Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 05:28 AM EDT

PDB ID	:	5IRD
BMRB ID	:	30034
Title	:	Solution structure of Rv1466 from Mycobacterium tuberculosis, a protein associated with [Fe-S] complex assembly and repair - Seattle Structural Genomics Center for Infectious Disease target MytuD.17486.a
Authors	:	Buchko, G.W.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2016-03-13

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
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 (1)) were used in the production of this report:

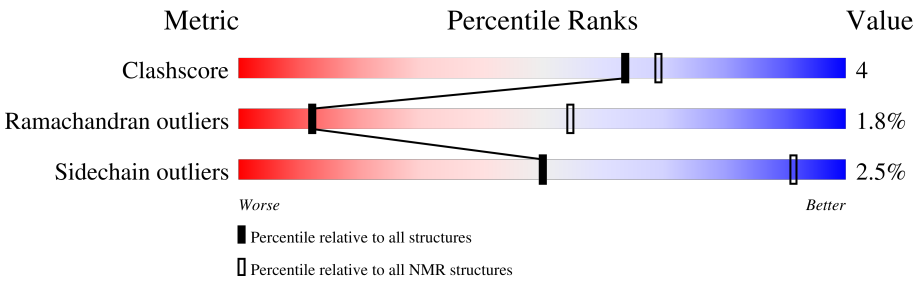
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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	119	

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:10-A:103 (94)	1.20	8

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

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

The models can be grouped into 3 clusters and 11 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1747 atoms, of which 858 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	119	1747	552	858	144	189	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A5U2G9
A	2	PRO	-	expression tag	UNP A5U2G9
A	3	GLY	-	expression tag	UNP A5U2G9
A	4	SER	-	expression tag	UNP A5U2G9

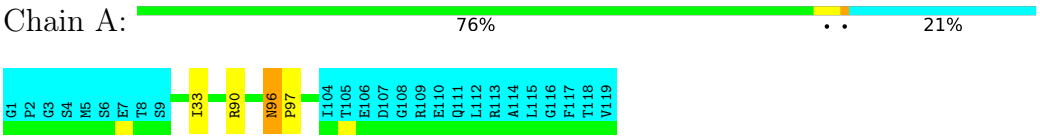
4 Residue-property plots (i)

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: Uncharacterized protein

Chain A:



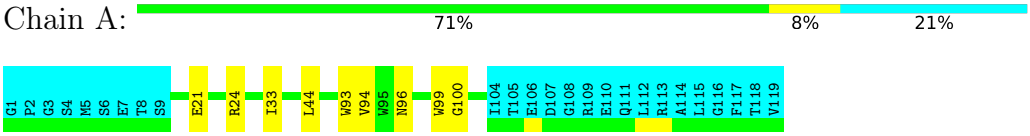
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Uncharacterized protein

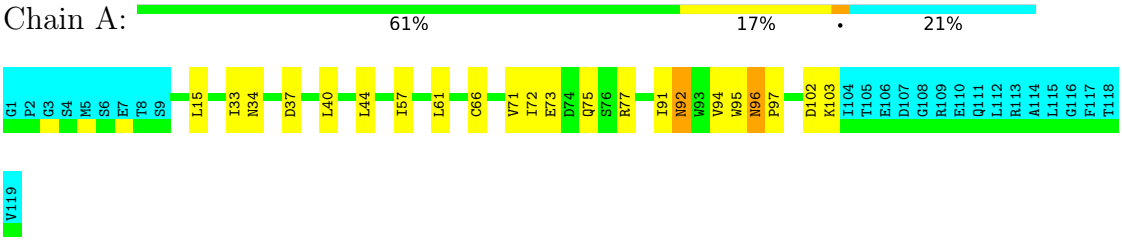
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Uncharacterized protein

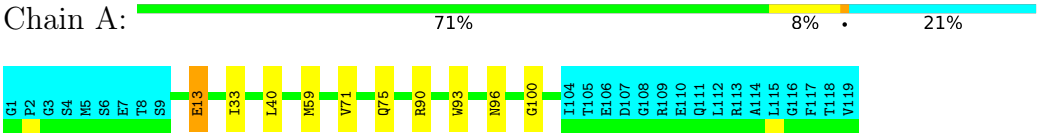
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein

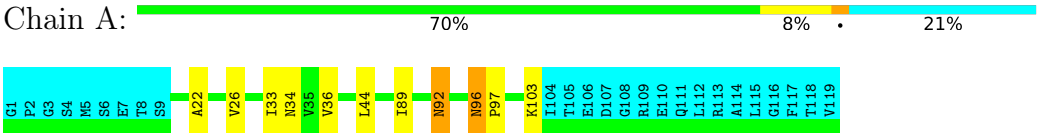
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein

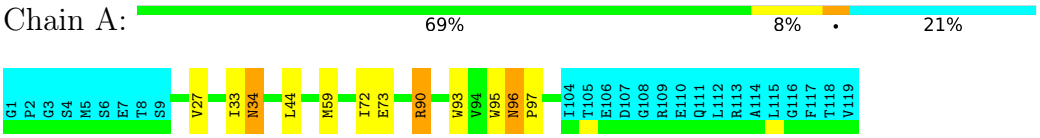
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein

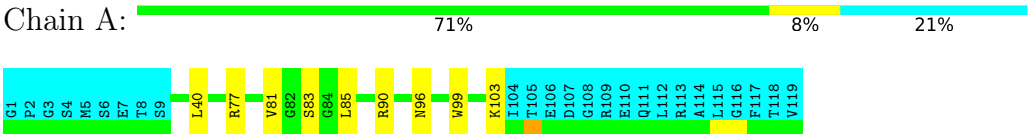
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein

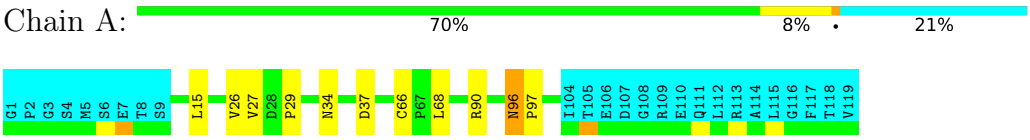
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein

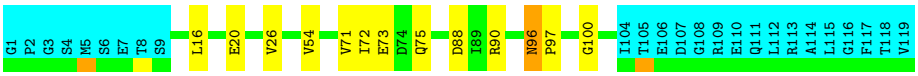
Chain A:



4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Uncharacterized protein

Chain A: 68% 10% • 21%



4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein

Chain A: 70% 9% 21%

4.2.10 Score per residue for model 10

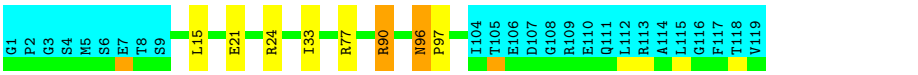
- Molecule 1: Uncharacterized protein

Chain A: 67% 9% • 21%

4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein

Chain A: 72% 5% • 21%



4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein

Chain A: 68% 8% • 21%

4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein

Chain A: 61% 17% • 21%

G1 P2 G3 S4 M5 S6 E7 T8 S9 A17 E21 V26 I33 L40 I57 D58 M59 T60 L61 T69 D70 V71 I72 E73 R90 I91 N92 W93 N96 P97 P98 D102 K103 I104 T105 E106 D107 G108 R109 E110 Q111 L112 R113 A114 L115 G116 F117 T118 V119

4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein

Chain A: 66% 12% • 21%

G1 P2 G3 S4 M5 S6 E7 T8 S9 A10 M23 V27 D28 P29 V41 D48 T53 M59 T60 L61 C66 R77 V81 I89 N96 G100 I104 T105 E106 D107 G108 R109 E110 Q111 L112 R113 A114 L115 G116 F117 T118 V119

4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein

Chain A: 66% 11% • 21%

G1 P2 G3 S4 M5 S6 E7 T8 S9 V19 M23 R24 D25 V26 I33 L44 V54 V71 Q75 D88 I89 R90 N96 P97 D102 K103 I104 T105 E106 D107 G108 R109 E110 Q111 L112 R113 A114 L115 G116 F117 T118 V119

4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein

Chain A: 63% 16% 21%

G1 P2 G3 S4 M5 S6 E7 T8 S9 E21 R24 V27 D28 P29 L56 I57 C66 P67 L68 T69 D70 V71 I72 E73 D74 Q75 R90 I91 N92 N96 K103 I104 T105 E106 D107 G108 R109 E110 Q111 L112 R113 A114 L115 G116 F117 T118 V119

4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized protein

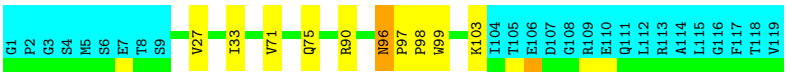
Chain A: 69% 8% • 21%

G1 P2 G3 S4 M5 S6 E7 T8 S9 I33 D48 T53 D58 T69 D70 V71 I72 E73 D74 Q75 V94 W95 N96 P97 G100 I104 T105 E106 D107 G108 R109 E110 Q111 L112 R113 A114 L115 G116 F117 T118 V119

4.2.18 Score per residue for model 18

- Molecule 1: Uncharacterized protein

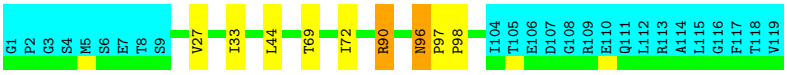
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein

Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein

Chain A:

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	**Classification**	**Version**
CYANA	structure calculation	2.1
CNS	refinement	1.1

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	1255
Number of shifts mapped to atoms	1255
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	705	680	680	6±3
All	All	14100	13600	13600	120

