



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:34 PM UTC

PDB ID : 6XQJ / pdb_00006xqj
BMRB ID : 30769
Title : Structure of HIV-1 Vpr in complex with the human nucleotide excision repair protein hHR23A
Authors : Byeon, I.-J.L.; Calero, G.; Wu, Y.; Byeon, C.H.; Gronenborn, A.M.
Deposited on : 2020-07-09

This is a wwPDB NMR Structure Validation Summary 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 ⓘ 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

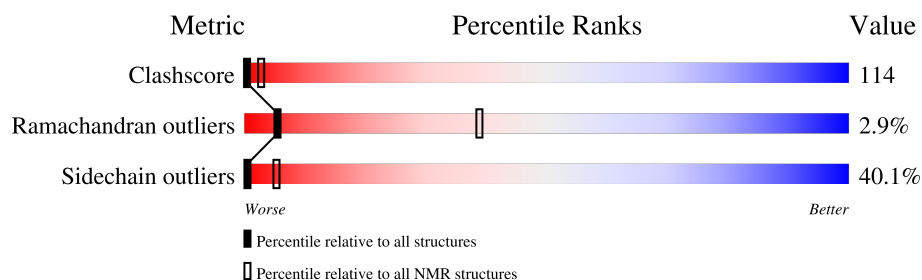
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

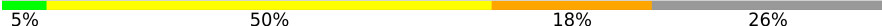
The overall completeness of chemical shifts assignment is 82%.

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	234	 5% 50% 18% 26%

2 Ensemble composition and analysis

This entry contains 55 models. Model 43 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:14-A:79, A:230-A:288, A:314-A:360 (172)	0.90	43

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 13 clusters and 2 single-model clusters were found.

Cluster number	Models
1	7, 16, 21, 22, 26, 28, 36, 38, 48, 53
2	5, 19, 23, 25, 27, 32, 43, 45, 50
3	3, 4, 6, 14, 15, 34, 41
4	2, 8, 11, 12, 29, 47
5	35, 37, 46, 51
6	1, 9, 42
7	17, 54
8	24, 44
9	33, 39
10	10, 13
11	18, 49
12	31, 55
13	20, 52
Single-model clusters	30; 40

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2856 atoms, of which 1415 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein Vpr,UV excision repair protein RAD23 homolog A.

Mol	Chain	Residues	Atoms						Trace
1	A	173	Total	C	H	N	O	S	0
			2855	925	1415	252	259	4	

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	GLY	-	linker	UNP P12520
A	81	GLY	-	linker	UNP P12520
A	82	SER	-	linker	UNP P12520
A	83	GLY	-	linker	UNP P12520
A	84	GLY	-	linker	UNP P12520
A	85	SER	-	linker	UNP P12520
A	364	LEU	-	expression tag	UNP P54725
A	365	GLU	-	expression tag	UNP P54725
A	366	HIS	-	expression tag	UNP P54725
A	367	HIS	-	expression tag	UNP P54725
A	368	HIS	-	expression tag	UNP P54725
A	369	HIS	-	expression tag	UNP P54725
A	370	HIS	-	expression tag	UNP P54725
A	371	HIS	-	expression tag	UNP P54725

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

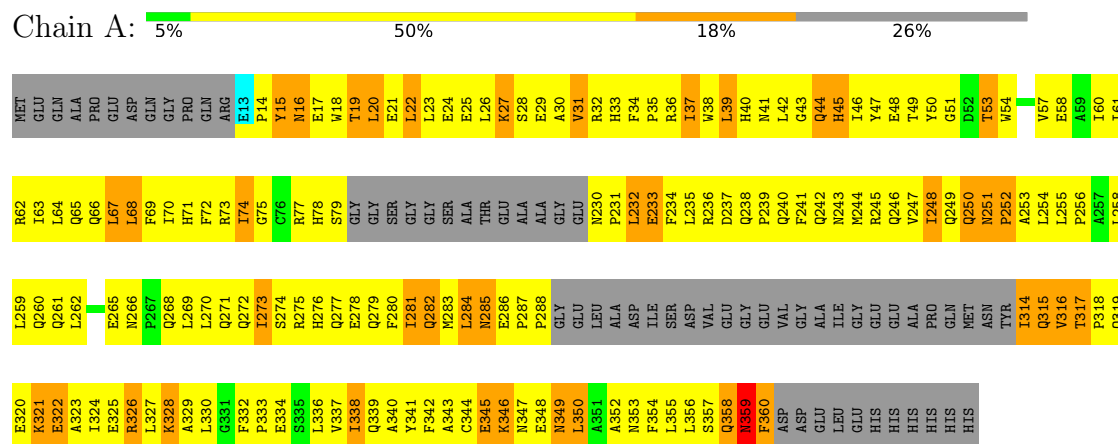
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

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.

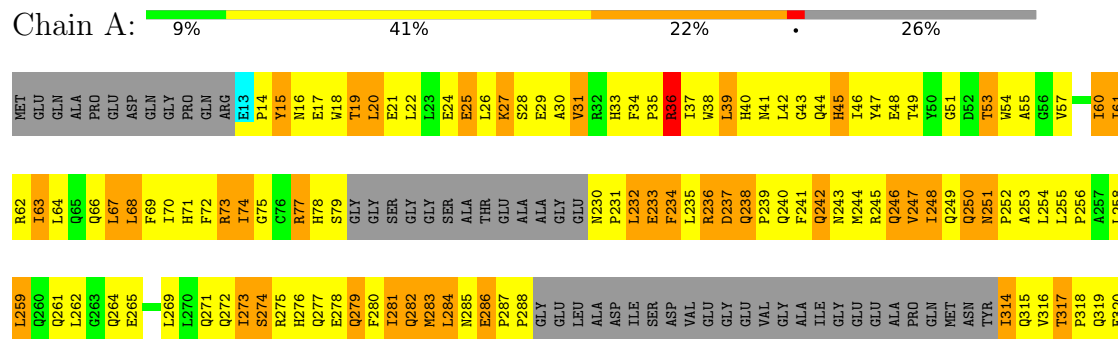
- Molecule 1: Protein Vpr,UV excision repair protein RAD23 homolog A



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 43. Colouring as in section 4.1 above.

- Molecule 1: Protein Vpr,UV excision repair protein RAD23 homolog A



K321	E322	A323	I324	E325	R326	L327	K328	A329	L330	G331	F332	P333	E334	S335	L336	Y337	I338	Q339	K340	Y341	F342	A343	C344	E345	K346	N347	E348	N349	L350	K351	A352	N353	F354	L355	L356	S357	Q358	N359	F360	ASP	ASP	GLU	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

5 Refinement protocol and experimental data overview

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

Of the 960 calculated structures, 55 were deposited, based on the following criterion: *lowest energy structures*.

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	2.48

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	2569
Number of shifts mapped to atoms	2067
Number of unparsed shifts	0
Number of shifts with mapping errors	502
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.60±0.00	0±0/1465 (0.0± 0.0%)	1.12±0.01	0±0/1985 (0.0± 0.0%)
All	All	0.60	0/80575 (0.0%)	1.12	4/109175 (0.0%)

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	360	PHE	CA-CB-CG	-5.12	108.67	113.80	49	1
1	A	241	PHE	CA-CB-CG	-5.12	108.68	113.80	40	2
1	A	342	PHE	CA-CB-CG	-5.10	108.70	113.80	24	1

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	1431	1409	1410	323±24
All	All	78760	77495	77550	17789

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 114.

5 of 3930 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:VAL:HG23	1:A:39:LEU:HD22	1.12	1.18	54	14
1:A:316:VAL:HG13	1:A:342:PHE:CZ	1.09	1.81	52	38
1:A:31:VAL:HG22	1:A:39:LEU:HD21	1.07	1.15	55	10
1:A:258:LEU:HD13	1:A:259:LEU:N	1.07	1.63	26	1
1:A:248:ILE:HD11	1:A:255:LEU:HD13	1.07	1.19	51	10

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	167/234 (71%)	137±4 (82±2%)	25±4 (15±2%)	5±1 (3±1%)	5	39
All	All	9185/12870 (71%)	7533 (82%)	1385 (15%)	267 (3%)	5	39

5 of 26 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	359	ASN	51
1	A	15	TYR	37
1	A	252	PRO	37
1	A	315	GLN	26
1	A	322	GLU	24

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	155/200 (78%)	91±13 (59±9%)	61±10 (39±6%)	0	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	8370/11000 (76%)	5014 (60%)	3356 (40%)	0 5

5 of 131 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	HIS	54
1	A	281	ILE	54
1	A	321	LYS	54
1	A	19	THR	53
1	A	284	LEU	53

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 82% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *BMRB_PDBdep_temp.txt*

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	2569
Number of shifts mapped to atoms	2067
Number of unparsed shifts	0
Number of shifts with mapping errors	502
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- No matching atom found in the structure. First 5 (of 502) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	HA	4.003	0.000	1
1	A	1	MET	HE1	2.109	0.003	1
1	A	1	MET	HE2	2.109	0.003	1
1	A	1	MET	HE3	2.109	0.003	1
1	A	1	MET	CA	55.482	0.000	1
1	A	1	MET	CE	16.793	0.032	1
1	A	2	GLU	HA	4.385	0.004	1
1	A	2	GLU	CA	56.543	0.000	1
1	A	3	GLN	H	8.53	0.005	1
1	A	3	GLN	HA	4.355	0.005	1
1	A	3	GLN	HB2	2.088	0.016	2
1	A	3	GLN	HB3	1.992	0.010	2
1	A	3	GLN	HE21	7.534	0.002	1
1	A	3	GLN	HE22	6.85	0.014	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	GLN	HG3	2.37	0.004	1
1	A	3	GLN	CA	55.586	0.048	1
1	A	3	GLN	CB	29.382	0.068	1
1	A	3	GLN	CG	33.859	0.007	1
1	A	3	GLN	N	121.976	0.095	1
1	A	3	GLN	NE2	112.599	0.039	1
1	A	4	ALA	H	8.557	0.004	1
1	A	4	ALA	HA	4.599	0.013	1
1	A	4	ALA	HB1	1.39	0.009	1
1	A	4	ALA	HB2	1.39	0.009	1
1	A	4	ALA	HB3	1.39	0.009	1
1	A	4	ALA	CA	50.568	0.033	1
1	A	4	ALA	CB	18.101	0.071	1
1	A	4	ALA	N	127.823	0.031	1
1	A	5	PRO	HA	4.412	0.004	1
1	A	5	PRO	HB2	1.936	0.009	2
1	A	5	PRO	HB3	2.312	0.005	2
1	A	5	PRO	HD2	3.821	0.007	2
1	A	5	PRO	HD3	3.673	0.006	2
1	A	5	PRO	HG2	2.029	0.002	1
1	A	5	PRO	CA	63.402	0.023	1
1	A	5	PRO	CB	32.064	0.066	1
1	A	5	PRO	CD	50.349	0.040	1
1	A	5	PRO	CG	27.07	0.019	1
1	A	6	GLU	H	8.669	0.007	1
1	A	6	GLU	HA	4.243	0.007	1
1	A	6	GLU	HB2	1.95	0.001	2
1	A	6	GLU	HB3	2.052	0.001	2
1	A	6	GLU	HG3	2.303	0.004	1
1	A	6	GLU	CA	56.942	0.110	1
1	A	6	GLU	CB	30.128	0.003	1
1	A	6	GLU	CG	36.309	0.000	1
1	A	6	GLU	N	120.519	0.075	1
1	A	7	ASP	H	8.314	0.007	1
1	A	7	ASP	HA	4.614	0.007	1
1	A	7	ASP	HB2	2.72	0.001	2
1	A	7	ASP	HB3	2.676	0.012	2
1	A	7	ASP	CA	54.529	0.049	1
1	A	7	ASP	CB	41.224	0.087	1
1	A	7	ASP	N	121.175	0.038	1
1	A	8	GLN	H	8.296	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	GLN	HA	4.374	0.006	1
1	A	8	GLN	HB2	2.207	0.002	2
1	A	8	GLN	HB3	1.977	0.012	2
1	A	8	GLN	HE21	7.536	0.004	1
1	A	8	GLN	HE22	6.834	0.002	1
1	A	8	GLN	HG3	2.389	0.006	1
1	A	8	GLN	CA	55.855	0.024	1
1	A	8	GLN	CB	29.458	0.031	1
1	A	8	GLN	CG	33.891	0.076	1
1	A	8	GLN	N	120.802	0.068	1
1	A	9	GLY	H	8.33	0.004	1
1	A	9	GLY	HA3	4.099	0.007	1
1	A	9	GLY	CA	44.79	0.047	1
1	A	9	GLY	N	109.856	0.057	1
1	A	10	PRO	HA	4.428	0.004	1
1	A	10	PRO	HB3	2.274	0.001	1
1	A	10	PRO	HD3	3.624	0.005	1
1	A	10	PRO	HG2	1.994	0.002	1
1	A	10	PRO	CA	63.461	0.076	1
1	A	10	PRO	CB	31.973	0.057	1
1	A	10	PRO	CD	49.843	0.080	1
1	A	10	PRO	CG	27.318	0.008	1
1	A	11	GLN	H	8.536	0.006	1
1	A	11	GLN	HA	4.314	0.008	1
1	A	11	GLN	HB2	1.99	0.008	2
1	A	11	GLN	HB3	2.115	0.005	2
1	A	11	GLN	HE21	7.482	0.005	1
1	A	11	GLN	HE22	6.827	0.005	1
1	A	11	GLN	HG3	2.365	0.008	1
1	A	11	GLN	CA	55.886	0.037	1
1	A	11	GLN	CB	29.52	0.021	1
1	A	11	GLN	CG	33.816	0.022	1
1	A	11	GLN	N	120.468	0.048	1
1	A	11	GLN	NE2	112.749	0.067	1
1	A	12	ARG	H	8.365	0.008	1
1	A	12	ARG	HA	4.371	0.004	1
1	A	12	ARG	HB2	1.748	0.005	2
1	A	12	ARG	HB3	1.848	0.007	2
1	A	12	ARG	HD2	3.177	0.005	1
1	A	12	ARG	HE	7.273	0.013	1
1	A	12	ARG	HG2	1.639	0.011	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	ARG	HG3	1.599	0.006	2
1	A	12	ARG	CA	55.811	0.038	1
1	A	12	ARG	CB	31.098	0.106	1
1	A	12	ARG	CD	43.294	0.036	1
1	A	12	ARG	CG	27.192	0.094	1
1	A	12	ARG	N	122.095	0.057	1
1	A	12	ARG	NE	84.664	0.078	1
1	A	80	GLY	H	8.636	0.013	1
1	A	80	GLY	HA3	4.04	0.013	1
1	A	80	GLY	CA	45.498	0.025	1
1	A	80	GLY	N	111.087	0.051	1
1	A	81	GLY	H	8.435	0.005	1
1	A	81	GLY	HA3	4.077	0.005	1
1	A	81	GLY	CA	45.398	0.083	1
1	A	81	GLY	N	109.033	0.066	1
1	A	82	SER	H	8.528	0.004	1
1	A	82	SER	HA	4.524	0.019	1
1	A	82	SER	HB3	3.913	0.002	1
1	A	82	SER	CA	58.779	0.037	1
1	A	82	SER	CB	63.857	0.024	1
1	A	82	SER	N	116.142	0.092	1
1	A	83	GLY	H	8.624	0.014	1
1	A	83	GLY	HA3	4.044	0.012	1
1	A	83	GLY	CA	45.443	0.050	1
1	A	83	GLY	N	111.107	0.032	1
1	A	84	GLY	H	8.308	0.004	1
1	A	84	GLY	HA3	4.028	0.005	1
1	A	84	GLY	CA	45.218	0.075	1
1	A	84	GLY	N	108.993	0.090	1
1	A	85	SER	H	8.302	0.005	1
1	A	85	SER	HA	4.506	0.006	1
1	A	85	SER	HB2	3.94	0.011	2
1	A	85	SER	HB3	3.892	0.004	2
1	A	85	SER	CA	58.413	0.063	1
1	A	85	SER	CB	63.981	0.068	1
1	A	85	SER	N	115.914	0.058	1
1	A	223	ALA	H	8.502	0.004	1
1	A	223	ALA	HA	4.412	0.005	1
1	A	223	ALA	HB1	1.454	0.006	1
1	A	223	ALA	HB2	1.454	0.006	1
1	A	223	ALA	HB3	1.454	0.006	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	223	ALA	CA	53.06	0.049	1
1	A	223	ALA	CB	19.135	0.076	1
1	A	223	ALA	N	125.912	0.035	1
1	A	224	THR	H	8.079	0.007	1
1	A	224	THR	HA	4.324	0.002	1
1	A	224	THR	HB	4.278	0.003	1
1	A	224	THR	HG21	1.216	0.008	1
1	A	224	THR	HG22	1.216	0.008	1
1	A	224	THR	HG23	1.216	0.008	1
1	A	224	THR	CA	62.135	0.084	1
1	A	224	THR	CB	69.717	0.092	1
1	A	224	THR	CG2	21.664	0.085	1
1	A	224	THR	N	112.12	0.092	1
1	A	225	GLU	H	8.266	0.010	1
1	A	225	GLU	HA	4.305	0.002	1
1	A	225	GLU	HB2	1.97	0.009	2
1	A	225	GLU	HB3	2.09	0.011	2
1	A	225	GLU	HG3	2.28	0.009	1
1	A	225	GLU	CA	56.71	0.072	1
1	A	225	GLU	CB	29.723	0.020	1
1	A	225	GLU	CG	36.229	0.065	1
1	A	225	GLU	N	122.872	0.068	1
1	A	226	ALA	H	8.292	0.005	1
1	A	226	ALA	HA	4.312	0.004	1
1	A	226	ALA	HB1	1.4	0.007	1
1	A	226	ALA	HB2	1.4	0.007	1
1	A	226	ALA	HB3	1.4	0.007	1
1	A	226	ALA	CA	52.516	0.023	1
1	A	226	ALA	CB	19.126	0.096	1
1	A	226	ALA	N	124.925	0.045	1
1	A	227	ALA	H	8.268	0.003	1
1	A	227	ALA	HA	4.322	0.004	1
1	A	227	ALA	HB1	1.429	0.005	1
1	A	227	ALA	HB2	1.429	0.005	1
1	A	227	ALA	HB3	1.429	0.005	1
1	A	227	ALA	CA	52.684	0.039	1
1	A	227	ALA	CB	19.124	0.084	1
1	A	227	ALA	N	123.458	0.057	1
1	A	228	GLY	H	8.307	0.004	1
1	A	228	GLY	HA2	3.995	0.004	2
1	A	228	GLY	HA3	3.958	0.002	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	228	GLY	CA	45.167	0.063	1
1	A	228	GLY	N	108.136	0.081	1
1	A	229	GLU	H	8.166	0.004	1
1	A	229	GLU	HA	4.258	0.005	1
1	A	229	GLU	HB2	1.905	0.005	2
1	A	229	GLU	HB3	1.989	0.011	2
1	A	229	GLU	HG2	2.214	0.004	2
1	A	229	GLU	HG3	2.176	0.009	2
1	A	229	GLU	CA	56.127	0.044	1
1	A	229	GLU	CB	30.536	0.065	1
1	A	229	GLU	CG	36.127	0.035	1
1	A	229	GLU	N	120.238	0.064	1
1	A	289	GLY	H	8.311	0.005	1
1	A	289	GLY	HA2	4.012	0.008	2
1	A	289	GLY	HA3	3.87	0.008	2
1	A	289	GLY	CA	45.171	0.122	1
1	A	289	GLY	N	108.612	0.090	1
1	A	290	GLU	H	8.347	0.006	1
1	A	290	GLU	HA	4.283	0.006	1
1	A	290	GLU	HB2	1.937	0.006	2
1	A	290	GLU	HB3	2.049	0.007	2
1	A	290	GLU	HG3	2.256	0.007	1
1	A	290	GLU	CA	56.447	0.068	1
1	A	290	GLU	CB	30.116	0.013	1
1	A	290	GLU	CG	36.119	0.006	1
1	A	290	GLU	N	120.469	0.069	1
1	A	291	LEU	H	8.321	0.006	1
1	A	291	LEU	HA	4.351	0.009	1
1	A	291	LEU	HB2	1.595	0.007	2
1	A	291	LEU	HB3	1.642	0.003	2
1	A	291	LEU	HD11	0.932	0.003	2
1	A	291	LEU	HD12	0.932	0.003	2
1	A	291	LEU	HD13	0.932	0.003	2
1	A	291	LEU	HD21	0.876	0.007	2
1	A	291	LEU	HD22	0.876	0.007	2
1	A	291	LEU	HD23	0.876	0.007	2
1	A	291	LEU	HG	1.636	0.004	1
1	A	291	LEU	CA	55.005	0.057	1
1	A	291	LEU	CB	42.287	0.098	1
1	A	291	LEU	CD1	25.227	0.067	2
1	A	291	LEU	CD2	23.529	0.086	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	291	LEU	CG	27.037	0.089	1
1	A	291	LEU	N	123.417	0.056	1
1	A	292	ALA	H	8.234	0.006	1
1	A	292	ALA	HA	4.31	0.002	1
1	A	292	ALA	HB1	1.383	0.008	1
1	A	292	ALA	HB2	1.383	0.008	1
1	A	292	ALA	HB3	1.383	0.008	1
1	A	292	ALA	CA	52.573	0.039	1
1	A	292	ALA	CB	19.393	0.083	1
1	A	292	ALA	N	124.714	0.035	1
1	A	293	ASP	H	8.287	0.005	1
1	A	293	ASP	HA	4.614	0.006	1
1	A	293	ASP	HB2	2.729	0.004	2
1	A	293	ASP	HB3	2.593	0.009	2
1	A	293	ASP	CA	54.435	0.057	1
1	A	293	ASP	CB	41.269	0.068	1
1	A	293	ASP	N	119.673	0.064	1
1	A	294	ILE	H	8.067	0.008	1
1	A	294	ILE	HA	4.259	0.006	1
1	A	294	ILE	HB	1.93	0.006	1
1	A	294	ILE	HD11	0.867	0.003	1
1	A	294	ILE	HD12	0.867	0.003	1
1	A	294	ILE	HD13	0.867	0.003	1
1	A	294	ILE	HG12	1.192	0.010	2
1	A	294	ILE	HG13	1.437	0.008	2
1	A	294	ILE	HG21	0.915	0.006	1
1	A	294	ILE	HG22	0.915	0.006	1
1	A	294	ILE	HG23	0.915	0.006	1
1	A	294	ILE	CA	61.127	0.078	1
1	A	294	ILE	CB	38.788	0.054	1
1	A	294	ILE	CD1	13.244	0.041	1
1	A	294	ILE	CG1	27.1	0.048	1
1	A	294	ILE	CG2	17.752	0.040	1
1	A	294	ILE	N	120.83	0.075	1
1	A	295	SER	H	8.414	0.008	1
1	A	295	SER	HA	4.462	0.008	1
1	A	295	SER	HB2	3.881	0.006	2
1	A	295	SER	HB3	3.852	0.006	2
1	A	295	SER	CA	58.591	0.061	1
1	A	295	SER	CB	63.968	0.081	1
1	A	295	SER	N	119.705	0.104	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	296	ASP	H	8.38	0.006	1
1	A	296	ASP	HA	4.66	0.004	1
1	A	296	ASP	HB2	2.715	0.007	2
1	A	296	ASP	HB3	2.652	0.010	2
1	A	296	ASP	CA	54.366	0.091	1
1	A	296	ASP	CB	41.196	0.064	1
1	A	296	ASP	N	122.752	0.045	1
1	A	297	VAL	H	8.03	0.007	1
1	A	297	VAL	HA	4.123	0.007	1
1	A	297	VAL	HB	2.1	0.007	1
1	A	297	VAL	HG11	0.923	0.003	2
1	A	297	VAL	HG12	0.923	0.003	2
1	A	297	VAL	HG13	0.923	0.003	2
1	A	297	VAL	HG21	0.931	0.006	2
1	A	297	VAL	HG22	0.931	0.006	2
1	A	297	VAL	HG23	0.931	0.006	2
1	A	297	VAL	CA	62.46	0.050	1
1	A	297	VAL	CB	32.677	0.101	1
1	A	297	VAL	CG1	21.222	0.086	2
1	A	297	VAL	CG2	20.488	0.032	2
1	A	297	VAL	N	119.747	0.071	1
1	A	298	GLU	H	8.456	0.005	1
1	A	298	GLU	HA	4.285	0.009	1
1	A	298	GLU	HB2	2.067	0.002	2
1	A	298	GLU	HB3	1.977	0.005	2
1	A	298	GLU	HG3	2.277	0.010	1
1	A	298	GLU	CA	56.869	0.025	1
1	A	298	GLU	CB	30.013	0.005	1
1	A	298	GLU	N	124.397	0.039	1
1	A	299	GLY	H	8.35	0.004	1
1	A	299	GLY	HA3	3.971	0.009	1
1	A	299	GLY	CA	45.156	0.031	1
1	A	299	GLY	N	110.105	0.042	1
1	A	300	GLU	H	8.261	0.006	1
1	A	300	GLU	HA	4.352	0.007	1
1	A	300	GLU	HB2	1.944	0.003	2
1	A	300	GLU	HB3	2.071	0.011	2
1	A	300	GLU	HG2	2.257	0.008	2
1	A	300	GLU	HG3	2.243	0.010	2
1	A	300	GLU	CA	56.366	0.043	1
1	A	300	GLU	CB	30.205	0.088	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	300	GLU	CG	36.099	0.004	1
1	A	300	GLU	N	120.81	0.050	1
1	A	301	VAL	H	8.287	0.005	1
1	A	301	VAL	HA	4.114	0.008	1
1	A	301	VAL	HB	2.1	0.005	1
1	A	301	VAL	HG11	0.952	0.008	2
1	A	301	VAL	HG12	0.952	0.008	2
1	A	301	VAL	HG13	0.952	0.008	2
1	A	301	VAL	HG21	0.965	0.003	2
1	A	301	VAL	HG22	0.965	0.003	2
1	A	301	VAL	HG23	0.965	0.003	2
1	A	301	VAL	CA	62.65	0.123	1
1	A	301	VAL	CB	32.533	0.113	1
1	A	301	VAL	CG1	20.765	0.081	2
1	A	301	VAL	CG2	21.128	0.085	2
1	A	301	VAL	N	121.553	0.082	1
1	A	302	GLY	H	8.491	0.007	1
1	A	302	GLY	HA2	3.914	0.002	2
1	A	302	GLY	HA3	3.972	0.008	2
1	A	302	GLY	CA	45.17	0.065	1
1	A	302	GLY	N	112.473	0.032	1
1	A	303	ALA	H	8.13	0.005	1
1	A	303	ALA	HA	4.368	0.004	1
1	A	303	ALA	HB1	1.37	0.005	1
1	A	303	ALA	HB2	1.37	0.005	1
1	A	303	ALA	HB3	1.37	0.005	1
1	A	303	ALA	CA	52.302	0.056	1
1	A	303	ALA	CB	19.371	0.052	1
1	A	303	ALA	N	123.987	0.049	1
1	A	304	ILE	H	8.198	0.005	1
1	A	304	ILE	HA	4.18	0.006	1
1	A	304	ILE	HB	1.882	0.008	1
1	A	304	ILE	HD11	0.885	0.017	1
1	A	304	ILE	HD12	0.885	0.017	1
1	A	304	ILE	HD13	0.885	0.017	1
1	A	304	ILE	HG12	1.205	0.005	2
1	A	304	ILE	HG13	1.503	0.007	2
1	A	304	ILE	HG21	0.926	0.009	1
1	A	304	ILE	HG22	0.926	0.009	1
1	A	304	ILE	HG23	0.926	0.009	1
1	A	304	ILE	CA	61.313	0.065	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	304	ILE	CB	38.76	0.053	1
1	A	304	ILE	CD1	13.11	0.099	1
1	A	304	ILE	CG1	27.351	0.091	1
1	A	304	ILE	CG2	17.478	0.076	1
1	A	304	ILE	N	120.301	0.112	1
1	A	305	GLY	H	8.482	0.006	1
1	A	305	GLY	HA3	3.979	0.011	1
1	A	305	GLY	CA	45.23	0.063	1
1	A	305	GLY	N	112.991	0.037	1
1	A	306	GLU	H	8.26	0.008	1
1	A	306	GLU	HA	4.312	0.006	1
1	A	306	GLU	HB2	2.063	0.006	2
1	A	306	GLU	HB3	1.931	0.003	2
1	A	306	GLU	HG3	2.258	0.007	1
1	A	306	GLU	CA	56.429	0.073	1
1	A	306	GLU	CB	30.413	0.046	1
1	A	306	GLU	CG	36.024	0.000	1
1	A	306	GLU	N	120.758	0.088	1
1	A	307	GLU	H	8.495	0.006	1
1	A	307	GLU	HA	4.292	0.007	1
1	A	307	GLU	HB2	1.941	0.007	2
1	A	307	GLU	HB3	2.065	0.006	2
1	A	307	GLU	HG3	2.257	0.010	1
1	A	307	GLU	CA	56.321	0.037	1
1	A	307	GLU	CB	30.088	0.041	1
1	A	307	GLU	CG	36.276	0.043	1
1	A	307	GLU	N	121.947	0.048	1
1	A	308	ALA	H	8.341	0.006	1
1	A	308	ALA	HA	4.594	0.005	1
1	A	308	ALA	HB1	1.368	0.007	1
1	A	308	ALA	HB2	1.368	0.007	1
1	A	308	ALA	HB3	1.368	0.007	1
1	A	308	ALA	CA	50.597	0.088	1
1	A	308	ALA	CB	18.197	0.056	1
1	A	308	ALA	N	126.559	0.051	1
1	A	309	PRO	HA	4.421	0.005	1
1	A	309	PRO	HB2	1.894	0.010	2
1	A	309	PRO	HB3	2.293	0.012	2
1	A	309	PRO	HD2	3.807	0.009	2
1	A	309	PRO	HD3	3.646	0.006	2
1	A	309	PRO	HG2	2.03	0.008	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	309	PRO	CA	63.215	0.038	1
1	A	309	PRO	CB	32.023	0.083	1
1	A	309	PRO	CD	50.443	0.066	1
1	A	309	PRO	CG	27.364	0.124	1
1	A	310	GLN	H	8.51	0.005	1
1	A	310	GLN	HA	4.281	0.009	1
1	A	310	GLN	HB2	2.108	0.013	2
1	A	310	GLN	HB3	1.98	0.004	2
1	A	310	GLN	HE21	7.535	0.011	1
1	A	310	GLN	HE22	6.849	0.010	1
1	A	310	GLN	HG3	2.388	0.005	1
1	A	310	GLN	CA	55.985	0.091	1
1	A	310	GLN	CB	29.108	0.038	1
1	A	310	GLN	CG	33.798	0.076	1
1	A	310	GLN	N	120.298	0.049	1
1	A	310	GLN	NE2	111.84	0.073	1
1	A	311	MET	H	8.401	0.008	1
1	A	311	MET	HA	4.412	0.010	1
1	A	311	MET	HB2	1.964	0.006	1
1	A	311	MET	HG2	2.474	0.004	2
1	A	311	MET	HG3	2.527	0.004	2
1	A	311	MET	CA	55.668	0.054	1
1	A	311	MET	CB	32.422	0.082	1
1	A	311	MET	CG	32.127	0.092	1
1	A	311	MET	N	121.119	0.103	1
1	A	312	ASN	H	8.333	0.007	1
1	A	312	ASN	HA	4.633	0.005	1
1	A	312	ASN	HB2	2.704	0.005	2
1	A	312	ASN	HB3	2.654	0.005	2
1	A	312	ASN	HD21	7.534	0.007	1
1	A	312	ASN	HD22	6.864	0.011	1
1	A	312	ASN	CA	53.383	0.039	1
1	A	312	ASN	CB	38.724	0.075	1
1	A	312	ASN	N	119.069	0.074	1
1	A	312	ASN	ND2	112.552	0.104	1
1	A	313	TYR	H	8.011	0.008	1
1	A	313	TYR	HA	4.531	0.007	1
1	A	313	TYR	HB2	2.928	0.005	2
1	A	313	TYR	HB3	3.021	0.009	2
1	A	313	TYR	HD1	7.046	0.007	3
1	A	313	TYR	HD2	7.046	0.007	3

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	313	TYR	HE1	6.815	0.009	3
1	A	313	TYR	HE2	6.815	0.009	3
1	A	313	TYR	CA	57.803	0.060	1
1	A	313	TYR	CB	38.671	0.068	1
1	A	313	TYR	CD1	133.107	0.025	3
1	A	313	TYR	CD2	133.107	0.025	3
1	A	313	TYR	CE1	118.271	0.025	3
1	A	313	TYR	CE2	118.271	0.025	3
1	A	313	TYR	N	119.9	0.108	1
1	A	361	ASP	H	8.415	0.005	1
1	A	361	ASP	HA	4.609	0.004	1
1	A	361	ASP	HB2	2.744	0.004	2
1	A	361	ASP	HB3	2.63	0.002	2
1	A	361	ASP	CA	54.637	0.101	1
1	A	361	ASP	CB	41.357	0.089	1
1	A	361	ASP	N	122.236	0.065	1
1	A	362	ASP	H	8.292	0.010	1
1	A	362	ASP	HA	4.561	0.005	1
1	A	362	ASP	HB3	2.697	0.006	1
1	A	362	ASP	CA	54.702	0.070	1
1	A	362	ASP	CB	41.208	0.107	1
1	A	362	ASP	N	121.037	0.044	1
1	A	363	GLU	H	8.437	0.010	1
1	A	363	GLU	HA	4.209	0.011	1
1	A	363	GLU	HB2	2.088	0.001	2
1	A	363	GLU	HB3	2.0	0.010	2
1	A	363	GLU	HG2	2.304	0.004	2
1	A	363	GLU	HG3	2.259	0.006	2
1	A	363	GLU	CA	57.253	0.072	1
1	A	363	GLU	CB	29.669	0.118	1
1	A	363	GLU	CG	36.186	0.028	1
1	A	363	GLU	N	120.617	0.043	1
1	A	364	LEU	H	8.145	0.008	1
1	A	364	LEU	HA	4.212	0.011	1
1	A	364	LEU	HB2	1.654	0.003	2
1	A	364	LEU	HB3	1.503	0.005	2
1	A	364	LEU	HD11	0.82	0.003	2
1	A	364	LEU	HD12	0.82	0.003	2
1	A	364	LEU	HD13	0.82	0.003	2
1	A	364	LEU	HD21	0.873	0.007	2
1	A	364	LEU	HD22	0.873	0.007	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	364	LEU	HD23	0.873	0.007	2
1	A	364	LEU	HG	1.6	0.002	1
1	A	364	LEU	CA	55.855	0.075	1
1	A	364	LEU	CB	42.129	0.069	1
1	A	364	LEU	CD1	23.43	0.022	2
1	A	364	LEU	CD2	25.057	0.049	2
1	A	364	LEU	CG	27.09	0.016	1
1	A	364	LEU	N	121.475	0.098	1
1	A	365	GLU	H	8.191	0.011	1
1	A	365	GLU	HA	4.153	0.004	1
1	A	365	GLU	HB2	1.908	0.000	1
1	A	365	GLU	HG3	2.168	0.005	1
1	A	365	GLU	CA	57.019	0.040	1
1	A	365	GLU	N	119.612	0.110	1
1	A	366	HIS	H	8.173	0.008	1
1	A	366	HIS	HA	4.563	0.012	1
1	A	366	HIS	HB2	3.054	0.008	2
1	A	366	HIS	HB3	2.996	0.003	2
1	A	366	HIS	HD2	6.978	0.016	1
1	A	366	HIS	HE1	7.941	0.003	1
1	A	366	HIS	CA	56.172	0.047	1
1	A	366	HIS	CB	30.495	0.037	1
1	A	366	HIS	CE1	138.021	0.005	1
1	A	366	HIS	N	118.845	0.040	1
1	A	367	HIS	H	7.958	0.015	1
1	A	370	HIS	HA	4.607	0.007	1
1	A	370	HIS	HB2	3.175	0.004	2
1	A	370	HIS	HB3	3.073	0.000	2
1	A	370	HIS	HD2	7.003	0.000	1
1	A	370	HIS	CA	56.047	0.059	1
1	A	371	HIS	H	8.064	0.009	1
1	A	371	HIS	HA	4.438	0.012	1
1	A	371	HIS	HB2	3.063	0.002	1
1	A	371	HIS	HD2	7.024	0.024	1
1	A	371	HIS	CA	57.398	0.040	1
1	A	371	HIS	CB	30.415	0.165	1
1	A	371	HIS	N	125.52	0.060	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	231	-0.48 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	209	0.47 ± 0.05	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	206	0.54 ± 0.30	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 2056 atoms were assigned a chemical shift out of a possible 2514. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	661/844 (78%)	336/339 (99%)	172/344 (50%)	153/161 (95%)
Sidechain	1217/1459 (83%)	833/945 (88%)	350/450 (78%)	34/64 (53%)
Aromatic	178/211 (84%)	90/108 (83%)	85/97 (88%)	3/6 (50%)
Overall	2056/2514 (82%)	1259/1392 (90%)	607/891 (68%)	190/231 (82%)

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	317	THR	HG1	5.69	0.08 – 2.19	21.6
1	A	53	THR	HG1	5.35	0.08 – 2.19	19.9
1	A	346	LYS	HA	1.71	2.15 – 6.37	-6.0

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:

