



wwPDB NMR Structure Validation Summary Report ⓘ

Jun 6, 2023 – 06:44 pm BST

PDB ID : 6R1V
BMRB ID : 34379
Title : Solution structure of sortase A from *S. aureus* in complex with 2-(aminomethyl)-3-hydroxy-4H-pyran-4-one based prodrug
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Deposited on : 2019-03-15

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

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<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
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

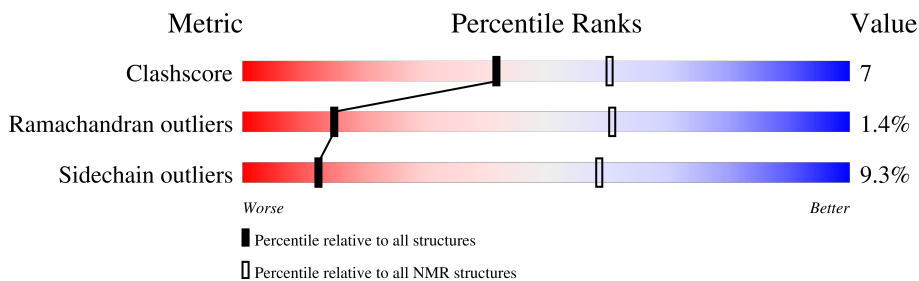
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	148	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	A	JPT	201	-	1

2 Ensemble composition and analysis i

This entry contains 20 models. Model 16 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:4-A:148 (145)	1.18	16

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 2 clusters and 5 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2389 atoms, of which 1192 are hydrogens and 0 are deuteriums.

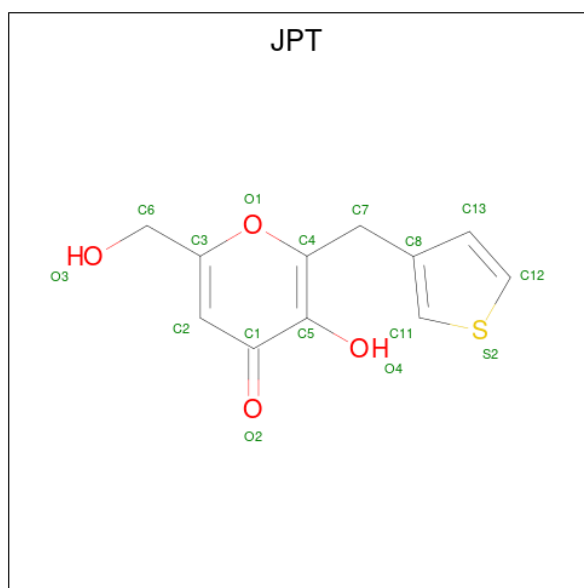
- Molecule 1 is a protein called Sortase A.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	148	2364	746	1183	199	232	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q2FV99
A	109	GLU	GLY	conflict	UNP Q2FV99

- Molecule 2 is 6-(hydroxymethyl)-3-oxidanyl-2-(thiophen-3-ylmethyl)pyran-4-one (three-letter code: JPT) (formula: C₁₁H₁₀O₄S).



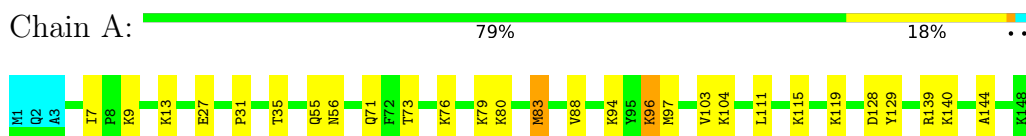
Mol	Chain	Residues	Atoms				
			Total	C	H	O	S
2	A	1	25	11	9	4	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

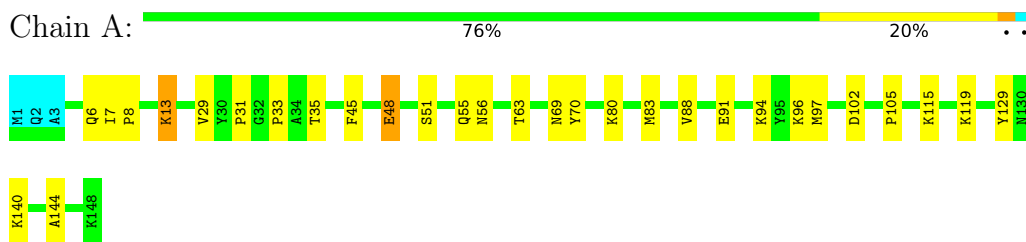
- Molecule 1: Sortase A



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

The representative model is number 16. Colouring as in section 4.1 above.

- Molecule 1: Sortase A



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, 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
CNS	refinement	1.2
CYANA	structure calculation	2.1

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	1867
Number of shifts mapped to atoms	1866
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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	1159	1162	1162	17±4
2	A	16	9	0	1±1
All	All	23500	23420	23240	341

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 7.

5 of 202 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:LYS:HA	1:A:132:LYS:HE2	0.84	1.46	16	1
1:A:43:VAL:HB	1:A:71:GLN:HG3	0.84	1.48	14	1
1:A:105:PRO:HA	2:A:201:JPT:O2	0.78	1.79	16	1
1:A:51:SER:HB3	1:A:54:ASP:HB2	0.76	1.57	20	1
1:A:102:ASP:HB3	1:A:140:LYS:HG3	0.75	1.59	9	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	144/148 (97%)	127±2 (88±2%)	15±2 (10±2%)	2±1 (1±1%)	15	61
All	All	2880/2960 (97%)	2543 (88%)	297 (10%)	40 (1%)	15	61

5 of 13 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	71	GLN	11
1	A	83	MET	10
1	A	4	LYS	5
1	A	128	ASP	3
1	A	90	ASN	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	129/131 (98%)	117±2 (91±2%)	12±2 (9±2%)	12	59
All	All	2580/2620 (98%)	2340 (91%)	240 (9%)	12	59

5 of 55 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	76	LYS	16
1	A	83	MET	16
1	A	94	LYS	15
1	A	96	LYS	15
1	A	104	LYS	15

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	JPT	A	201	1	16,17,17	2.63±0.03	8±0 (49±2%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	JPT	A	201	1	18,23,23	3.84±0.10	9±0 (50±2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	JPT	A	201	1	-	0±0,6,6,6	0±0,2,2,2

5 of 8 unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	201	JPT	C5-C4	5.08	1.39	1.35	18	20
2	A	201	JPT	C6-C3	4.74	1.39	1.50	16	20
2	A	201	JPT	C5-C1	4.24	1.36	1.45	20	20
2	A	201	JPT	C7-C4	4.09	1.38	1.49	20	20
2	A	201	JPT	C11-S2	3.75	1.66	1.70	11	20

5 of 10 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	201	JPT	C8-C11-S2	9.92	105.90	112.29	4	20
2	A	201	JPT	C4-O1-C3	9.36	113.39	119.52	14	20
2	A	201	JPT	O1-C4-C7	6.31	118.04	109.31	3	20
2	A	201	JPT	O1-C3-C6	5.19	116.02	111.35	14	20
2	A	201	JPT	C6-C3-C2	3.89	120.40	126.74	16	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 93% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

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	1867
Number of shifts mapped to atoms	1866
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	201	JPT	H7	5.13	0.020	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	147	-0.14 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	138	-0.02 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	136	0.09 ± 0.08	None needed (< 0.5 ppm)
^{15}N	135	-0.18 ± 0.22	None needed (< 0.5 ppm)

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 93%, i.e. 1839 atoms were assigned a chemical shift out of a possible 1987. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	701/715 (98%)	288/289 (100%)	279/290 (96%)	134/136 (99%)
Sidechain	1028/1149 (89%)	693/736 (94%)	322/366 (88%)	13/47 (28%)
Aromatic	110/123 (89%)	55/59 (93%)	54/62 (87%)	1/2 (50%)
Overall	1839/1987 (93%)	1036/1084 (96%)	655/718 (91%)	148/185 (80%)

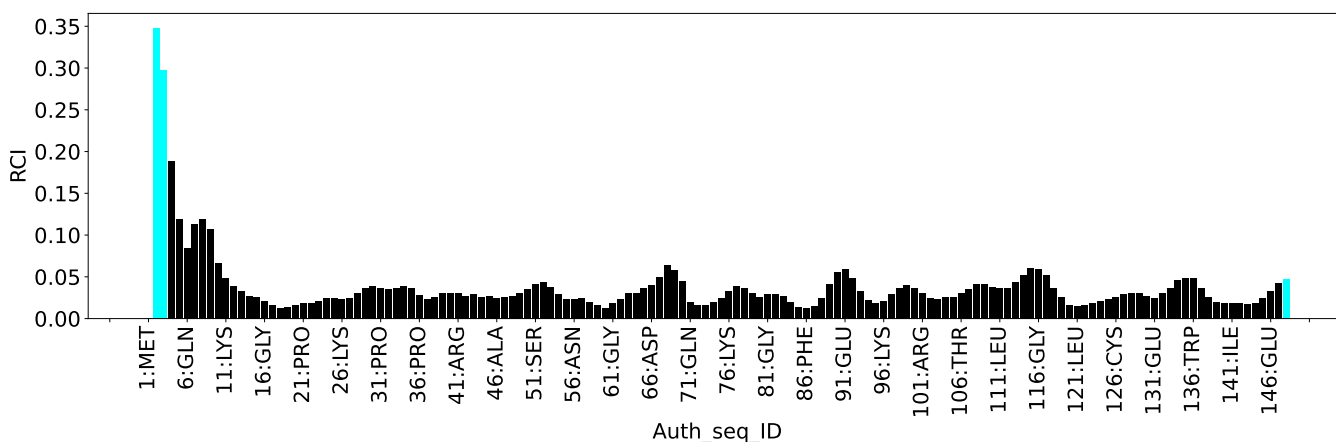
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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:



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	2172
Intra-residue ($ i-j =0$)	583
Sequential ($ i-j =1$)	621
Medium range ($ i-j >1$ and $ i-j <5$)	259
Long range ($ i-j \geq 5$)	709
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	14.7
Number of long range restraints per residue ¹	4.8

¹Long 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)	22.5	0.2
0.2-0.5 (Medium)	5.0	0.48
>0.5 (Large)	0.1	0.82

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis [i](#)

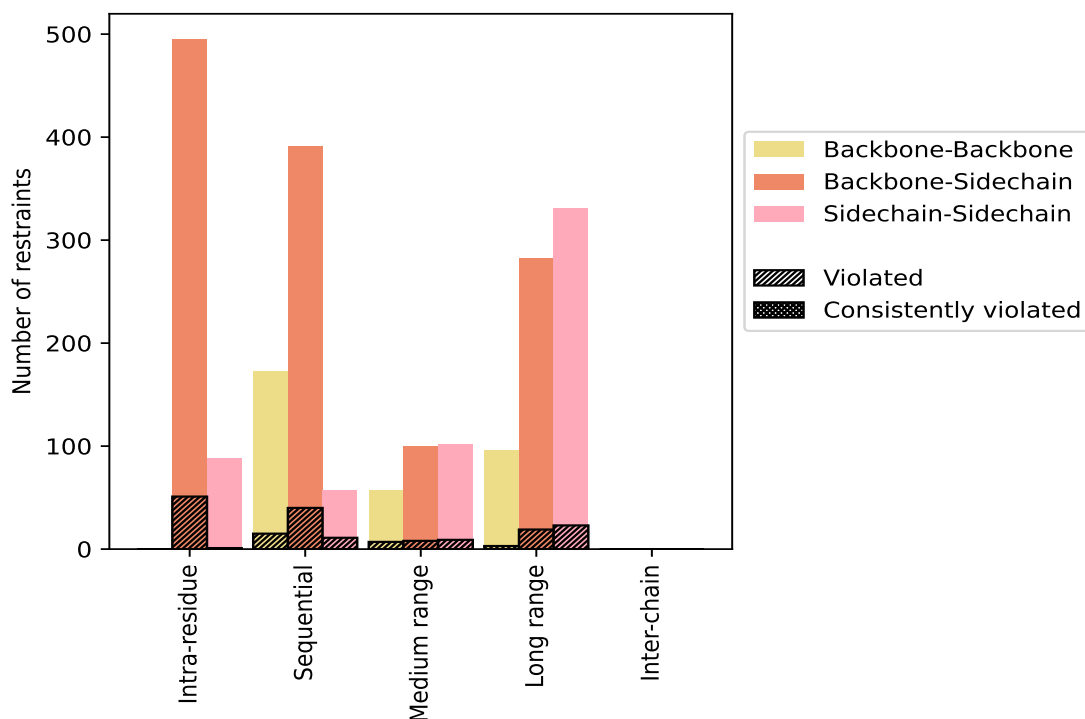
9.1 Summary of distance violations [i](#)

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	583	26.8	52	8.9	2.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	495	22.8	51	10.3	2.3	0	0.0	0.0
Sidechain-Sidechain	88	4.1	1	1.1	0.0	0	0.0	0.0
Sequential ($i-j =1$)	621	28.6	66	10.6	3.0	0	0.0	0.0
Backbone-Backbone	173	8.0	15	8.7	0.7	0	0.0	0.0
Backbone-Sidechain	391	18.0	40	10.2	1.8	0	0.0	0.0
Sidechain-Sidechain	57	2.6	11	19.3	0.5	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	259	11.9	24	9.3	1.1	0	0.0	0.0
Backbone-Backbone	57	2.6	7	12.3	0.3	0	0.0	0.0
Backbone-Sidechain	100	4.6	8	8.0	0.4	0	0.0	0.0
Sidechain-Sidechain	102	4.7	9	8.8	0.4	0	0.0	0.0
Long range ($i-j \geq 5$)	709	32.6	45	6.3	2.1	0	0.0	0.0
Backbone-Backbone	96	4.4	3	3.1	0.1	0	0.0	0.0
Backbone-Sidechain	282	13.0	19	6.7	0.9	0	0.0	0.0
Sidechain-Sidechain	331	15.2	23	6.9	1.1	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	2172	100.0	187	8.6	8.6	0	0.0	0.0
Backbone-Backbone	326	15.0	25	7.7	1.2	0	0.0	0.0
Backbone-Sidechain	1268	58.4	118	9.3	5.4	0	0.0	0.0
Sidechain-Sidechain	578	26.6	44	7.6	2.0	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 disulfid 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	7	7	2	6	0	22	0.17	0.29	0.05	0.16
2	6	11	6	5	0	28	0.17	0.35	0.06	0.16
3	6	15	1	9	0	31	0.15	0.3	0.04	0.14
4	12	10	6	6	0	34	0.17	0.41	0.06	0.16
5	9	9	5	7	0	30	0.16	0.28	0.05	0.14
6	9	10	3	7	0	29	0.17	0.39	0.06	0.17
7	10	11	2	9	0	32	0.16	0.43	0.07	0.14
8	7	6	3	4	0	20	0.16	0.35	0.06	0.13
9	10	15	2	6	0	33	0.18	0.48	0.08	0.15
10	7	9	3	10	0	29	0.17	0.48	0.08	0.14
11	10	10	5	3	0	28	0.16	0.28	0.04	0.16

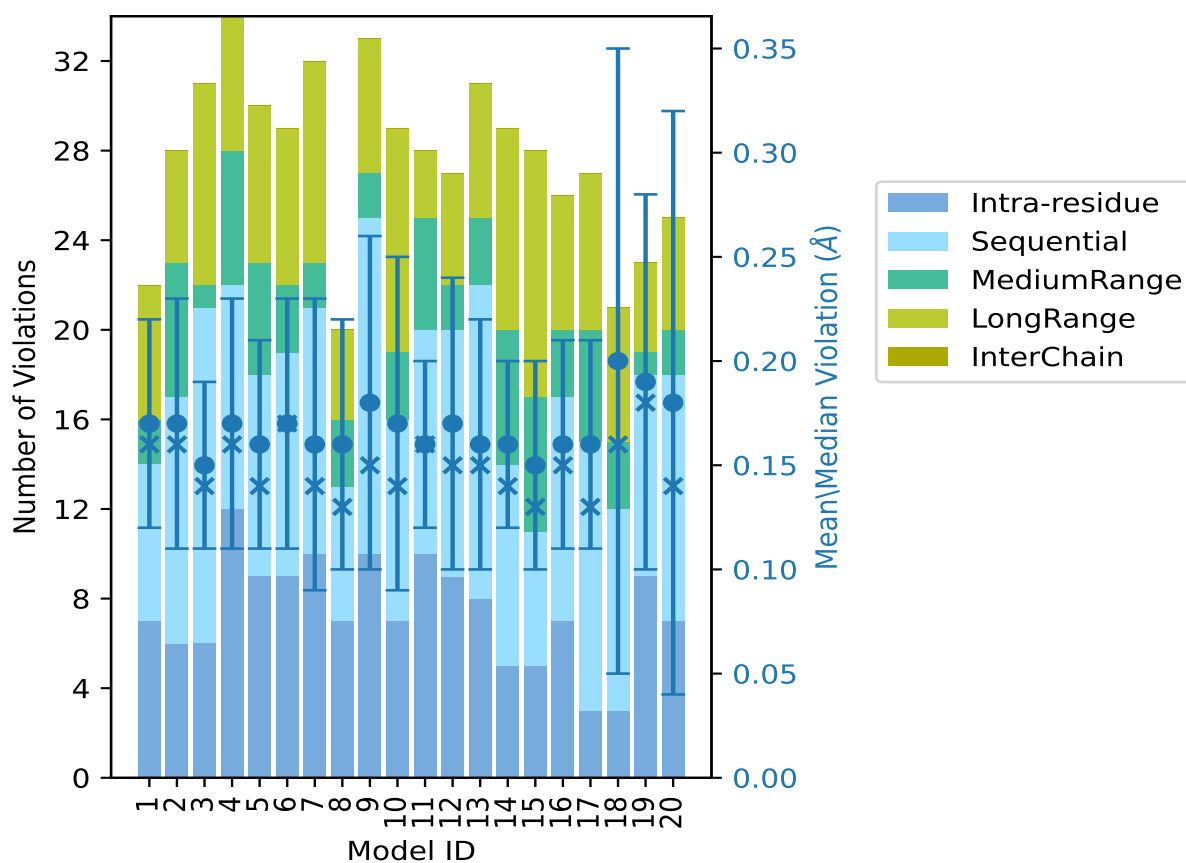
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
12	9	11	2	5	0	27	0.17	0.39	0.07	0.15
13	8	14	3	6	0	31	0.16	0.34	0.06	0.15
14	5	9	6	9	0	29	0.16	0.27	0.04	0.14
15	5	6	6	11	0	28	0.15	0.31	0.05	0.13
16	7	10	3	6	0	26	0.16	0.3	0.05	0.15
17	3	12	5	7	0	27	0.16	0.29	0.05	0.13
18	3	9	3	6	0	21	0.2	0.82	0.15	0.16
19	9	9	1	4	0	23	0.19	0.46	0.09	0.18
20	7	11	2	5	0	25	0.18	0.81	0.14	0.14

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

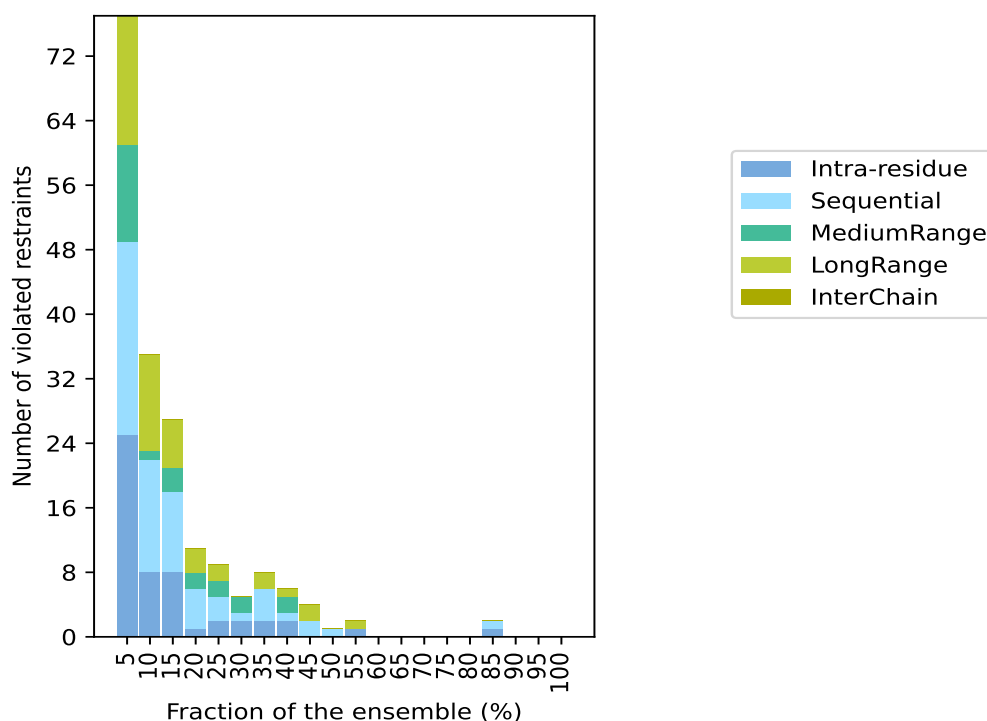
9.3 Distance violation statistics for the ensemble

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, 1985(IR:531, SQ:555, MR:235, LR:664, 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	%
25	24	12	16	0	77	1	5.0
8	14	1	12	0	35	2	10.0
8	10	3	6	0	27	3	15.0
1	5	2	3	0	11	4	20.0
2	3	2	2	0	9	5	25.0
2	1	2	0	0	5	6	30.0
2	4	0	2	0	8	7	35.0
2	1	2	1	0	6	8	40.0
0	2	0	2	0	4	9	45.0
0	1	0	0	0	1	10	50.0
1	0	0	1	0	2	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
1	1	0	0	0	2	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

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

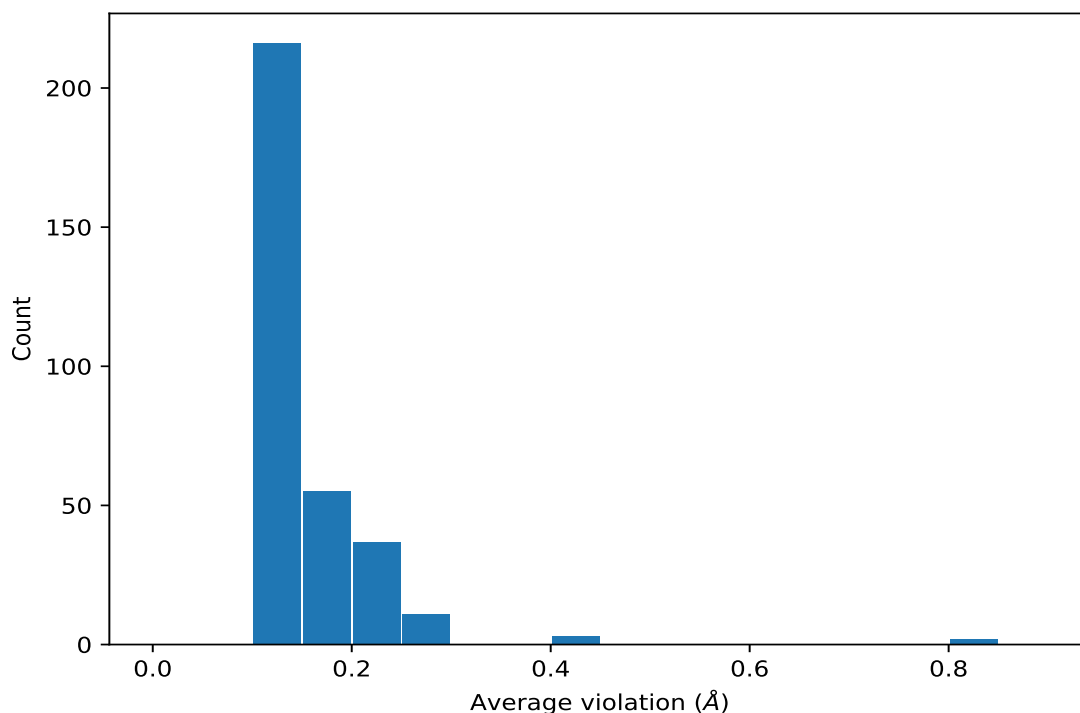
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 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)
(1,533)	1:A:33:PRO:HB3	1:A:34:ALA:H	17	0.2	0.03	0.2
(1,269)	1:A:132:LYS:H	1:A:132:LYS:HB3	17	0.2	0.03	0.21
(1,643)	1:A:148:LYS:H	1:A:148:LYS:HD2	11	0.16	0.03	0.16
(1,643)	1:A:148:LYS:H	1:A:148:LYS:HD3	11	0.16	0.03	0.16
(1,784)	1:A:121:LEU:H	1:A:143:VAL:HA	11	0.12	0.01	0.12
(1,1186)	1:A:18:ILE:HG21	1:A:19:GLU:H	10	0.14	0.02	0.14
(1,1186)	1:A:18:ILE:HG22	1:A:19:GLU:H	10	0.14	0.02	0.14
(1,1186)	1:A:18:ILE:HG23	1:A:19:GLU:H	10	0.14	0.02	0.14
(1,1942)	1:A:96:LYS:HG2	1:A:147:VAL:HG11	9	0.17	0.02	0.16
(1,1942)	1:A:96:LYS:HG2	1:A:147:VAL:HG12	9	0.17	0.02	0.16
(1,1942)	1:A:96:LYS:HG2	1:A:147:VAL:HG13	9	0.17	0.02	0.16
(1,1942)	1:A:96:LYS:HG2	1:A:147:VAL:HG21	9	0.17	0.02	0.16
(1,1942)	1:A:96:LYS:HG2	1:A:147:VAL:HG22	9	0.17	0.02	0.16
(1,1942)	1:A:96:LYS:HG2	1:A:147:VAL:HG23	9	0.17	0.02	0.16
(1,1942)	1:A:96:LYS:HG3	1:A:147:VAL:HG11	9	0.17	0.02	0.16
(1,1942)	1:A:96:LYS:HG3	1:A:147:VAL:HG12	9	0.17	0.02	0.16

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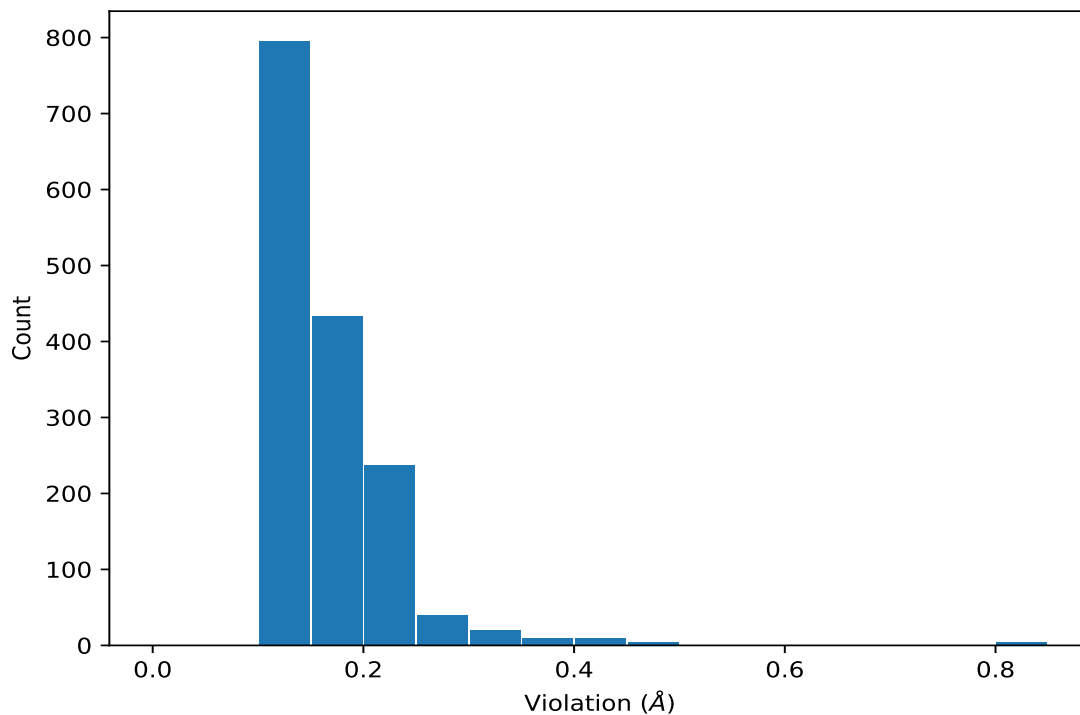
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1942)	1:A:96:LYS:HG3	1:A:147:VAL:HG13	9	0.17	0.02	0.16
(1,1942)	1:A:96:LYS:HG3	1:A:147:VAL:HG21	9	0.17	0.02	0.16
(1,1942)	1:A:96:LYS:HG3	1:A:147:VAL:HG22	9	0.17	0.02	0.16
(1,1942)	1:A:96:LYS:HG3	1:A:147:VAL:HG23	9	0.17	0.02	0.16
(1,641)	1:A:13:LYS:HD2	1:A:14:VAL:H	9	0.16	0.04	0.16
(1,641)	1:A:13:LYS:HD3	1:A:14:VAL:H	9	0.16	0.04	0.16
(1,1848)	1:A:81:GLY:HA2	1:A:96:LYS:HB2	9	0.14	0.02	0.13
(1,1848)	1:A:81:GLY:HA2	1:A:96:LYS:HB3	9	0.14	0.02	0.13
(1,1848)	1:A:81:GLY:HA3	1:A:96:LYS:HB2	9	0.14	0.02	0.13
(1,1848)	1:A:81:GLY:HA3	1:A:96:LYS:HB3	9	0.14	0.02	0.13
(1,47)	1:A:107:ASP:H	1:A:108:VAL:H	9	0.13	0.02	0.13
(1,987)	1:A:115:LYS:HA	1:A:117:LYS:H	8	0.29	0.02	0.29

¹Number of violated models, ²Standard 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)
(1,1134)	1:A:64:PHE:HA	1:A:64:PHE:HE1	18	0.82
(1,1134)	1:A:64:PHE:HA	1:A:64:PHE:HE2	18	0.82
(1,1134)	1:A:64:PHE:HA	1:A:64:PHE:HE1	20	0.81
(1,1134)	1:A:64:PHE:HA	1:A:64:PHE:HE2	20	0.81
(1,1069)	1:A:2:GLN:HA	1:A:3:ALA:H	9	0.48
(1,1069)	1:A:2:GLN:HA	1:A:3:ALA:H	10	0.48
(1,439)	1:A:112:ASP:HB2	1:A:113:GLU:H	19	0.46
(1,439)	1:A:112:ASP:HB3	1:A:113:GLU:H	19	0.46
(1,923)	1:A:110:VAL:H	1:A:110:VAL:HG21	9	0.44
(1,923)	1:A:110:VAL:H	1:A:110:VAL:HG22	9	0.44
(1,923)	1:A:110:VAL:H	1:A:110:VAL:HG23	9	0.44
(1,923)	1:A:110:VAL:H	1:A:110:VAL:HG21	7	0.43
(1,923)	1:A:110:VAL:H	1:A:110:VAL:HG22	7	0.43
(1,923)	1:A:110:VAL:H	1:A:110:VAL:HG23	7	0.43
(1,923)	1:A:110:VAL:H	1:A:110:VAL:HG21	4	0.41
(1,923)	1:A:110:VAL:H	1:A:110:VAL:HG22	4	0.41
(1,923)	1:A:110:VAL:H	1:A:110:VAL:HG23	4	0.41
(1,644)	1:A:132:LYS:HA	1:A:132:LYS:HD2	12	0.39
(1,644)	1:A:132:LYS:HA	1:A:132:LYS:HD3	12	0.39
(1,1079)	1:A:110:VAL:H	1:A:110:VAL:HG11	6	0.39

10 Dihedral-angle violation analysis

No dihedral-angle restraints found