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:LEU:HB3	1:A:66:CYS:SG	0.65	2.31	2	1
1:A:99:TRP:HB3	1:A:103:LYS:HD2	0.60	1.74	6	1
1:A:77:ARG:HD2	1:A:89:ILE:HG12	0.54	1.80	14	1
1:A:72:ILE:HD12	1:A:73:GLU:N	0.54	2.17	8	5
1:A:83:SER:HB3	1:A:85:LEU:HG	0.54	1.80	6	1
1:A:68:LEU:HD23	1:A:71:VAL:HB	0.54	1.79	12	1
1:A:69:THR:O	1:A:73:GLU:HB2	0.54	2.03	17	1
1:A:92:ASN:HB2	1:A:103:LYS:HG2	0.53	1.79	4	1
1:A:92:ASN:HD22	1:A:93:TRP:N	0.52	2.03	10	1
1:A:96:ASN:HB3	1:A:97:PRO:HD3	0.52	1.81	2	6
1:A:77:ARG:O	1:A:81:VAL:HG12	0.52	2.05	6	1
1:A:17:ALA:O	1:A:21:GLU:HG2	0.51	2.06	13	1
1:A:94:VAL:HG11	1:A:99:TRP:CD1	0.51	2.40	1	1
1:A:41:VAL:HG22	1:A:59:MET:SD	0.50	2.46	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:VAL:O	1:A:29:PRO:HD3	0.50	2.07	7	4
1:A:40:LEU:HD21	1:A:94:VAL:HG23	0.49	1.84	2	1
1:A:56:LEU:HD22	1:A:103:LYS:O	0.49	2.07	16	1
1:A:96:ASN:H	1:A:97:PRO:HD2	0.49	1.66	20	2
1:A:69:THR:HA	1:A:72:ILE:HG12	0.49	1.83	19	1
1:A:60:THR:HG22	1:A:94:VAL:O	0.49	2.07	20	1
1:A:99:TRP:HB3	1:A:103:LYS:HD3	0.49	1.84	18	1
1:A:71:VAL:O	1:A:75:GLN:HG2	0.49	2.07	16	6
1:A:59:MET:O	1:A:93:TRP:HA	0.48	2.08	5	3
1:A:96:ASN:N	1:A:97:PRO:HD2	0.48	2.24	20	5
1:A:66:CYS:SG	1:A:68:LEU:HB2	0.48	2.48	16	1
1:A:21:GLU:O	1:A:24:ARG:HB3	0.48	2.09	16	3
1:A:69:THR:O	1:A:73:GLU:HG3	0.48	2.09	12	1
1:A:23:MET:O	1:A:27:VAL:HG12	0.48	2.08	14	1
1:A:34:ASN:HD22	1:A:34:ASN:N	0.47	2.06	5	2
1:A:26:VAL:O	1:A:26:VAL:HG12	0.47	2.08	20	4
1:A:92:ASN:HB2	1:A:103:LYS:HD3	0.47	1.86	2	2
1:A:92:ASN:ND2	1:A:102:ASP:HB2	0.47	2.25	2	1
1:A:22:ALA:O	1:A:26:VAL:HG22	0.47	2.10	10	2
1:A:33:ILE:HD12	1:A:33:ILE:N	0.47	2.25	5	8
1:A:58:ASP:OD2	1:A:92:ASN:HB3	0.46	2.10	13	1
1:A:90:ARG:NH1	1:A:102:ASP:O	0.46	2.49	15	1
1:A:92:ASN:OD1	1:A:102:ASP:HB2	0.45	2.11	13	1
1:A:48:ASP:HA	1:A:53:THR:HA	0.45	1.88	14	3
1:A:27:VAL:HG22	1:A:33:ILE:O	0.45	2.11	18	1
1:A:61:LEU:HG	1:A:93:TRP:CZ3	0.45	2.46	13	1
1:A:47:GLN:NE2	1:A:56:LEU:HD11	0.45	2.26	12	1
1:A:57:ILE:O	1:A:91:ILE:HA	0.44	2.12	16	3
1:A:40:LEU:HD12	1:A:59:MET:HA	0.44	1.88	13	1
1:A:61:LEU:HD13	1:A:66:CYS:O	0.44	2.11	14	1
1:A:44:LEU:HD12	1:A:44:LEU:O	0.44	2.12	4	4
1:A:54:VAL:HA	1:A:88:ASP:O	0.44	2.13	8	2
1:A:69:THR:HG23	1:A:70:ASP:N	0.44	2.28	16	3
1:A:96:ASN:HB2	1:A:97:PRO:HD3	0.44	1.88	11	1
1:A:27:VAL:HG23	1:A:34:ASN:HA	0.44	1.90	5	1
1:A:66:CYS:HB3	1:A:68:LEU:HD13	0.44	1.89	7	2
1:A:34:ASN:O	1:A:37:ASP:HB3	0.44	2.13	2	2
1:A:96:ASN:N	1:A:97:PRO:CD	0.43	2.81	15	2
1:A:16:LEU:O	1:A:20:GLU:HG3	0.43	2.14	8	1
1:A:58:ASP:OD2	1:A:94:VAL:HG23	0.42	2.13	17	1
1:A:13:GLU:H	1:A:13:GLU:CD	0.42	2.18	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ILE:HD12	1:A:93:TRP:HH2	0.42	1.75	12	1
1:A:77:ARG:O	1:A:81:VAL:HG22	0.42	2.15	14	1
1:A:34:ASN:OD1	1:A:36:VAL:HB	0.42	2.14	4	1
1:A:33:ILE:N	1:A:33:ILE:HD12	0.41	2.30	20	1
1:A:71:VAL:O	1:A:75:GLN:HG3	0.41	2.15	3	1
1:A:74:ASP:O	1:A:77:ARG:HG3	0.41	2.16	10	1
1:A:90:ARG:NH1	1:A:91:ILE:O	0.41	2.54	16	1
1:A:46:VAL:HA	1:A:55:ALA:HA	0.41	1.92	20	1
1:A:95:TRP:CD1	1:A:95:TRP:N	0.40	2.89	5	1
1:A:19:VAL:O	1:A:23:MET:HG2	0.40	2.16	15	1
1:A:23:MET:HA	1:A:26:VAL:HG22	0.40	1.93	15	1
1:A:89:ILE:O	1:A:90:ARG:NH1	0.40	2.54	20	1
1:A:90:ARG:HG3	1:A:103:LYS:O	0.40	2.16	20	1

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	94/119 (79%)	86±2 (92±2%)	6±2 (6±2%)	2±1 (2±1%)	12	54
All	All	1880/2380 (79%)	1726 (92%)	121 (6%)	33 (2%)	12	54

All 8 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	96	ASN	20
1	A	100	GLY	5
1	A	98	PRO	3
1	A	95	TRP	1
1	A	99	TRP	1
1	A	26	VAL	1
1	A	10	ALA	1
1	A	27	VAL	1

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	78/98 (80%)	76±1 (98±2%)	2±1 (2±2%)	50 91
All	All	1560/1960 (80%)	1521 (98%)	39 (2%)	50 91

All 19 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	90	ARG	7
1	A	92	ASN	4
1	A	33	ILE	4
1	A	89	ILE	3
1	A	44	LEU	2
1	A	77	ARG	2
1	A	40	LEU	2
1	A	34	ASN	2
1	A	24	ARG	2
1	A	102	ASP	2
1	A	93	TRP	1
1	A	13	GLU	1
1	A	30	GLU	1
1	A	69	THR	1
1	A	20	GLU	1
1	A	68	LEU	1
1	A	72	ILE	1
1	A	25	ASP	1
1	A	73	GLU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *TB86c_BMRB_Deposit3_1.txt*

