wwPDB NMR Structure Validation Summary Report

Jun 5, 2023 – 05:50 PM JST

PDB ID	:	6JTF
BMRB ID	:	36245
Title	:	Complex of MarH and L-Trp
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Deposited on	:	2019-04-10

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:

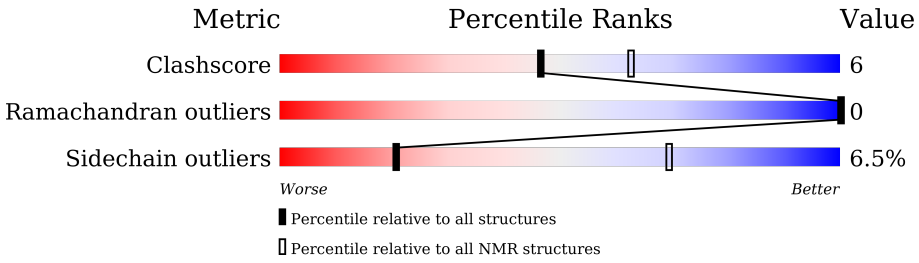
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 59%.

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	126	81% 14%

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:7-A:129 (123)	0.01	2

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. No single-model clusters were found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1863 atoms, of which 930 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cupin superfamily protein.

Mol	Chain	Residues	Atoms						Trace
1	A	123	Total	C	H	N	O	S	0
			1835	589	918	156	168	4	

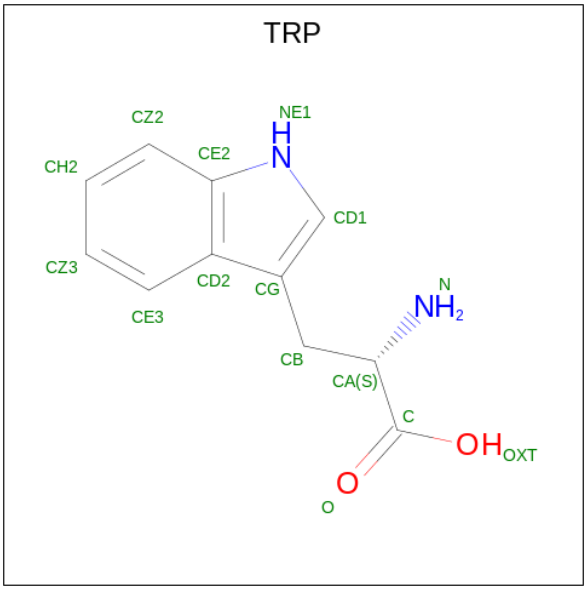
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLY	-	expression tag	UNP X2D812
A	5	SER	-	expression tag	UNP X2D812

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

Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				
3	A	1	Total	C	H	N	O
			27	11	12	2	2

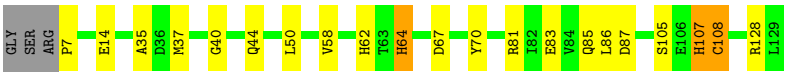
4 Residue-property plots (i)

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: Cupin superfamily protein

Chain A:

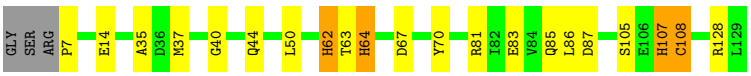


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: Cupin superfamily protein

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 200 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
X-PLOR NIH	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	978
Number of shifts mapped to atoms	967
Number of unparsed shifts	0
Number of shifts with mapping errors	11
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	59%

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	1.22±0.01	3±1/942 (0.3± 0.1%)	1.15±0.00	6±1/1285 (0.5± 0.0%)
All	All	1.22	63/18840 (0.3%)	1.15	126/25700 (0.5%)

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	0.3±0.5
All	All	0	7

5 of 6 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
1	A	53	LEU	N-CA	8.06	1.62	1.46	11	1
1	A	40	GLY	N-CA	-5.90	1.37	1.46	1	20
1	A	70	TYR	C-N	5.72	1.47	1.34	11	1
1	A	108	CYS	CB-SG	-5.61	1.72	1.81	1	20
1	A	52	THR	C-N	-5.35	1.21	1.34	11	1

5 of 8 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
1	A	37	MET	CG-SD-CE	8.26	113.42	100.20	1	20
1	A	81	ARG	NE-CZ-NH2	7.67	124.14	120.30	1	20
1	A	87	ASP	CB-CG-OD2	-6.10	112.81	118.30	1	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	67	ASP	CB-CG-OD2	-5.91	112.98	118.30	1	20
1	A	67	ASP	CB-CG-OD1	5.66	123.39	118.30	1	20

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	107	HIS	Sidechain	7

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	917	918	917	12±2
3	A	15	12	9	0±0
All	All	18660	18600	18520	240

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 6.

5 of 28 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:HIS:N	1:A:64:HIS:ND1	0.88	2.20	2	15
1:A:70:TYR:OH	1:A:107:HIS:CE1	0.76	2.37	4	20
1:A:107:HIS:C	1:A:107:HIS:ND1	0.76	2.39	12	15
1:A:107:HIS:HD1	1:A:108:CYS:N	0.71	1.83	12	16
1:A:107:HIS:ND1	1:A:108:CYS:N	0.67	2.42	13	20

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	121/126 (96%)	120±0 (99±0%)	1±0 (1±0%)	0±0 (0±0%)	100	100
All	All	2420/2520 (96%)	2400 (99%)	20 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	97/99 (98%)	91±1 (94±1%)	6±1 (6±1%)	21	69
All	All	1940/1980 (98%)	1814 (94%)	126 (6%)	21	69

5 of 9 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	7	PRO	20
1	A	50	LEU	20
1	A	62	HIS	20
1	A	64	HIS	20
1	A	128	ARG	20

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

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
3	TRP	A	202	2	14,16,16	1.04±0.03	1±0 (7±1%)

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
3	TRP	A	202	2	16,22,22	0.85±0.08	0±0 (1±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
3	TRP	A	202	2	-	0±0,7,8,8	0±0,2,2,2

All 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
3	A	202	TRP	OXT-C	2.53	1.22	1.30	18	20
3	A	202	TRP	CZ3-CE3	2.08	1.41	1.36	18	1

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	202	TRP	CB-CG-CD1	2.07	125.41	127.97	12	5

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

The completeness of assignment taking into account all chemical shift lists is 59% for the well-defined parts and 59% 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

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	978
Number of shifts mapped to atoms	967
Number of unparsed shifts	0
Number of shifts with mapping errors	11
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- No matching atom found in the structure. First 5 (of 11) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	6	ARG	H	8.461	0.026	1
1	A	6	ARG	HA	4.697	0.005	1
1	A	6	ARG	HB2	1.76	0.012	2
1	A	6	ARG	HB3	1.842	0.010	2
1	A	6	ARG	HG2	1.68	0.016	2
1	A	6	ARG	HD2	3.212	0.009	2
1	A	6	ARG	CA	54.057	0.091	1
1	A	6	ARG	CB	30.499	0.091	1
1	A	6	ARG	CG	26.89	0.089	1
1	A	6	ARG	CD	43.518	0.070	1
1	A	6	ARG	N	123.674	0.026	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	118	0.16 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	102	-0.30 ± 0.29	None needed (< 0.5 ppm)
$^{13}C'$	99	0.40 ± 0.11	None needed (< 0.5 ppm)
^{15}N	103	-0.43 ± 0.52	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 59%, i.e. 967 atoms were assigned a chemical shift out of a possible 1636. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	530/608 (87%)	212/249 (85%)	216/248 (87%)	102/111 (92%)
Sidechain	437/907 (48%)	266/602 (44%)	171/284 (60%)	0/21 (0%)
Aromatic	0/121 (0%)	0/62 (0%)	0/52 (0%)	0/7 (0%)
Overall	967/1636 (59%)	478/913 (52%)	387/584 (66%)	102/139 (73%)

7.1.4 Statistically unusual chemical shifts (i)

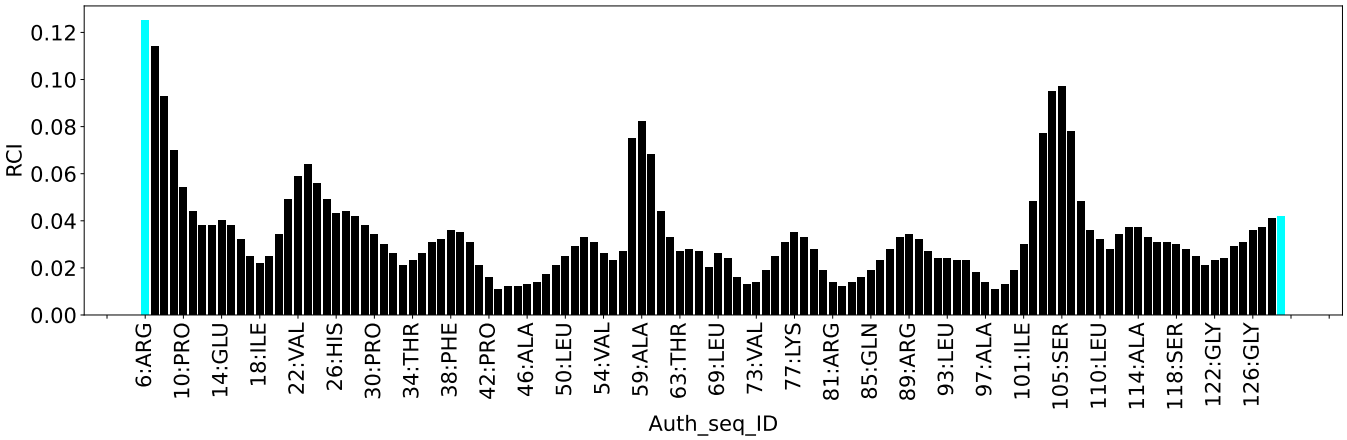
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	46	ALA	HB1	-0.04	0.14 – 2.58	-5.7
1	A	46	ALA	HB2	-0.04	0.14 – 2.58	-5.7
1	A	46	ALA	HB3	-0.04	0.14 – 2.58	-5.7

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	20
Intra-residue (|i-j|=0)	11
Sequential (|i-j|=1)	2
Medium range (|i-j|>1 and |i-j|<5)	3
Long range (|i-j|≥5)	4
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	0.2
Number of long range restraints per residue[1]	0.0

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

8.2 Residual restraint violations

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)	None	None
0.2-0.5 (Medium)	1.4	0.41
>0.5 (Large)	7.0	10.99

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)

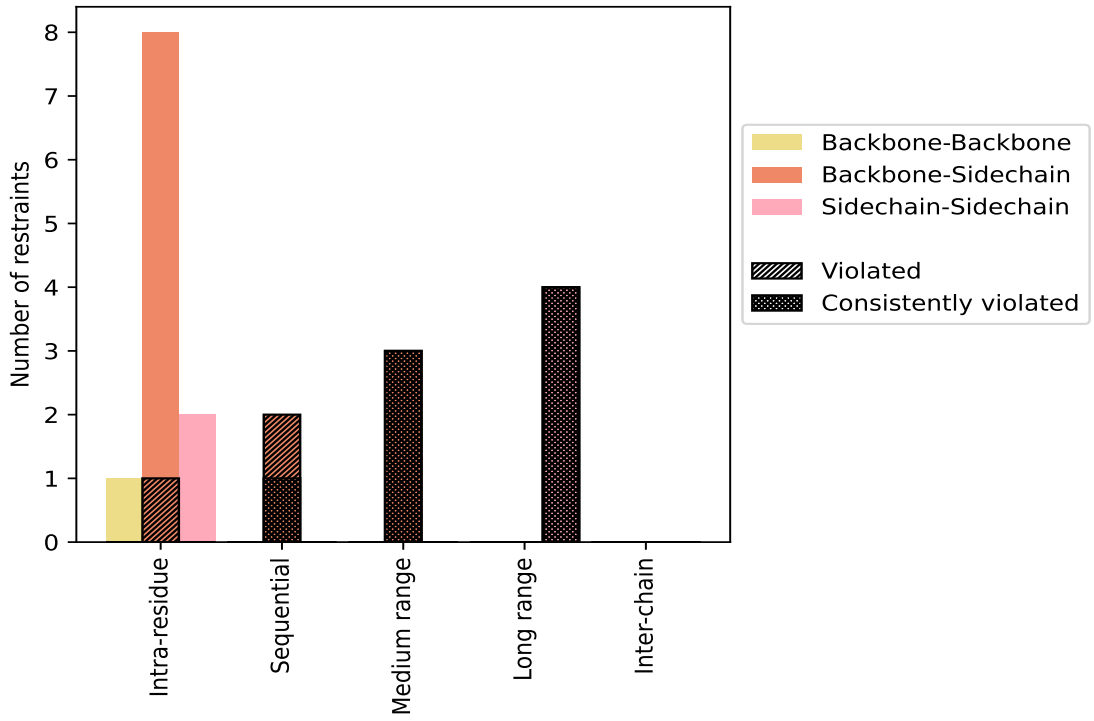
9.1 Summary of distance violations (i)

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)	11	55.0	1	9.1	5.0	0	0.0	0.0
Backbone-Backbone	1	5.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	8	40.0	1	12.5	5.0	0	0.0	0.0
Sidechain-Sidechain	2	10.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	2	10.0	2	100.0	10.0	1	50.0	5.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	10.0	2	100.0	10.0	1	50.0	5.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	3	15.0	3	100.0	15.0	3	100.0	15.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	3	15.0	3	100.0	15.0	3	100.0	15.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	4	20.0	4	100.0	20.0	4	100.0	20.0
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	4	20.0	4	100.0	20.0	4	100.0	20.0
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	20	100.0	10	50.0	50.0	8	40.0	40.0
Backbone-Backbone	1	5.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	13	65.0	6	46.2	30.0	4	30.8	20.0
Sidechain-Sidechain	6	30.0	4	66.7	20.0	4	66.7	20.0

[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



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	1	3	4	0	8	5.99	10.84	3.07	5.79
2	0	1	3	4	0	8	5.99	10.87	3.08	5.79
3	0	1	3	4	0	8	5.99	10.87	3.08	5.79
4	0	1	3	4	0	8	5.99	10.87	3.08	5.79
5	0	1	3	4	0	8	6.0	10.88	3.09	5.79
6	0	1	3	4	0	8	5.99	10.83	3.07	5.79
7	0	1	3	4	0	8	5.99	10.86	3.08	5.79
8	0	1	3	4	0	8	6.0	10.88	3.09	5.79
9	0	1	3	4	0	8	5.99	10.82	3.07	5.79
10	0	1	3	4	0	8	5.99	10.87	3.08	5.79
11	0	1	3	4	0	8	5.99	10.85	3.07	5.79

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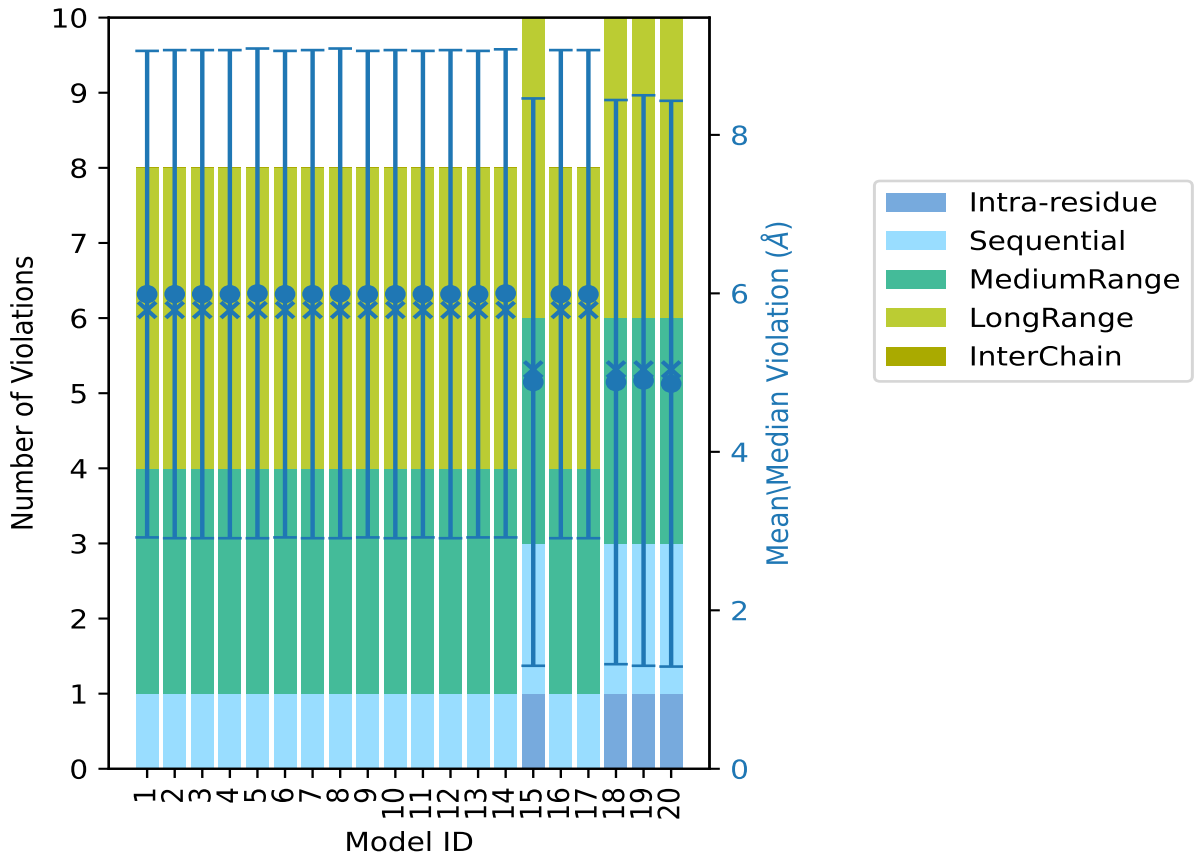
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	1	3	4	0	8	5.99	10.86	3.08	5.79
13	0	1	3	4	0	8	5.99	10.86	3.07	5.79
14	0	1	3	4	0	8	6.0	10.87	3.08	5.79
15	1	2	3	4	0	10	4.88	10.9	3.58	5.04
16	0	1	3	4	0	8	5.99	10.83	3.08	5.79
17	0	1	3	4	0	8	5.99	10.86	3.08	5.79
18	1	2	3	4	0	10	4.88	10.85	3.56	5.04
19	1	2	3	4	0	10	4.9	10.99	3.6	5.04
20	1	2	3	4	0	10	4.86	10.84	3.57	5.04

[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

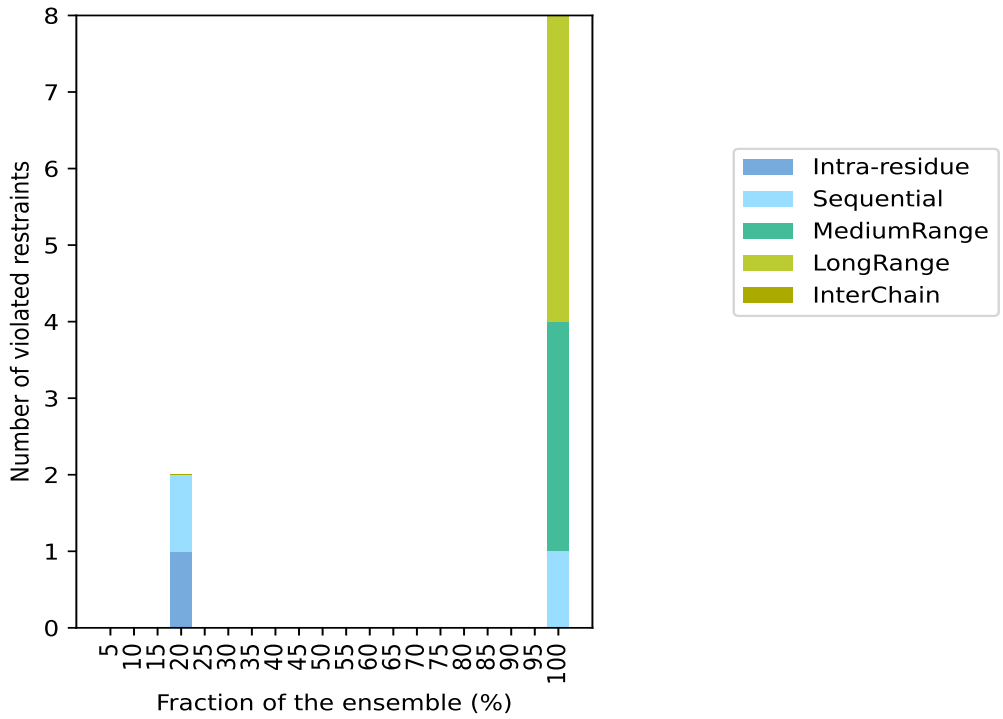
9.3 Distance violation statistics for the ensemble (i)

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, 10(IR:10, SQ:0, MR:0, LR:0, 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	0	0	0	0	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
1	1	0	0	0	2	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	1	3	4	0	8	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

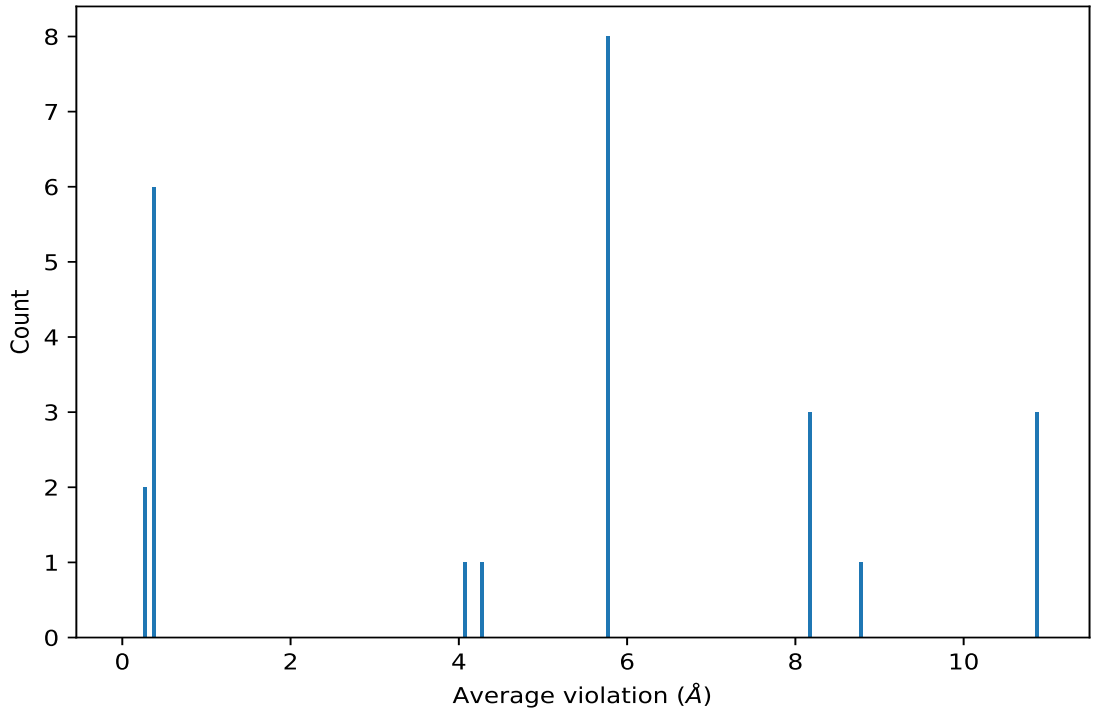
9.3.1 Bar graph : Distance violation statistics for the ensemble



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)
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD21	20	10.86	0.03	10.86
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD22	20	10.86	0.03	10.86
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD23	20	10.86	0.03	10.86
(1,19)	1:A:61:PRO:HG3	1:A:58:VAL:HA	20	8.76	0.02	8.76
(1,12)	1:A:53:LEU:HD21	1:A:61:PRO:HG3	20	8.19	0.08	8.17
(1,12)	1:A:53:LEU:HD22	1:A:61:PRO:HG3	20	8.19	0.08	8.17
(1,12)	1:A:53:LEU:HD23	1:A:61:PRO:HG3	20	8.19	0.08	8.17
(1,3)	1:A:32:TYR:HB2	1:A:49:GLU:HB2	20	5.79	0.0	5.79
(1,3)	1:A:32:TYR:HB2	1:A:49:GLU:HB3	20	5.79	0.0	5.79
(1,3)	1:A:32:TYR:HB3	1:A:49:GLU:HB2	20	5.79	0.0	5.79
(1,3)	1:A:32:TYR:HB3	1:A:49:GLU:HB3	20	5.79	0.0	5.79
(1,4)	1:A:49:GLU:HB2	1:A:32:TYR:HB2	20	5.79	0.0	5.79
(1,4)	1:A:49:GLU:HB2	1:A:32:TYR:HB3	20	5.79	0.0	5.79
(1,4)	1:A:49:GLU:HB3	1:A:32:TYR:HB2	20	5.79	0.0	5.79
(1,4)	1:A:49:GLU:HB3	1:A:32:TYR:HB3	20	5.79	0.0	5.79
(1,18)	1:A:61:PRO:HG2	1:A:59:ALA:H	20	4.28	0.0	4.28

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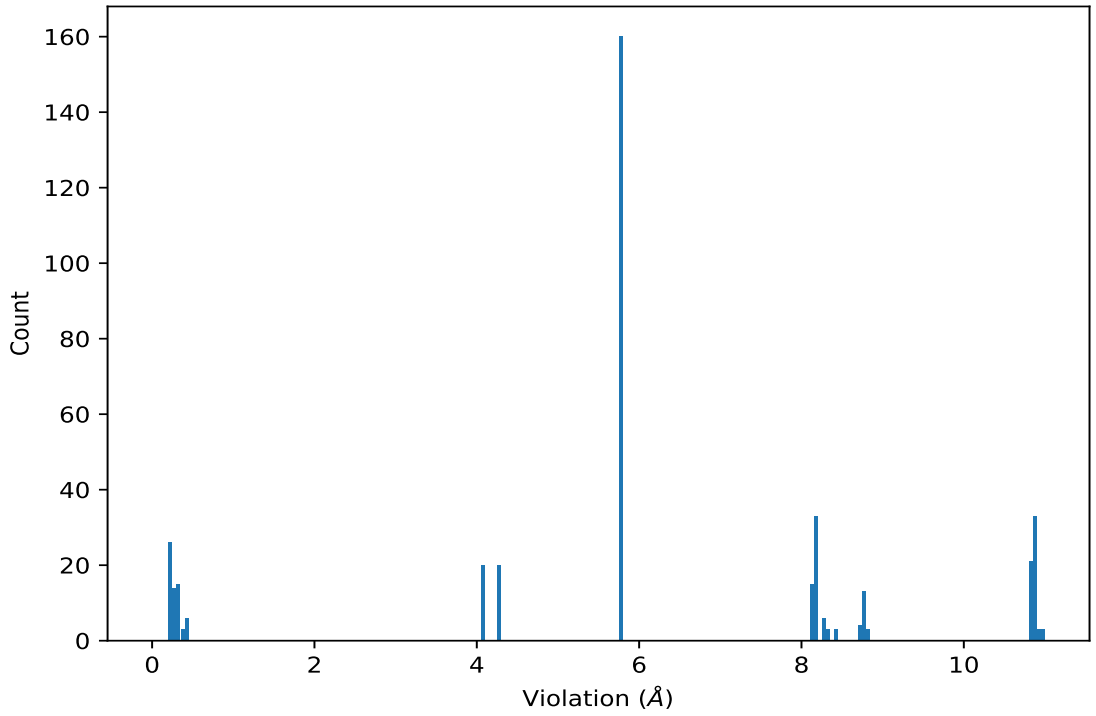
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,17)	1:A:61:PRO:HG2	1:A:59:ALA:HA	20	4.05	0.0	4.05
(1,7)	1:A:49:GLU:HB2	1:A:50:LEU:H	20	0.25	0.01	0.24
(1,7)	1:A:49:GLU:HB3	1:A:50:LEU:H	20	0.25	0.01	0.24
(1,10)	1:A:53:LEU:HD11	1:A:54:VAL:H	4	0.36	0.03	0.34
(1,10)	1:A:53:LEU:HD12	1:A:54:VAL:H	4	0.36	0.03	0.34
(1,10)	1:A:53:LEU:HD13	1:A:54:VAL:H	4	0.36	0.03	0.34
(1,11)	1:A:53:LEU:HD11	1:A:53:LEU:HA	4	0.36	0.03	0.36

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

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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

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)
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD21	19	10.99
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD22	19	10.99
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD23	19	10.99
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD21	15	10.9
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD22	15	10.9
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD23	15	10.9
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD21	5	10.88
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD22	5	10.88
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD23	5	10.88
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD21	8	10.88
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD22	8	10.88
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD23	8	10.88
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD21	2	10.87
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD22	2	10.87
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD23	2	10.87
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD21	3	10.87
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD22	3	10.87
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD23	3	10.87
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD21	4	10.87
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD22	4	10.87
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD23	4	10.87
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD21	10	10.87
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD22	10	10.87
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD23	10	10.87
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD21	14	10.87
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD22	14	10.87
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD23	14	10.87
(1,16)	1:A:61:PRO:HG2	1:A:53:LEU:HD21	7	10.86

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found