wwPDB NMR Structure Validation Summary Report

Aug 24, 2023 – 10:10 AM JST

PDB ID	:	7XX9
BMRB ID	:	36491
Title	:	Solution structure of RRM2 of Human SART3
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Deposited on	:	2022-05-29

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

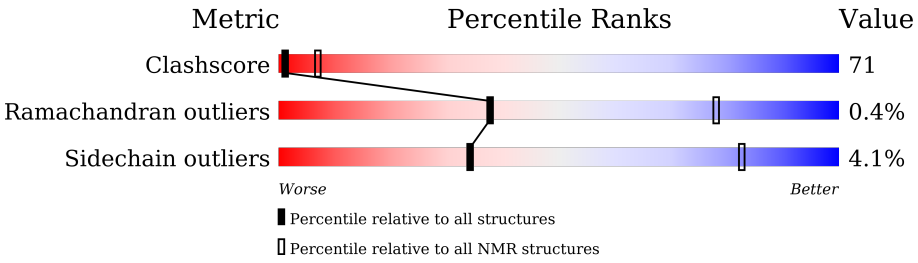
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 89%.

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	84	21% 69% • 8%

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 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:801-A:877 (77)	0.58	14

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 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1318 atoms, of which 668 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Squamous cell carcinoma antigen recognized by T-cells 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	84	1318	408	668	112	124	6	0

There are 4 discrepancies between the modelled and reference sequences:

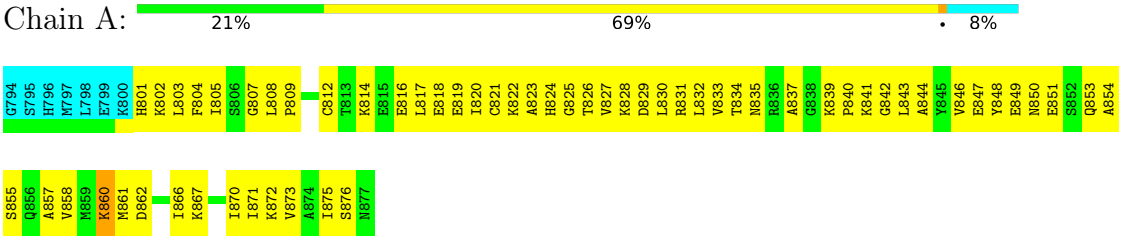
Chain	Residue	Modelled	Actual	Comment	Reference
A	794	GLY	-	expression tag	UNP Q15020
A	795	SER	-	expression tag	UNP Q15020
A	796	HIS	-	expression tag	UNP Q15020
A	797	MET	-	expression tag	UNP Q15020

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.

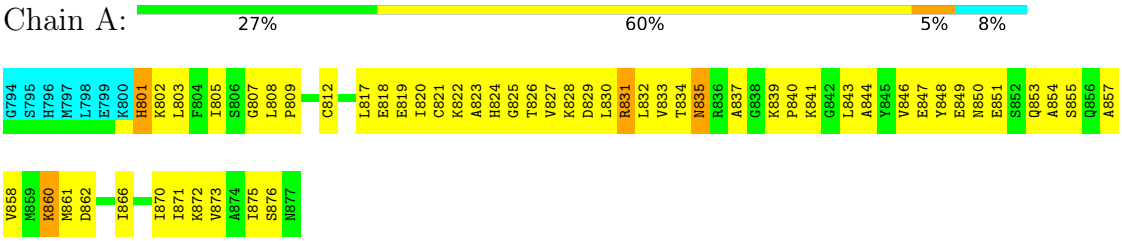
• Molecule 1: Squamous cell carcinoma antigen recognized by T-cells 3



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

The representative model is number 14. Colouring as in section 4.1 above.

• Molecule 1: Squamous cell carcinoma antigen recognized by T-cells 3



5 Refinement protocol and experimental data overview

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

Of the 1000 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
CYANA	structure calculation	
X-PLOR NIH	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	1
Total number of shifts	1076
Number of shifts mapped to atoms	1076
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

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	596	615	615	86±9
All	All	11920	12300	12300	1728

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 71.