7.1.1 Bookkeeping (i)

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

Total number of shifts	1255
Number of shifts mapped to atoms	1255
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	114	-0.08 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	104	0.10 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	91	0.16 ± 0.15	None needed (< 0.5 ppm)
^{15}N	105	0.64 ± 0.50	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 86%, i.e. 1034 atoms were assigned a chemical shift out of a possible 1205. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	431/466 (92%)	179/190 (94%)	168/188 (89%)	84/88 (95%)
Sidechain	576/694 (83%)	387/455 (85%)	183/224 (82%)	6/15 (40%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	27/45 (60%)	14/22 (64%)	10/20 (50%)	3/3 (100%)
Overall	1034/1205 (86%)	580/667 (87%)	361/432 (84%)	93/106 (88%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1254 atoms were assigned a chemical shift out of a possible 1515. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	533/593 (90%)	223/243 (92%)	205/238 (86%)	105/112 (94%)
Sidechain	694/867 (80%)	463/567 (82%)	224/278 (81%)	7/22 (32%)
Aromatic	27/55 (49%)	14/27 (52%)	10/25 (40%)	3/3 (100%)
Overall	1254/1515 (83%)	700/837 (84%)	439/541 (81%)	115/137 (84%)

7.1.4 Statistically unusual chemical shifts (i)

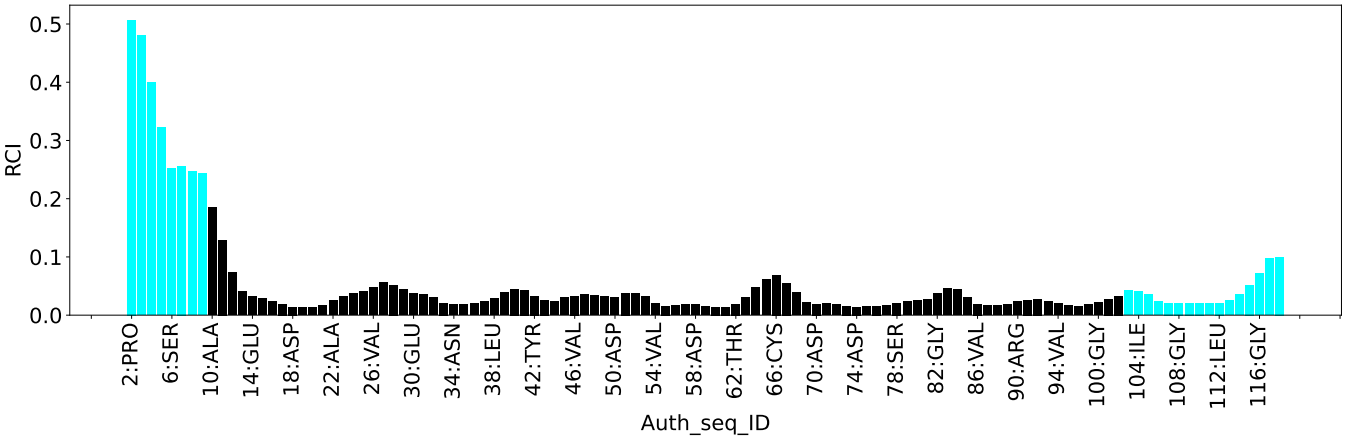
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	90	ARG	NH1	8.87	49.05 – 99.42	-13.0
1	A	30	GLU	HB2	3.36	1.00 – 3.05	6.5
1	A	30	GLU	HB3	3.17	0.95 – 3.05	5.6
1	A	91	ILE	HG21	-0.64	-0.56 – 2.11	-5.3
1	A	91	ILE	HG22	-0.64	-0.56 – 2.11	-5.3
1	A	91	ILE	HG23	-0.64	-0.56 – 2.11	-5.3
1	A	62	THR	HG21	0.03	0.08 – 2.19	-5.2
1	A	62	THR	HG22	0.03	0.08 – 2.19	-5.2
1	A	62	THR	HG23	0.03	0.08 – 2.19	-5.2

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:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
2:PRO
6:SER
10:ALA
14:GLU
18:ASP
22:ALA
26:VAL
30:GLU
34:ASN
38:LEU
42:TYR
46:VAL
50:ASP
54:VAL
58:ASP
62:THR
66:CYS
70:ASP
74:ASP
78:SER
82:GLY
86:VAL
90:ARG
94:VAL
100:GLY
104:ILE
108:GLY
112:LEU
116:GLY
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1111
Intra-residue (|i-j|=0)	322
Sequential (|i-j|=1)	345
Medium range (|i-j|>1 and |i-j|<5)	158
Long range (|i-j|≥5)	210
Inter-chain	0
Hydrogen bond restraints	76
Disulfide bond restraints	0
Total dihedral-angle restraints	158
Number of unmapped restraints	0
Number of restraints per residue	10.7
Number of long range restraints per residue[1]	2.0

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations (i)

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model (i)

Distance violations less than 0.1 Å are not included in the calculation.There are no distance violations

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	2.0	2.3

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Bins (°)	Average number of violations per model	Max (°)
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

