Full wwPDB NMR Structure Validation Report (i)

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Title	:	Chemical Shift Assignments for MIP and MDM2 in bound state
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Deposited on	:	2014-06-03

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:

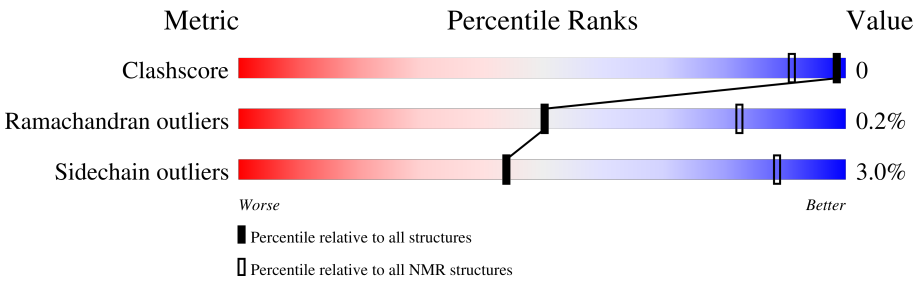
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 91%.

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	131	67% • 31%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 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:-8-A:1, A:33-A:113 (91)	0.47	11

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

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

The models can be grouped into 4 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2107 atoms, of which 1055 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E3 ubiquitin-protein ligase Mdm2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	131	2107	676	1055	172	194	10	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q00987
A	-10	PRO	-	expression tag	UNP Q00987
A	-9	ARG	-	expression tag	UNP Q00987
A	-8	PHE	-	expression tag	UNP Q00987
A	-7	TRP	-	expression tag	UNP Q00987
A	-6	GLU	-	expression tag	UNP Q00987
A	-5	TYR	-	expression tag	UNP Q00987
A	-4	TRP	-	expression tag	UNP Q00987
A	-3	LEU	-	expression tag	UNP Q00987
A	-2	ARG	-	expression tag	UNP Q00987
A	-1	LEU	-	expression tag	UNP Q00987
A	0	MET	-	expression tag	UNP Q00987
A	1	GLU	-	expression tag	UNP Q00987
A	2	GLY	-	expression tag	UNP Q00987
A	3	GLY	-	expression tag	UNP Q00987
A	4	GLY	-	expression tag	UNP Q00987
A	5	GLU	-	expression tag	UNP Q00987
A	6	ASN	-	expression tag	UNP Q00987
A	7	LEU	-	expression tag	UNP Q00987
A	8	TYR	-	expression tag	UNP Q00987
A	9	PHE	-	expression tag	UNP Q00987
A	10	GLN	-	expression tag	UNP Q00987
A	11	GLY	-	expression tag	UNP Q00987
A	109	MET	-	expression tag	UNP Q00987
A	110	ALA	-	expression tag	UNP Q00987
A	111	SER	-	expression tag	UNP Q00987
A	112	MET	-	expression tag	UNP Q00987
A	113	THR	-	expression tag	UNP Q00987
A	114	GLY	-	expression tag	UNP Q00987
A	115	GLY	-	expression tag	UNP Q00987
A	116	GLN	-	expression tag	UNP Q00987

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Chain	Residue	Modelled	Actual	Comment	Reference
A	117	GLN	-	expression tag	UNP Q00987
A	118	MET	-	expression tag	UNP Q00987
A	119	GLY	-	expression tag	UNP Q00987

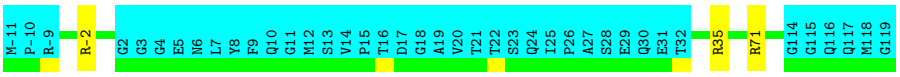
4 Residue-property plots (i)

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: E3 ubiquitin-protein ligase Mdm2

Chain A: 67% • 31%



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

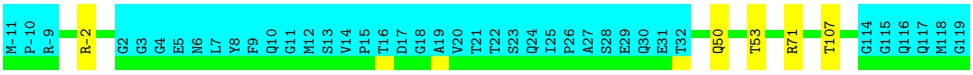
• Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 66% • • 31%