5 of 521 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:807:GLY:C	1:A:808:LEU:HD22	1.03	1.74	6	2
1:A:807:GLY:C	1:A:808:LEU:HD12	1.00	1.76	12	9
1:A:803:LEU:HD21	1:A:854:ALA:HB1	0.99	1.32	16	2
1:A:829:ASP:O	1:A:846:VAL:HG23	0.97	1.60	2	17
1:A:857:ALA:HB1	1:A:861:MET:HE2	0.97	1.35	3	12

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	76/84 (90%)	72±1 (95±1%)	4±1 (5±1%)	0±0 (0±1%)	38 78
All	All	1520/1680 (90%)	1438 (95%)	76 (5%)	6 (0%)	38 78

All 2 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	807	GLY	4
1	A	842	GLY	2

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	66/72 (92%)	63±1 (96±2%)	3±1 (4±2%)	34 82
All	All	1320/1440 (92%)	1266 (96%)	54 (4%)	34 82

5 of 22 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	860	LYS	12
1	A	801	HIS	5
1	A	808	LEU	4
1	A	802	LYS	3
1	A	814	LYS	3

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

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *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	1076
Number of shifts mapped to atoms	1076
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

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. First 5 (of 0) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	798	LEU	HD12	0.912	0.01	.
1	A	798	LEU	HD13	0.912	0.01	.
1	A	798	LEU	HD22	0.855	0.01	.
1	A	798	LEU	HD23	0.855	0.01	.
1	A	803	LEU	HD12	0.994	0.01	.
1	A	803	LEU	HD13	0.994	0.01	.
1	A	803	LEU	HD22	0.871	0.00	.
1	A	803	LEU	HD23	0.871	0.00	.
1	A	805	ILE	HD12	0.659	0.01	.
1	A	805	ILE	HD13	0.659	0.01	.
1	A	805	ILE	HG22	0.759	0.01	.
1	A	805	ILE	HG23	0.759	0.01	.
1	A	808	LEU	HD12	0.826	0.01	.
1	A	808	LEU	HD13	0.826	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	808	LEU	HD22	0.566	0.01	.
1	A	808	LEU	HD23	0.566	0.01	.
1	A	817	LEU	HD12	0.762	0.01	.
1	A	817	LEU	HD13	0.762	0.01	.
1	A	817	LEU	HD22	0.635	0.00	.
1	A	817	LEU	HD23	0.635	0.00	.
1	A	820	ILE	HD12	0.865	0.01	.
1	A	820	ILE	HD13	0.865	0.01	.
1	A	820	ILE	HG22	1.029	0.00	.
1	A	820	ILE	HG23	1.029	0.00	.
1	A	823	ALA	HB2	0.925	0.01	.
1	A	823	ALA	HB3	0.925	0.01	.
1	A	827	VAL	HG12	0.596	0.01	.
1	A	827	VAL	HG13	0.596	0.01	.
1	A	827	VAL	HG22	0.533	0.01	.
1	A	827	VAL	HG23	0.533	0.01	.
1	A	830	LEU	HD12	0.771	0.00	.
1	A	830	LEU	HD13	0.771	0.00	.
1	A	830	LEU	HD22	0.782	0.01	.
1	A	830	LEU	HD23	0.782	0.01	.
1	A	832	LEU	HD12	0.851	0.01	.
1	A	832	LEU	HD13	0.851	0.01	.
1	A	832	LEU	HD22	0.745	0.01	.
1	A	832	LEU	HD23	0.745	0.01	.
1	A	833	VAL	HG12	1.048	0.01	.
1	A	833	VAL	HG13	1.048	0.01	.
1	A	833	VAL	HG22	1.027	0.01	.
1	A	833	VAL	HG23	1.027	0.01	.
1	A	834	THR	HG22	0.981	0.01	.
1	A	834	THR	HG23	0.981	0.01	.
1	A	837	ALA	HB2	1.432	0.01	.
1	A	837	ALA	HB3	1.432	0.01	.
1	A	843	LEU	HD12	1.028	0.00	.
1	A	843	LEU	HD13	1.028	0.00	.
1	A	843	LEU	HD22	0.972	0.01	.
1	A	843	LEU	HD23	0.972	0.01	.
1	A	844	ALA	HB2	1.088	0.01	.
1	A	844	ALA	HB3	1.088	0.01	.
1	A	846	VAL	HG12	0.816	0.01	.
1	A	846	VAL	HG13	0.816	0.01	.
1	A	846	VAL	HG22	0.741	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	846	VAL	HG23	0.741	0.01	.
1	A	854	ALA	HB2	1.500	0.01	.
1	A	854	ALA	HB3	1.500	0.01	.
1	A	857	ALA	HB2	1.327	0.01	.
1	A	857	ALA	HB3	1.327	0.01	.
1	A	858	VAL	HG12	0.982	0.01	.
1	A	858	VAL	HG13	0.982	0.01	.
1	A	858	VAL	HG22	0.982	0.01	.
1	A	858	VAL	HG23	0.982	0.01	.
1	A	865	THR	HG22	0.977	0.01	.
1	A	865	THR	HG23	0.977	0.01	.
1	A	866	ILE	HD12	0.764	0.01	.
1	A	866	ILE	HD13	0.764	0.01	.
1	A	866	ILE	HG22	0.771	0.01	.
1	A	866	ILE	HG23	0.771	0.01	.
1	A	870	ILE	HD12	0.795	0.01	.
1	A	870	ILE	HD13	0.795	0.01	.
1	A	870	ILE	HG22	0.765	0.00	.
1	A	870	ILE	HG23	0.765	0.00	.
1	A	871	ILE	HD12	0.636	0.01	.
1	A	871	ILE	HD13	0.636	0.01	.
1	A	871	ILE	HG22	0.696	0.01	.
1	A	871	ILE	HG23	0.696	0.01	.
1	A	873	VAL	HG12	0.917	0.01	.
1	A	873	VAL	HG13	0.917	0.01	.
1	A	873	VAL	HG22	0.876	0.01	.
1	A	873	VAL	HG23	0.876	0.01	.
1	A	874	ALA	HB2	1.454	0.03	.
1	A	874	ALA	HB3	1.454	0.03	.
1	A	875	ILE	HD12	0.825	0.01	.
1	A	875	ILE	HD13	0.825	0.01	.
1	A	875	ILE	HG22	1.006	0.01	.
1	A	875	ILE	HG23	1.006	0.01	.

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	82	-0.70 ± 0.18	Should be applied
$^{13}C_{\beta}$	77	-0.59 ± 0.18	Should be applied

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C'$	82	2.74 ± 0.26	Should be applied
^{15}N	78	0.25 ± 0.42	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 89%, i.e. 925 atoms were assigned a chemical shift out of a possible 1044. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	384/386 (99%)	156/157 (99%)	154/154 (100%)	74/75 (99%)
Sidechain	516/606 (85%)	350/394 (89%)	160/191 (84%)	6/21 (29%)
Aromatic	25/52 (48%)	16/26 (62%)	9/24 (38%)	0/2 (0%)
Overall	925/1044 (89%)	522/577 (90%)	323/369 (88%)	80/98 (82%)

7.1.4 Statistically unusual chemical shifts

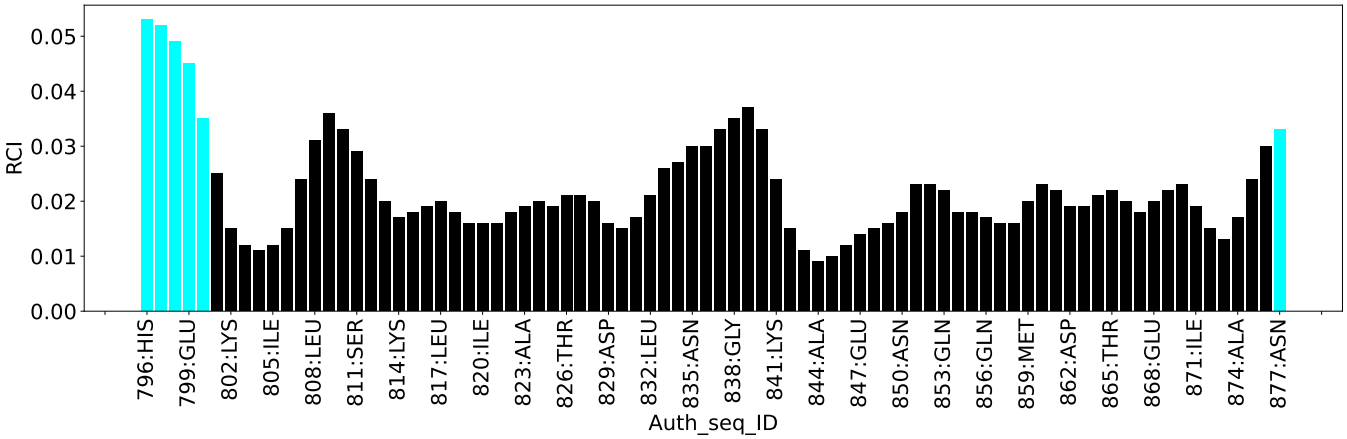
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	828	LYS	HE2	1.61	1.95 – 3.88	-6.8
1	A	828	LYS	HE3	1.61	1.92 – 3.89	-6.6