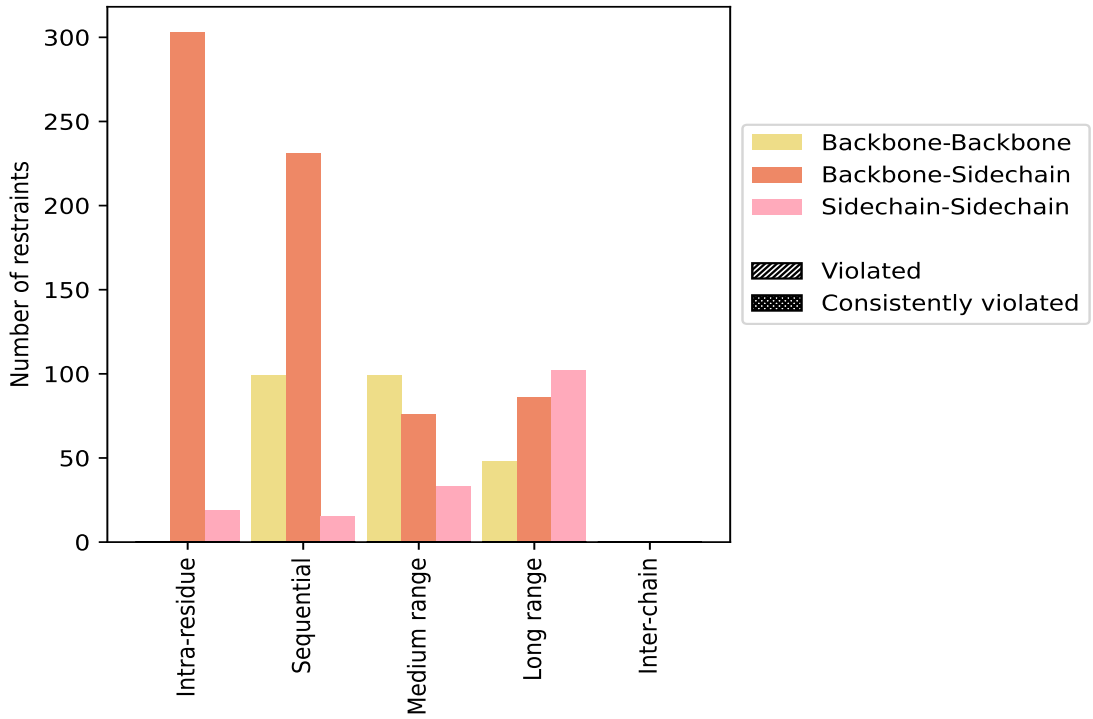
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	322	29.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	303	27.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	19	1.7	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	345	31.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	99	8.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	231	20.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	15	1.4	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	158	14.2	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	49	4.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	76	6.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	33	3.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	210	18.9	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	22	2.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	86	7.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	102	9.2	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	76	6.8	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1111	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	246	22.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	696	62.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	169	15.2	0	0.0	0.0	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations (i)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

No violations found

9.3 Distance violation statistics for the ensemble (i)

No violations found

9.4 Most violated distance restraints in the ensemble (i)

No violations found

9.5 All violated distance restraints (i)

No violations found

10 Dihedral-angle violation analysis (i)

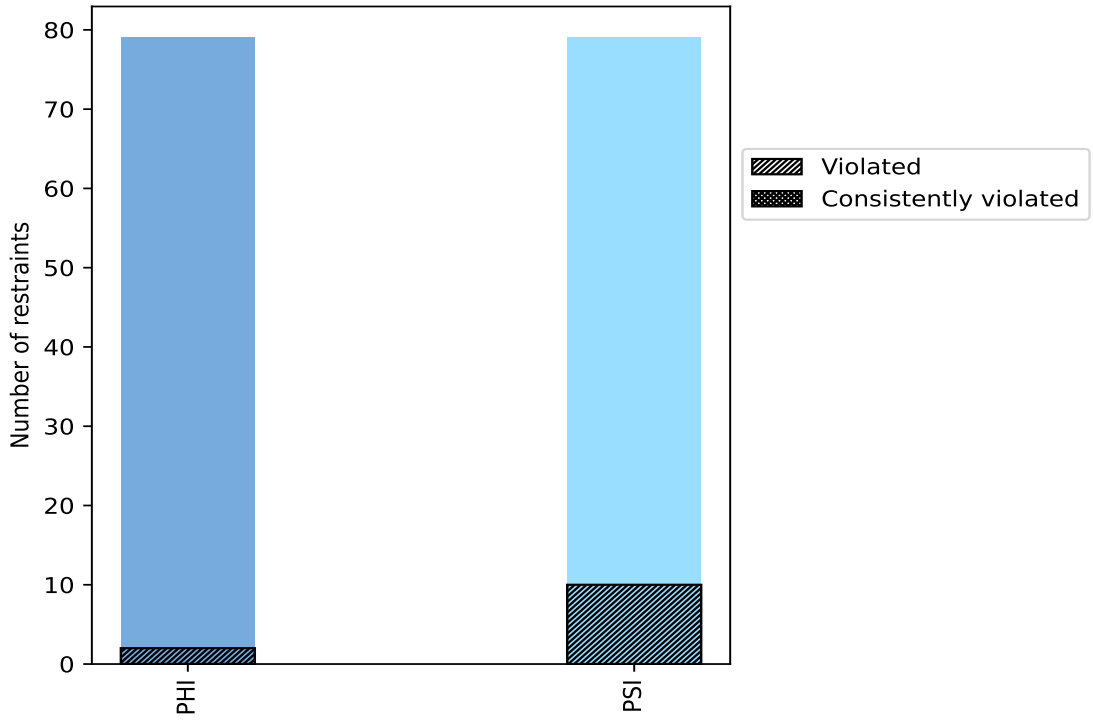
10.1 Summary of dihedral-angle violations (i)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	79	50.0	2	2.5	1.3	0	0.0	0.0
PSI	79	50.0	10	12.7	6.3	0	0.0	0.0
Total	158	100.0	12	7.6	7.6	0	0.0	0.0

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations (i)