4.2.2 Score per residue for model 2

• Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 66% • 31%



4.2.3 Score per residue for model 3

• Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 66% • 31%

M-11 P-10 R-9 R-2 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 T55 R71 T113 G114 G115 Q116 Q117 M118 G119

4.2.4 Score per residue for model 4

• Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 65% 5% 31%

M-11 P-10 R-9 R-2 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 R35 T53 R71 R103 T113 G114 G115 Q116 Q117 M118 G119

4.2.5 Score per residue for model 5

• Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 69% • 31%

M-11 P-10 R-9 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 N85 G114 G115 Q116 Q117 M118 G119

4.2.6 Score per residue for model 6

• Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 64% 5% • 31%

M-11 P-10 R-9 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 L40 T53 Y54 T55 R71 H102 T107 M112 T113 G114 G115 Q116 Q117 M118 G119

4.2.7 Score per residue for model 7

• Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 66% • 31%

M-11 P-10 R-9 R-2 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 L40 R71 C83 M112 T113 G114 G115 Q116 Q117 M118 G119

4.2.8 Score per residue for model 8

- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 66% • 31%

M-11 P-10 R-9 R-2 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 K45 R103 T107 T113 G114 G115 Q116 Q117 M118 G119

4.2.9 Score per residue for model 9

- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 65% • • 31%

M-11 P-10 R-9 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 T53 Y54 T55 Q78 V99 R103 T107 G114 G115 Q116 Q117 M118 G119

4.2.10 Score per residue for model 10

- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 69% • 31%

M-11 P-10 R-9 R-2 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 G114 G115 Q116 Q117 M118 G119

4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 66% • • 31%

M-11 P-10 R-9 R-2 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 R35 P36 K37 T107 G114 G115 Q116 Q117 M118 G119

4.2.12 Score per residue for model 12

- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 66% • • 31%

M-11 P-10 R-9 R-2 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 R35 R71 N85 R103 G114 G115 Q116 Q117 M118 G119

4.2.13 Score per residue for model 13

- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 68% • 31%

M-11 P-10 R-9 R-2 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 R35 G114 G115 Q116 Q117 M118 G119

4.2.14 Score per residue for model 14

- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 67% •• 31%

M-11 P-10 R-9 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 R35 R71 R103 G114 G115 Q116 Q117 M118 G119

4.2.15 Score per residue for model 15

- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 66% • 31%

M-11 P-10 R-9 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 L40 R103 T107 M112 T113 G114 G115 Q116 Q117 M118 G119

4.2.16 Score per residue for model 16

- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 67% • 31%

M-11 P-10 R-9 L-1 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 T53 T113 G114 G115 Q116 Q117 M118 G119

4.2.17 Score per residue for model 17

- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 66% •• 31%

M-11 P-10 R-9 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 R35 T55 Q77 T107 G114 G115 Q116 Q117 M118 G119

4.2.18 Score per residue for model 18

- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 64% 5% • 31%

M-11 P-10 R-9 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 R35 L41 K42 L43 L44 K45 K57 R71 R103 G114 G115 Q116 Q117 M118 G119

4.2.19 Score per residue for model 19

- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 65% • • 31%

M-11 P-10 R-9 R-2 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 R35 R71 N85 Y106 T107 G114 G115 Q116 Q117 M118 G119

4.2.20 Score per residue for model 20

- Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain A: 66% • • 31%

M-11 P-10 R-9 G2 G3 G4 E5 N6 L7 Y8 F9 Q10 G11 M12 S13 V14 P15 T16 D17 G18 A19 V20 T21 T22 S23 Q24 I25 P26 A27 S28 E29 Q30 E31 T32 R71 T107 M108 M109 T113 G114 G115 Q116 Q117 M118 G119

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry*.

