A	128	LEU	HB2	1.44	-1.0	2
A	95	LEU	CA	57.9	-1.0	1
A	117	ASP	N	123.11	-1.0	1
A	117	ASP	HB3	2.73	-1.0	2
A	28	PHE	HA	4.55	-1.0	1
A	95	LEU	HD11	0.91	-1.0	2
A	93	PRO	HB3	2.05	-1.0	2
A	101	ASN	HA	4.56	-1.0	1
A	133	ALA	HB2	1.47	-1.0	1
A	117	ASP	HA	4.74	-1.0	1
A	127	HIS	H	8.51	-1.0	1
A	118	THR	C	174.63	-1.0	1
A	113	CYS	HA	5.0	-1.0	1
A	123	GLU	CA	55.37	-1.0	1
A	27	VAL	HG23	0.74	-1.0	1
A	119	LYS	N	121.8	-1.0	1
A	29	GLN	HG2	2.07	-1.0	2
A	121	ILE	C	173.42	-1.0	1
A	31	ASP	CA	59.29	-1.0	1
A	21	SER	HA	4.46	-1.0	1
A	112	GLU	C	177.17	-1.0	1
A	132	MET	HB3	2.33	-1.0	2
A	115	LYS	N	125.25	-1.0	1
A	132	MET	N	128.95	-1.0	1
A	136	ALA	HB2	1.39	-1.0	1
A	130	LYS	CA	54.2	-1.0	1
A	117	ASP	C	176.67	-1.0	1
A	109	ILE	C	175.36	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	108	VAL	HG11	0.54	-1.0	2
A	94	GLU	N	115.56	-1.0	1
A	130	LYS	C	173.5	-1.0	1
A	118	THR	HG22	1.01	-1.0	1
A	121	ILE	HB	1.84	-1.0	1
A	140	ILE	HA	4.17	-1.0	1
A	21	SER	HB2	3.84	-1.0	2
A	107	TYR	HE1	6.81	-1.0	3
A	118	THR	H	8.25	-1.0	1
A	114	GLY	H	8.37	-1.0	1
A	26	TYR	HE1	6.74	-1.0	3
A	100	ILE	HA	3.84	-1.0	1
A	121	ILE	HG23	0.81	-1.0	4
A	110	CYS	C	173.5	-1.0	1
A	109	ILE	HG21	0.55	-1.0	4
A	127	HIS	C	173.86	-1.0	1
A	124	GLY	N	116.08	-1.0	1
A	137	ILE	CA	59.7	-1.0	1
A	136	ALA	N	126.91	-1.0	1
A	91	ILE	HG12	1.74	-1.0	2
A	27	VAL	HG13	0.7	-1.0	1
A	109	ILE	H	8.01	-1.0	1
A	130	LYS	H	9.25	-1.0	1
A	28	PHE	CA	58.11	-1.0	1
A	30	LYS	HB2	1.25	-1.0	2
A	118	THR	CA	58.95	-1.0	1
A	121	ILE	HG22	0.81	-1.0	4
A	100	ILE	CA	58.87	-1.0	1
A	94	GLU	C	177.51	-1.0	1
A	108	VAL	HB	2.06	-1.0	1
A	94	GLU	HB2	1.97	-1.0	2
A	127	HIS	HA	5.18	-1.0	1
A	25	ASP	HB2	2.76	-1.0	2
A	97	LYS	CA	61.0	-1.0	1
A	99	ARG	CA	55.88	-1.0	1
A	137	ILE	H	8.3	-1.0	1
A	119	LYS	CA	54.89	-1.0	1
A	113	CYS	CA	58.6	-1.0	1
A	109	ILE	HG23	0.55	-1.0	4
A	95	LEU	N	122.76	-1.0	1
A	125	ARG	C	175.41	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	92	SER	CA	65.74	-1.0	1
A	137	ILE	HG21	0.82	-1.0	4
A	97	LYS	C	178.04	-1.0	1
A	23	ILE	HG21	0.95	-1.0	4
A	93	PRO	HB2	1.88	-1.0	2
A	112	GLU	HB2	1.84	-1.0	2
A	103	PHE	HB2	3.02	-1.0	2
A	133	ALA	CA	54.66	-1.0	1
A	95	LEU	HA	4.2	-1.0	1
A	109	ILE	HB	1.04	-1.0	1
A	26	TYR	HD1	6.98	-1.0	3
A	105	ARG	HA	4.06	-1.0	1
A	94	GLU	H	8.43	-1.0	1
A	107	TYR	HA	4.44	-1.0	1
A	115	LYS	HB2	1.33	-1.0	2