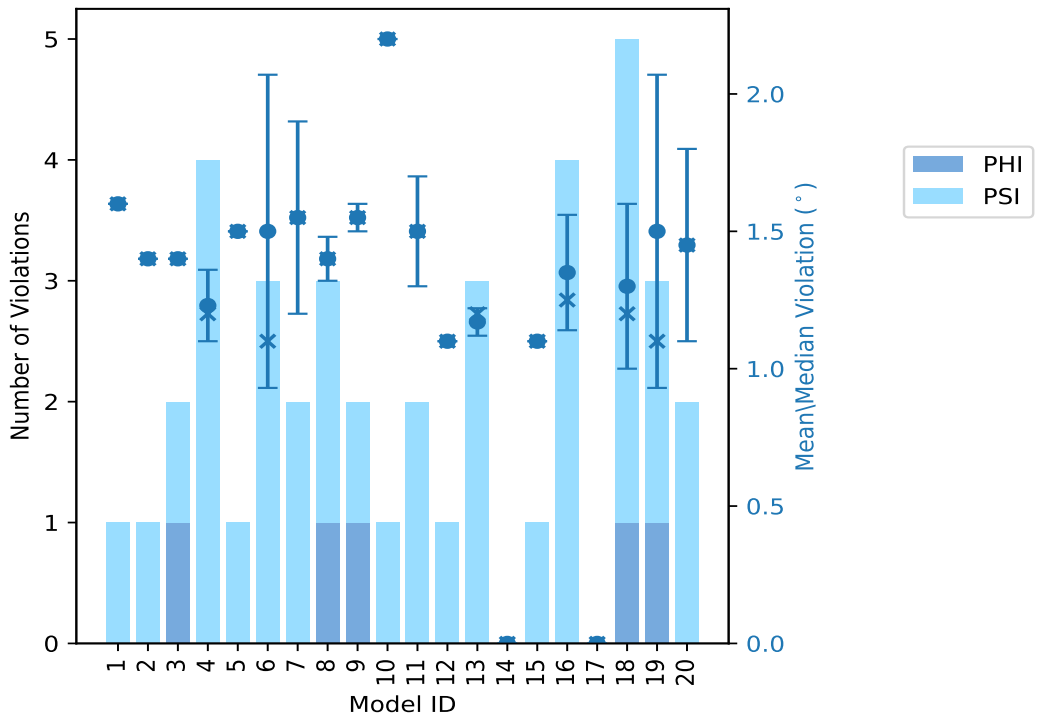
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	1	1	1.6	1.6	0.0	1.6
2	0	1	1	1.4	1.4	0.0	1.4
3	1	1	2	1.4	1.4	0.0	1.4
4	0	4	4	1.23	1.4	0.13	1.2
5	0	1	1	1.5	1.5	0.0	1.5
6	0	3	3	1.5	2.3	0.57	1.1
7	0	2	2	1.55	1.9	0.35	1.55
8	1	2	3	1.4	1.5	0.08	1.4
9	1	1	2	1.55	1.6	0.05	1.55
10	0	1	1	2.2	2.2	0.0	2.2
11	0	2	2	1.5	1.7	0.2	1.5
12	0	1	1	1.1	1.1	0.0	1.1
13	0	3	3	1.17	1.2	0.05	1.2
14	0	0	0	0.0	0.0	0.0	0.0
15	0	1	1	1.1	1.1	0.0	1.1
16	0	4	4	1.35	1.7	0.21	1.25
17	0	0	0	0.0	0.0	0.0	0.0
18	1	4	5	1.3	1.9	0.3	1.2
19	1	2	3	1.5	2.3	0.57	1.1
20	0	2	2	1.45	1.8	0.35	1.45

10.2.1 Bar graph : Dihedral violation statistics for each model (i)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

10.3 Dihedral-angle violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
1	5	6	1	5.0
0	1	1	2	10.0
0	0	0	3	15.0
1	1	2	4	20.0
0	1	1	5	25.0
0	1	1	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

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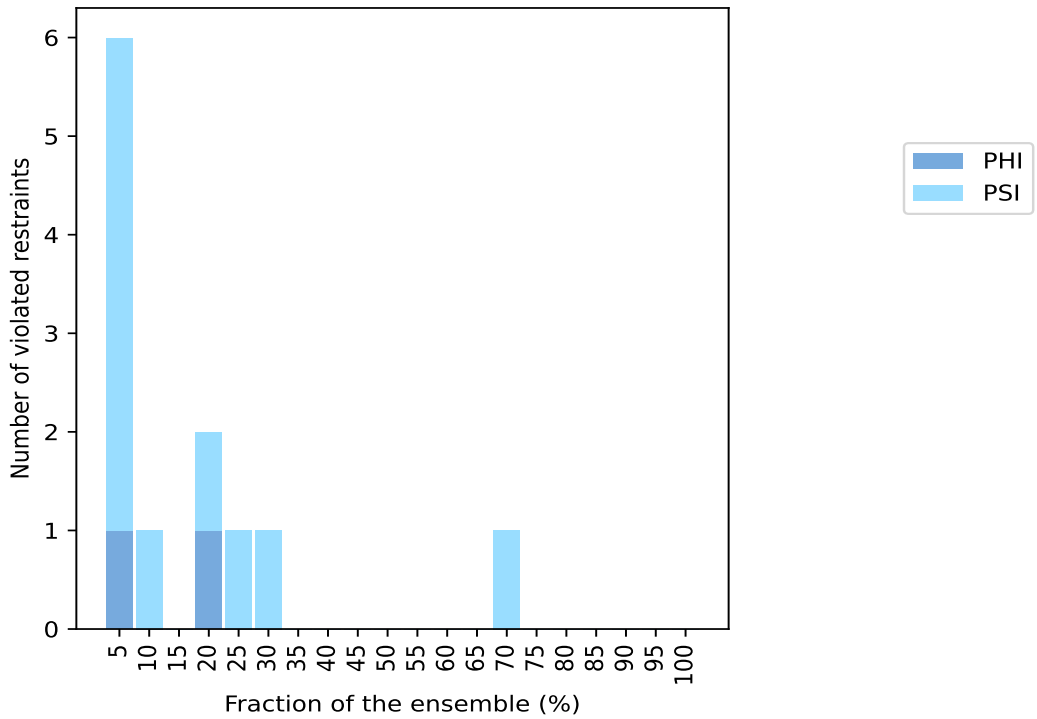
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	1	1	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)

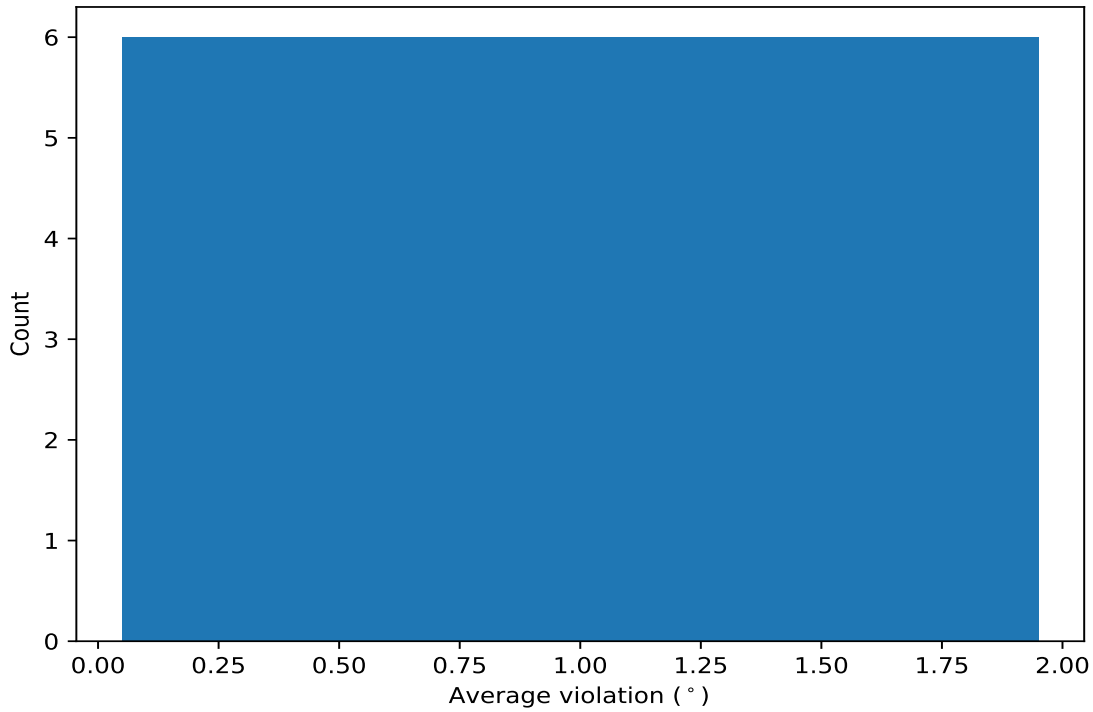


10.4 Most violated dihedral-angle restraints in the ensemble (i)

10.4.1 Histogram : Distribution of mean dihedral-angle violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints (i)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

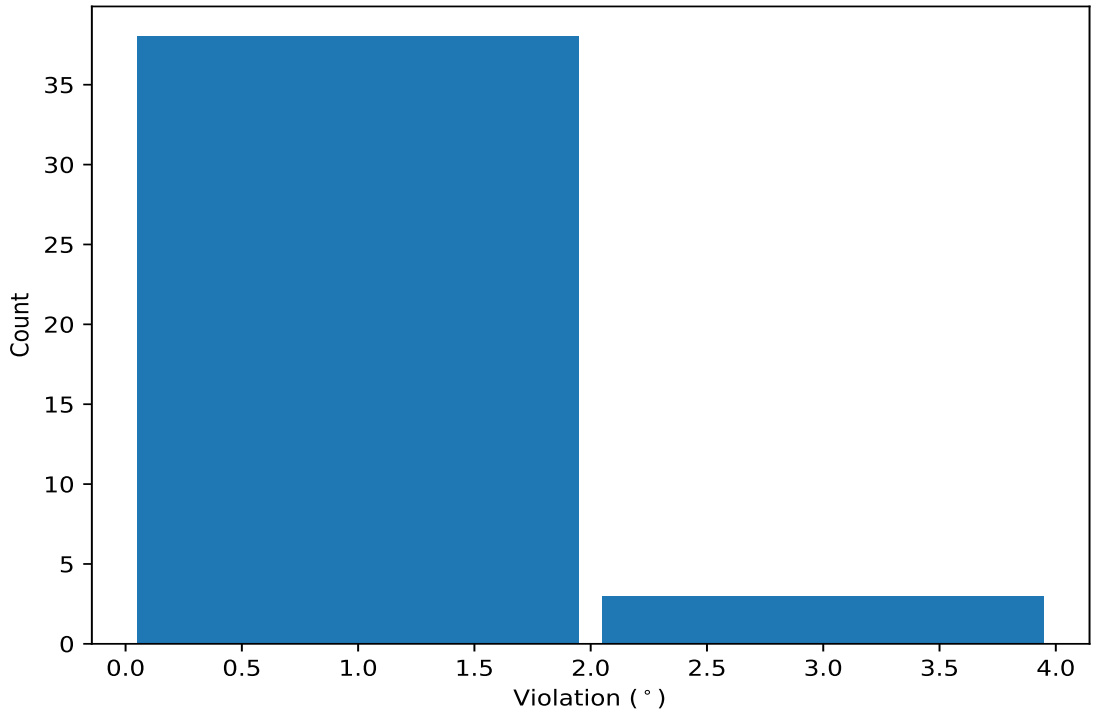
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,112)	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	1:A:80:LEU:N	14	1.67	0.39	1.6
(1,48)	1:A:39:GLY:N	1:A:39:GLY:CA	1:A:39:GLY:C	1:A:40:LEU:N	6	1.37	0.19	1.35
(1,116)	1:A:81:VAL:N	1:A:81:VAL:CA	1:A:81:VAL:C	1:A:82:GLY:N	5	1.14	0.08	1.1
(1,49)	1:A:39:GLY:C	1:A:40:LEU:N	1:A:40:LEU:CA	1:A:40:LEU:C	4	1.4	0.12	1.45
(1,24)	1:A:23:MET:N	1:A:23:MET:CA	1:A:23:MET:C	1:A:24:ARG:N	4	1.2	0.07	1.2
(1,152)	1:A:110:GLU:N	1:A:110:GLU:CA	1:A:110:GLU:C	1:A:111:GLN:N	2	1.45	0.25	1.45

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,112)	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	1:A:80:LEU:N	6	2.3
(1,112)	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	1:A:80:LEU:N	19	2.3
(1,112)	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	1:A:80:LEU:N	10	2.2
(1,112)	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	1:A:80:LEU:N	7	1.9
(1,112)	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	1:A:80:LEU:N	18	1.9
(1,112)	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	1:A:80:LEU:N	20	1.8
(1,152)	1:A:110:GLU:N	1:A:110:GLU:CA	1:A:110:GLU:C	1:A:111:GLN:N	11	1.7
(1,112)	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	1:A:80:LEU:N	16	1.7
(1,48)	1:A:39:GLY:N	1:A:39:GLY:CA	1:A:39:GLY:C	1:A:40:LEU:N	1	1.6
(1,48)	1:A:39:GLY:N	1:A:39:GLY:CA	1:A:39:GLY:C	1:A:40:LEU:N	9	1.6
(1,49)	1:A:39:GLY:C	1:A:40:LEU:N	1:A:40:LEU:CA	1:A:40:LEU:C	8	1.5
(1,49)	1:A:39:GLY:C	1:A:40:LEU:N	1:A:40:LEU:CA	1:A:40:LEU:C	9	1.5
(1,112)	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	1:A:80:LEU:N	5	1.5
(1,49)	1:A:39:GLY:C	1:A:40:LEU:N	1:A:40:LEU:CA	1:A:40:LEU:C	3	1.4
(1,48)	1:A:39:GLY:N	1:A:39:GLY:CA	1:A:39:GLY:C	1:A:40:LEU:N	8	1.4
(1,112)	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	1:A:80:LEU:N	2	1.4
(1,112)	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	1:A:80:LEU:N	3	1.4
(1,112)	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	1:A:80:LEU:N	4	1.4
(1,48)	1:A:39:GLY:N	1:A:39:GLY:CA	1:A:39:GLY:C	1:A:40:LEU:N	4	1.3
(1,24)	1:A:23:MET:N	1:A:23:MET:CA	1:A:23:MET:C	1:A:24:ARG:N	8	1.3
(1,116)	1:A:81:VAL:N	1:A:81:VAL:CA	1:A:81:VAL:C	1:A:82:GLY:N	16	1.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,112)	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	1:A:80:LEU:N	11	1.3
(1,49)	1:A:39:GLY:C	1:A:40:LEU:N	1:A:40:LEU:CA	1:A:40:LEU:C	18	1.2
(1,48)	1:A:39:GLY:N	1:A:39:GLY:CA	1:A:39:GLY:C	1:A:40:LEU:N	7	1.2
(1,24)	1:A:23:MET:N	1:A:23:MET:CA	1:A:23:MET:C	1:A:24:ARG:N	13	1.2
(1,24)	1:A:23:MET:N	1:A:23:MET:CA	1:A:23:MET:C	1:A:24:ARG:N	16	1.2
(1,152)	1:A:110:GLU:N	1:A:110:GLU:CA	1:A:110:GLU:C	1:A:111:GLN:N	18	1.2
(1,142)	1:A:105:THR:N	1:A:105:THR:CA	1:A:105:THR:C	1:A:106:GLU:N	16	1.2
(1,112)	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	1:A:80:LEU:N	13	1.2
(1,96)	1:A:71:VAL:N	1:A:71:VAL:CA	1:A:71:VAL:C	1:A:72:ILE:N	15	1.1
(1,86)	1:A:64:ALA:N	1:A:64:ALA:CA	1:A:64:ALA:C	1:A:65:ALA:N	18	1.1
(1,48)	1:A:39:GLY:N	1:A:39:GLY:CA	1:A:39:GLY:C	1:A:40:LEU:N	6	1.1
(1,4)	1:A:13:GLU:N	1:A:13:GLU:CA	1:A:13:GLU:C	1:A:14:GLU:N	13	1.1
(1,24)	1:A:23:MET:N	1:A:23:MET:CA	1:A:23:MET:C	1:A:24:ARG:N	4	1.1
(1,144)	1:A:106:GLU:N	1:A:106:GLU:CA	1:A:106:GLU:C	1:A:107:ASP:N	20	1.1
(1,116)	1:A:81:VAL:N	1:A:81:VAL:CA	1:A:81:VAL:C	1:A:82:GLY:N	4	1.1
(1,116)	1:A:81:VAL:N	1:A:81:VAL:CA	1:A:81:VAL:C	1:A:82:GLY:N	6	1.1
(1,116)	1:A:81:VAL:N	1:A:81:VAL:CA	1:A:81:VAL:C	1:A:82:GLY:N	18	1.1
(1,116)	1:A:81:VAL:N	1:A:81:VAL:CA	1:A:81:VAL:C	1:A:82:GLY:N	19	1.1
(1,112)	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	1:A:80:LEU:N	12	1.1
(1,111)	1:A:78:SER:C	1:A:79:ALA:N	1:A:79:ALA:CA	1:A:79:ALA:C	19	1.1