Of the 200 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
Amber	refinement	12
CYANA	structure solution	2.0.14

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	1553
Number of shifts mapped to atoms	1553
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality (i)

6.1 Standard geometry (i)

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	0.75±0.00	0±0/786 (0.0± 0.0%)	1.03±0.02	2±1/1059 (0.2± 0.1%)
All	All	0.75	0/15720 (0.0%)	1.03	38/21180 (0.2%)

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	-2	ARG	NE-CZ-NH1	8.29	124.44	120.30	3	11
1	A	103	ARG	NE-CZ-NH1	6.97	123.78	120.30	18	6
1	A	71	ARG	NE-CZ-NH1	6.36	123.48	120.30	3	11
1	A	35	ARG	NE-CZ-NH1	6.07	123.33	120.30	1	8
1	A	106	TYR	CB-CG-CD2	-5.53	117.68	121.00	19	1
1	A	-2	ARG	NE-CZ-NH2	-5.16	117.72	120.30	3	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	766	789	789	0±0
All	All	15320	15780	15780	4

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:HD11	1:A:45:LYS:HE2	0.46	1.87	18	1
1:A:40:LEU:HD22	1:A:112:MET:HB3	0.45	1.88	6	3

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	91/131 (69%)	87±2 (95±2%)	4±2 (5±2%)	0±0 (0±0%)	50	82
All	All	1820/2620 (69%)	1734 (95%)	82 (5%)	4 (0%)	50	82

All 4 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	50	GLN	1
1	A	102	HIS	1
1	A	83	CYS	1
1	A	85	ASN	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	85/115 (74%)	82±2 (97±2%)	3±2 (3±2%)	44	89
All	All	1700/2300 (74%)	1649 (97%)	51 (3%)	44	89

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	107	THR	9
1	A	53	THR	6
1	A	35	ARG	5
1	A	113	THR	5
1	A	71	ARG	5
1	A	55	THR	4
1	A	103	ARG	3
1	A	85	ASN	2
1	A	-2	ARG	2
1	A	50	GLN	1
1	A	45	LYS	1
1	A	78	GLN	1
1	A	99	VAL	1
1	A	37	LYS	1
1	A	-1	LEU	1
1	A	77	GLN	1
1	A	43	LEU	1
1	A	57	LYS	1
1	A	109	MET	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 91% for the well-defined parts and 85% 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 (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	1553
Number of shifts mapped to atoms	1553
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	126	-0.44 ± 0.15	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	114	0.34 ± 0.14	None needed (< 0.5 ppm)
$^{13}C'$	118	-0.29 ± 0.11	None needed (< 0.5 ppm)
^{15}N	112	0.73 ± 0.34	Should be applied

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 91%, i.e. 1230 atoms were assigned a chemical shift out of a possible 1350. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	433/453 (96%)	177/183 (97%)	175/182 (96%)	81/88 (92%)
Sidechain	674/756 (89%)	459/495 (93%)	215/235 (91%)	0/26 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	123/141 (87%)	62/68 (91%)	59/69 (86%)	2/4 (50%)
Overall	1230/1350 (91%)	698/746 (94%)	449/486 (92%)	83/118 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1550 atoms were assigned a chemical shift out of a possible 1821. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	595/655 (91%)	239/268 (89%)	244/262 (93%)	112/125 (90%)
Sidechain	820/1006 (82%)	553/657 (84%)	266/314 (85%)	1/35 (3%)
Aromatic	135/160 (84%)	68/77 (88%)	65/79 (82%)	2/4 (50%)
Overall	1550/1821 (85%)	860/1002 (86%)	575/655 (88%)	115/164 (70%)

7.1.4 Statistically unusual chemical shifts (i)

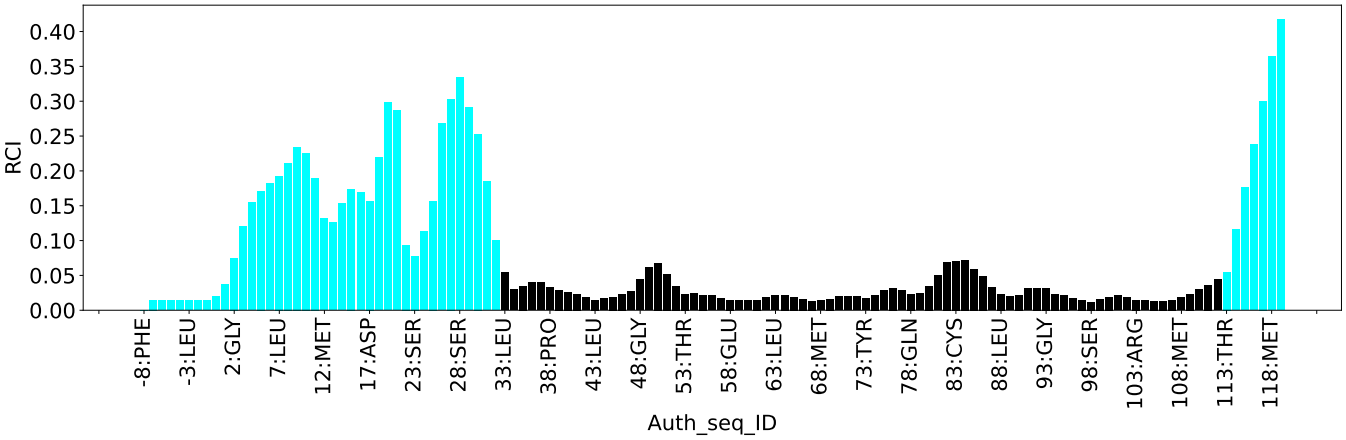
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	113	THR	HG1	4.72	0.08 – 2.19	17.0
1	A	81	VAL	HB	0.32	0.43 – 3.54	-5.4

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
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-8:PHE
-3:LEU
2:GLY
7:LEU
12:MET
17:ASP
23:SER
28:SER
33:LEU
38:PRO
43:LEU
48:GLY
53:THR
58:GLU
63:LEU
68:MET
73:TYR
78:GLN
83:CYS
88:LEU
93:GLY
98:SER
103:ARG
108:MET
113:THR
118:MET
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	1522
Intra-residue (|i-j|=0)	396
Sequential (|i-j|=1)	347
Medium range (|i-j|>1 and |i-j|<5)	329
Long range (|i-j|≥5)	450
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	11.6
Number of long range restraints per residue[1]	3.4

[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.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.2	0.18
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

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

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

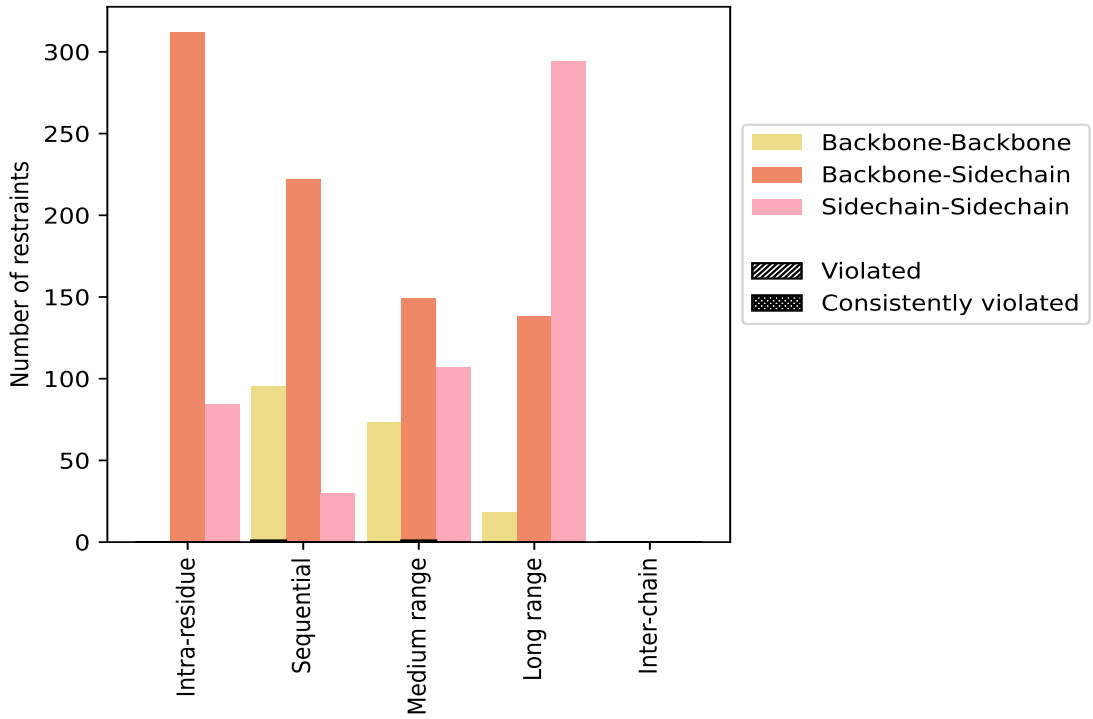
9.1 Summary of distance violations (i)

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)	396	26.0	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	312	20.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	84	5.5	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	347	22.8	1	0.3	0.1	0	0.0	0.0
Backbone-Backbone	95	6.2	1	1.1	0.1	0	0.0	0.0
Backbone-Sidechain	222	14.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	30	2.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	329	21.6	1	0.3	0.1	0	0.0	0.0
Backbone-Backbone	73	4.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	149	9.8	1	0.7	0.1	0	0.0	0.0
Sidechain-Sidechain	107	7.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	450	29.6	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	18	1.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	138	9.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	294	19.3	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	0	0.0	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	1522	100.0	2	0.1	0.1	0	0.0	0.0
Backbone-Backbone	186	12.2	1	0.5	0.1	0	0.0	0.0
Backbone-Sidechain	821	53.9	1	0.1	0.1	0	0.0	0.0
Sidechain-Sidechain	515	33.8	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)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	1	0	0	0	1	0.14	0.14	0.0	0.14
7	0	0	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	1	0	0	0	1	0.18	0.18	0.0	0.18
10	0	0	1	0	0	1	0.12	0.12	0.0	0.12
11	0	1	0	0	0	1	0.13	0.13	0.0	0.13

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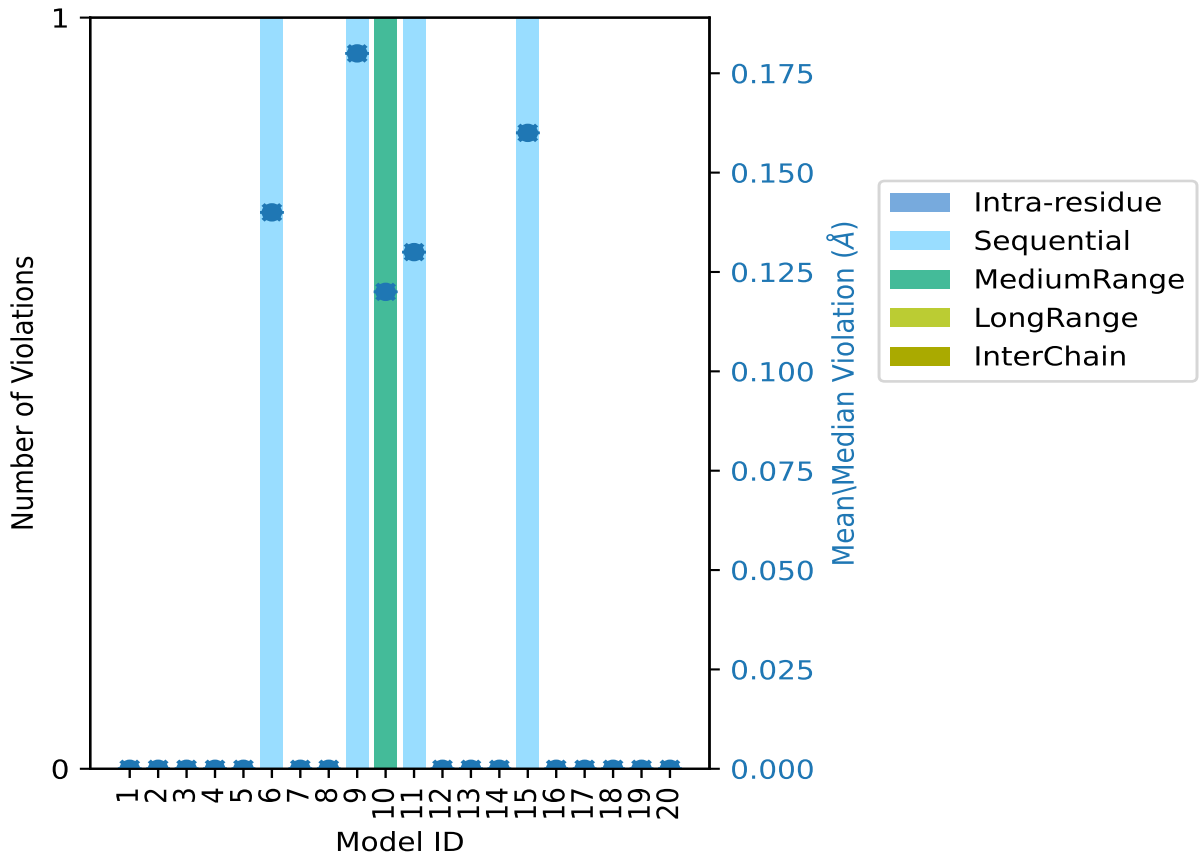
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0	0	0.0	0.0	0.0	0.0
15	0	1	0	0	0	1	0.16	0.16	0.0	0.16
16	0	0	0	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0	0	0	0.0	0.0	0.0	0.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance 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

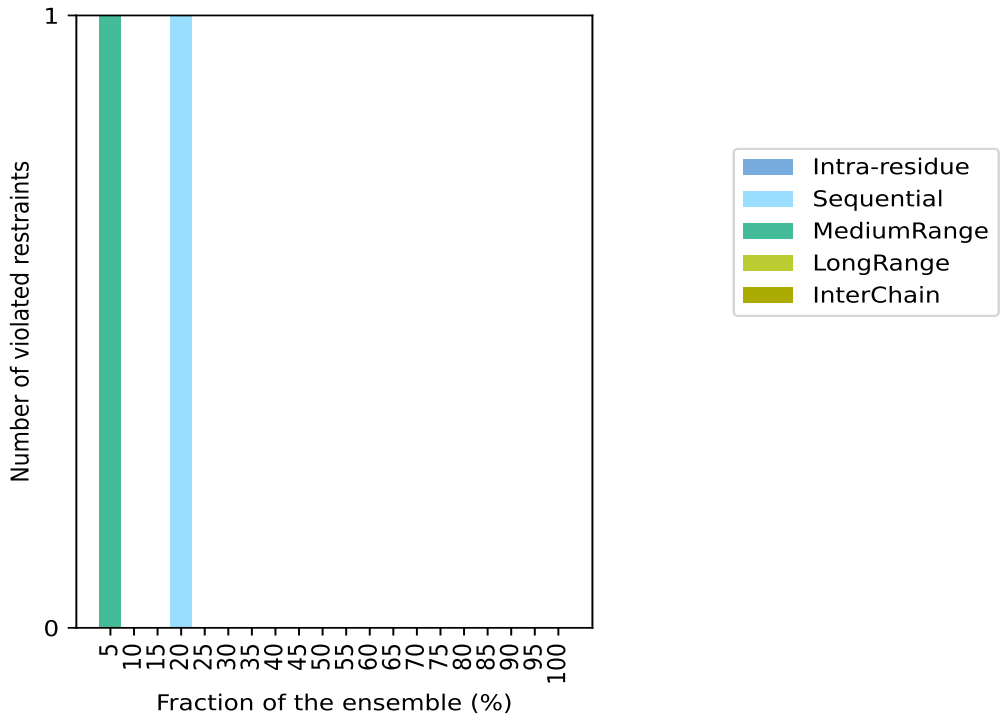
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in 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 the ensemble. In total, 1520(IR:396, SQ:346, MR:328, LR:450, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	1	0	0	1	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	1	0	0	0	1	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

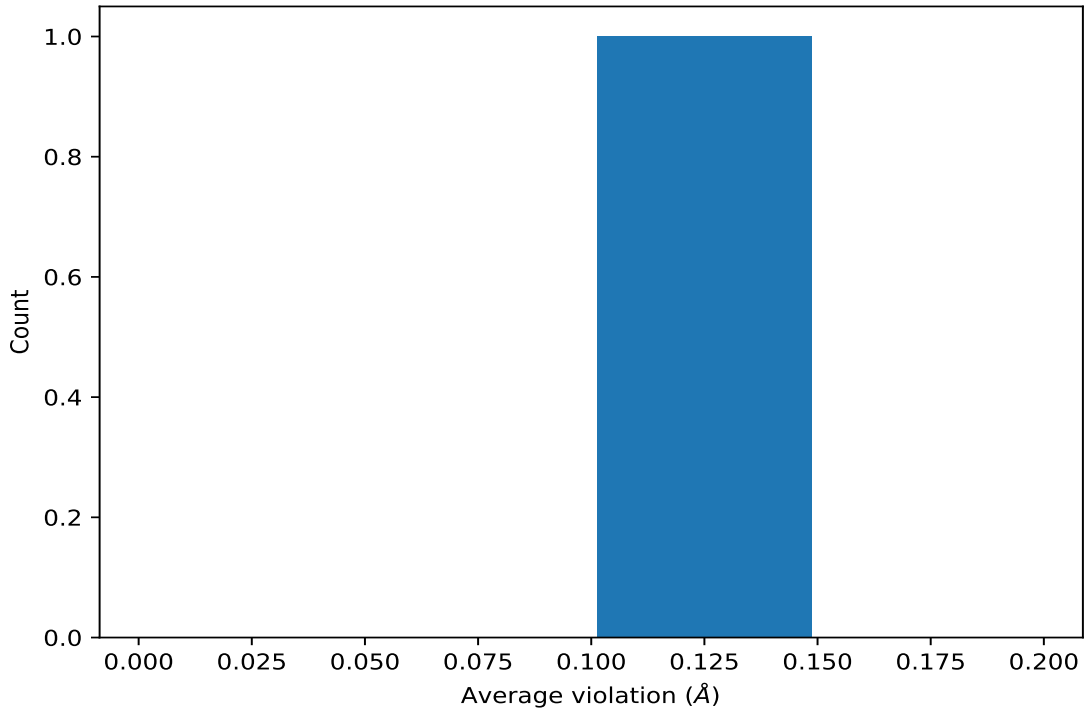
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance 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



9.4.2 Table: Most violated distance 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. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,234)	1:A:13:SER:HA	1:A:14:VAL:H	4	0.15	0.02	0.15

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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

9.5.2 Table : All distance violations (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. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:A:13:SER:HA	1:A:14:VAL:H	9	0.18
(1,234)	1:A:13:SER:HA	1:A:14:VAL:H	15	0.16
(1,234)	1:A:13:SER:HA	1:A:14:VAL:H	6	0.14
(1,234)	1:A:13:SER:HA	1:A:14:VAL:H	11	0.13
(1,1065)	1:A:74:ASP:HB2	1:A:77:GLN:H	10	0.12

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value