A	26	TYR	H	7.82	-1.0	1
A	137	ILE	C	175.07	-1.0	1
A	31	ASP	N	111.98	-1.0	1
A	133	ALA	C	178.09	-1.0	1
A	118	THR	HB	3.8	-1.0	1
A	111	ARG	CA	58.08	-1.0	1
A	132	MET	CA	55.93	-1.0	1
A	128	LEU	HD23	0.76	-1.0	2
A	132	MET	HB2	2.02	-1.0	2
A	119	LYS	H	9.28	-1.0	1
A	128	LEU	HD22	0.76	-1.0	2
A	91	ILE	CA	59.54	-1.0	1
A	94	GLU	CA	59.97	-1.0	1
A	108	VAL	HG12	0.54	-1.0	2
A	106	GLU	CA	57.87	-1.0	1
A	111	ARG	C	175.86	-1.0	1
A	25	ASP	H	8.22	-1.0	1
A	26	TYR	CA	58.47	-1.0	1
A	108	VAL	CA	64.7	-1.0	1
A	115	LYS	CA	52.37	-1.0	1
A	95	LEU	H	7.49	-1.0	1
A	30	LYS	H	8.16	-1.0	1
A	93	PRO	CA	65.83	-1.0	1
A	112	GLU	HB3	2.12	-1.0	2
A	31	ASP	HB2	1.46	-1.0	2
A	103	PHE	CA	62.18	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	27	VAL	H	7.71	-1.0	1
A	26	TYR	HB3	2.96	-1.0	2
A	129	LEU	HA	4.85	-1.0	1
A	140	ILE	N	115.8	-1.0	1
A	136	ALA	CA	54.18	-1.0	1
A	33	PHE	CA	61.68	-1.0	1
A	120	ILE	CA	55.73	-1.0	1
A	27	VAL	HG12	0.7	-1.0	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
$^{13}\text{C}_\alpha$	107	-0.58 ± 0.21	Should be applied
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	74	0.38 ± 0.24	None needed (< 0.5 ppm)
^{15}N	103	-0.22 ± 0.43	None needed (< 0.5 ppm)

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 51%, i.e. 324 atoms were assigned a chemical shift out of a possible 638. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	219/245 (89%)	94/98 (96%)	77/98 (79%)	48/49 (98%)
Sidechain	105/358 (29%)	105/208 (50%)	0/127 (0%)	0/23 (0%)
Aromatic	0/35 (0%)	0/19 (0%)	0/16 (0%)	0/0 (—%)
Overall	324/638 (51%)	199/325 (61%)	77/241 (32%)	48/72 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 50%, i.e. 347 atoms were assigned a chemical shift out of a possible 696. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	234/260 (90%)	100/104 (96%)	83/104 (80%)	51/52 (98%)
Sidechain	113/401 (28%)	113/234 (48%)	0/138 (0%)	0/29 (0%)
Aromatic	0/35 (0%)	0/19 (0%)	0/16 (0%)	0/0 (—%)

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	Total	¹ H	¹³ C	¹⁵ N
Overall	347/696 (50%)	213/357 (60%)	83/258 (32%)	51/81 (63%)

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, ppm	Expected range, ppm	Z-score
1	A	84	ARG	HG2	3.23	2.92 – 0.22	6.1

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:

