wwPDB NMR Structure Validation Summary Report ⓘ

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BMRB ID	:	34121
Title	:	NMR solution structure of lysostaphin
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Deposited on	:	2017-04-07

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 ⓘ 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:

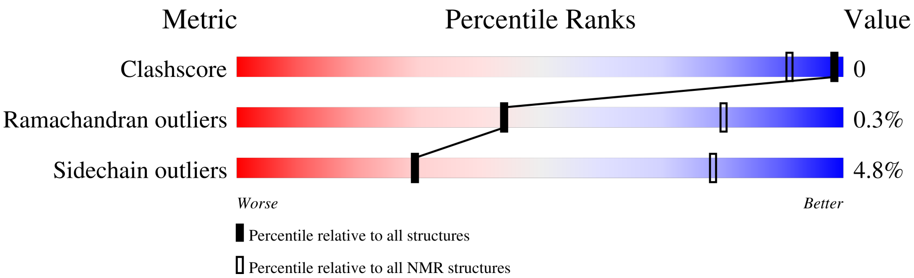
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 85%.

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	245	

2 Ensemble composition and analysis ⓘ

This entry contains 15 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:253-A:268, A:278-A:304, A:313-A:350, A:360-A:388 (110)	0.53	10
2	A:402-A:465, A:470-A:493 (88)	0.44	6

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 5 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 3, 7, 14
2	8, 9, 10, 15
3	1, 11, 12
4	5, 13
5	4, 6

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3722 atoms, of which 1823 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Lysostaphin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	245	3721	1208	1823	331	352	7	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	GLY	-	expression tag	UNP P10547
A	250	SER	-	expression tag	UNP P10547

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

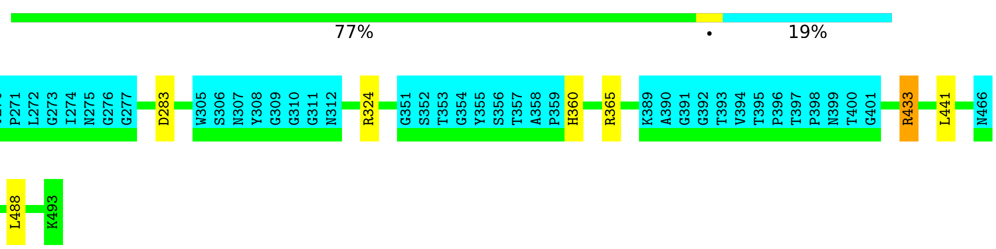
4 Residue-property plots (i)

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: Lysostaphin

Chain A:

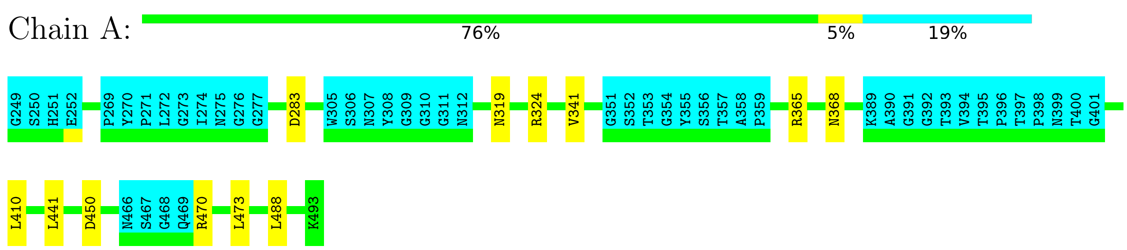


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 10. Colouring as in section 4.1 above.

- Molecule 1: Lysostaphin

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 15 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	
Amber	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	2622
Number of shifts mapped to atoms	2622
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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: ZN

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±0/1627 (0.0± 0.0%)	1.05±0.02	5±1/2205 (0.2± 0.1%)
All	All	0.75	0/24405 (0.0%)	1.05	75/33075 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.7±1.2
All	All	0	10

There are no bond-length outliers.

5 of 12 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	470	ARG	NE-CZ-NH1	10.01	125.30	120.30	1	13
1	A	365	ARG	NE-CZ-NH1	9.65	125.13	120.30	9	9
1	A	433	ARG	NE-CZ-NH1	9.14	124.87	120.30	6	7
1	A	427	ARG	NE-CZ-NH1	8.95	124.78	120.30	6	4
1	A	324	ARG	NE-CZ-NH1	8.62	124.61	120.30	6	10

There are no chirality outliers.

5 of 6 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	365	ARG	Sidechain	3

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	433	ARG	Sidechain	2
1	A	470	ARG	Sidechain	2
1	A	261	TYR	Sidechain	1
1	A	333	TYR	Sidechain	1

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	1579	1538	1538	0±1
All	All	23700	23070	23070	5

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:402:TRP:CH2	1:A:454:LYS:HE3	0.49	2.43	5	1
1:A:402:TRP:CZ2	1:A:412:LYS:HE2	0.49	2.43	12	1
1:A:402:TRP:CE2	1:A:412:LYS:HE3	0.44	2.48	4	1
1:A:332:LYS:HE3	1:A:349:TRP:CZ3	0.43	2.47	5	1
1:A:402:TRP:CZ2	1:A:412:LYS:HE3	0.43	2.48	5	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	197/245 (80%)	190±1 (96±1%)	7±1 (3±1%)	1±1 (0±0%)	44	80
All	All	2955/3675 (80%)	2848 (96%)	99 (3%)	8 (0%)	44	80

5 of 6 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	368	ASN	3
1	A	319	ASN	1
1	A	388	GLY	1
1	A	253	HIS	1
1	A	350	SER	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	167/199 (84%)	159±2 (95±1%)	8±2 (5±1%)	29	78
All	All	2505/2985 (84%)	2385 (95%)	120 (5%)	29	78

5 of 43 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	433	ARG	14
1	A	441	LEU	13
1	A	488	LEU	11
1	A	360	HIS	8
1	A	473	LEU	5

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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 85% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *LSSv3.1.bmrb*

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	2622
Number of shifts mapped to atoms	2622
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	25

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	235	-1.16 ± 0.17	Should be applied
$^{13}C_{\beta}$	206	-1.53 ± 0.09	Should be applied
$^{13}C'$	0	—	None (insufficient data)
^{15}N	207	0.05 ± 0.37	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 85%, i.e. 2275 atoms were assigned a chemical shift out of a possible 2683. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	791/999 (79%)	407/412 (99%)	198/396 (50%)	186/191 (97%)
Sidechain	1244/1357 (92%)	848/885 (96%)	373/419 (89%)	23/53 (43%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	240/327 (73%)	143/161 (89%)	87/151 (58%)	10/15 (67%)
Overall	2275/2683 (85%)	1398/1458 (96%)	658/966 (68%)	219/259 (85%)

7.1.4 Statistically unusual chemical shifts (i)

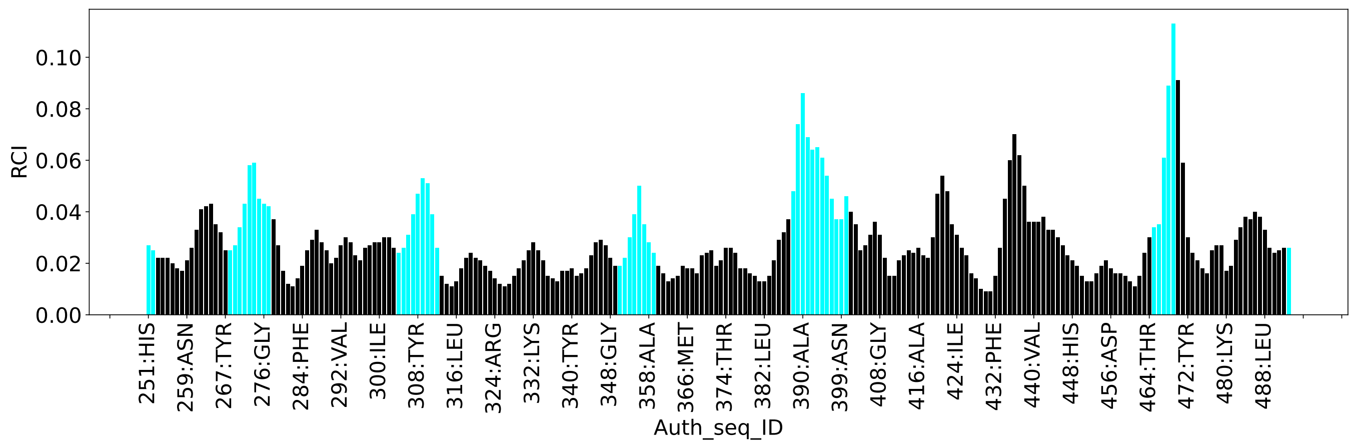
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	454	LYS	HB3	-1.02	0.46 – 3.04	-10.8
1	A	454	LYS	HE3	0.98	1.92 – 3.89	-9.8
1	A	454	LYS	HD3	-0.36	0.54 – 2.65	-9.3
1	A	293	LYS	HB3	-0.64	0.46 – 3.04	-9.3
1	A	449	TYR	CD1	120.26	125.84 – 139.60	-9.1
1	A	454	LYS	HD2	0.10	0.58 – 2.64	-7.3
1	A	324	ARG	HD3	1.30	1.81 – 4.39	-7.0
1	A	454	LYS	HE2	1.59	1.95 – 3.88	-6.8
1	A	474	PRO	HB3	-0.39	0.25 – 3.76	-6.8
1	A	258	LEU	HG	-0.71	-0.13 – 3.16	-6.7
1	A	372	ASN	HB3	0.59	1.12 – 4.38	-6.6
1	A	412	LYS	HD3	0.25	0.54 – 2.65	-6.4
1	A	431	PRO	HA	2.39	2.78 – 6.00	-6.2
1	A	258	LEU	HD21	-0.96	-0.65 – 2.13	-6.1
1	A	258	LEU	HD22	-0.96	-0.65 – 2.13	-6.1
1	A	258	LEU	HD23	-0.96	-0.65 – 2.13	-6.1
1	A	324	ARG	HB3	0.16	0.43 – 3.11	-6.0
1	A	315	GLY	HA2	6.13	2.15 – 5.77	6.0
1	A	324	ARG	HB2	0.29	0.52 – 3.08	-5.9
1	A	412	LYS	HD2	0.40	0.58 – 2.64	-5.8
1	A	454	LYS	HB2	0.45	0.58 – 2.97	-5.6
1	A	293	LYS	H	4.94	5.24 – 11.12	-5.5
1	A	431	PRO	HB3	0.09	0.25 – 3.76	-5.5
1	A	431	PRO	HB2	0.26	0.37 – 3.78	-5.3
1	A	324	ARG	HD2	1.97	1.97 – 4.26	-5.0

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	3569
Intra-residue (|i-j|=0)	656
Sequential (|i-j|=1)	821
Medium range (|i-j|>1 and |i-j|<5)	391
Long range (|i-j|≥5)	1613
Inter-chain	0
Hydrogen bond restraints	88
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	14.6
Number of long range restraints per residue[1]	6.9

[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)	18.9	0.2
0.2-0.5 (Medium)	15.5	0.5
>0.5 (Large)	1.6	1.63

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)

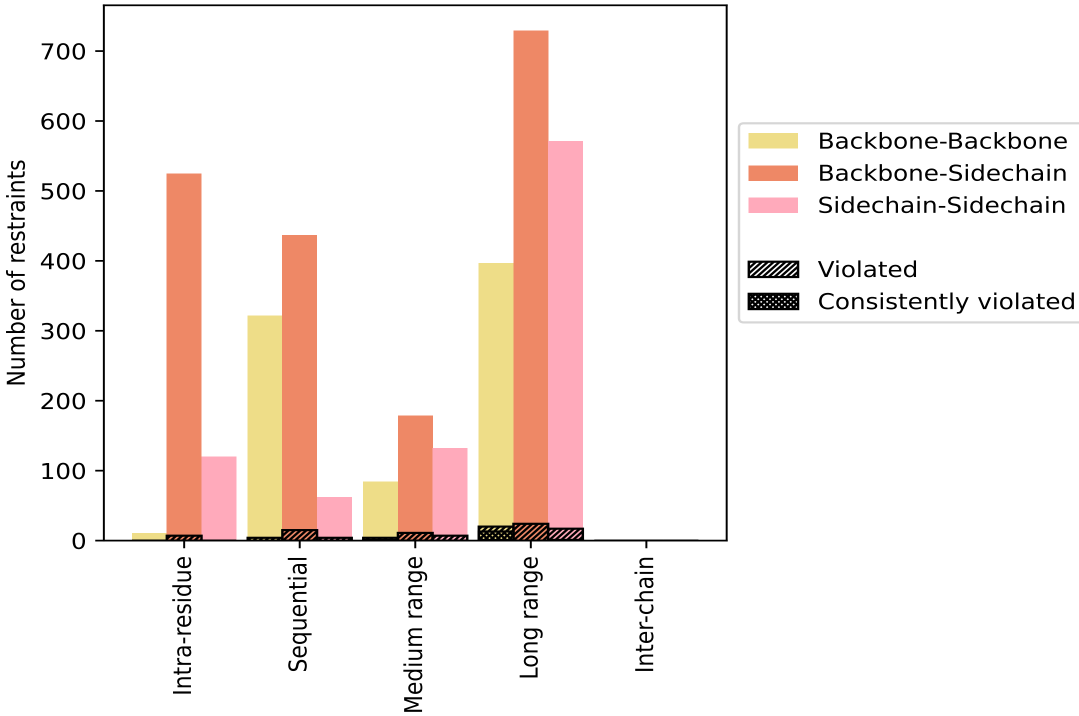
9.1 Summary of distance violations (i)

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)	656	18.4	7	1.1	0.2	0	0.0	0.0
Backbone-Backbone	11	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	525	14.7	7	1.3	0.2	0	0.0	0.0
Sidechain-Sidechain	120	3.4	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	821	23.0	23	2.8	0.6	0	0.0	0.0
Backbone-Backbone	322	9.0	4	1.2	0.1	0	0.0	0.0
Backbone-Sidechain	437	12.2	15	3.4	0.4	0	0.0	0.0
Sidechain-Sidechain	62	1.7	4	6.5	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	391	11.0	20	5.1	0.6	0	0.0	0.0
Backbone-Backbone	80	2.2	2	2.5	0.1	0	0.0	0.0
Backbone-Sidechain	179	5.0	11	6.1	0.3	0	0.0	0.0
Sidechain-Sidechain	132	3.7	7	5.3	0.2	0	0.0	0.0
Long range (|i-j|≥5)	1613	45.2	42	2.6	1.2	1	0.1	0.0
Backbone-Backbone	313	8.8	1	0.3	0.0	0	0.0	0.0
Backbone-Sidechain	729	20.4	24	3.3	0.7	0	0.0	0.0
Sidechain-Sidechain	571	16.0	17	3.0	0.5	1	0.2	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	88	2.5	21	23.9	0.6	14	15.9	0.4
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3569	100.0	113	3.2	3.2	15	0.4	0.4
Backbone-Backbone	814	22.8	28	3.4	0.8	14	1.7	0.4
Backbone-Sidechain	1870	52.4	57	3.0	1.6	0	0.0	0.0
Sidechain-Sidechain	885	24.8	28	3.2	0.8	1	0.1	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	1	4	2	30	0	37	0.22	0.48	0.08	0.21
2	3	2	5	26	0	36	0.21	0.66	0.11	0.17
3	1	4	5	31	0	41	0.24	0.9	0.14	0.2
4	1	3	6	32	0	42	0.23	0.59	0.12	0.19
5	2	1	4	23	0	30	0.24	1.29	0.21	0.2
6	0	2	7	24	0	33	0.31	1.29	0.27	0.23
7	0	5	5	31	0	41	0.27	1.54	0.23	0.21
8	1	2	8	25	0	36	0.25	1.5	0.22	0.2
9	0	2	8	25	0	35	0.2	0.32	0.06	0.2
10	1	4	3	29	0	37	0.22	0.62	0.11	0.2
11	0	5	2	28	0	35	0.22	0.66	0.1	0.2

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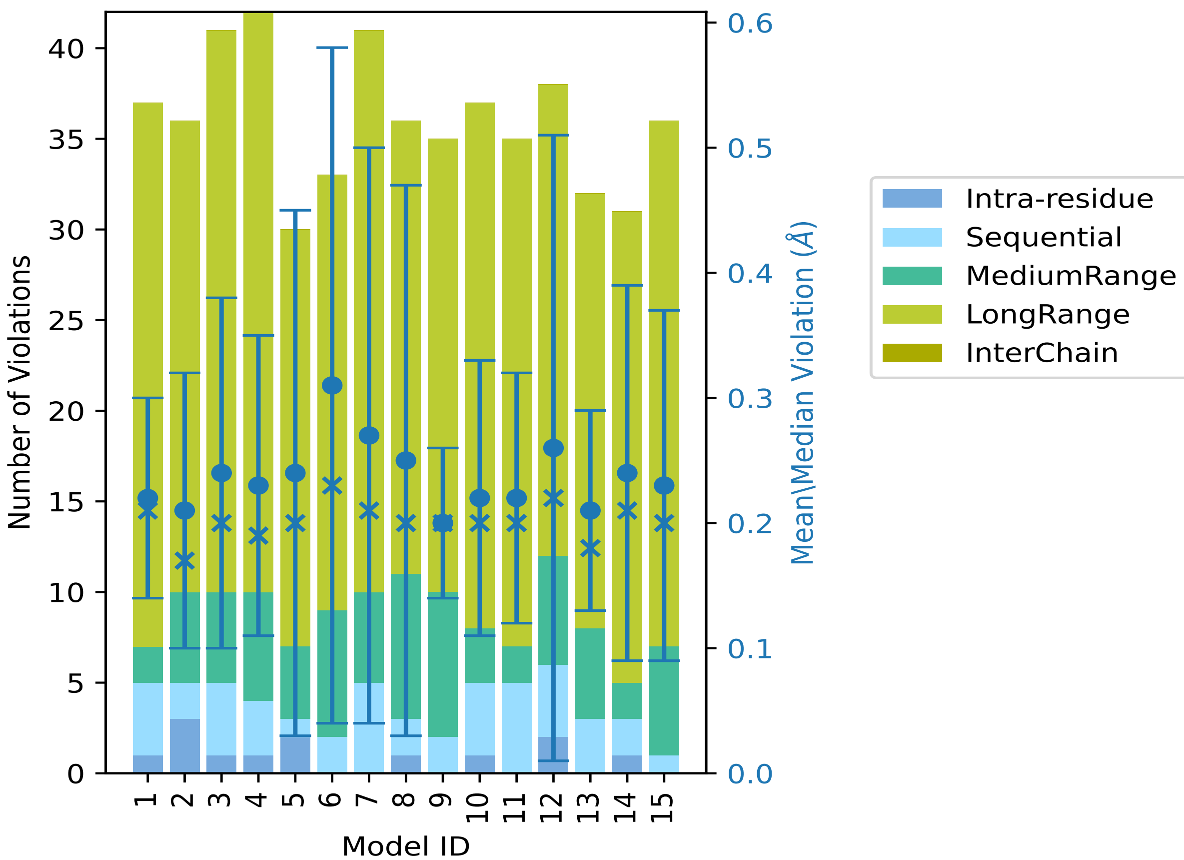
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	2	4	6	26	0	38	0.26	1.63	0.25	0.22
13	0	3	5	24	0	32	0.21	0.51	0.08	0.18
14	1	2	2	26	0	31	0.24	0.89	0.15	0.21
15	0	1	6	29	0	36	0.23	0.77	0.14	0.2

[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

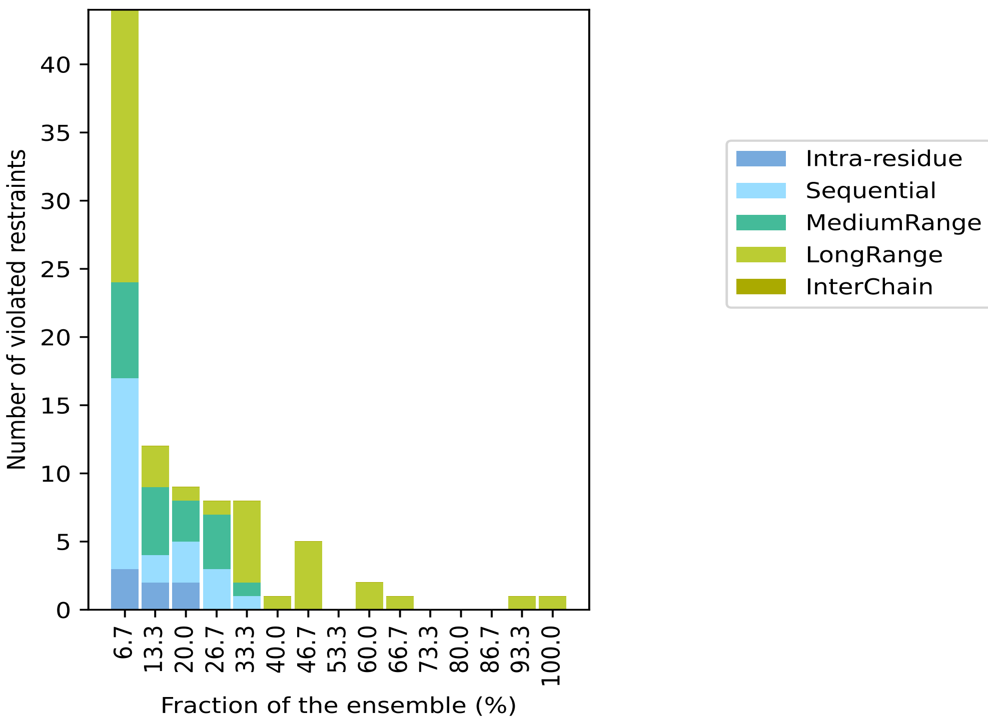
9.3 Distance violation statistics for the ensemble (i)

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, 3389(IR:649, SQ:798, MR:371, LR:1571, 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]	%
3	14	7	20	0	44	1	6.7
2	2	5	3	0	12	2	13.3
2	3	3	1	0	9	3	20.0
0	3	4	1	0	8	4	26.7
0	1	1	6	0	8	5	33.3
0	0	0	1	0	1	6	40.0
0	0	0	5	0	5	7	46.7
0	0	0	0	0	0	8	53.3
0	0	0	2	0	2	9	60.0
0	0	0	1	0	1	10	66.7
0	0	0	0	0	0	11	73.3
0	0	0	0	0	0	12	80.0
0	0	0	0	0	0	13	86.7
0	0	0	1	0	1	14	93.3
0	0	0	1	0	1	15	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

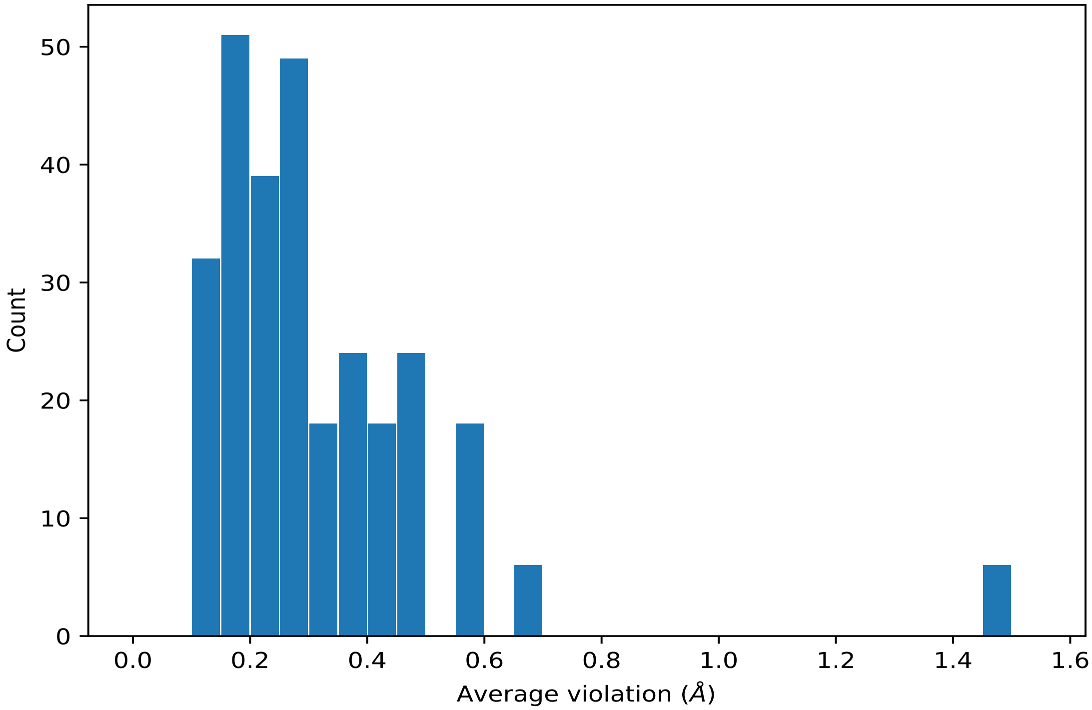
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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 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.

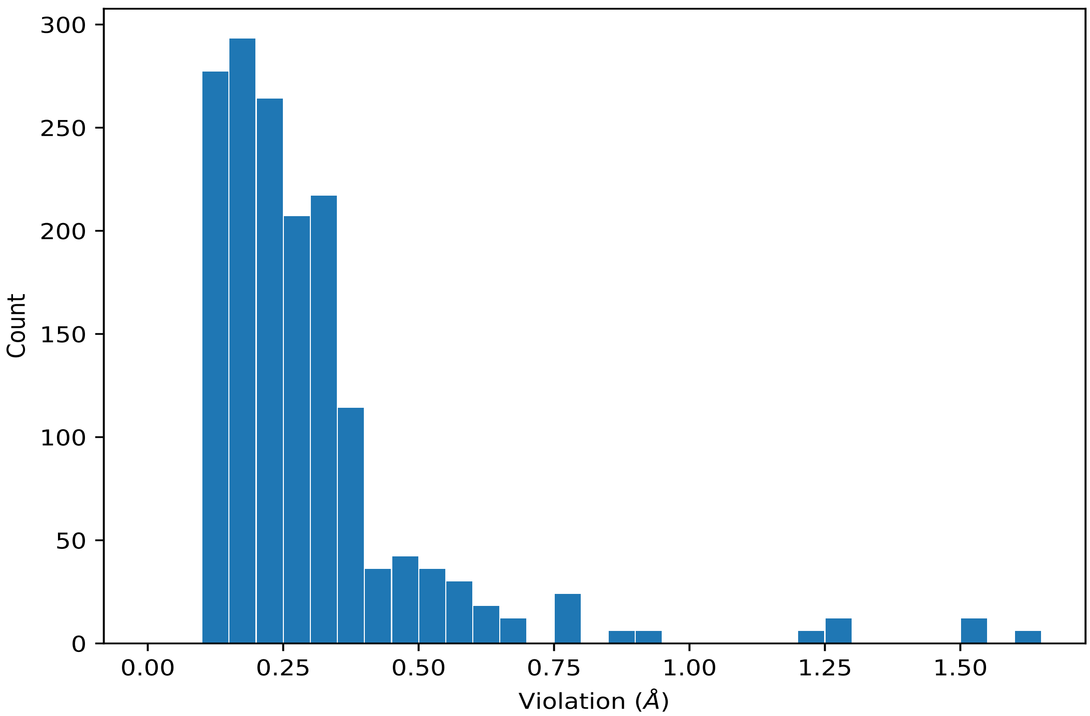
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,20)	1:A:473:LEU:N	1:A:461:VAL:O	15	0.3	0.01	0.31
(2,3)	1:A:362:HIS:ND1	2:A:501:ZN:ZN	15	0.3	0.04	0.3
(4,8)	1:A:314:ILE:O	1:A:327:TYR:N	15	0.27	0.04	0.28
(4,3)	1:A:364:GLN:N	1:A:326:TRP:O	15	0.27	0.03	0.28
(4,14)	1:A:350:SER:N	1:A:290:THR:O	15	0.26	0.06	0.28
(4,9)	1:A:316:LEU:N	1:A:325:GLN:O	15	0.25	0.04	0.26
(4,11)	1:A:299:LYS:N	1:A:317:ILE:O	15	0.25	0.05	0.25
(4,1)	1:A:282:VAL:N	1:A:363:PHE:O	15	0.22	0.03	0.21
(4,2)	1:A:282:VAL:O	1:A:363:PHE:N	15	0.22	0.03	0.22
(4,18)	1:A:424:ILE:N	1:A:441:LEU:O	15	0.19	0.02	0.19

[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)
(1,3414)	1:A:487:VAL:HG11	1:A:489:TRP:HE1	12	1.63
(1,3414)	1:A:487:VAL:HG12	1:A:489:TRP:HE1	12	1.63
(1,3414)	1:A:487:VAL:HG13	1:A:489:TRP:HE1	12	1.63
(1,3414)	1:A:487:VAL:HG21	1:A:489:TRP:HE1	12	1.63
(1,3414)	1:A:487:VAL:HG22	1:A:489:TRP:HE1	12	1.63
(1,3414)	1:A:487:VAL:HG23	1:A:489:TRP:HE1	12	1.63
(1,3414)	1:A:487:VAL:HG11	1:A:489:TRP:HE1	7	1.54
(1,3414)	1:A:487:VAL:HG12	1:A:489:TRP:HE1	7	1.54
(1,3414)	1:A:487:VAL:HG13	1:A:489:TRP:HE1	7	1.54
(1,3414)	1:A:487:VAL:HG21	1:A:489:TRP:HE1	7	1.54
(1,3414)	1:A:487:VAL:HG22	1:A:489:TRP:HE1	7	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3414)	1:A:487:VAL:HG23	1:A:489:TRP:HE1	7	1.54
(1,3414)	1:A:487:VAL:HG11	1:A:489:TRP:HE1	8	1.5
(1,3414)	1:A:487:VAL:HG12	1:A:489:TRP:HE1	8	1.5
(1,3414)	1:A:487:VAL:HG13	1:A:489:TRP:HE1	8	1.5
(1,3414)	1:A:487:VAL:HG21	1:A:489:TRP:HE1	8	1.5
(1,3414)	1:A:487:VAL:HG22	1:A:489:TRP:HE1	8	1.5
(1,3414)	1:A:487:VAL:HG23	1:A:489:TRP:HE1	8	1.5
(1,930)	1:A:313:GLN:HA	1:A:330:LEU:HD11	6	1.29
(1,930)	1:A:313:GLN:HA	1:A:330:LEU:HD12	6	1.29
(1,930)	1:A:313:GLN:HA	1:A:330:LEU:HD13	6	1.29
(1,930)	1:A:313:GLN:HA	1:A:330:LEU:HD21	6	1.29
(1,930)	1:A:313:GLN:HA	1:A:330:LEU:HD22	6	1.29
(1,930)	1:A:313:GLN:HA	1:A:330:LEU:HD23	6	1.29
(1,3414)	1:A:487:VAL:HG11	1:A:489:TRP:HE1	5	1.29
(1,3414)	1:A:487:VAL:HG12	1:A:489:TRP:HE1	5	1.29
(1,3414)	1:A:487:VAL:HG13	1:A:489:TRP:HE1	5	1.29
(1,3414)	1:A:487:VAL:HG21	1:A:489:TRP:HE1	5	1.29
(1,3414)	1:A:487:VAL:HG22	1:A:489:TRP:HE1	5	1.29
(1,3414)	1:A:487:VAL:HG23	1:A:489:TRP:HE1	5	1.29
(1,957)	1:A:314:ILE:H	1:A:330:LEU:HD11	6	1.2
(1,957)	1:A:314:ILE:H	1:A:330:LEU:HD12	6	1.2
(1,957)	1:A:314:ILE:H	1:A:330:LEU:HD13	6	1.2
(1,957)	1:A:314:ILE:H	1:A:330:LEU:HD21	6	1.2
(1,957)	1:A:314:ILE:H	1:A:330:LEU:HD22	6	1.2
(1,957)	1:A:314:ILE:H	1:A:330:LEU:HD23	6	1.2
(1,1997)	1:A:410:LEU:HD11	1:A:478:TRP:HE1	3	0.9
(1,1997)	1:A:410:LEU:HD12	1:A:478:TRP:HE1	3	0.9
(1,1997)	1:A:410:LEU:HD13	1:A:478:TRP:HE1	3	0.9
(1,1997)	1:A:410:LEU:HD21	1:A:478:TRP:HE1	3	0.9
(1,1997)	1:A:410:LEU:HD22	1:A:478:TRP:HE1	3	0.9
(1,1997)	1:A:410:LEU:HD23	1:A:478:TRP:HE1	3	0.9
(1,1997)	1:A:410:LEU:HD11	1:A:478:TRP:HE1	14	0.89
(1,1997)	1:A:410:LEU:HD12	1:A:478:TRP:HE1	14	0.89
(1,1997)	1:A:410:LEU:HD13	1:A:478:TRP:HE1	14	0.89
(1,1997)	1:A:410:LEU:HD21	1:A:478:TRP:HE1	14	0.89
(1,1997)	1:A:410:LEU:HD22	1:A:478:TRP:HE1	14	0.89
(1,1997)	1:A:410:LEU:HD23	1:A:478:TRP:HE1	14	0.89
(1,2644)	1:A:437:GLN:HE21	1:A:440:VAL:HG11	15	0.77
(1,2644)	1:A:437:GLN:HE21	1:A:440:VAL:HG12	15	0.77
(1,2644)	1:A:437:GLN:HE21	1:A:440:VAL:HG13	15	0.77
(1,2644)	1:A:437:GLN:HE21	1:A:440:VAL:HG21	15	0.77
(1,2644)	1:A:437:GLN:HE21	1:A:440:VAL:HG22	15	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2644)	1:A:437:GLN:HE21	1:A:440:VAL:HG23	15	0.77
(1,2644)	1:A:437:GLN:HE22	1:A:440:VAL:HG11	15	0.77
(1,2644)	1:A:437:GLN:HE22	1:A:440:VAL:HG12	15	0.77
(1,2644)	1:A:437:GLN:HE22	1:A:440:VAL:HG13	15	0.77
(1,2644)	1:A:437:GLN:HE22	1:A:440:VAL:HG21	15	0.77
(1,2644)	1:A:437:GLN:HE22	1:A:440:VAL:HG22	15	0.77
(1,2644)	1:A:437:GLN:HE22	1:A:440:VAL:HG23	15	0.77
(1,1215)	1:A:330:LEU:HD11	1:A:333:TYR:HE1	6	0.77

10 Dihedral-angle violation analysis (i)

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