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:


RCI
0.05
0.04
0.03
0.02
0.01
0.00
796:HIS
799:GLU
802:LYS
805:ILE
808:LEU
811:SER
814:LYS
817:LEU
820:ILE
823:ALA
826:THR
829:ASP
832:LEU
835:ASN
838:GLY
841:LYS
844:ALA
847:GLU
850:ASN
853:GLN
856:GLN
859:MET
862:ASP
865:THR
868:GLU
871:ILE
874:ALA
877:ASN
Auth_seq_ID

8 NMR restraints analysis

8.1 Conformationally restricting restraints

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	1215
Intra-residue (|i-j|=0)	304
Sequential (|i-j|=1)	362
Medium range (|i-j|>1 and |i-j|<5)	175
Long range (|i-j|≥5)	374
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	14.5
Number of long range restraints per residue[1]	4.5

[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

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

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)	9.9	0.2
0.2-0.5 (Medium)	4.1	0.41
>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)

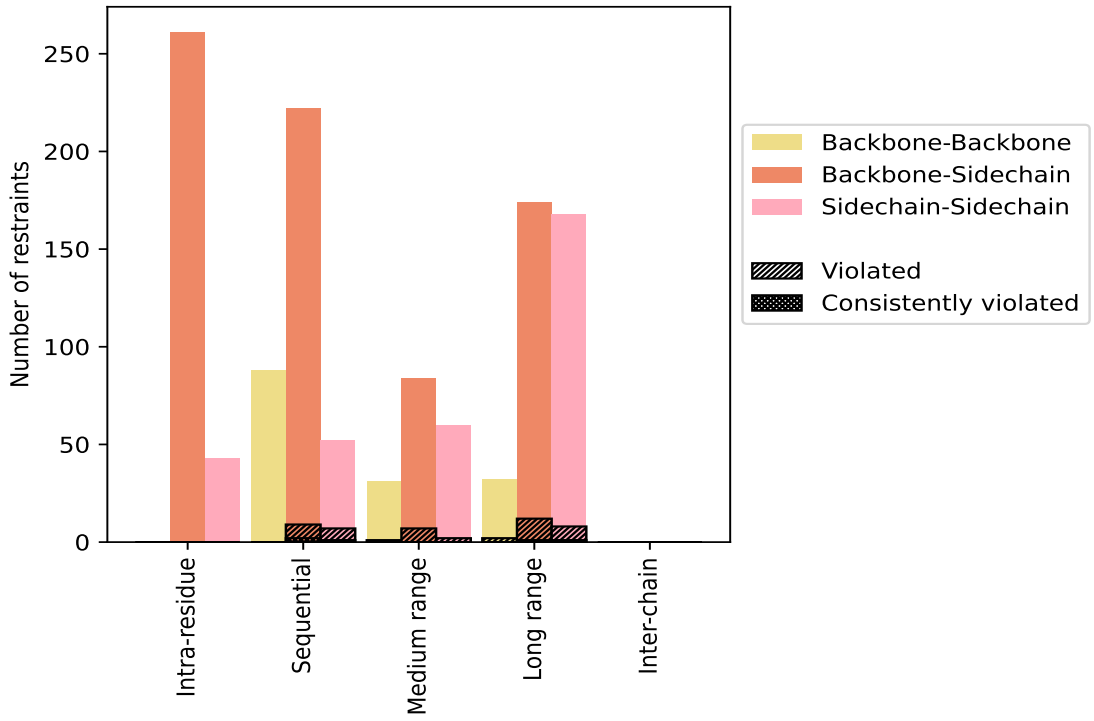
9.1 Summary of distance violations (i)

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)	304	25.0	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	261	21.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	43	3.5	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	362	29.8	16	4.4	1.3	3	0.8	0.2
Backbone-Backbone	88	7.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	222	18.3	9	4.1	0.7	2	0.9	0.2
Sidechain-Sidechain	52	4.3	7	13.5	0.6	1	1.9	0.1
Medium range (|i-j|>1 & |i-j|<5)	175	14.4	10	5.7	0.8	0	0.0	0.0
Backbone-Backbone	31	2.6	1	3.2	0.1	0	0.0	0.0
Backbone-Sidechain	84	6.9	7	8.3	0.6	0	0.0	0.0
Sidechain-Sidechain	60	4.9	2	3.3	0.2	0	0.0	0.0
Long range (|i-j|≥5)	374	30.8	22	5.9	1.8	2	0.5	0.2
Backbone-Backbone	32	2.6	2	6.2	0.2	0	0.0	0.0
Backbone-Sidechain	174	14.3	12	6.9	1.0	1	0.6	0.1
Sidechain-Sidechain	168	13.8	8	4.8	0.7	1	0.6	0.1
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	1215	100.0	48	4.0	4.0	5	0.4	0.4
Backbone-Backbone	151	12.4	3	2.0	0.2	0	0.0	0.0
Backbone-Sidechain	741	61.0	28	3.8	2.3	3	0.4	0.2
Sidechain-Sidechain	323	26.6	17	5.3	1.4	2	0.6	0.2

[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



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

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	5	4	8	0	17	0.19	0.38	0.08	0.17
2	0	6	3	8	0	17	0.17	0.41	0.08	0.15
3	0	4	5	5	0	14	0.19	0.39	0.07	0.17
4	0	4	4	5	0	13	0.19	0.37	0.08	0.16
5	0	6	3	5	0	14	0.17	0.38	0.07	0.16
6	0	5	2	6	0	13	0.17	0.37	0.07	0.14
7	0	3	5	7	0	15	0.18	0.41	0.08	0.15
8	0	4	5	8	0	17	0.17	0.38	0.07	0.16
9	0	4	3	7	0	14	0.18	0.38	0.08	0.15
10	0	4	5	6	0	15	0.19	0.38	0.08	0.16
11	0	5	5	5	0	15	0.2	0.38	0.07	0.17

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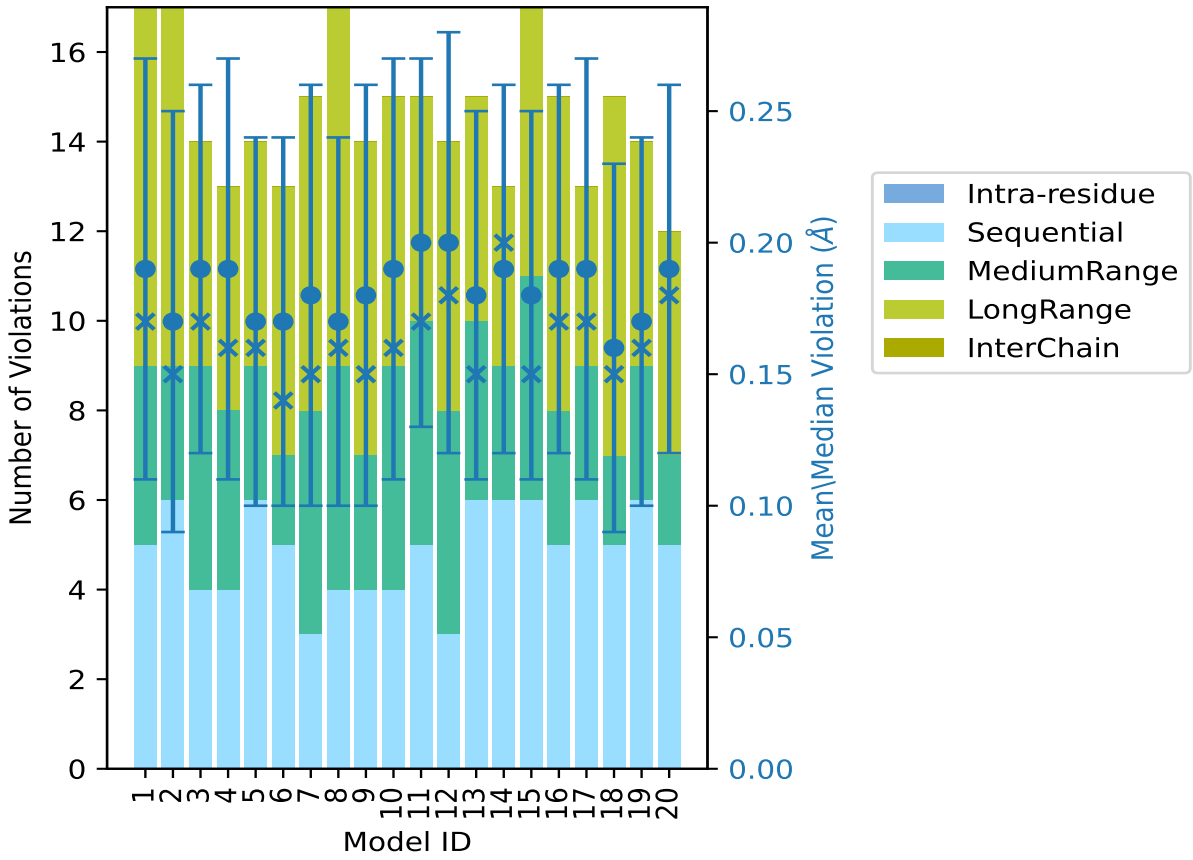
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	3	5	6	0	14	0.2	0.38	0.08	0.18
13	0	6	4	5	0	15	0.18	0.33	0.07	0.15
14	0	6	3	4	0	13	0.19	0.39	0.07	0.2
15	0	6	5	6	0	17	0.18	0.38	0.07	0.15
16	0	5	3	7	0	15	0.19	0.36	0.07	0.17
17	0	6	3	4	0	13	0.19	0.38	0.08	0.17
18	0	5	2	8	0	15	0.16	0.38	0.07	0.15
19	0	6	3	5	0	14	0.17	0.37	0.07	0.16
20	0	5	2	5	0	12	0.19	0.37	0.07	0.18

[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



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

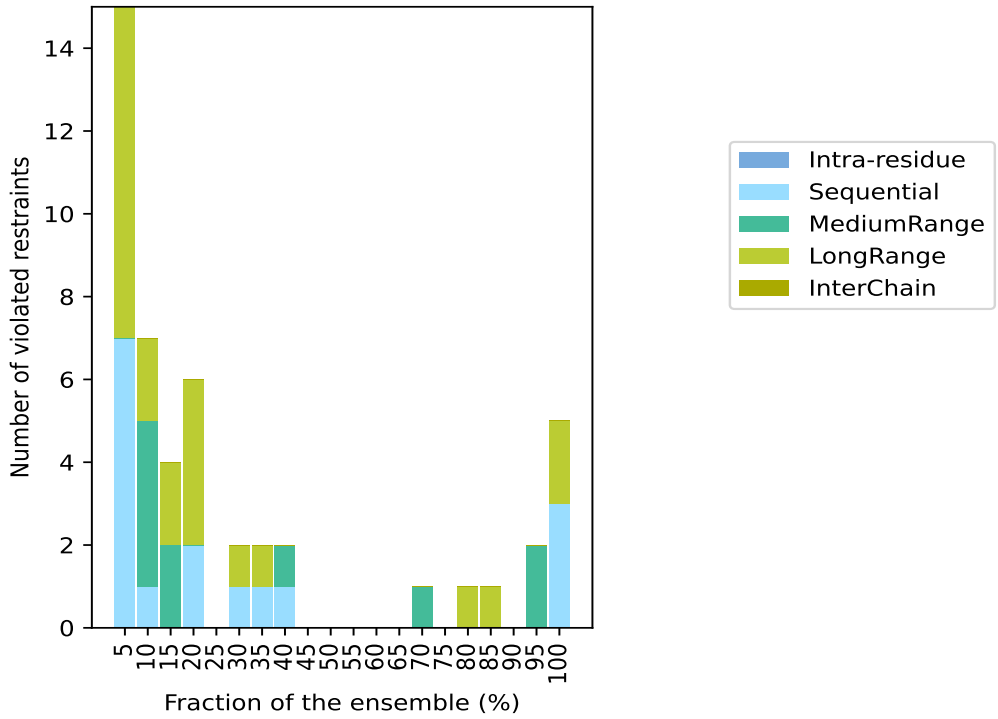
9.3 Distance violation statistics for the ensemble (i)

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, 1167(IR:304, SQ:346, MR:165, LR:352, 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	7	0	8	0	15	1	5.0
0	1	4	2	0	7	2	10.0
0	0	2	2	0	4	3	15.0
0	2	0	4	0	6	4	20.0
0	0	0	0	0	0	5	25.0
0	1	0	1	0	2	6	30.0
0	1	0	1	0	2	7	35.0
0	1	1	0	0	2	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	1	0	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	1	0	1	16	80.0
0	0	0	1	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	2	0	0	2	19	95.0
0	3	0	2	0	5	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

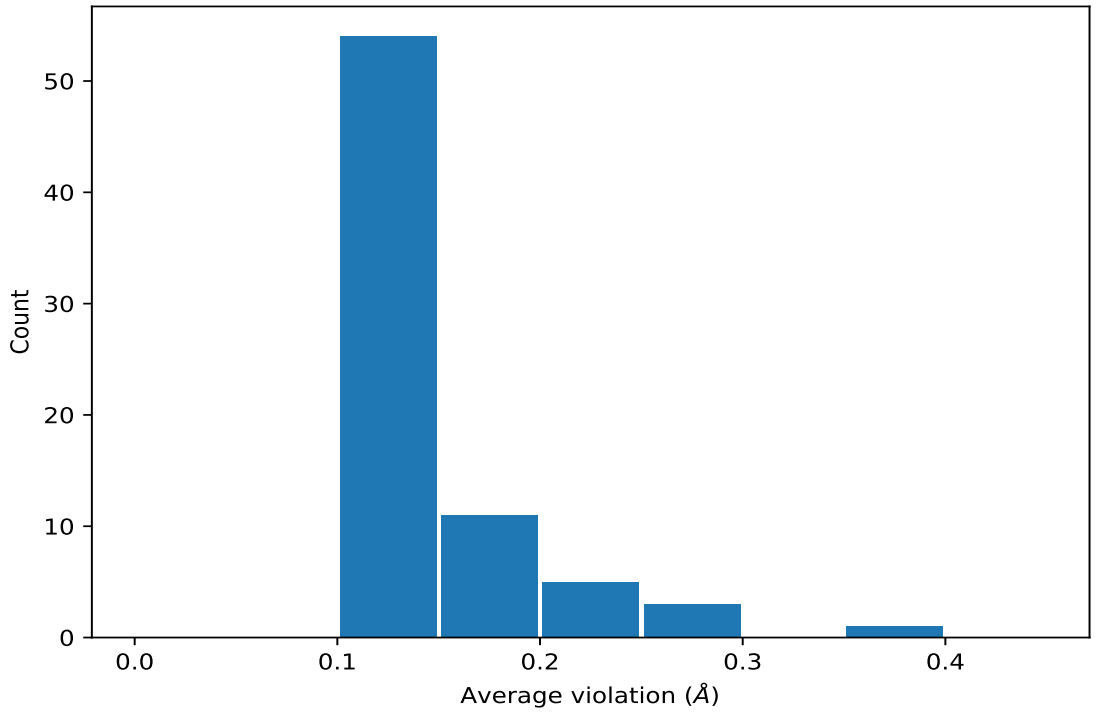
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation 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)
(1,266)	1:813:A:THR:HB	1:814:A:LYS:HA	20	0.38	0.02	0.38
(1,659)	1:833:A:VAL:HG11	1:844:A:ALA:H	20	0.24	0.03	0.24
(1,659)	1:833:A:VAL:HG12	1:844:A:ALA:H	20	0.24	0.03	0.24
(1,659)	1:833:A:VAL:HG13	1:844:A:ALA:H	20	0.24	0.03	0.24
(1,733)	1:840:A:PRO:HD3	1:841:A:LYS:HG2	20	0.2	0.04	0.22
(1,733)	1:840:A:PRO:HD3	1:841:A:LYS:HG3	20	0.2	0.04	0.22
(1,521)	1:827:A:VAL:HA	1:828:A:LYS:HB3	20	0.19	0.02	0.2
(1,819)	1:848:A:TYR:HE1	1:853:A:GLN:HB3	20	0.18	0.04	0.17
(1,819)	1:848:A:TYR:HE2	1:853:A:GLN:HB3	20	0.18	0.04	0.17
(1,1082)	1:865:A:THR:HG21	1:867:A:LYS:H	19	0.28	0.06	0.29
(1,1082)	1:865:A:THR:HG22	1:867:A:LYS:H	19	0.28	0.06	0.29
(1,1082)	1:865:A:THR:HG23	1:867:A:LYS:H	19	0.28	0.06	0.29
(1,905)	1:855:A:SER:HA	1:858:A:VAL:HA	19	0.15	0.02	0.14
(1,424)	1:821:A:CYS:HA	1:827:A:VAL:HA	17	0.14	0.03	0.14
(1,651)	1:833:A:VAL:HG11	1:842:A:GLY:H	16	0.14	0.02	0.13
(1,651)	1:833:A:VAL:HG12	1:842:A:GLY:H	16	0.14	0.02	0.13

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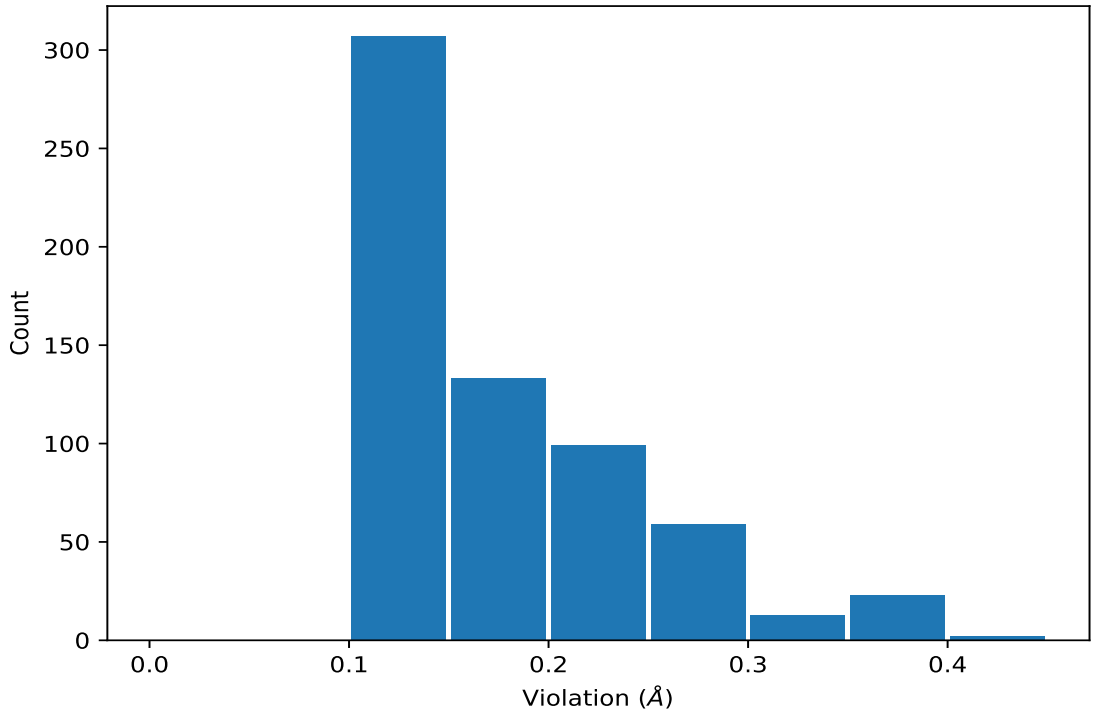
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,651)	1:833:A:VAL:HG13	1:842:A:GLY:H	16	0.14	0.02	0.13
(1,651)	1:833:A:VAL:HG21	1:842:A:GLY:H	16	0.14	0.02	0.13
(1,651)	1:833:A:VAL:HG22	1:842:A:GLY:H	16	0.14	0.02	0.13
(1,651)	1:833:A:VAL:HG23	1:842:A:GLY:H	16	0.14	0.02	0.13
(1,1105)	1:866:A:ILE:HD11	1:869:A:ASN:H	14	0.15	0.03	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.



9.5.2 Table : All distance violations (i)

The following table provides the 10 worst performing restraints, sorted by the violation 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)
(1,266)	1:813:A:THR:HB	1:814:A:LYS:HA	2	0.41
(1,266)	1:813:A:THR:HB	1:814:A:LYS:HA	7	0.41
(1,266)	1:813:A:THR:HB	1:814:A:LYS:HA	3	0.39
(1,266)	1:813:A:THR:HB	1:814:A:LYS:HA	14	0.39
(1,1082)	1:865:A:THR:HG21	1:867:A:LYS:H	10	0.38
(1,1082)	1:865:A:THR:HG22	1:867:A:LYS:H	10	0.38
(1,1082)	1:865:A:THR:HG23	1:867:A:LYS:H	10	0.38
(1,266)	1:813:A:THR:HB	1:814:A:LYS:HA	1	0.38
(1,266)	1:813:A:THR:HB	1:814:A:LYS:HA	5	0.38
(1,266)	1:813:A:THR:HB	1:814:A:LYS:HA	8	0.38
(1,266)	1:813:A:THR:HB	1:814:A:LYS:HA	9	0.38
(1,266)	1:813:A:THR:HB	1:814:A:LYS:HA	11	0.38

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found