wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2MA9
BMRB ID	:	19333
Title	:	HIV-1 Vif SOCS-box and Elongin BC solution structure
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Deposited on	:	2013-07-01

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 (i) symbol.

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

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

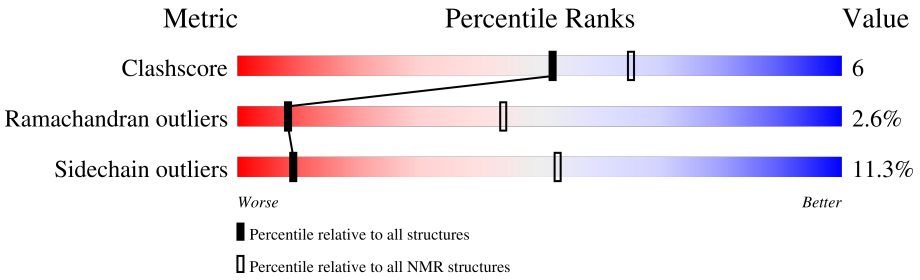
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 25%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	36	50% 31% 8% 11%
2	B	118	82% 17% .
3	C	91	81% 19%

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:6-A:37, B:1-B:118, C:1-C:91 (241)	0.35	2

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 3 single-model clusters were found.

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2307 atoms, of which 412 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Virion infectivity factor.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	32	316	169	59	45	43	0

- Molecule 2 is a protein called Transcription elongation factor B polypeptide 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	118	1124	575	204	156	184	5	0

- Molecule 3 is a protein called Transcription elongation factor B polypeptide 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
3	C	91	867	460	149	117	137	4	0

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

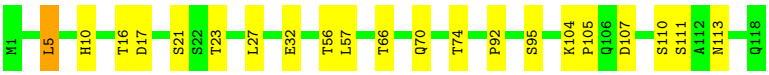
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for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

• Molecule 1: Virion infectivity factor

Chain A:

• Molecule 2: Transcription elongation factor B polypeptide 2

Chain B:



• Molecule 3: Transcription elongation factor B polypeptide 1

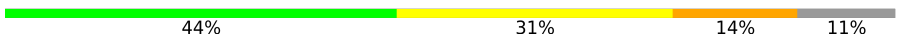
Chain C:

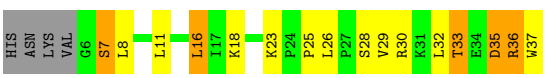
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 2. Colouring as in section 4.1 above.

• Molecule 1: Virion infectivity factor

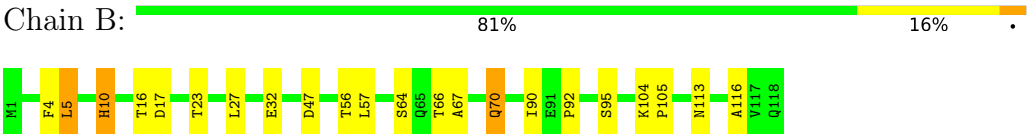
Chain A:





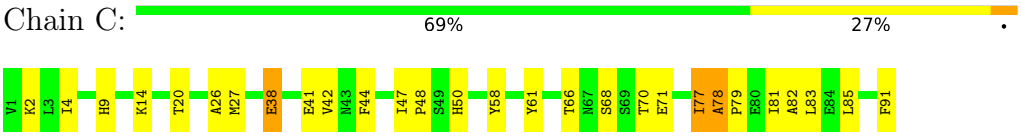
• Molecule 2: Transcription elongation factor B polypeptide 2

Chain B:



• Molecule 3: Transcription elongation factor B polypeptide 1

Chain C:



5 Refinement protocol and experimental data overview

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

Of the 200 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
CS-ROSETTA	structure solution	
CS-ROSETTA	refinement	
HADDOCK	structure solution	
HADDOCK	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	3
Total number of shifts	827
Number of shifts mapped to atoms	726
Number of unparsed shifts	0
Number of shifts with mapping errors	101
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	25%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	257	59	282	8±3
2	B	920	204	908	10±2
3	C	718	149	714	10±4
All	All	37900	8240	38080	434

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

5 of 121 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:LYS:HD3	1:A:24:PRO:HD2	0.92	1.41	15	11
1:A:23:LYS:HD2	1:A:35:ASP:HB3	0.90	1.43	2	6
1:A:23:LYS:HG3	1:A:35:ASP:HB3	0.90	1.41	11	14
2:B:17:ASP:HB3	3:C:14:LYS:HD2	0.83	1.50	4	13
1:A:23:LYS:HG2	1:A:24:PRO:HD2	0.82	1.50	8	2

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	30/36 (83%)	23±1 (77±5%)	4±2 (12±5%)	3±1 (10±3%)	1 9
2	B	116/118 (98%)	110±1 (95±1%)	4±1 (4±1%)	2±1 (1±1%)	16 63
3	C	89/91 (98%)	78±2 (88±2%)	10±2 (11±2%)	2±1 (2±1%)	12 54
All	All	4700/4900 (96%)	4224 (90%)	353 (8%)	123 (3%)	8 44

5 of 16 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	36	ARG	20
1	A	29	VAL	19
2	B	10	HIS	18
3	C	77	ILE	16
1	A	35	ASP	12

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	28/32 (88%)	21±2 (76±6%)	7±2 (24±6%)	2 27
2	B	103/103 (100%)	94±2 (91±2%)	9±2 (9±2%)	13 60
3	C	80/80 (100%)	72±2 (90±2%)	8±2 (10±2%)	11 57
All	All	4220/4300 (98%)	3743 (89%)	477 (11%)	9 53

5 of 74 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	36	ARG	20
3	C	70	THR	20
1	A	7	SER	19
1	A	28	SER	19
2	B	5	LEU	19

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 monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 25% for the well-defined parts and 25% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	152
Number of shifts mapped to atoms	106
Number of unparsed shifts	0
Number of shifts with mapping errors	46
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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 46) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	HIS	CB	30.77	.	.
1	A	2	HIS	CA	57.08	.	.
1	A	2	HIS	HA	4.43	.	.
1	A	3	ASN	CB	32.97	.	.
1	A	4	LYS	N	120.98	.	.
1	A	4	LYS	CB	30.54	.	.
1	A	4	LYS	CA	56.31	.	.
1	A	4	LYS	H	8.23	.	.
1	A	4	LYS	HA	4.14	.	.
1	A	5	VAL	N	121.2	.	.
1	A	5	VAL	CB	33.02	.	.
1	A	5	VAL	CA	62.61	.	.
1	A	5	VAL	H	8.15	.	.
1	A	5	VAL	HA	3.98	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	6	GLY	HA2	4.0	.	.
1	A	6	GLY	HA3	4.0	.	.
1	A	7	SER	HA	4.47	.	.
1	A	8	LEU	HA	4.2	.	.
1	A	9	GLN	HA	4.23	.	.
1	A	11	LEU	HA	4.59	.	.
1	A	12	ALA	HA	4.26	.	.
1	A	13	LEU	HA	4.25	.	.
1	A	14	ALA	HA	4.2	.	.
1	A	15	ALA	HA	4.28	.	.
1	A	16	LEU	HA	4.32	.	.
1	A	17	ILE	HA	4.17	.	.
1	A	18	LYS	HA	4.62	.	.
1	A	19	PRO	HA	4.47	.	.
1	A	20	LYS	HA	4.6	.	.
1	A	21	GLN	HA	4.24	.	.
1	A	22	ILE	HA	4.26	.	.
1	A	23	LYS	HA	4.81	.	.
1	A	24	PRO	HA	4.7	.	.
1	A	25	PRO	HA	4.4	.	.
1	A	26	LEU	HA	4.31	.	.
1	A	27	PRO	HA	4.44	.	.
1	A	28	SER	HA	4.44	.	.
1	A	29	VAL	HA	4.14	.	.
1	A	30	ARG	HA	4.33	.	.
1	A	31	LYS	HA	4.65	.	.
1	A	32	LEU	HA	4.61	.	.
1	A	33	THR	HA	4.33	.	.
1	A	34	GLU	HA	5.03	.	.
1	A	35	ASP	HA	4.48	.	.
1	A	36	ARG	HA	4.47	.	.
1	A	37	TRP	HA	4.68	.	.

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	33	0.46 ± 0.75	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	32	0.59 ± 0.76	None needed (imprecise)
$^{13}C'$	0	—	None (insufficient data)

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
^{15}N	26	-0.40 ± 0.73	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 4%, i.e. 138 atoms were assigned a chemical shift out of a possible 3290. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	110/1180 (9%)	56/475 (12%)	30/482 (6%)	24/223 (11%)
Sidechain	28/1895 (1%)	0/1233 (0%)	28/594 (5%)	0/68 (0%)
Aromatic	0/215 (0%)	0/107 (0%)	0/103 (0%)	0/5 (0%)
Overall	138/3290 (4%)	56/1815 (3%)	58/1179 (5%)	24/296 (8%)

7.1.4 Statistically unusual chemical shifts

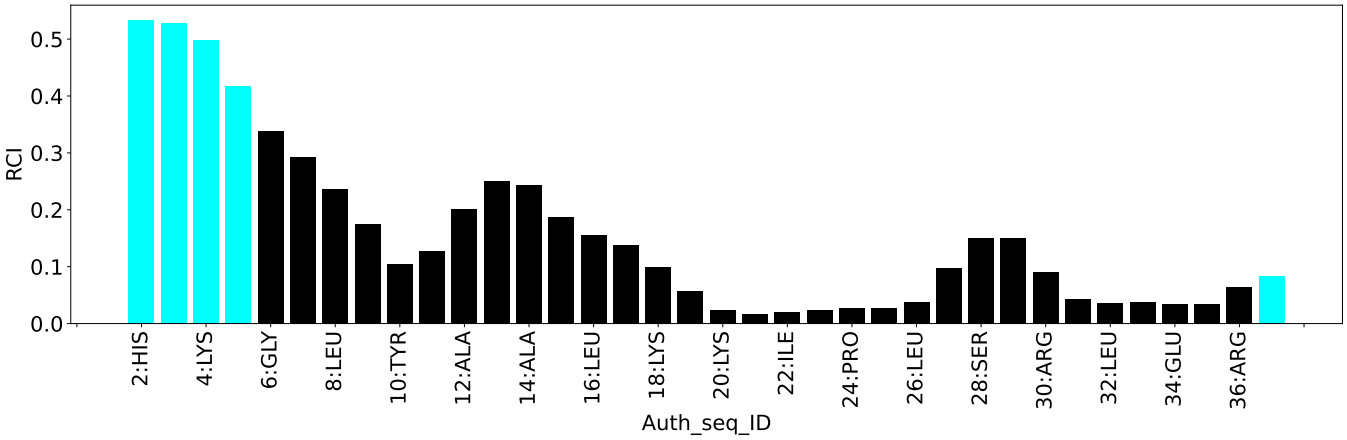
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	20	LYS	CB	41.78	24.03 – 41.47	5.2
1	A	26	LEU	CB	32.94	33.11 – 51.34	-5.1

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.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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	468
Number of shifts mapped to atoms	431
Number of unparsed shifts	0
Number of shifts with mapping errors	37
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.

- No matching atom found in the structure. First 5 (of 37) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	11	LYS	HA	4.35	.	.
2	B	22	SER	HA	4.05	.	.
2	B	26	GLU	HA	4.37	.	.
2	B	30	ILE	HA	4.05	.	.
2	B	32	GLU	HA	4.11	.	.
2	B	33	GLY	HA2	3.6	.	.
2	B	33	GLY	HA3	3.6	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	35	LEU	HA	4.19	.	.
2	B	54	GLY	HA2	3.26	.	.
2	B	54	GLY	HA3	3.26	.	.
2	B	55	LYS	HA	4.32	.	.
2	B	58	GLY	HA2	3.84	.	.
2	B	58	GLY	HA3	3.84	.	.
2	B	61	GLY	HA2	3.82	.	.
2	B	61	GLY	HA3	3.82	.	.
2	B	65	GLN	HA	4.23	.	.
2	B	78	ALA	HA	4.25	.	.
2	B	90	ILE	HA	4.14	.	.
2	B	100	PRO	HA	4.35	.	.
2	B	101	ASP	HA	4.48	.	.
2	B	102	VAL	HA	4.02	.	.
2	B	103	MET	HA	4.4	.	.
2	B	104	LYS	HA	4.51	.	.
2	B	106	GLN	HA	4.22	.	.
2	B	107	ASP	HA	4.59	.	.
2	B	108	SER	HA	4.37	.	.
2	B	109	GLY	HA2	3.94	.	.
2	B	109	GLY	HA3	3.94	.	.
2	B	110	SER	HA	4.44	.	.
2	B	111	SER	HA	4.41	.	.
2	B	112	ALA	HA	4.25	.	.
2	B	113	ASN	HA	4.61	.	.
2	B	114	GLU	HA	4.19	.	.
2	B	115	GLN	HA	4.24	.	.
2	B	116	ALA	HA	4.27	.	.
2	B	117	VAL	HA	4.05	.	.
2	B	118	GLN	HA	4.11	.	.

7.2.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	106	-0.11 ± 0.18	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	46	-0.19 ± 0.40	None needed (< 0.5 ppm)
$^{13}C'$	97	0.51 ± 0.10	Should be applied
^{15}N	91	-0.76 ± 0.52	None needed (imprecise)

7.2.3 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 14%, i.e. 468 atoms were assigned a chemical shift out of a possible 3290. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	422/1180 (36%)	128/475 (27%)	203/482 (42%)	91/223 (41%)
Sidechain	46/1895 (2%)	0/1233 (0%)	46/594 (8%)	0/68 (0%)
Aromatic	0/215 (0%)	0/107 (0%)	0/103 (0%)	0/5 (0%)
Overall	468/3290 (14%)	128/1815 (7%)	249/1179 (21%)	91/296 (31%)

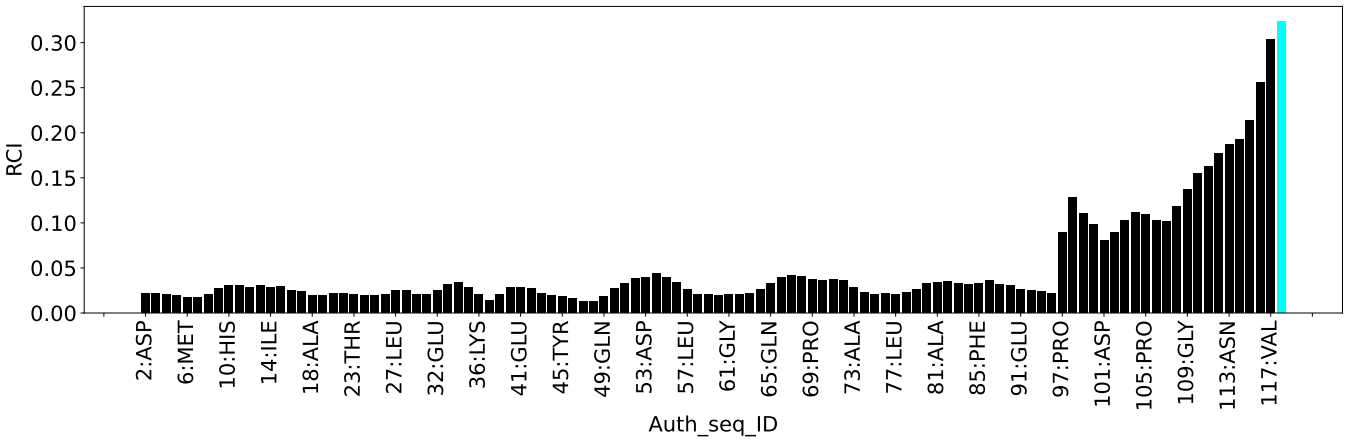
7.2.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.2.5 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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain B:



7.3 Chemical shift list 3

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_3*

7.3.1 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	207
Number of shifts mapped to atoms	189
Number of unparsed shifts	0
Number of shifts with mapping errors	18
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.

- No matching atom found in the structure. First 5 (of 18) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3	C	8	GLY	HA2	4.01	.	.
3	C	8	GLY	HA3	4.01	.	.
3	C	11	PHE	HA	4.6	.	.
3	C	17	HIS	HA	4.7	.	.
3	C	22	GLY	HA2	4.17	.	.
3	C	22	GLY	HA3	4.17	.	.
3	C	25	LYS	HA	4.33	.	.
3	C	30	GLY	HA2	4.6	.	.
3	C	30	GLY	HA3	4.6	.	.
3	C	35	ALA	HA	4.81	.	.
3	C	44	PHE	HA	4.69	.	.
3	C	45	ARG	HA	4.3	.	.
3	C	50	HIS	HA	4.56	.	.
3	C	60	THR	HA	4.5	.	.
3	C	82	ALA	HA	4.63	.	.
3	C	83	LEU	HA	4.0	.	.
3	C	89	ALA	HA	4.44	.	.
3	C	90	ASN	HA	4.38	.	.

7.3.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	53	-0.57 ± 0.55	None needed (imprecise)
$^{13}C_{\beta}$	16	—	None (insufficient data)
$^{13}C'$	34	-0.04 ± 0.23	None needed (< 0.5 ppm)
^{15}N	43	-0.23 ± 0.41	None needed (< 0.5 ppm)

7.3.3 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 6%, i.e. 207 atoms were assigned a chemical shift out of a possible 3290. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	191/1180 (16%)	61/475 (13%)	87/482 (18%)	43/223 (19%)
Sidechain	16/1895 (1%)	0/1233 (0%)	16/594 (3%)	0/68 (0%)
Aromatic	0/215 (0%)	0/107 (0%)	0/103 (0%)	0/5 (0%)
Overall	207/3290 (6%)	61/1815 (3%)	103/1179 (9%)	43/296 (15%)

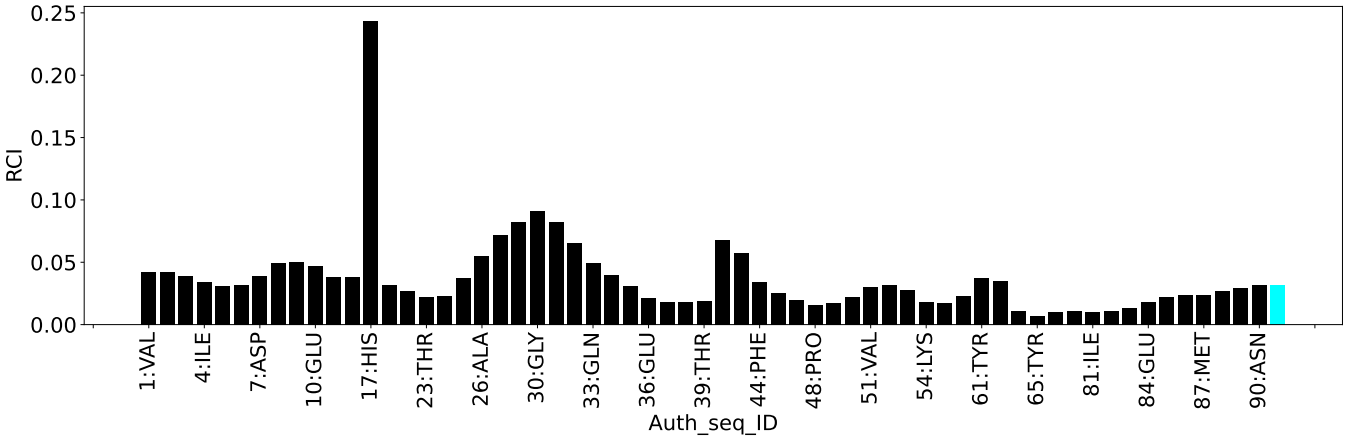
7.3.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.3.5 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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain C:


RCI
0.25
0.20
0.15
0.10
0.05
0.00
1:VAL
4:ILE
7:ASP
10:GLU
17:HIS
23:THR
26:ALA
30:GLY
33:GLN
36:GLU
39:THR
44:PHE
48:PRO
51:VAL
54:LYS
61:TYR
65:TYR
81:ILE
84:GLU
87:MET
90:ASN
Auth_seq_ID