Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	8PXX
BMRB ID	:	34840
Title	:	Structure of the WW domain tandem of PRPF40A in complex with SF1
Authors	:	Martinez-Lumbreras, S.; Sattler, M.
Deposited on	:	2023-07-24

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

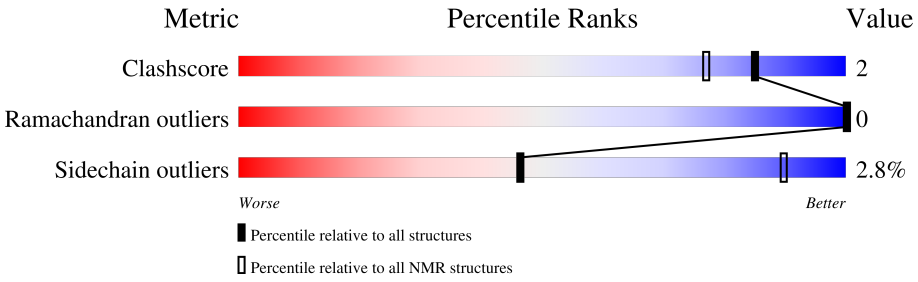
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 87%.

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	99	59% · 37%
2	B	27	11% · 85%

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:146-A:174, B:575-B:578 (33)	0.12	14
2	A:186-A:218 (33)	0.16	15

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 3 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1916 atoms, of which 940 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Pre-mRNA-processing factor 40 homolog A.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	99	1582	508	776	132	163	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	GLY	-	expression tag	UNP O75400
A	139	ALA	-	expression tag	UNP O75400
A	140	MET	-	expression tag	UNP O75400

- Molecule 2 is a protein called Splicing factor 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	27	334	108	164	28	33	1	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	569	GLY	-	expression tag	UNP Q15637
B	570	ALA	-	expression tag	UNP Q15637
B	571	MET	-	expression tag	UNP Q15637
B	572	SER	-	expression tag	UNP Q15637
B	573	GLY	-	expression tag	UNP Q15637
B	574	SER	-	expression tag	UNP Q15637
B	591	SER	-	expression tag	UNP Q15637
B	592	GLY	-	expression tag	UNP Q15637
B	593	SER	-	expression tag	UNP Q15637
B	594	GLY	-	expression tag	UNP Q15637
B	595	ASN	-	expression tag	UNP Q15637

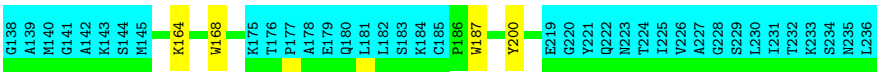
4 Residue-property plots (i)

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.

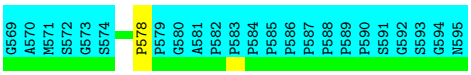
• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



• Molecule 2: Splicing factor 1

Chain B:



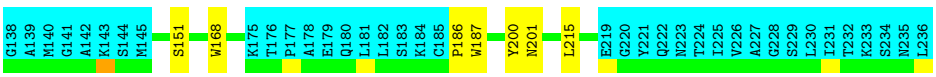
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

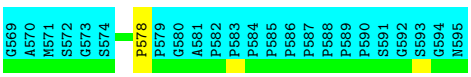
• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



• Molecule 2: Splicing factor 1

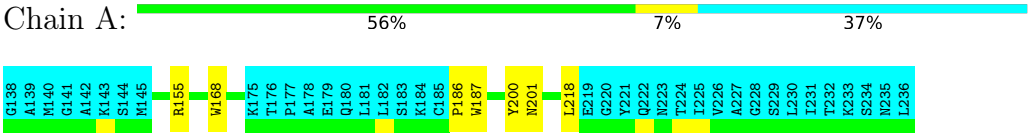
Chain B:



4.2.2 Score per residue for model 2

• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



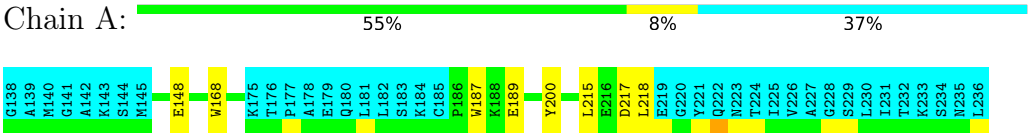
• Molecule 2: Splicing factor 1

Chain B:

4.2.3 Score per residue for model 3

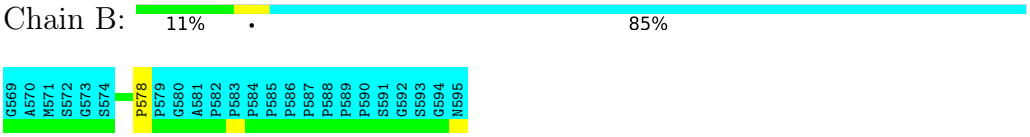
• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



• Molecule 2: Splicing factor 1

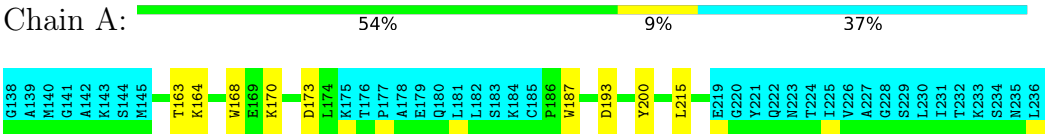
Chain B:



4.2.4 Score per residue for model 4

• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



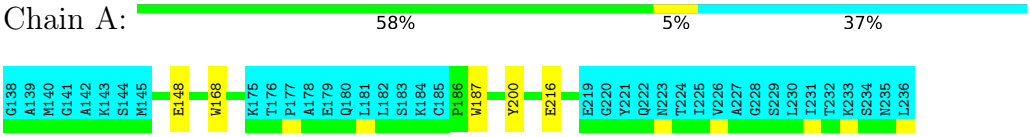
• Molecule 2: Splicing factor 1

Chain B:

4.2.5 Score per residue for model 5

• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



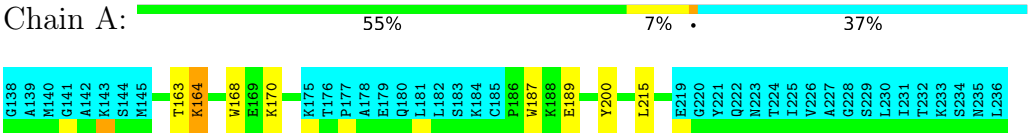
• Molecule 2: Splicing factor 1

Chain B:

4.2.6 Score per residue for model 6

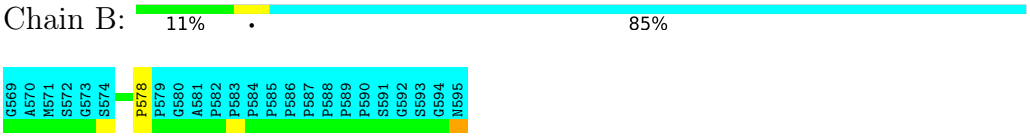
• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



• Molecule 2: Splicing factor 1

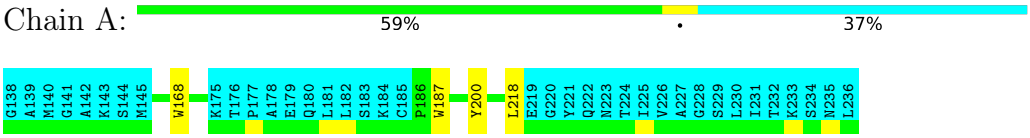
Chain B:



4.2.7 Score per residue for model 7

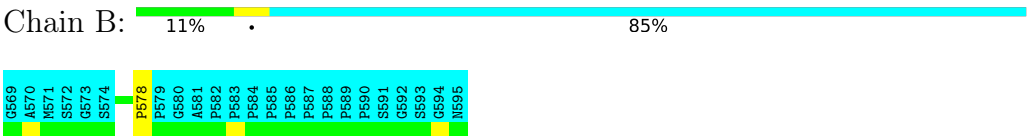
• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



• Molecule 2: Splicing factor 1

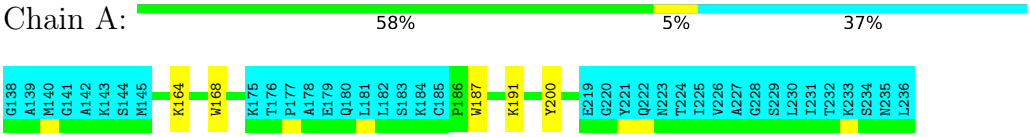
Chain B:



4.2.8 Score per residue for model 8

• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



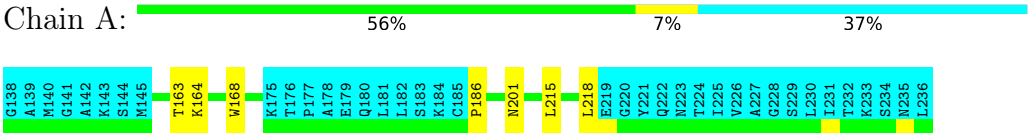
• Molecule 2: Splicing factor 1

Chain B:

4.2.9 Score per residue for model 9

• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



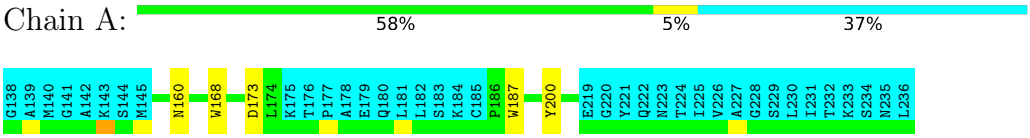
• Molecule 2: Splicing factor 1

Chain B:

4.2.10 Score per residue for model 10

• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



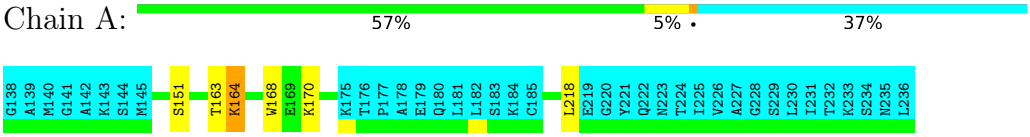
• Molecule 2: Splicing factor 1

Chain B:

4.2.11 Score per residue for model 11

• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



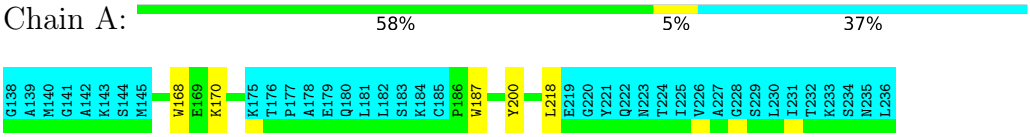
• Molecule 2: Splicing factor 1

Chain B:

4.2.12 Score per residue for model 12

• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



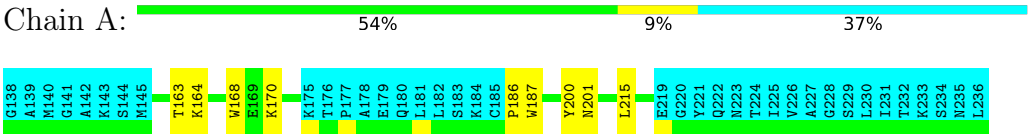
• Molecule 2: Splicing factor 1

Chain B:

4.2.13 Score per residue for model 13

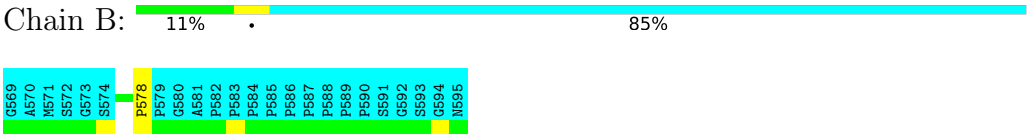
• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



• Molecule 2: Splicing factor 1

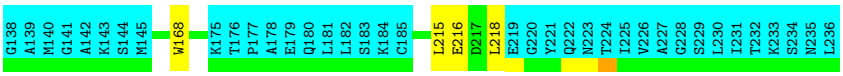
Chain B:



4.2.14 Score per residue for model 14 (medoid)

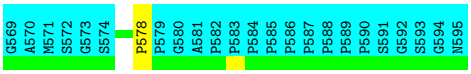
• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



• Molecule 2: Splicing factor 1

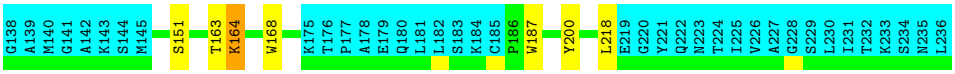
Chain B:



4.2.15 Score per residue for model 15

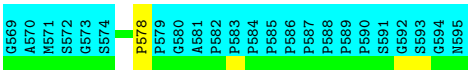
• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



• Molecule 2: Splicing factor 1

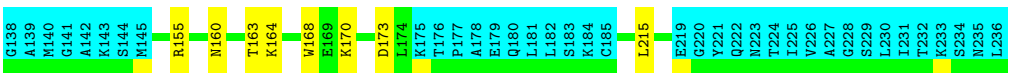
Chain B:



4.2.16 Score per residue for model 16

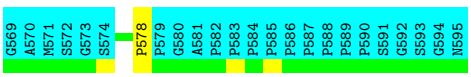
• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



• Molecule 2: Splicing factor 1

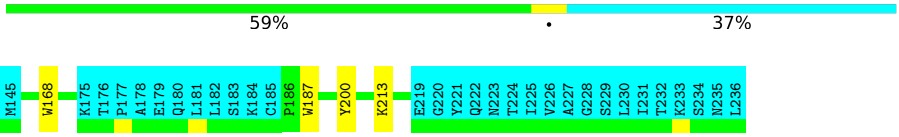
Chain B:



4.2.17 Score per residue for model 17

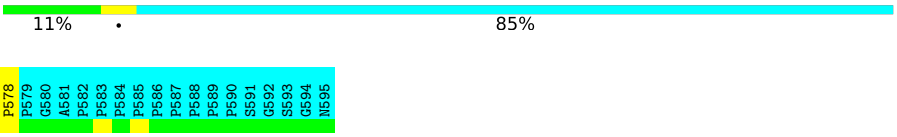
• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



• Molecule 2: Splicing factor 1

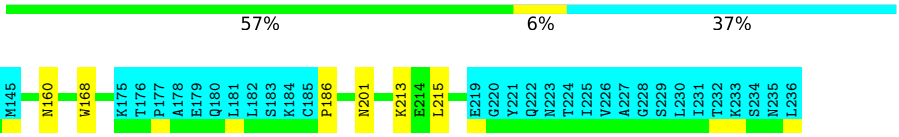
Chain B:



4.2.18 Score per residue for model 18

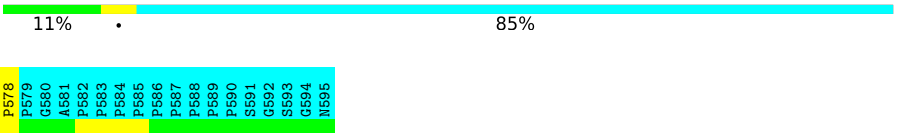
• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



• Molecule 2: Splicing factor 1

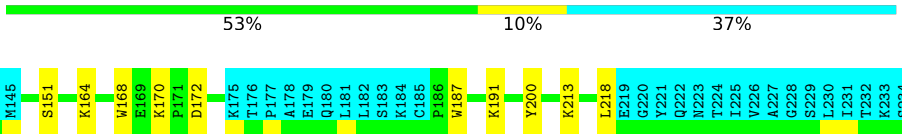
Chain B:



4.2.19 Score per residue for model 19

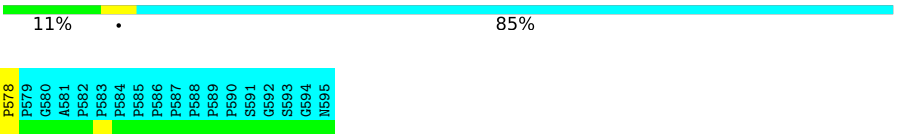
• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



• Molecule 2: Splicing factor 1

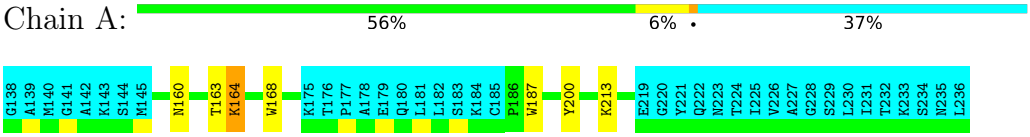
Chain B:



4.2.20 Score per residue for model 20

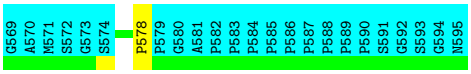
• Molecule 1: Pre-mRNA-processing factor 40 homolog A

Chain A:



• Molecule 2: Splicing factor 1

Chain B:



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
ARIA	structure calculation	

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	1455
Number of shifts mapped to atoms	1455
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

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	540	495	494	2±1
2	B	29	32	32	1±0
All	All	11380	10540	10520	48

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:TRP:CE2	2:B:578:PRO:HG2	0.52	2.40	17	20
1:A:187:TRP:HA	1:A:200:TYR:O	0.48	2.08	10	15
1:A:186:PRO:O	1:A:201:ASN:HA	0.46	2.09	1	5
1:A:163:THR:O	1:A:164:LYS:HB2	0.46	2.11	9	8

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	62/99 (63%)	59±0 (96±1%)	3±0 (4±1%)	0±0 (0±0%)	100	100
2	B	4/27 (15%)	4±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	1320/2520 (52%)	1269 (96%)	51 (4%)	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	59/88 (67%)	57±1 (97±2%)	2±1 (3±2%)	44	89
2	B	4/20 (20%)	4±0 (100±0%)	0±0 (0±0%)	100	100
All	All	1260/2160 (58%)	1225 (97%)	35 (3%)	46	90

All 12 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	218	LEU	6
1	A	164	LYS	6
1	A	151	SER	4
1	A	213	LYS	4
1	A	173	ASP	3
1	A	155	ARG	2
1	A	148	GLU	2
1	A	189	GLU	2
1	A	216	GLU	2
1	A	191	LYS	2
1	A	193	ASP	1
1	A	172	ASP	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	1455
Number of shifts mapped to atoms	1455
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

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

- Chemical shift has been reported more than once. All 82 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	139	ALA	HB2	1.459	0.000	1
1	A	139	ALA	HB3	1.459	0.000	1
1	A	140	MET	HE2	2.161	0.000	1
1	A	140	MET	HE3	2.161	0.000	1
1	A	142	ALA	HB2	1.459	0.000	1
1	A	142	ALA	HB3	1.459	0.000	1
1	A	145	MET	HE2	2.090	0.000	1
1	A	145	MET	HE3	2.090	0.000	1
1	A	147	THR	HG22	1.336	0.000	1
1	A	147	THR	HG23	1.336	0.000	1
1	A	156	THR	HG22	1.024	0.000	1
1	A	156	THR	HG23	1.024	0.000	1
1	A	161	THR	HG22	1.449	0.000	1
1	A	161	THR	HG23	1.449	0.000	1
1	A	163	THR	HG22	1.034	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	163	THR	HG23	1.034	0.000	1
1	A	167	THR	HG22	1.402	0.000	1
1	A	167	THR	HG23	1.402	0.000	1
1	A	174	LEU	HD12	0.951	0.000	2
1	A	174	LEU	HD13	0.951	0.000	2
1	A	174	LEU	HD22	0.841	0.000	2
1	A	174	LEU	HD23	0.841	0.000	2
1	A	176	THR	HG22	1.428	0.000	1
1	A	176	THR	HG23	1.428	0.000	1
1	A	178	ALA	HB2	1.466	0.000	1
1	A	178	ALA	HB3	1.466	0.000	1
1	A	181	LEU	HD12	0.929	0.000	2
1	A	181	LEU	HD13	0.929	0.000	2
1	A	181	LEU	HD22	0.915	0.000	2
1	A	181	LEU	HD23	0.915	0.000	2
1	A	182	LEU	HD12	0.997	0.000	2
1	A	182	LEU	HD13	0.997	0.000	2
1	A	182	LEU	HD22	0.968	0.000	2
1	A	182	LEU	HD23	0.968	0.000	2
1	A	204	THR	HG22	1.034	0.000	1
1	A	204	THR	HG23	1.034	0.000	1
1	A	210	ALA	HB2	1.346	0.000	1
1	A	210	ALA	HB3	1.346	0.000	1
1	A	215	LEU	HD12	1.028	0.000	2
1	A	215	LEU	HD13	1.028	0.000	2
1	A	215	LEU	HD22	0.995	0.000	2
1	A	215	LEU	HD23	0.995	0.000	2
1	A	218	LEU	HD12	1.066	0.000	2
1	A	218	LEU	HD13	1.066	0.000	2
1	A	218	LEU	HD22	0.979	0.000	2
1	A	218	LEU	HD23	0.979	0.000	2
1	A	224	THR	HG22	1.243	0.000	1
1	A	224	THR	HG23	1.243	0.000	1
1	A	225	ILE	HD12	0.859	0.000	1
1	A	225	ILE	HD13	0.859	0.000	1
1	A	225	ILE	HG22	0.901	0.000	1
1	A	225	ILE	HG23	0.901	0.000	1
1	A	226	VAL	HG12	0.989	0.000	2
1	A	226	VAL	HG13	0.989	0.000	2
1	A	226	VAL	HG22	0.977	0.000	2
1	A	226	VAL	HG23	0.977	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	227	ALA	HB2	1.458	0.000	1
1	A	227	ALA	HB3	1.458	0.000	1
1	A	230	LEU	HD12	0.964	0.000	2
1	A	230	LEU	HD13	0.964	0.000	2
1	A	230	LEU	HD22	0.908	0.000	2
1	A	230	LEU	HD23	0.908	0.000	2
1	A	231	ILE	HD12	0.902	0.000	1
1	A	231	ILE	HD13	0.902	0.000	1
1	A	231	ILE	HG22	0.950	0.000	1
1	A	231	ILE	HG23	0.950	0.000	1
1	A	232	THR	HG22	1.243	0.000	1
1	A	232	THR	HG23	1.243	0.000	1
1	A	236	LEU	HD12	0.950	0.000	2
1	A	236	LEU	HD13	0.950	0.000	2
1	A	236	LEU	HD22	0.909	0.000	2
1	A	236	LEU	HD23	0.909	0.000	2
1	B	570	ALA	HB2	1.417	0.000	1
1	B	570	ALA	HB3	1.417	0.000	1
1	B	571	MET	HE2	2.109	0.000	1
1	B	571	MET	HE3	2.109	0.000	1
1	B	577	LEU	HD12	0.865	0.000	2
1	B	577	LEU	HD13	0.865	0.000	2
1	B	577	LEU	HD22	0.471	0.000	2
1	B	577	LEU	HD23	0.471	0.000	2
1	B	581	ALA	HB2	1.262	0.000	1
1	B	581	ALA	HB3	1.262	0.000	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
$^{13}C_{\alpha}$	123	0.28 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	112	0.14 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	102	0.01 ± 0.29	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 87%, i.e. 791 atoms were assigned a chemical

shift out of a possible 909. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	248/316 (78%)	125/126 (99%)	66/132 (50%)	57/58 (98%)
Sidechain	435/474 (92%)	291/299 (97%)	138/156 (88%)	6/19 (32%)
Aromatic	108/119 (91%)	54/56 (96%)	50/57 (88%)	4/6 (67%)
Overall	791/909 (87%)	470/481 (98%)	254/345 (74%)	67/83 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1373 atoms were assigned a chemical shift out of a possible 1601. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	461/603 (76%)	236/244 (97%)	123/252 (49%)	102/107 (95%)
Sidechain	796/870 (91%)	537/561 (96%)	248/281 (88%)	11/28 (39%)
Aromatic	116/128 (91%)	58/60 (97%)	54/62 (87%)	4/6 (67%)
Overall	1373/1601 (86%)	831/865 (96%)	425/595 (71%)	117/141 (83%)

7.1.4 Statistically unusual chemical shifts (i)

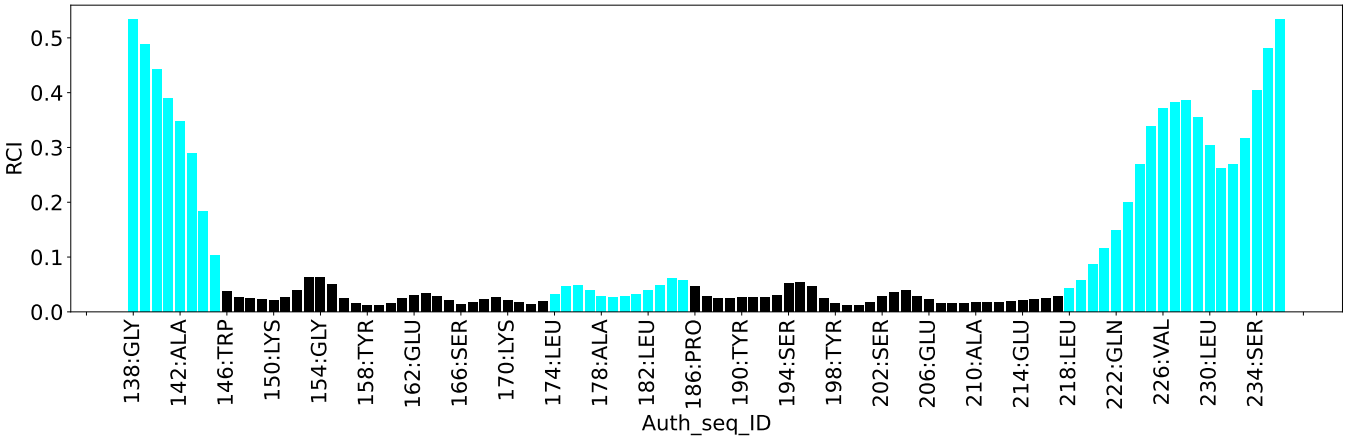
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	201	ASN	HB3	-0.43	1.12 – 4.38	-9.8
1	A	160	ASN	HB3	-0.02	1.12 – 4.38	-8.5
1	A	149	HIS	HB3	0.90	1.18 – 4.91	-5.8
1	A	171	PRO	HG3	0.11	0.33 – 3.48	-5.7
1	A	212	PRO	HG3	0.22	0.33 – 3.48	-5.3
1	A	171	PRO	HG2	0.38	0.41 – 3.45	-5.1

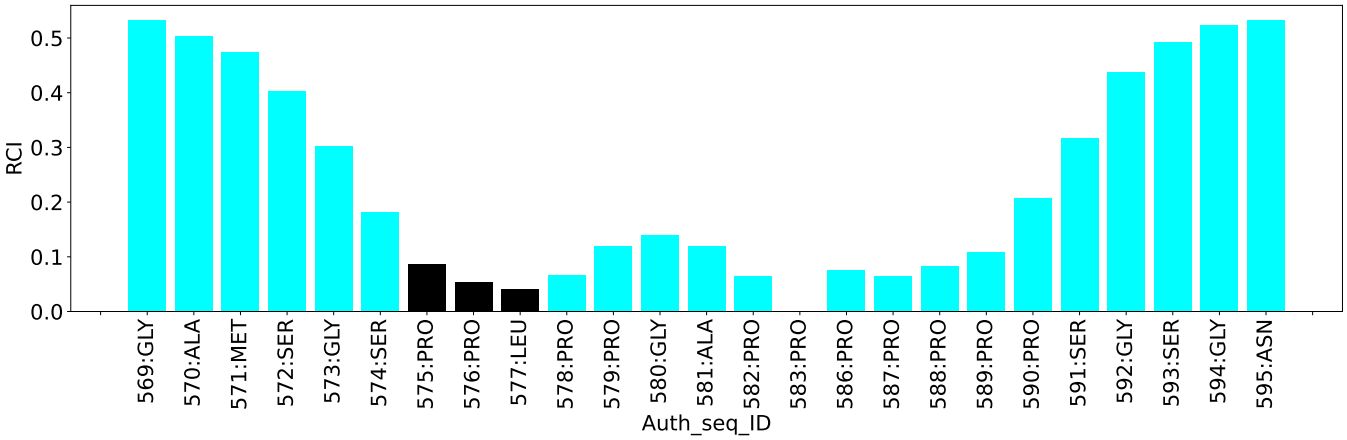
7.1.5 Random Coil Index (RCI) plots (i)

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:



Random coil index (RCI) for chain B:



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	3897
Intra-residue (|i-j|=0)	1225
Sequential (|i-j|=1)	746
Medium range (|i-j|>1 and |i-j|<5)	567
Long range (|i-j|≥5)	1080
Inter-chain	279
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	169
Number of unmapped restraints	0
Number of restraints per residue	32.3
Number of long range restraints per residue[1]	8.6

[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)	16.1	0.2
0.2-0.5 (Medium)	27.1	0.5
>0.5 (Large)	5.1	0.78

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	15.0	8.04
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

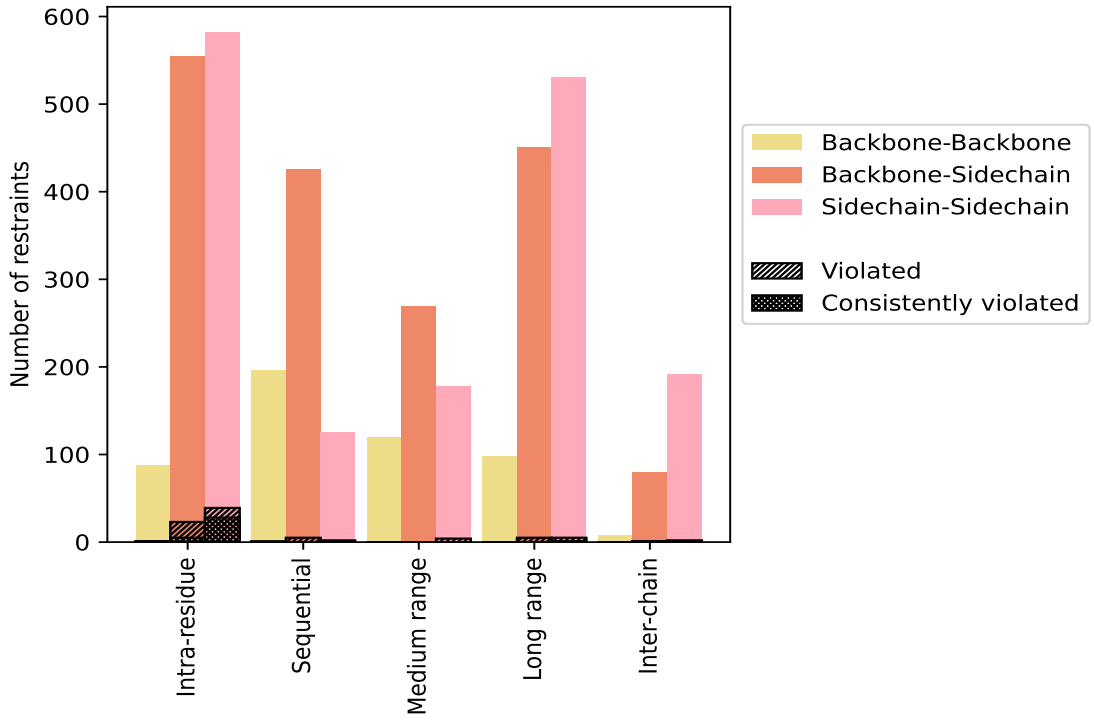
9.1 Summary of distance violations (i)

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)	1225	31.4	63	5.1	1.6	34	2.8	0.9
Backbone-Backbone	88	2.3	1	1.1	0.0	1	1.1	0.0
Backbone-Sidechain	555	14.2	23	4.1	0.6	5	0.9	0.1
Sidechain-Sidechain	582	14.9	39	6.7	1.0	28	4.8	0.7
Sequential (|i-j|=1)	746	19.1	8	1.1	0.2	0	0.0	0.0
Backbone-Backbone	196	5.0	1	0.5	0.0	0	0.0	0.0
Backbone-Sidechain	425	10.9	5	1.2	0.1	0	0.0	0.0
Sidechain-Sidechain	125	3.2	2	1.6	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	567	14.5	4	0.7	0.1	0	0.0	0.0
Backbone-Backbone	120	3.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	269	6.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	178	4.6	4	2.2	0.1	0	0.0	0.0
Long range (|i-j|≥5)	1080	27.7	10	0.9	0.3	1	0.1	0.0
Backbone-Backbone	98	2.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	451	11.6	5	1.1	0.1	0	0.0	0.0
Sidechain-Sidechain	531	13.6	5	0.9	0.1	1	0.2	0.0
Inter-chain	279	7.2	3	1.1	0.1	1	0.4	0.0
Backbone-Backbone	8	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	80	2.1	1	1.2	0.0	1	1.2	0.0
Sidechain-Sidechain	191	4.9	2	1.0	0.1	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	3897	100.0	88	2.3	2.3	36	0.9	0.9
Backbone-Backbone	510	13.1	2	0.4	0.1	1	0.2	0.0
Backbone-Sidechain	1780	45.7	34	1.9	0.9	6	0.3	0.2
Sidechain-Sidechain	1607	41.2	52	3.2	1.3	29	1.8	0.7

[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	42	1	0	2	2	47	0.3	0.66	0.15	0.27
2	39	0	0	1	3	43	0.3	0.58	0.13	0.29
3	43	3	0	2	2	50	0.29	0.6	0.15	0.26
4	46	1	2	2	3	54	0.28	0.63	0.14	0.24
5	44	2	2	3	3	54	0.3	0.66	0.16	0.26
6	42	2	0	1	3	48	0.3	0.64	0.15	0.26
7	40	2	1	1	3	47	0.3	0.66	0.15	0.27
8	42	1	1	2	3	49	0.28	0.56	0.13	0.26
9	44	0	0	2	3	49	0.32	0.69	0.17	0.29
10	43	0	1	1	3	48	0.3	0.61	0.13	0.28
11	43	0	1	1	2	47	0.3	0.62	0.14	0.27

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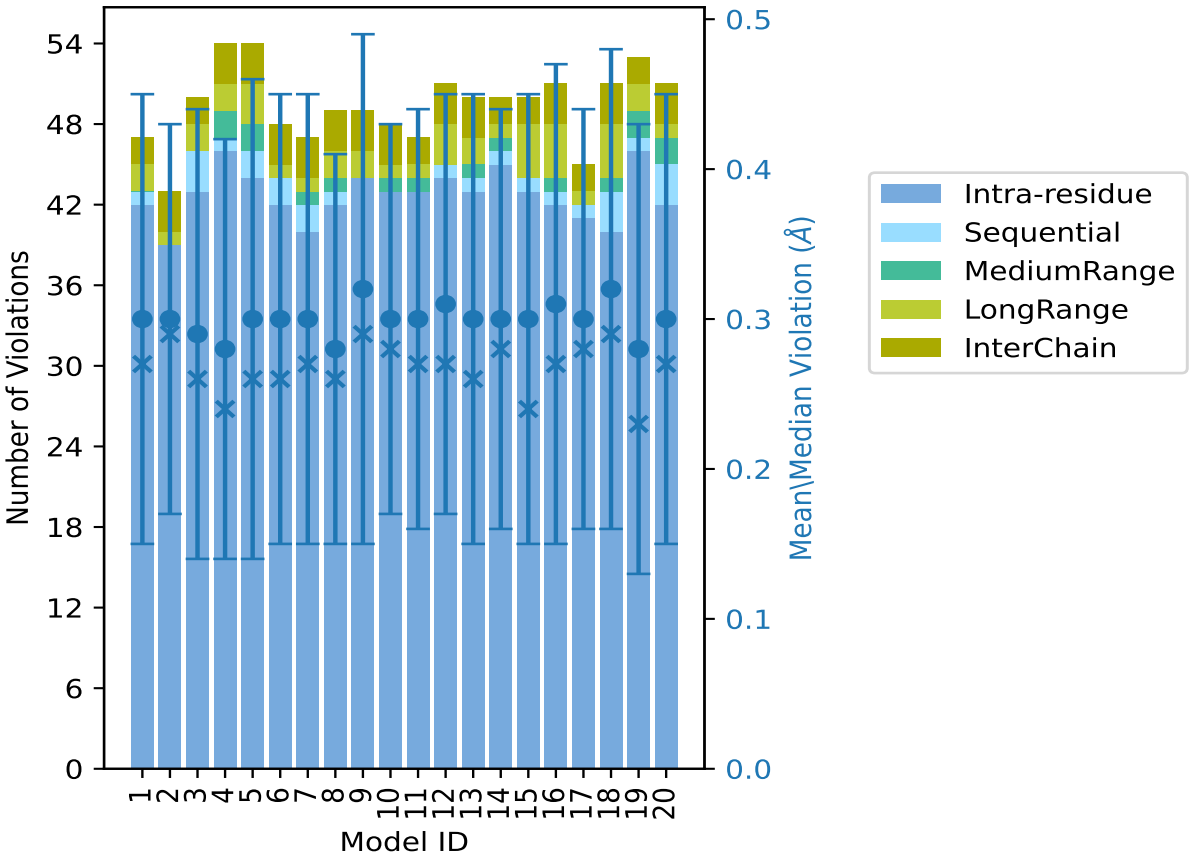
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	44	1	0	3	3	51	0.31	0.63	0.14	0.27
13	43	1	1	2	3	50	0.3	0.63	0.15	0.26
14	45	1	1	1	2	50	0.3	0.63	0.14	0.28
15	43	1	0	4	2	50	0.3	0.62	0.15	0.24
16	42	1	1	4	3	51	0.31	0.78	0.16	0.27
17	41	1	0	1	2	45	0.3	0.63	0.14	0.28
18	40	3	1	4	3	51	0.32	0.69	0.16	0.29
19	46	1	2	2	2	53	0.28	0.64	0.15	0.23
20	42	3	2	1	3	51	0.3	0.64	0.15	0.27

[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

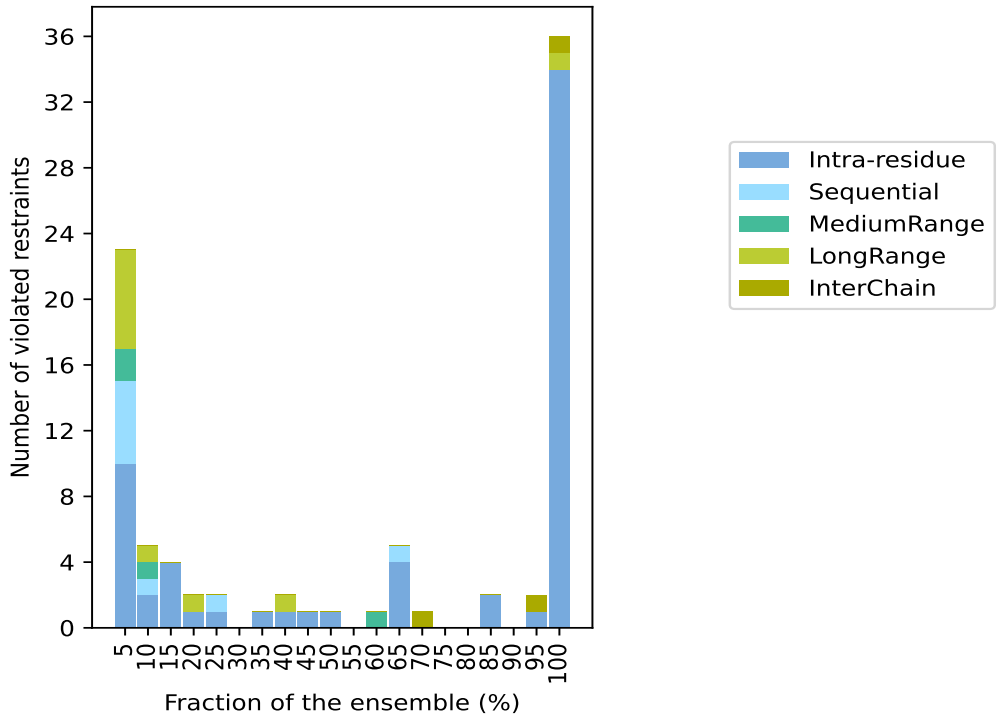
9.3 Distance violation statistics for the ensemble (i)

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, 3809(IR:1162, SQ:738, MR:563, LR:1070, IC:276) 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]	%
10	5	2	6	0	23	1	5.0
2	1	1	1	0	5	2	10.0
4	0	0	0	0	4	3	15.0
1	0	0	1	0	2	4	20.0
1	1	0	0	0	2	5	25.0
0	0	0	0	0	0	6	30.0
1	0	0	0	0	1	7	35.0
1	0	0	1	0	2	8	40.0
1	0	0	0	0	1	9	45.0
1	0	0	0	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	1	0	0	1	12	60.0
4	1	0	0	0	5	13	65.0
0	0	0	0	1	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
2	0	0	0	0	2	17	85.0
0	0	0	0	0	0	18	90.0
1	0	0	0	1	2	19	95.0
34	0	0	1	1	36	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

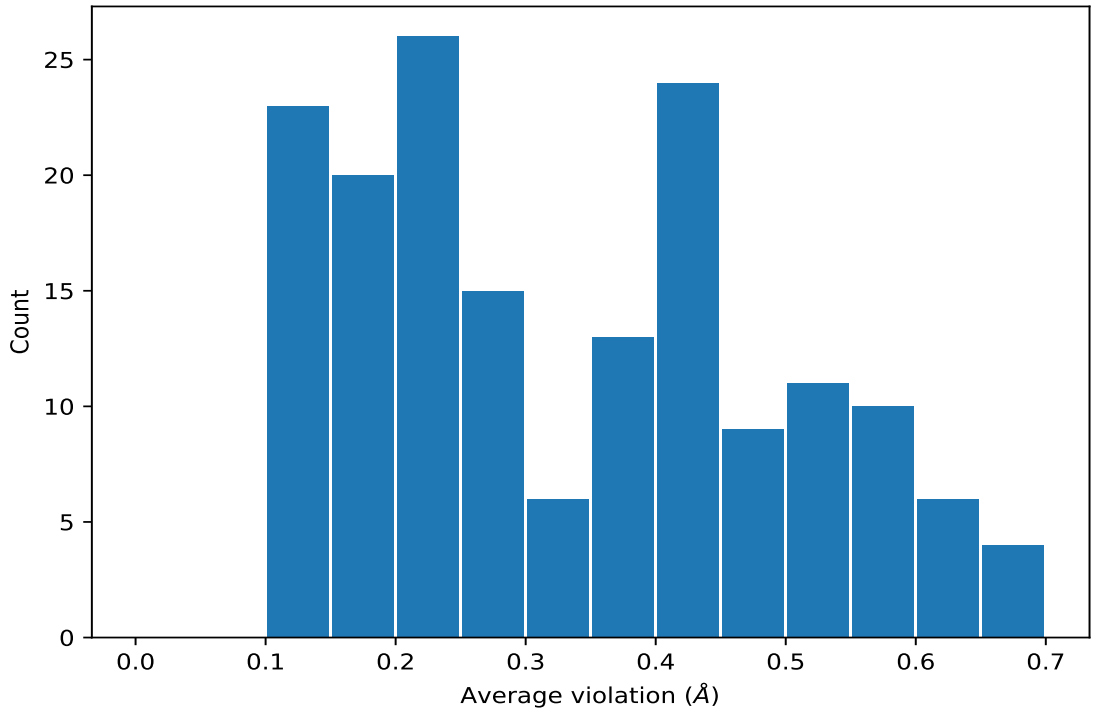
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 (i)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1050)	1:182:A:LEU:HD12	1:182:A:LEU:HB3	20	0.6	0.05	0.61
(1,1050)	1:182:A:LEU:HD11	1:182:A:LEU:HB3	20	0.6	0.05	0.61
(1,1050)	1:182:A:LEU:HD13	1:182:A:LEU:HB3	20	0.6	0.05	0.61
(1,3429)	1:181:A:LEU:HD23	1:181:A:LEU:HG	20	0.56	0.02	0.56
(1,3429)	1:181:A:LEU:HD11	1:181:A:LEU:HG	20	0.56	0.02	0.56
(1,3429)	1:181:A:LEU:HD13	1:181:A:LEU:HG	20	0.56	0.02	0.56
(1,3429)	1:181:A:LEU:HD12	1:181:A:LEU:HG	20	0.56	0.02	0.56
(1,3429)	1:181:A:LEU:HD21	1:181:A:LEU:HG	20	0.56	0.02	0.56
(1,3200)	1:163:A:THR:HG22	1:163:A:THR:HB	20	0.54	0.01	0.54
(1,3200)	1:163:A:THR:HG23	1:163:A:THR:HB	20	0.54	0.01	0.54
(1,3200)	1:163:A:THR:HG21	1:163:A:THR:HB	20	0.54	0.01	0.54
(1,3200)	1:204:A:THR:HG21	1:204:A:THR:HB	20	0.54	0.01	0.54
(1,3200)	1:204:A:THR:HG22	1:204:A:THR:HB	20	0.54	0.01	0.54
(1,3171)	1:226:A:VAL:HG23	1:226:A:VAL:HB	20	0.5	0.01	0.5
(1,3171)	1:226:A:VAL:HG13	1:226:A:VAL:HB	20	0.5	0.01	0.5
(1,3171)	1:226:A:VAL:HG12	1:226:A:VAL:HB	20	0.5	0.01	0.5

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3171)	1:226:A:VAL:HG11	1:226:A:VAL:HB	20	0.5	0.01	0.5
(1,3171)	1:226:A:VAL:HG22	1:226:A:VAL:HB	20	0.5	0.01	0.5
(1,3171)	1:226:A:VAL:HG21	1:226:A:VAL:HB	20	0.5	0.01	0.5
(1,7)	1:232:A:THR:HG22	1:232:A:THR:HB	20	0.44	0.03	0.45
(1,7)	1:232:A:THR:HG21	1:232:A:THR:HB	20	0.44	0.03	0.45
(1,7)	1:232:A:THR:HG23	1:232:A:THR:HB	20	0.44	0.03	0.45
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD23	20	0.44	0.01	0.44
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD22	20	0.44	0.01	0.44
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD21	20	0.44	0.01	0.44
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG23	20	0.44	0.01	0.44
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG22	20	0.44	0.01	0.44
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG21	20	0.44	0.01	0.44
(1,260)	1:218:A:LEU:HD13	1:218:A:LEU:HG	20	0.43	0.01	0.44
(1,260)	1:218:A:LEU:HD12	1:218:A:LEU:HG	20	0.43	0.01	0.44
(1,260)	1:218:A:LEU:HD11	1:218:A:LEU:HG	20	0.43	0.01	0.44
(1,1370)	1:218:A:LEU:HD23	1:218:A:LEU:HG	20	0.43	0.02	0.44
(1,1370)	1:218:A:LEU:HD21	1:218:A:LEU:HG	20	0.43	0.02	0.44
(1,1370)	1:218:A:LEU:HD22	1:218:A:LEU:HG	20	0.43	0.02	0.44
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG22	20	0.42	0.02	0.42
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG21	20	0.42	0.02	0.42
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG23	20	0.42	0.02	0.42
(1,1458)	1:156:A:THR:HG22	1:156:A:THR:HB	20	0.42	0.01	0.42
(1,1458)	1:156:A:THR:HG23	1:156:A:THR:HB	20	0.42	0.01	0.42
(1,1458)	1:156:A:THR:HG21	1:156:A:THR:HB	20	0.42	0.01	0.42
(1,1367)	1:182:A:LEU:HD13	1:182:A:LEU:HG	20	0.42	0.02	0.42
(1,1367)	1:182:A:LEU:HD12	1:182:A:LEU:HG	20	0.42	0.02	0.42
(1,1367)	1:182:A:LEU:HD11	1:182:A:LEU:HG	20	0.42	0.02	0.42
(1,307)	1:178:A:ALA:HB2	1:178:A:ALA:HA	20	0.39	0.02	0.4
(1,307)	1:178:A:ALA:HB1	1:178:A:ALA:HA	20	0.39	0.02	0.4
(1,307)	1:178:A:ALA:HB3	1:178:A:ALA:HA	20	0.39	0.02	0.4
(1,331)	1:147:A:THR:HG21	1:147:A:THR:HB	20	0.37	0.01	0.37
(1,331)	1:147:A:THR:HG22	1:147:A:THR:HB	20	0.37	0.01	0.37
(1,331)	1:147:A:THR:HG23	1:147:A:THR:HB	20	0.37	0.01	0.37
(1,29)	1:230:A:LEU:HD13	1:230:A:LEU:HG	20	0.37	0.03	0.36
(1,29)	1:230:A:LEU:HD12	1:230:A:LEU:HG	20	0.37	0.03	0.36
(1,29)	1:230:A:LEU:HD11	1:230:A:LEU:HG	20	0.37	0.03	0.36
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD12	20	0.37	0.01	0.37
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD13	20	0.37	0.01	0.37
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD11	20	0.37	0.01	0.37
(1,264)	1:174:A:LEU:HD23	1:174:A:LEU:HG	20	0.31	0.01	0.31
(1,264)	1:174:A:LEU:HD22	1:174:A:LEU:HG	20	0.31	0.01	0.31
(1,264)	1:174:A:LEU:HD21	1:174:A:LEU:HG	20	0.31	0.01	0.31

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1479)	1:161:A:THR:HG21	1:161:A:THR:HB	20	0.3	0.01	0.3
(1,1479)	1:161:A:THR:HG22	1:161:A:THR:HB	20	0.3	0.01	0.3
(1,1479)	1:161:A:THR:HG23	1:161:A:THR:HB	20	0.3	0.01	0.3
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB2	20	0.29	0.03	0.29
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB3	20	0.29	0.03	0.29
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB1	20	0.29	0.03	0.29
(1,315)	1:227:A:ALA:HB2	1:227:A:ALA:HA	20	0.28	0.01	0.28
(1,315)	1:227:A:ALA:HB1	1:227:A:ALA:HA	20	0.28	0.01	0.28
(1,315)	1:227:A:ALA:HB3	1:227:A:ALA:HA	20	0.28	0.01	0.28
(1,1482)	1:176:A:THR:HG22	1:176:A:THR:HB	20	0.27	0.01	0.27
(1,1482)	1:176:A:THR:HG21	1:176:A:THR:HB	20	0.27	0.01	0.27
(1,1482)	1:176:A:THR:HG23	1:176:A:THR:HB	20	0.27	0.01	0.27
(1,316)	1:142:A:ALA:HB1	1:142:A:ALA:HA	20	0.23	0.01	0.23
(1,316)	1:142:A:ALA:HB2	1:142:A:ALA:HA	20	0.23	0.01	0.23
(1,316)	1:142:A:ALA:HB3	1:142:A:ALA:HA	20	0.23	0.01	0.23
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG21	20	0.23	0.02	0.23
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG23	20	0.23	0.02	0.23
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG22	20	0.23	0.02	0.23
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	20	0.23	0.04	0.22
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB2	20	0.23	0.04	0.22
(1,1489)	1:167:A:THR:HG22	1:167:A:THR:HB	20	0.23	0.01	0.23
(1,1489)	1:167:A:THR:HG21	1:167:A:THR:HB	20	0.23	0.01	0.23
(1,1489)	1:167:A:THR:HG23	1:167:A:THR:HB	20	0.23	0.01	0.23
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG22	20	0.23	0.03	0.24
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG23	20	0.23	0.03	0.24
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG21	20	0.23	0.03	0.24
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE3	20	0.22	0.01	0.22
(1,3406)	1:205:A:LYS:HD2	1:205:A:LYS:HE3	20	0.22	0.01	0.22
(1,3406)	1:205:A:LYS:HD2	1:205:A:LYS:HE2	20	0.22	0.01	0.22
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE2	20	0.22	0.01	0.22
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD11	20	0.21	0.01	0.21
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD12	20	0.21	0.01	0.21
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD13	20	0.21	0.01	0.21
(1,943)	1:225:A:ILE:HD13	1:225:A:ILE:HG12	20	0.18	0.02	0.19
(1,943)	1:225:A:ILE:HD12	1:225:A:ILE:HG12	20	0.18	0.02	0.19
(1,943)	1:225:A:ILE:HD11	1:225:A:ILE:HG12	20	0.18	0.02	0.19
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	20	0.18	0.0	0.18
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD22	20	0.17	0.03	0.17
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD23	20	0.17	0.03	0.17
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD21	20	0.17	0.03	0.17
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	20	0.16	0.01	0.16
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	20	0.15	0.0	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	20	0.15	0.0	0.15
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	20	0.13	0.01	0.13
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	20	0.11	0.0	0.11
(1,706)	2:577:B:LEU:HD13	1:168:A:TRP:HH2	19	0.29	0.06	0.28
(1,706)	2:577:B:LEU:HD12	1:168:A:TRP:HH2	19	0.29	0.06	0.28
(1,706)	2:577:B:LEU:HD11	1:168:A:TRP:HH2	19	0.29	0.06	0.28
(1,942)	1:225:A:ILE:HD12	1:225:A:ILE:HG13	19	0.12	0.01	0.13
(1,942)	1:225:A:ILE:HD11	1:225:A:ILE:HG13	19	0.12	0.01	0.13
(1,942)	1:225:A:ILE:HD13	1:225:A:ILE:HG13	19	0.12	0.01	0.13
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD12	17	0.18	0.05	0.16
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD11	17	0.18	0.05	0.16
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD13	17	0.18	0.05	0.16
(1,28)	1:230:A:LEU:HD23	1:230:A:LEU:HG	17	0.12	0.01	0.12
(1,28)	1:230:A:LEU:HD22	1:230:A:LEU:HG	17	0.12	0.01	0.12
(1,28)	1:230:A:LEU:HD21	1:230:A:LEU:HG	17	0.12	0.01	0.12
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD12	14	0.15	0.04	0.15
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD11	14	0.15	0.04	0.15
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD13	14	0.15	0.04	0.15
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG22	13	0.46	0.07	0.44
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG23	13	0.46	0.07	0.44
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG21	13	0.46	0.07	0.44
(1,3576)	1:156:A:THR:H	1:155:A:ARG:HG2	13	0.35	0.07	0.37
(1,143)	1:213:A:LYS:HA	1:213:A:LYS:HD2	13	0.15	0.02	0.16
(1,149)	1:218:A:LEU:HA	1:218:A:LEU:HG	13	0.13	0.01	0.13
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG21	13	0.11	0.01	0.11
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG23	13	0.11	0.01	0.11
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG22	13	0.11	0.01	0.11
(1,1488)	1:167:A:THR:HG23	1:171:A:PRO:HG3	12	0.14	0.02	0.15
(1,1488)	1:167:A:THR:HG22	1:171:A:PRO:HG3	12	0.14	0.02	0.15
(1,1488)	1:167:A:THR:HG21	1:171:A:PRO:HG3	12	0.14	0.02	0.15
(1,3145)	1:188:A:LYS:HB2	1:188:A:LYS:HE3	10	0.29	0.19	0.18
(1,944)	1:225:A:ILE:HG13	1:225:A:ILE:HG21	9	0.59	0.02	0.59
(1,944)	1:225:A:ILE:HG13	1:225:A:ILE:HG22	9	0.59	0.02	0.59
(1,944)	1:225:A:ILE:HG13	1:225:A:ILE:HG23	9	0.59	0.02	0.59
(1,3281)	1:215:A:LEU:HD21	1:188:A:LYS:HA	8	0.47	0.18	0.53
(1,3281)	1:182:A:LEU:HD11	1:188:A:LYS:HA	8	0.47	0.18	0.53
(1,3281)	1:215:A:LEU:HD22	1:188:A:LYS:HA	8	0.47	0.18	0.53
(1,3281)	1:215:A:LEU:HD23	1:188:A:LYS:HA	8	0.47	0.18	0.53
(1,3407)	1:164:A:LYS:HD2	1:164:A:LYS:HA	8	0.17	0.05	0.14
(1,3407)	1:164:A:LYS:HD3	1:164:A:LYS:HA	8	0.17	0.05	0.14
(1,18)	1:231:A:ILE:HA	1:231:A:ILE:HG22	7	0.61	0.03	0.61
(1,18)	1:231:A:ILE:HA	1:231:A:ILE:HG23	7	0.61	0.03	0.61

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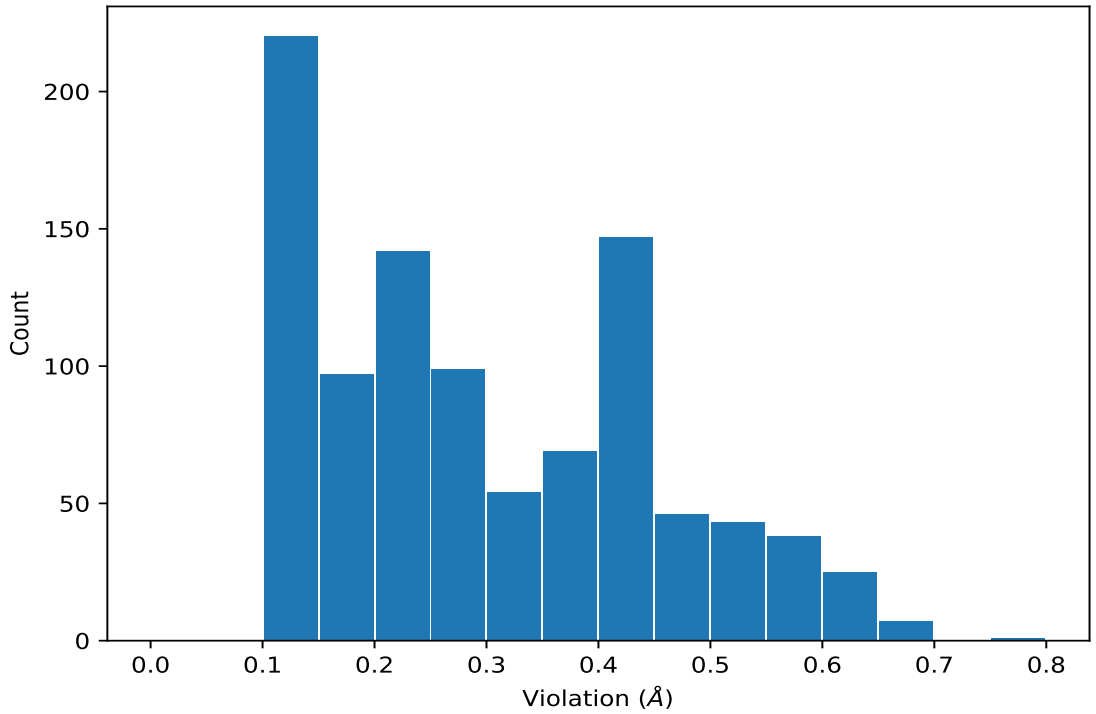
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,18)	1:231:A:ILE:HA	1:231:A:ILE:HG21	7	0.61	0.03	0.61
(1,3137)	1:222:A:GLN:HG3	1:222:A:GLN:HA	5	0.22	0.03	0.22
(1,3137)	1:222:A:GLN:HG2	1:222:A:GLN:HA	5	0.22	0.03	0.22
(1,2451)	1:182:A:LEU:H	1:181:A:LEU:HD13	5	0.14	0.02	0.15
(1,2451)	1:182:A:LEU:H	1:181:A:LEU:HD12	5	0.14	0.02	0.15
(1,3177)	1:156:A:THR:HG22	1:150:A:LYS:HE3	4	0.65	0.03	0.64
(1,3177)	1:156:A:THR:HG23	1:150:A:LYS:HE3	4	0.65	0.03	0.64
(1,306)	1:230:A:LEU:HD13	1:230:A:LEU:HA	4	0.65	0.03	0.64
(1,306)	1:230:A:LEU:HD12	1:230:A:LEU:HA	4	0.65	0.03	0.64
(1,3713)	1:205:A:LYS:H	1:205:A:LYS:HD2	3	0.25	0.11	0.25
(1,3713)	1:205:A:LYS:H	1:205:A:LYS:HD3	3	0.25	0.11	0.25
(1,222)	1:211:A:LYS:HD3	1:211:A:LYS:HE2	3	0.2	0.0	0.2
(1,2968)	1:225:A:ILE:H	1:225:A:ILE:HG22	3	0.14	0.01	0.14
(1,2968)	1:225:A:ILE:H	1:225:A:ILE:HG21	3	0.14	0.01	0.14
(1,2968)	1:225:A:ILE:H	1:225:A:ILE:HG23	3	0.14	0.01	0.14
(1,3290)	1:233:A:LYS:HG2	1:233:A:LYS:HE3	3	0.1	0.0	0.1
(1,3290)	1:233:A:LYS:HG3	1:233:A:LYS:HE3	3	0.1	0.0	0.1
(1,6)	1:232:A:THR:HG21	1:232:A:THR:HA	2	0.57	0.06	0.57
(1,6)	1:232:A:THR:HG22	1:232:A:THR:HA	2	0.57	0.06	0.57
(1,3449)	1:167:A:THR:HG22	1:169:A:GLU:HG3	2	0.45	0.05	0.45
(1,3449)	1:167:A:THR:HG23	1:169:A:GLU:HG2	2	0.45	0.05	0.45
(1,3747)	1:226:A:VAL:H	1:226:A:VAL:HG22	2	0.2	0.05	0.2
(1,3747)	1:226:A:VAL:H	1:226:A:VAL:HG23	2	0.2	0.05	0.2
(1,2948)	1:223:A:ASN:H	1:222:A:GLN:HB2	2	0.18	0.08	0.18
(1,3387)	1:211:A:LYS:HE3	1:216:A:GLU:HB2	2	0.14	0.02	0.14

[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 lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:231:A:ILE:HG12	1:231:A:ILE:HG23	16	0.78
(1,3742)	1:221:A:TYR:H	1:181:A:LEU:HD11	18	0.69
(1,3177)	1:156:A:THR:HG22	1:150:A:LYS:HE3	16	0.69
(1,306)	1:230:A:LEU:HD13	1:230:A:LEU:HA	9	0.69
(1,3177)	1:156:A:THR:HG23	1:150:A:LYS:HE3	1	0.66
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG23	9	0.66
(1,306)	1:230:A:LEU:HD12	1:230:A:LEU:HA	5	0.66
(1,18)	1:231:A:ILE:HA	1:231:A:ILE:HG23	7	0.66
(1,3281)	1:215:A:LEU:HD22	1:188:A:LYS:HA	9	0.64
(1,1050)	1:182:A:LEU:HD12	1:182:A:LEU:HB3	6	0.64
(1,1050)	1:182:A:LEU:HD12	1:182:A:LEU:HB3	19	0.64
(1,18)	1:231:A:ILE:HA	1:231:A:ILE:HG21	20	0.64
(1,6)	1:232:A:THR:HG22	1:232:A:THR:HA	5	0.64
(1,3281)	1:215:A:LEU:HD22	1:188:A:LYS:HA	16	0.63
(1,3177)	1:156:A:THR:HG23	1:150:A:LYS:HE3	4	0.63
(1,1050)	1:182:A:LEU:HD12	1:182:A:LEU:HB3	12	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1050)	1:182:A:LEU:HD12	1:182:A:LEU:HB3	13	0.63
(1,1050)	1:182:A:LEU:HD12	1:182:A:LEU:HB3	14	0.63
(1,1050)	1:182:A:LEU:HD13	1:182:A:LEU:HB3	17	0.63
(1,1050)	1:182:A:LEU:HD12	1:182:A:LEU:HB3	20	0.63
(1,3281)	1:215:A:LEU:HD23	1:188:A:LYS:HA	15	0.62
(1,3177)	1:156:A:THR:HG23	1:150:A:LYS:HE3	13	0.62
(1,1050)	1:182:A:LEU:HD12	1:182:A:LEU:HB3	1	0.62
(1,1050)	1:182:A:LEU:HD11	1:182:A:LEU:HB3	4	0.62
(1,306)	1:230:A:LEU:HD13	1:230:A:LEU:HA	11	0.62
(1,306)	1:230:A:LEU:HD12	1:230:A:LEU:HA	18	0.62
(1,18)	1:231:A:ILE:HA	1:231:A:ILE:HG23	19	0.62
(1,1050)	1:182:A:LEU:HD13	1:182:A:LEU:HB3	5	0.61
(1,1050)	1:182:A:LEU:HD13	1:182:A:LEU:HB3	10	0.61
(1,1050)	1:182:A:LEU:HD11	1:182:A:LEU:HB3	15	0.61
(1,944)	1:225:A:ILE:HG13	1:225:A:ILE:HG23	7	0.61
(1,944)	1:225:A:ILE:HG13	1:225:A:ILE:HG22	20	0.61
(1,18)	1:231:A:ILE:HA	1:231:A:ILE:HG21	15	0.61
(1,3429)	1:181:A:LEU:HD21	1:181:A:LEU:HG	14	0.6
(1,3429)	1:181:A:LEU:HD21	1:181:A:LEU:HG	15	0.6
(1,3145)	1:188:A:LYS:HB2	1:188:A:LYS:HE3	3	0.6
(1,1050)	1:182:A:LEU:HD11	1:182:A:LEU:HB3	3	0.6
(1,1050)	1:182:A:LEU:HD12	1:182:A:LEU:HB3	9	0.6
(1,944)	1:225:A:ILE:HG13	1:225:A:ILE:HG22	18	0.6
(1,18)	1:231:A:ILE:HA	1:231:A:ILE:HG22	6	0.6
(1,3429)	1:181:A:LEU:HD13	1:181:A:LEU:HG	9	0.59
(1,3429)	1:181:A:LEU:HD23	1:181:A:LEU:HG	12	0.59
(1,3429)	1:181:A:LEU:HD11	1:181:A:LEU:HG	16	0.59
(1,3145)	1:188:A:LYS:HB2	1:188:A:LYS:HE3	9	0.59
(1,1050)	1:182:A:LEU:HD13	1:182:A:LEU:HB3	7	0.59
(1,944)	1:225:A:ILE:HG13	1:225:A:ILE:HG21	5	0.59
(1,944)	1:225:A:ILE:HG13	1:225:A:ILE:HG21	13	0.59
(1,3429)	1:181:A:LEU:HD23	1:181:A:LEU:HG	1	0.58
(1,1050)	1:182:A:LEU:HD11	1:182:A:LEU:HB3	2	0.58
(1,944)	1:225:A:ILE:HG13	1:225:A:ILE:HG22	6	0.58
(1,18)	1:231:A:ILE:HA	1:231:A:ILE:HG21	17	0.58
(1,18)	1:231:A:ILE:HA	1:231:A:ILE:HG21	18	0.58
(1,3429)	1:181:A:LEU:HD11	1:181:A:LEU:HG	4	0.57
(1,944)	1:225:A:ILE:HG13	1:225:A:ILE:HG22	14	0.57
(1,944)	1:225:A:ILE:HG13	1:225:A:ILE:HG22	15	0.57
(1,3429)	1:181:A:LEU:HD11	1:181:A:LEU:HG	3	0.56
(1,3429)	1:181:A:LEU:HD13	1:181:A:LEU:HG	5	0.56
(1,3429)	1:181:A:LEU:HD13	1:181:A:LEU:HG	6	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1050)	1:182:A:LEU:HD12	1:182:A:LEU:HB3	8	0.56
(1,944)	1:225:A:ILE:HG13	1:225:A:ILE:HG23	12	0.56
(1,3429)	1:181:A:LEU:HD11	1:181:A:LEU:HG	2	0.55
(1,3429)	1:181:A:LEU:HD13	1:181:A:LEU:HG	7	0.55
(1,3429)	1:181:A:LEU:HD12	1:181:A:LEU:HG	10	0.55
(1,3429)	1:181:A:LEU:HD11	1:181:A:LEU:HG	11	0.55
(1,3429)	1:181:A:LEU:HD13	1:181:A:LEU:HG	18	0.55
(1,3281)	1:215:A:LEU:HD21	1:188:A:LYS:HA	3	0.55
(1,3200)	1:163:A:THR:HG22	1:163:A:THR:HB	10	0.55
(1,3200)	1:204:A:THR:HG21	1:204:A:THR:HB	13	0.55
(1,3200)	1:204:A:THR:HG22	1:204:A:THR:HB	15	0.55
(1,3200)	1:163:A:THR:HG22	1:163:A:THR:HB	19	0.55
(1,3145)	1:188:A:LYS:HB2	1:188:A:LYS:HE3	14	0.55
(1,3429)	1:181:A:LEU:HD13	1:181:A:LEU:HG	8	0.54
(1,3429)	1:181:A:LEU:HD11	1:181:A:LEU:HG	17	0.54
(1,3429)	1:181:A:LEU:HD12	1:181:A:LEU:HG	19	0.54
(1,3429)	1:181:A:LEU:HD12	1:181:A:LEU:HG	20	0.54
(1,3200)	1:163:A:THR:HG23	1:163:A:THR:HB	4	0.54
(1,3200)	1:163:A:THR:HG21	1:163:A:THR:HB	5	0.54
(1,3200)	1:163:A:THR:HG23	1:163:A:THR:HB	6	0.54
(1,3200)	1:163:A:THR:HG21	1:163:A:THR:HB	9	0.54
(1,3200)	1:163:A:THR:HG23	1:163:A:THR:HB	11	0.54
(1,3200)	1:163:A:THR:HG23	1:163:A:THR:HB	14	0.54
(1,3200)	1:163:A:THR:HG22	1:163:A:THR:HB	20	0.54
(1,1050)	1:182:A:LEU:HD11	1:182:A:LEU:HB3	11	0.54
(1,1050)	1:182:A:LEU:HD11	1:182:A:LEU:HB3	18	0.54
(1,3429)	1:181:A:LEU:HD13	1:181:A:LEU:HG	13	0.53
(1,3200)	1:163:A:THR:HG22	1:163:A:THR:HB	1	0.53
(1,3200)	1:163:A:THR:HG22	1:163:A:THR:HB	2	0.53
(1,3200)	1:163:A:THR:HG21	1:163:A:THR:HB	12	0.53
(1,3200)	1:163:A:THR:HG21	1:163:A:THR:HB	16	0.53
(1,3200)	1:163:A:THR:HG23	1:163:A:THR:HB	18	0.53
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG22	1	0.53
(1,3200)	1:163:A:THR:HG23	1:163:A:THR:HB	3	0.52
(1,3200)	1:163:A:THR:HG22	1:163:A:THR:HB	7	0.52
(1,3200)	1:163:A:THR:HG21	1:163:A:THR:HB	8	0.52
(1,3200)	1:163:A:THR:HG23	1:163:A:THR:HB	17	0.52
(1,3281)	1:215:A:LEU:HD22	1:188:A:LYS:HA	18	0.51
(1,3171)	1:226:A:VAL:HG12	1:226:A:VAL:HB	3	0.51
(1,3171)	1:226:A:VAL:HG11	1:226:A:VAL:HB	4	0.51
(1,3171)	1:226:A:VAL:HG11	1:226:A:VAL:HB	8	0.51
(1,3171)	1:226:A:VAL:HG13	1:226:A:VAL:HB	17	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3171)	1:226:A:VAL:HG13	1:226:A:VAL:HB	19	0.51
(1,6)	1:232:A:THR:HG21	1:232:A:THR:HA	19	0.51
(1,3449)	1:167:A:THR:HG23	1:169:A:GLU:HG2	5	0.5
(1,3171)	1:226:A:VAL:HG23	1:226:A:VAL:HB	1	0.5
(1,3171)	1:226:A:VAL:HG22	1:226:A:VAL:HB	7	0.5
(1,3171)	1:226:A:VAL:HG13	1:226:A:VAL:HB	9	0.5
(1,3171)	1:226:A:VAL:HG11	1:226:A:VAL:HB	10	0.5
(1,3171)	1:226:A:VAL:HG22	1:226:A:VAL:HB	11	0.5
(1,3171)	1:226:A:VAL:HG11	1:226:A:VAL:HB	13	0.5
(1,3171)	1:226:A:VAL:HG13	1:226:A:VAL:HB	14	0.5
(1,3171)	1:226:A:VAL:HG11	1:226:A:VAL:HB	15	0.5
(1,3171)	1:226:A:VAL:HG13	1:226:A:VAL:HB	16	0.5
(1,3171)	1:226:A:VAL:HG11	1:226:A:VAL:HB	18	0.5
(1,3171)	1:226:A:VAL:HG12	1:226:A:VAL:HB	20	0.5
(1,3171)	1:226:A:VAL:HG12	1:226:A:VAL:HB	6	0.49
(1,3171)	1:226:A:VAL:HG13	1:226:A:VAL:HB	2	0.48
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG22	12	0.48
(1,3281)	1:182:A:LEU:HD11	1:188:A:LYS:HA	12	0.47
(1,3171)	1:226:A:VAL:HG22	1:226:A:VAL:HB	5	0.47
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG21	20	0.47
(1,7)	1:232:A:THR:HG22	1:232:A:THR:HB	11	0.47
(1,7)	1:232:A:THR:HG23	1:232:A:THR:HB	17	0.47
(1,3171)	1:226:A:VAL:HG21	1:226:A:VAL:HB	12	0.46
(1,1367)	1:182:A:LEU:HD12	1:182:A:LEU:HG	16	0.46
(1,1367)	1:182:A:LEU:HD12	1:182:A:LEU:HG	18	0.46
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD22	11	0.46
(1,7)	1:232:A:THR:HG22	1:232:A:THR:HB	3	0.46
(1,7)	1:232:A:THR:HG23	1:232:A:THR:HB	8	0.46
(1,7)	1:232:A:THR:HG21	1:232:A:THR:HB	13	0.46
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG21	13	0.45
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG23	14	0.45
(1,1370)	1:218:A:LEU:HD22	1:218:A:LEU:HG	4	0.45
(1,1370)	1:218:A:LEU:HD23	1:218:A:LEU:HG	5	0.45
(1,1370)	1:218:A:LEU:HD23	1:218:A:LEU:HG	6	0.45
(1,1370)	1:218:A:LEU:HD22	1:218:A:LEU:HG	8	0.45
(1,1370)	1:218:A:LEU:HD23	1:218:A:LEU:HG	10	0.45
(1,1370)	1:218:A:LEU:HD21	1:218:A:LEU:HG	17	0.45
(1,1370)	1:218:A:LEU:HD23	1:218:A:LEU:HG	20	0.45
(1,1050)	1:182:A:LEU:HD13	1:182:A:LEU:HB3	16	0.45
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG22	7	0.45
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG21	18	0.45
(1,260)	1:218:A:LEU:HD13	1:218:A:LEU:HG	3	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,260)	1:218:A:LEU:HD13	1:218:A:LEU:HG	4	0.45
(1,260)	1:218:A:LEU:HD11	1:218:A:LEU:HG	9	0.45
(1,260)	1:218:A:LEU:HD13	1:218:A:LEU:HG	16	0.45
(1,260)	1:218:A:LEU:HD12	1:218:A:LEU:HG	18	0.45
(1,260)	1:218:A:LEU:HD13	1:218:A:LEU:HG	20	0.45
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD23	7	0.45
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD22	12	0.45
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD23	13	0.45
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD22	14	0.45
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD21	16	0.45
(1,7)	1:232:A:THR:HG22	1:232:A:THR:HB	1	0.45
(1,7)	1:232:A:THR:HG21	1:232:A:THR:HB	2	0.45
(1,7)	1:232:A:THR:HG22	1:232:A:THR:HB	4	0.45
(1,7)	1:232:A:THR:HG22	1:232:A:THR:HB	6	0.45
(1,7)	1:232:A:THR:HG21	1:232:A:THR:HB	9	0.45
(1,7)	1:232:A:THR:HG23	1:232:A:THR:HB	10	0.45
(1,7)	1:232:A:THR:HG22	1:232:A:THR:HB	15	0.45
(1,7)	1:232:A:THR:HG22	1:232:A:THR:HB	18	0.45
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG23	2	0.44
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG23	8	0.44
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG21	10	0.44
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG21	11	0.44
(1,1370)	1:218:A:LEU:HD23	1:218:A:LEU:HG	1	0.44
(1,1370)	1:218:A:LEU:HD23	1:218:A:LEU:HG	13	0.44
(1,1370)	1:218:A:LEU:HD21	1:218:A:LEU:HG	14	0.44
(1,1370)	1:218:A:LEU:HD21	1:218:A:LEU:HG	19	0.44
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG23	2	0.44
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG22	3	0.44
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG23	5	0.44
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG23	9	0.44
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG22	10	0.44
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG23	11	0.44
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG22	12	0.44
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG23	13	0.44
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG21	14	0.44
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG23	16	0.44
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG23	17	0.44
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG22	19	0.44
(1,260)	1:218:A:LEU:HD13	1:218:A:LEU:HG	1	0.44
(1,260)	1:218:A:LEU:HD12	1:218:A:LEU:HG	11	0.44
(1,260)	1:218:A:LEU:HD11	1:218:A:LEU:HG	14	0.44
(1,260)	1:218:A:LEU:HD12	1:218:A:LEU:HG	17	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD22	2	0.44
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD21	4	0.44
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD23	5	0.44
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD21	6	0.44
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD22	8	0.44
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD22	9	0.44
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD21	10	0.44
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD21	15	0.44
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD21	17	0.44
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD21	18	0.44
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD21	19	0.44
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD23	20	0.44
(1,15)	1:231:A:ILE:HG13	1:231:A:ILE:HG21	10	0.44
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG21	12	0.44
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG22	20	0.44
(1,7)	1:232:A:THR:HG22	1:232:A:THR:HB	7	0.44
(1,7)	1:232:A:THR:HG21	1:232:A:THR:HB	12	0.44
(1,7)	1:232:A:THR:HG23	1:232:A:THR:HB	14	0.44
(1,7)	1:232:A:THR:HG22	1:232:A:THR:HB	16	0.44
(1,7)	1:232:A:THR:HG22	1:232:A:THR:HB	20	0.44
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG23	3	0.43
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG23	5	0.43
(1,1458)	1:156:A:THR:HG22	1:156:A:THR:HB	6	0.43
(1,1458)	1:156:A:THR:HG22	1:156:A:THR:HB	7	0.43
(1,1458)	1:156:A:THR:HG23	1:156:A:THR:HB	14	0.43
(1,1458)	1:156:A:THR:HG22	1:156:A:THR:HB	17	0.43
(1,1370)	1:218:A:LEU:HD22	1:218:A:LEU:HG	3	0.43
(1,1370)	1:218:A:LEU:HD23	1:218:A:LEU:HG	7	0.43
(1,1370)	1:218:A:LEU:HD23	1:218:A:LEU:HG	9	0.43
(1,1370)	1:218:A:LEU:HD21	1:218:A:LEU:HG	12	0.43
(1,1370)	1:218:A:LEU:HD21	1:218:A:LEU:HG	15	0.43
(1,1367)	1:182:A:LEU:HD12	1:182:A:LEU:HG	4	0.43
(1,1367)	1:182:A:LEU:HD11	1:182:A:LEU:HG	5	0.43
(1,1367)	1:182:A:LEU:HD13	1:182:A:LEU:HG	6	0.43
(1,1367)	1:182:A:LEU:HD13	1:182:A:LEU:HG	20	0.43
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG23	1	0.43
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG21	4	0.43
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG21	6	0.43
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG21	8	0.43
(1,945)	1:225:A:ILE:HB	1:225:A:ILE:HG21	15	0.43
(1,307)	1:178:A:ALA:HB3	1:178:A:ALA:HA	10	0.43
(1,260)	1:218:A:LEU:HD13	1:218:A:LEU:HG	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,260)	1:218:A:LEU:HD11	1:218:A:LEU:HG	6	0.43
(1,260)	1:218:A:LEU:HD13	1:218:A:LEU:HG	8	0.43
(1,260)	1:218:A:LEU:HD11	1:218:A:LEU:HG	12	0.43
(1,260)	1:218:A:LEU:HD11	1:218:A:LEU:HG	15	0.43
(1,260)	1:218:A:LEU:HD13	1:218:A:LEU:HG	19	0.43
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD23	1	0.43
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG22	1	0.43
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG23	6	0.43
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG23	14	0.43
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG23	15	0.43
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG22	17	0.43
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG23	18	0.43
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG22	19	0.43
(1,1458)	1:156:A:THR:HG23	1:156:A:THR:HB	2	0.42
(1,1458)	1:156:A:THR:HG21	1:156:A:THR:HB	3	0.42
(1,1458)	1:156:A:THR:HG21	1:156:A:THR:HB	4	0.42
(1,1458)	1:156:A:THR:HG22	1:156:A:THR:HB	8	0.42
(1,1458)	1:156:A:THR:HG23	1:156:A:THR:HB	9	0.42
(1,1458)	1:156:A:THR:HG21	1:156:A:THR:HB	10	0.42
(1,1458)	1:156:A:THR:HG22	1:156:A:THR:HB	11	0.42
(1,1458)	1:156:A:THR:HG21	1:156:A:THR:HB	12	0.42
(1,1458)	1:156:A:THR:HG21	1:156:A:THR:HB	13	0.42
(1,1458)	1:156:A:THR:HG22	1:156:A:THR:HB	15	0.42
(1,1458)	1:156:A:THR:HG21	1:156:A:THR:HB	16	0.42
(1,1458)	1:156:A:THR:HG23	1:156:A:THR:HB	18	0.42
(1,1458)	1:156:A:THR:HG21	1:156:A:THR:HB	19	0.42
(1,1370)	1:218:A:LEU:HD22	1:218:A:LEU:HG	18	0.42
(1,1367)	1:182:A:LEU:HD13	1:182:A:LEU:HG	1	0.42
(1,1367)	1:182:A:LEU:HD13	1:182:A:LEU:HG	8	0.42
(1,1367)	1:182:A:LEU:HD13	1:182:A:LEU:HG	12	0.42
(1,1367)	1:182:A:LEU:HD13	1:182:A:LEU:HG	13	0.42
(1,1367)	1:182:A:LEU:HD13	1:182:A:LEU:HG	14	0.42
(1,1367)	1:182:A:LEU:HD11	1:182:A:LEU:HG	17	0.42
(1,1367)	1:182:A:LEU:HD13	1:182:A:LEU:HG	19	0.42
(1,307)	1:178:A:ALA:HB2	1:178:A:ALA:HA	1	0.42
(1,307)	1:178:A:ALA:HB3	1:178:A:ALA:HA	16	0.42
(1,307)	1:178:A:ALA:HB3	1:178:A:ALA:HA	17	0.42
(1,260)	1:218:A:LEU:HD12	1:218:A:LEU:HG	13	0.42
(1,258)	1:182:A:LEU:HG	1:182:A:LEU:HD22	3	0.42
(1,29)	1:230:A:LEU:HD11	1:230:A:LEU:HG	18	0.42
(1,13)	1:231:A:ILE:HB	1:231:A:ILE:HD13	16	0.42
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG22	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG21	3	0.42
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG21	7	0.42
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG23	8	0.42
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG23	9	0.42
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG23	10	0.42
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG23	13	0.42
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG21	16	0.42
(1,3576)	1:156:A:THR:H	1:155:A:ARG:HG2	1	0.41
(1,3576)	1:156:A:THR:H	1:155:A:ARG:HG2	12	0.41
(1,3576)	1:156:A:THR:H	1:155:A:ARG:HG2	17	0.41
(1,3576)	1:156:A:THR:H	1:155:A:ARG:HG2	19	0.41
(1,3449)	1:167:A:THR:HG22	1:169:A:GLU:HG3	20	0.41
(1,1458)	1:156:A:THR:HG23	1:156:A:THR:HB	5	0.41
(1,1458)	1:156:A:THR:HG22	1:156:A:THR:HB	20	0.41
(1,1370)	1:218:A:LEU:HD21	1:218:A:LEU:HG	2	0.41
(1,1370)	1:218:A:LEU:HD22	1:218:A:LEU:HG	16	0.41
(1,1367)	1:182:A:LEU:HD12	1:182:A:LEU:HG	3	0.41
(1,1367)	1:182:A:LEU:HD13	1:182:A:LEU:HG	11	0.41
(1,1367)	1:182:A:LEU:HD12	1:182:A:LEU:HG	15	0.41
(1,307)	1:178:A:ALA:HB2	1:178:A:ALA:HA	3	0.41
(1,307)	1:178:A:ALA:HB1	1:178:A:ALA:HA	20	0.41
(1,260)	1:218:A:LEU:HD11	1:218:A:LEU:HG	7	0.41
(1,260)	1:218:A:LEU:HD11	1:218:A:LEU:HG	10	0.41
(1,29)	1:230:A:LEU:HD13	1:230:A:LEU:HG	5	0.41
(1,29)	1:230:A:LEU:HD11	1:230:A:LEU:HG	11	0.41
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG22	4	0.41
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG21	11	0.41
(1,7)	1:232:A:THR:HG22	1:232:A:THR:HB	5	0.41
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG21	16	0.4
(1,1458)	1:156:A:THR:HG22	1:156:A:THR:HB	1	0.4
(1,1367)	1:182:A:LEU:HD13	1:182:A:LEU:HG	9	0.4
(1,307)	1:178:A:ALA:HB1	1:178:A:ALA:HA	2	0.4
(1,307)	1:178:A:ALA:HB1	1:178:A:ALA:HA	6	0.4
(1,307)	1:178:A:ALA:HB1	1:178:A:ALA:HA	9	0.4
(1,307)	1:178:A:ALA:HB1	1:178:A:ALA:HA	11	0.4
(1,307)	1:178:A:ALA:HB3	1:178:A:ALA:HA	12	0.4
(1,260)	1:218:A:LEU:HD12	1:218:A:LEU:HG	2	0.4
(1,29)	1:230:A:LEU:HD12	1:230:A:LEU:HG	8	0.4
(1,29)	1:230:A:LEU:HD13	1:230:A:LEU:HG	17	0.4
(1,3576)	1:156:A:THR:H	1:155:A:ARG:HG2	20	0.39
(1,1367)	1:182:A:LEU:HD11	1:182:A:LEU:HG	10	0.39
(1,706)	2:577:B:LEU:HD11	1:168:A:TRP:HH2	4	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,706)	2:577:B:LEU:HD13	1:168:A:TRP:HH2	11	0.39
(1,331)	1:147:A:THR:HG21	1:147:A:THR:HB	13	0.39
(1,307)	1:178:A:ALA:HB3	1:178:A:ALA:HA	5	0.39
(1,307)	1:178:A:ALA:HB1	1:178:A:ALA:HA	13	0.39
(1,29)	1:230:A:LEU:HD11	1:230:A:LEU:HG	9	0.39
(1,3713)	1:205:A:LYS:H	1:205:A:LYS:HD3	12	0.38
(1,3576)	1:156:A:THR:H	1:155:A:ARG:HG2	14	0.38
(1,2984)	1:231:A:ILE:H	1:231:A:ILE:HG22	4	0.38
(1,706)	2:577:B:LEU:HD11	1:168:A:TRP:HH2	9	0.38
(1,331)	1:147:A:THR:HG21	1:147:A:THR:HB	1	0.38
(1,331)	1:147:A:THR:HG21	1:147:A:THR:HB	3	0.38
(1,331)	1:147:A:THR:HG23	1:147:A:THR:HB	6	0.38
(1,331)	1:147:A:THR:HG22	1:147:A:THR:HB	7	0.38
(1,331)	1:147:A:THR:HG21	1:147:A:THR:HB	14	0.38
(1,331)	1:147:A:THR:HG23	1:147:A:THR:HB	16	0.38
(1,331)	1:147:A:THR:HG21	1:147:A:THR:HB	19	0.38
(1,307)	1:178:A:ALA:HB2	1:178:A:ALA:HA	7	0.38
(1,307)	1:178:A:ALA:HB3	1:178:A:ALA:HA	18	0.38
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD11	4	0.38
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD11	10	0.38
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD13	16	0.38
(1,3576)	1:156:A:THR:H	1:155:A:ARG:HG2	3	0.37
(1,1370)	1:218:A:LEU:HD22	1:218:A:LEU:HG	11	0.37
(1,1367)	1:182:A:LEU:HD12	1:182:A:LEU:HG	2	0.37
(1,1367)	1:182:A:LEU:HD11	1:182:A:LEU:HG	7	0.37
(1,706)	2:577:B:LEU:HD12	1:168:A:TRP:HH2	16	0.37
(1,331)	1:147:A:THR:HG22	1:147:A:THR:HB	2	0.37
(1,331)	1:147:A:THR:HG22	1:147:A:THR:HB	4	0.37
(1,331)	1:147:A:THR:HG21	1:147:A:THR:HB	5	0.37
(1,331)	1:147:A:THR:HG22	1:147:A:THR:HB	8	0.37
(1,331)	1:147:A:THR:HG23	1:147:A:THR:HB	9	0.37
(1,331)	1:147:A:THR:HG23	1:147:A:THR:HB	10	0.37
(1,331)	1:147:A:THR:HG21	1:147:A:THR:HB	11	0.37
(1,331)	1:147:A:THR:HG21	1:147:A:THR:HB	12	0.37
(1,331)	1:147:A:THR:HG23	1:147:A:THR:HB	15	0.37
(1,331)	1:147:A:THR:HG23	1:147:A:THR:HB	17	0.37
(1,331)	1:147:A:THR:HG22	1:147:A:THR:HB	18	0.37
(1,331)	1:147:A:THR:HG21	1:147:A:THR:HB	20	0.37
(1,307)	1:178:A:ALA:HB3	1:178:A:ALA:HA	8	0.37
(1,307)	1:178:A:ALA:HB3	1:178:A:ALA:HA	14	0.37
(1,307)	1:178:A:ALA:HB3	1:178:A:ALA:HA	19	0.37
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD13	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD13	7	0.37
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD11	8	0.37
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD11	9	0.37
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD12	13	0.37
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD12	14	0.37
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD11	15	0.37
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD13	20	0.37
(1,29)	1:230:A:LEU:HD12	1:230:A:LEU:HG	2	0.37
(1,3576)	1:156:A:THR:H	1:155:A:ARG:HG2	13	0.36
(1,1786)	2:585:B:PRO:HA	2:586:B:PRO:HD2	20	0.36
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD12	1	0.36
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD12	3	0.36
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD13	5	0.36
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD11	6	0.36
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD11	12	0.36
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD12	17	0.36
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD13	18	0.36
(1,29)	1:230:A:LEU:HD12	1:230:A:LEU:HG	3	0.36
(1,29)	1:230:A:LEU:HD12	1:230:A:LEU:HG	4	0.36
(1,29)	1:230:A:LEU:HD12	1:230:A:LEU:HG	6	0.36
(1,29)	1:230:A:LEU:HD12	1:230:A:LEU:HG	7	0.36
(1,29)	1:230:A:LEU:HD12	1:230:A:LEU:HG	12	0.36
(1,29)	1:230:A:LEU:HD12	1:230:A:LEU:HG	15	0.36
(1,29)	1:230:A:LEU:HD12	1:230:A:LEU:HG	20	0.36
(1,3576)	1:156:A:THR:H	1:155:A:ARG:HG2	18	0.35
(1,307)	1:178:A:ALA:HB1	1:178:A:ALA:HA	4	0.35
(1,307)	1:178:A:ALA:HB2	1:178:A:ALA:HA	15	0.35
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD12	11	0.35
(1,266)	1:174:A:LEU:HG	1:174:A:LEU:HD11	19	0.35
(1,29)	1:230:A:LEU:HD13	1:230:A:LEU:HG	1	0.35
(1,29)	1:230:A:LEU:HD11	1:230:A:LEU:HG	13	0.35
(1,1439)	1:181:A:LEU:HD13	1:221:A:TYR:HE1	12	0.34
(1,706)	2:577:B:LEU:HD11	1:168:A:TRP:HH2	18	0.34
(1,29)	1:230:A:LEU:HD11	1:230:A:LEU:HG	10	0.34
(1,29)	1:230:A:LEU:HD12	1:230:A:LEU:HG	16	0.34
(1,29)	1:230:A:LEU:HD13	1:230:A:LEU:HG	19	0.34
(1,11)	1:224:A:THR:HB	1:224:A:THR:HG23	5	0.34
(1,7)	1:232:A:THR:HG22	1:232:A:THR:HB	19	0.34
(1,3576)	1:156:A:THR:H	1:155:A:ARG:HG2	8	0.33
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB2	1	0.33
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB3	9	0.33
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB2	12	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:230:A:LEU:HD13	1:230:A:LEU:HG	14	0.33
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB3	6	0.32
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB3	16	0.32
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB3	17	0.32
(1,1479)	1:161:A:THR:HG21	1:161:A:THR:HB	1	0.32
(1,1479)	1:161:A:THR:HG22	1:161:A:THR:HB	13	0.32
(1,264)	1:174:A:LEU:HD22	1:174:A:LEU:HG	2	0.32
(1,264)	1:174:A:LEU:HD21	1:174:A:LEU:HG	5	0.32
(1,264)	1:174:A:LEU:HD21	1:174:A:LEU:HG	6	0.32
(1,264)	1:174:A:LEU:HD21	1:174:A:LEU:HG	7	0.32
(1,264)	1:174:A:LEU:HD23	1:174:A:LEU:HG	11	0.32
(1,264)	1:174:A:LEU:HD22	1:174:A:LEU:HG	13	0.32
(1,264)	1:174:A:LEU:HD21	1:174:A:LEU:HG	19	0.32
(1,3576)	1:156:A:THR:H	1:155:A:ARG:HG2	7	0.31
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB2	11	0.31
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB3	2	0.31
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB2	10	0.31
(1,1479)	1:161:A:THR:HG21	1:161:A:THR:HB	5	0.31
(1,1479)	1:161:A:THR:HG22	1:161:A:THR:HB	10	0.31
(1,1479)	1:161:A:THR:HG21	1:161:A:THR:HB	12	0.31
(1,1479)	1:161:A:THR:HG23	1:161:A:THR:HB	14	0.31
(1,1479)	1:161:A:THR:HG23	1:161:A:THR:HB	17	0.31
(1,706)	2:577:B:LEU:HD12	1:168:A:TRP:HH2	2	0.31
(1,706)	2:577:B:LEU:HD11	1:168:A:TRP:HH2	17	0.31
(1,264)	1:174:A:LEU:HD23	1:174:A:LEU:HG	1	0.31
(1,264)	1:174:A:LEU:HD21	1:174:A:LEU:HG	4	0.31
(1,264)	1:174:A:LEU:HD21	1:174:A:LEU:HG	8	0.31
(1,264)	1:174:A:LEU:HD23	1:174:A:LEU:HG	9	0.31
(1,264)	1:174:A:LEU:HD23	1:174:A:LEU:HG	10	0.31
(1,264)	1:174:A:LEU:HD22	1:174:A:LEU:HG	12	0.31
(1,264)	1:174:A:LEU:HD22	1:174:A:LEU:HG	14	0.31
(1,264)	1:174:A:LEU:HD21	1:174:A:LEU:HG	15	0.31
(1,264)	1:174:A:LEU:HD23	1:174:A:LEU:HG	16	0.31
(1,264)	1:174:A:LEU:HD21	1:174:A:LEU:HG	17	0.31
(1,264)	1:174:A:LEU:HD21	1:174:A:LEU:HG	18	0.31
(1,264)	1:174:A:LEU:HD21	1:174:A:LEU:HG	20	0.31
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB2	8	0.3
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB1	3	0.3
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB2	5	0.3
(1,1479)	1:161:A:THR:HG21	1:161:A:THR:HB	3	0.3
(1,1479)	1:161:A:THR:HG22	1:161:A:THR:HB	7	0.3
(1,1479)	1:161:A:THR:HG23	1:161:A:THR:HB	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1479)	1:161:A:THR:HG22	1:161:A:THR:HB	9	0.3
(1,1479)	1:161:A:THR:HG21	1:161:A:THR:HB	15	0.3
(1,1479)	1:161:A:THR:HG23	1:161:A:THR:HB	19	0.3
(1,315)	1:227:A:ALA:HB1	1:227:A:ALA:HA	2	0.3
(1,264)	1:174:A:LEU:HD22	1:174:A:LEU:HG	3	0.3
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD12	14	0.29
(1,1482)	1:176:A:THR:HG22	1:176:A:THR:HB	1	0.29
(1,1479)	1:161:A:THR:HG22	1:161:A:THR:HB	2	0.29
(1,1479)	1:161:A:THR:HG23	1:161:A:THR:HB	4	0.29
(1,1479)	1:161:A:THR:HG21	1:161:A:THR:HB	6	0.29
(1,1479)	1:161:A:THR:HG21	1:161:A:THR:HB	16	0.29
(1,1479)	1:161:A:THR:HG23	1:161:A:THR:HB	18	0.29
(1,1479)	1:161:A:THR:HG23	1:161:A:THR:HB	20	0.29
(1,706)	2:577:B:LEU:HD11	1:168:A:TRP:HH2	10	0.29
(1,706)	2:577:B:LEU:HD13	1:168:A:TRP:HH2	14	0.29
(1,315)	1:227:A:ALA:HB3	1:227:A:ALA:HA	7	0.29
(1,315)	1:227:A:ALA:HB3	1:227:A:ALA:HA	9	0.29
(1,315)	1:227:A:ALA:HB2	1:227:A:ALA:HA	10	0.29
(1,315)	1:227:A:ALA:HB1	1:227:A:ALA:HA	18	0.29
(1,3576)	1:156:A:THR:H	1:155:A:ARG:HG2	6	0.28
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB2	18	0.28
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB3	20	0.28
(1,1482)	1:176:A:THR:HG22	1:176:A:THR:HB	3	0.28
(1,1482)	1:176:A:THR:HG22	1:176:A:THR:HB	6	0.28
(1,1482)	1:176:A:THR:HG23	1:176:A:THR:HB	10	0.28
(1,1482)	1:176:A:THR:HG22	1:176:A:THR:HB	15	0.28
(1,1482)	1:176:A:THR:HG22	1:176:A:THR:HB	20	0.28
(1,706)	2:577:B:LEU:HD11	1:168:A:TRP:HH2	5	0.28
(1,315)	1:227:A:ALA:HB1	1:227:A:ALA:HA	3	0.28
(1,315)	1:227:A:ALA:HB2	1:227:A:ALA:HA	4	0.28
(1,315)	1:227:A:ALA:HB1	1:227:A:ALA:HA	5	0.28
(1,315)	1:227:A:ALA:HB3	1:227:A:ALA:HA	8	0.28
(1,315)	1:227:A:ALA:HB2	1:227:A:ALA:HA	11	0.28
(1,315)	1:227:A:ALA:HB1	1:227:A:ALA:HA	14	0.28
(1,315)	1:227:A:ALA:HB3	1:227:A:ALA:HA	15	0.28
(1,315)	1:227:A:ALA:HB1	1:227:A:ALA:HA	17	0.28
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG22	11	0.28
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB2	7	0.27
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB2	14	0.27
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB1	7	0.27
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB2	8	0.27
(1,1482)	1:176:A:THR:HG21	1:176:A:THR:HB	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1482)	1:176:A:THR:HG21	1:176:A:THR:HB	4	0.27
(1,1482)	1:176:A:THR:HG23	1:176:A:THR:HB	5	0.27
(1,1482)	1:176:A:THR:HG21	1:176:A:THR:HB	7	0.27
(1,1482)	1:176:A:THR:HG21	1:176:A:THR:HB	8	0.27
(1,1482)	1:176:A:THR:HG21	1:176:A:THR:HB	9	0.27
(1,1482)	1:176:A:THR:HG21	1:176:A:THR:HB	11	0.27
(1,1482)	1:176:A:THR:HG21	1:176:A:THR:HB	12	0.27
(1,1482)	1:176:A:THR:HG23	1:176:A:THR:HB	13	0.27
(1,1482)	1:176:A:THR:HG23	1:176:A:THR:HB	16	0.27
(1,1482)	1:176:A:THR:HG23	1:176:A:THR:HB	17	0.27
(1,1482)	1:176:A:THR:HG21	1:176:A:THR:HB	19	0.27
(1,1479)	1:161:A:THR:HG22	1:161:A:THR:HB	11	0.27
(1,706)	2:577:B:LEU:HD11	1:168:A:TRP:HH2	13	0.27
(1,315)	1:227:A:ALA:HB2	1:227:A:ALA:HA	1	0.27
(1,315)	1:227:A:ALA:HB1	1:227:A:ALA:HA	6	0.27
(1,315)	1:227:A:ALA:HB1	1:227:A:ALA:HA	12	0.27
(1,315)	1:227:A:ALA:HB1	1:227:A:ALA:HA	13	0.27
(1,315)	1:227:A:ALA:HB3	1:227:A:ALA:HA	16	0.27
(1,315)	1:227:A:ALA:HB3	1:227:A:ALA:HA	20	0.27
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG22	10	0.27
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	20	0.26
(1,3407)	1:164:A:LYS:HD3	1:164:A:LYS:HA	11	0.26
(1,3137)	1:222:A:GLN:HG3	1:222:A:GLN:HA	2	0.26
(1,2948)	1:223:A:ASN:H	1:222:A:GLN:HB2	18	0.26
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB3	11	0.26
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB2	14	0.26
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB2	19	0.26
(1,1482)	1:176:A:THR:HG22	1:176:A:THR:HB	14	0.26
(1,1482)	1:176:A:THR:HG22	1:176:A:THR:HB	18	0.26
(1,706)	2:577:B:LEU:HD11	1:168:A:TRP:HH2	8	0.26
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG22	14	0.26
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG23	16	0.26
(1,12)	1:231:A:ILE:HA	1:231:A:ILE:HD12	10	0.26
(1,3747)	1:226:A:VAL:H	1:226:A:VAL:HG22	12	0.25
(1,3713)	1:205:A:LYS:H	1:205:A:LYS:HD2	4	0.25
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	2	0.25
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB3	13	0.25
(1,1489)	1:167:A:THR:HG23	1:167:A:THR:HB	11	0.25
(1,706)	2:577:B:LEU:HD13	1:168:A:TRP:HH2	6	0.25
(1,706)	2:577:B:LEU:HD11	1:168:A:TRP:HH2	20	0.25
(1,316)	1:142:A:ALA:HB2	1:142:A:ALA:HA	2	0.25
(1,316)	1:142:A:ALA:HB1	1:142:A:ALA:HA	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	1:142:A:ALA:HB2	1:142:A:ALA:HA	5	0.25
(1,316)	1:142:A:ALA:HB2	1:142:A:ALA:HA	15	0.25
(1,315)	1:227:A:ALA:HB3	1:227:A:ALA:HA	19	0.25
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG22	4	0.25
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG22	7	0.25
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG22	1	0.25
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG23	2	0.25
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG21	9	0.25
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG23	14	0.25
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD11	5	0.24
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD11	10	0.24
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	15	0.24
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE2	20	0.24
(1,2729)	1:203:A:GLN:HE21	1:204:A:THR:HG23	3	0.24
(1,1489)	1:167:A:THR:HG22	1:167:A:THR:HB	2	0.24
(1,1489)	1:167:A:THR:HG23	1:167:A:THR:HB	4	0.24
(1,1489)	1:167:A:THR:HG21	1:167:A:THR:HB	10	0.24
(1,1489)	1:167:A:THR:HG22	1:167:A:THR:HB	18	0.24
(1,706)	2:577:B:LEU:HD13	1:168:A:TRP:HH2	19	0.24
(1,316)	1:142:A:ALA:HB3	1:142:A:ALA:HA	7	0.24
(1,316)	1:142:A:ALA:HB1	1:142:A:ALA:HA	17	0.24
(1,316)	1:142:A:ALA:HB3	1:142:A:ALA:HA	19	0.24
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG21	2	0.24
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG23	9	0.24
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG23	10	0.24
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG21	18	0.24
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG23	3	0.24
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG23	8	0.24
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG21	11	0.24
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG22	12	0.24
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG21	13	0.24
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	4	0.23
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	12	0.23
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	18	0.23
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE2	11	0.23
(1,3406)	1:205:A:LYS:HD2	1:205:A:LYS:HE3	17	0.23
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE3	18	0.23
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB3	4	0.23
(1,1489)	1:167:A:THR:HG22	1:167:A:THR:HB	1	0.23
(1,1489)	1:167:A:THR:HG21	1:167:A:THR:HB	3	0.23
(1,1489)	1:167:A:THR:HG23	1:167:A:THR:HB	7	0.23
(1,1489)	1:167:A:THR:HG21	1:167:A:THR:HB	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1489)	1:167:A:THR:HG21	1:167:A:THR:HB	12	0.23
(1,1489)	1:167:A:THR:HG23	1:167:A:THR:HB	14	0.23
(1,1489)	1:167:A:THR:HG23	1:167:A:THR:HB	16	0.23
(1,316)	1:142:A:ALA:HB2	1:142:A:ALA:HA	3	0.23
(1,316)	1:142:A:ALA:HB1	1:142:A:ALA:HA	6	0.23
(1,316)	1:142:A:ALA:HB1	1:142:A:ALA:HA	8	0.23
(1,316)	1:142:A:ALA:HB1	1:142:A:ALA:HA	9	0.23
(1,316)	1:142:A:ALA:HB1	1:142:A:ALA:HA	10	0.23
(1,316)	1:142:A:ALA:HB3	1:142:A:ALA:HA	13	0.23
(1,316)	1:142:A:ALA:HB2	1:142:A:ALA:HA	14	0.23
(1,316)	1:142:A:ALA:HB1	1:142:A:ALA:HA	16	0.23
(1,316)	1:142:A:ALA:HB2	1:142:A:ALA:HA	18	0.23
(1,316)	1:142:A:ALA:HB3	1:142:A:ALA:HA	20	0.23
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD13	4	0.23
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD13	10	0.23
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD13	16	0.23
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG21	1	0.23
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG21	5	0.23
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG21	8	0.23
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG22	13	0.23
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG23	15	0.23
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG21	19	0.23
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG22	4	0.23
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG23	5	0.23
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG22	17	0.23
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD12	6	0.22
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD13	8	0.22
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	9	0.22
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	17	0.22
(1,3407)	1:164:A:LYS:HD3	1:164:A:LYS:HA	15	0.22
(1,3407)	1:164:A:LYS:HD3	1:164:A:LYS:HA	19	0.22
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE3	1	0.22
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE3	3	0.22
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE3	7	0.22
(1,3406)	1:205:A:LYS:HD2	1:205:A:LYS:HE3	8	0.22
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE2	9	0.22
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE2	10	0.22
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE3	16	0.22
(1,3406)	1:205:A:LYS:HD2	1:205:A:LYS:HE2	19	0.22
(1,3137)	1:222:A:GLN:HG2	1:222:A:GLN:HA	6	0.22
(1,3137)	1:222:A:GLN:HG3	1:222:A:GLN:HA	9	0.22
(1,2360)	1:178:A:ALA:H	1:178:A:ALA:HB1	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD23	12	0.22
(1,1489)	1:167:A:THR:HG22	1:167:A:THR:HB	5	0.22
(1,1489)	1:167:A:THR:HG22	1:167:A:THR:HB	8	0.22
(1,1489)	1:167:A:THR:HG23	1:167:A:THR:HB	13	0.22
(1,1489)	1:167:A:THR:HG21	1:167:A:THR:HB	15	0.22
(1,1489)	1:167:A:THR:HG23	1:167:A:THR:HB	17	0.22
(1,1489)	1:167:A:THR:HG22	1:167:A:THR:HB	19	0.22
(1,1489)	1:167:A:THR:HG21	1:167:A:THR:HB	20	0.22
(1,706)	2:577:B:LEU:HD13	1:168:A:TRP:HH2	1	0.22
(1,706)	2:577:B:LEU:HD11	1:168:A:TRP:HH2	12	0.22
(1,706)	2:577:B:LEU:HD12	1:168:A:TRP:HH2	15	0.22
(1,316)	1:142:A:ALA:HB1	1:142:A:ALA:HA	1	0.22
(1,316)	1:142:A:ALA:HB2	1:142:A:ALA:HA	12	0.22
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD11	3	0.22
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD12	7	0.22
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD11	13	0.22
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD12	18	0.22
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG23	6	0.22
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG23	20	0.22
(1,3748)	1:227:A:ALA:H	1:226:A:VAL:HG23	5	0.21
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD11	4	0.21
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD11	15	0.21
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	5	0.21
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB2	10	0.21
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	13	0.21
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE3	2	0.21
(1,3406)	1:205:A:LYS:HD2	1:205:A:LYS:HE2	5	0.21
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE2	12	0.21
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE2	14	0.21
(1,3137)	1:222:A:GLN:HG2	1:222:A:GLN:HA	14	0.21
(1,1489)	1:167:A:THR:HG21	1:167:A:THR:HB	6	0.21
(1,316)	1:142:A:ALA:HB2	1:142:A:ALA:HA	11	0.21
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD11	1	0.21
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD13	6	0.21
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD13	8	0.21
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD13	9	0.21
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD13	15	0.21
(1,155)	1:188:A:LYS:HA	1:215:A:LEU:HD12	5	0.21
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG23	12	0.21
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG22	16	0.21
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG21	7	0.21
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	6	0.2
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	16	0.2
(1,3406)	1:205:A:LYS:HD2	1:205:A:LYS:HE3	4	0.2
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE3	6	0.2
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD22	1	0.2
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD22	3	0.2
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD21	15	0.2
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD22	19	0.2
(1,943)	1:225:A:ILE:HD11	1:225:A:ILE:HG12	14	0.2
(1,706)	2:577:B:LEU:HD12	1:168:A:TRP:HH2	7	0.2
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD12	2	0.2
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD12	5	0.2
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD11	11	0.2
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD13	12	0.2
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD11	14	0.2
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD11	17	0.2
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD13	19	0.2
(1,259)	1:174:A:LEU:HB3	1:174:A:LEU:HD12	20	0.2
(1,222)	1:211:A:LYS:HD3	1:211:A:LYS:HE2	12	0.2
(1,222)	1:211:A:LYS:HD3	1:211:A:LYS:HE2	17	0.2
(1,222)	1:211:A:LYS:HD3	1:211:A:LYS:HE2	19	0.2
(1,143)	1:213:A:LYS:HA	1:213:A:LYS:HD2	13	0.2
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG23	3	0.2
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG21	19	0.2
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG22	20	0.2
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD11	5	0.19
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD13	6	0.19
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE2	13	0.19
(1,3406)	1:205:A:LYS:HD3	1:205:A:LYS:HE2	15	0.19
(1,3145)	1:188:A:LYS:HB2	1:188:A:LYS:HE3	8	0.19
(1,3145)	1:188:A:LYS:HB2	1:188:A:LYS:HE3	13	0.19
(1,2983)	1:231:A:ILE:H	1:231:A:ILE:HB	10	0.19
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD21	14	0.19
(1,943)	1:225:A:ILE:HD13	1:225:A:ILE:HG12	1	0.19
(1,943)	1:225:A:ILE:HD12	1:225:A:ILE:HG12	4	0.19
(1,943)	1:225:A:ILE:HD12	1:225:A:ILE:HG12	5	0.19
(1,943)	1:225:A:ILE:HD12	1:225:A:ILE:HG12	6	0.19
(1,943)	1:225:A:ILE:HD11	1:225:A:ILE:HG12	7	0.19
(1,943)	1:225:A:ILE:HD13	1:225:A:ILE:HG12	9	0.19
(1,943)	1:225:A:ILE:HD12	1:225:A:ILE:HG12	11	0.19
(1,943)	1:225:A:ILE:HD11	1:225:A:ILE:HG12	12	0.19
(1,943)	1:225:A:ILE:HD13	1:225:A:ILE:HG12	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:225:A:ILE:HD13	1:225:A:ILE:HG12	16	0.19
(1,943)	1:225:A:ILE:HD13	1:225:A:ILE:HG12	18	0.19
(1,943)	1:225:A:ILE:HD11	1:225:A:ILE:HG12	19	0.19
(1,113)	1:158:A:TYR:HB2	1:167:A:THR:HG22	17	0.19
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG22	15	0.19
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD12	12	0.18
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	19	0.18
(1,3313)	1:215:A:LEU:HD22	1:189:A:GLU:HG2	16	0.18
(1,3281)	1:182:A:LEU:HD11	1:188:A:LYS:HA	19	0.18
(1,3145)	1:188:A:LYS:HB2	1:188:A:LYS:HE3	11	0.18
(1,3137)	1:222:A:GLN:HG3	1:222:A:GLN:HA	3	0.18
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	1	0.18
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	10	0.18
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	14	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	1	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	2	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	3	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	5	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	6	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	7	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	8	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	10	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	11	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	12	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	13	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	15	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	16	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	17	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	18	0.18
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	20	0.18
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD21	11	0.18
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD21	16	0.18
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD21	20	0.18
(1,1488)	1:167:A:THR:HG22	1:171:A:PRO:HG3	18	0.18
(1,943)	1:225:A:ILE:HD13	1:225:A:ILE:HG12	10	0.18
(1,943)	1:225:A:ILE:HD12	1:225:A:ILE:HG12	15	0.18
(1,943)	1:225:A:ILE:HD13	1:225:A:ILE:HG12	17	0.18
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD11	13	0.17
(1,3318)	1:150:A:LYS:HE2	1:148:A:GLU:HG2	4	0.17
(1,3145)	1:188:A:LYS:HB2	1:188:A:LYS:HE3	15	0.17
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	5	0.17
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	11	0.17
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	12	0.17
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	16	0.17
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	4	0.17
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	9	0.17
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	14	0.17
(1,2215)	1:165:A:GLN:HE22	1:165:A:GLN:HE21	19	0.17
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD23	2	0.17
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD23	9	0.17
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD21	17	0.17
(1,1568)	1:219:A:GLU:HG2	1:215:A:LEU:HD23	19	0.17
(1,943)	1:225:A:ILE:HD12	1:225:A:ILE:HG12	20	0.17
(1,143)	1:213:A:LYS:HA	1:213:A:LYS:HD2	2	0.17
(1,143)	1:213:A:LYS:HA	1:213:A:LYS:HD2	8	0.17
(1,143)	1:213:A:LYS:HA	1:213:A:LYS:HD2	11	0.17
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD12	9	0.16
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD13	17	0.16
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD12	19	0.16
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD12	20	0.16
(1,3576)	1:156:A:THR:H	1:155:A:ARG:HG2	16	0.16
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD11	4	0.16
(1,3387)	1:211:A:LYS:HE3	1:216:A:GLU:HB2	15	0.16
(1,3145)	1:188:A:LYS:HB2	1:188:A:LYS:HE3	1	0.16
(1,2968)	1:225:A:ILE:H	1:225:A:ILE:HG23	4	0.16
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	9	0.16
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	13	0.16
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	17	0.16
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	19	0.16
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	20	0.16
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD23	8	0.16
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD23	18	0.16
(1,1488)	1:167:A:THR:HG21	1:171:A:PRO:HG3	10	0.16
(1,1488)	1:167:A:THR:HG23	1:171:A:PRO:HG3	11	0.16
(1,943)	1:225:A:ILE:HD13	1:225:A:ILE:HG12	3	0.16
(1,943)	1:225:A:ILE:HD13	1:225:A:ILE:HG12	8	0.16
(1,143)	1:213:A:LYS:HA	1:213:A:LYS:HD2	3	0.16
(1,143)	1:213:A:LYS:HA	1:213:A:LYS:HD2	4	0.16
(1,143)	1:213:A:LYS:HA	1:213:A:LYS:HD2	16	0.16
(1,3747)	1:226:A:VAL:H	1:226:A:VAL:HG23	5	0.15
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD13	7	0.15
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD12	13	0.15
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD11	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD11	20	0.15
(1,3483)	2:572:B:SER:HA	2:572:B:SER:HB3	1	0.15
(1,3407)	1:164:A:LYS:HD2	1:164:A:LYS:HA	10	0.15
(1,3281)	1:182:A:LEU:HD11	1:188:A:LYS:HA	8	0.15
(1,3145)	1:188:A:LYS:HB2	1:188:A:LYS:HE3	4	0.15
(1,2451)	1:182:A:LEU:H	1:181:A:LEU:HD13	4	0.15
(1,2451)	1:182:A:LEU:H	1:181:A:LEU:HD12	6	0.15
(1,2451)	1:182:A:LEU:H	1:181:A:LEU:HD12	7	0.15
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	3	0.15
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	4	0.15
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	6	0.15
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	7	0.15
(1,1488)	1:167:A:THR:HG23	1:171:A:PRO:HG3	4	0.15
(1,1488)	1:167:A:THR:HG23	1:171:A:PRO:HG3	7	0.15
(1,1488)	1:167:A:THR:HG22	1:171:A:PRO:HG3	8	0.15
(1,1488)	1:167:A:THR:HG21	1:171:A:PRO:HG3	20	0.15
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	1	0.15
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	3	0.15
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	7	0.15
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	9	0.15
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	11	0.15
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	13	0.15
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	14	0.15
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	15	0.15
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	16	0.15
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	18	0.15
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	20	0.15
(1,149)	1:218:A:LEU:HA	1:218:A:LEU:HG	4	0.15
(1,149)	1:218:A:LEU:HA	1:218:A:LEU:HG	14	0.15
(1,149)	1:218:A:LEU:HA	1:218:A:LEU:HG	19	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	1	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	2	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	3	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	4	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	5	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	6	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	7	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	8	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	9	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	10	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	11	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	13	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	14	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	15	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	16	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	17	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	18	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	19	0.15
(1,19)	1:231:A:ILE:HG13	1:231:A:ILE:HG12	20	0.15
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG23	6	0.15
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD12	1	0.14
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD12	16	0.14
(1,2968)	1:225:A:ILE:H	1:225:A:ILE:HG22	16	0.14
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	2	0.14
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	15	0.14
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD21	6	0.14
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD22	10	0.14
(1,1488)	1:167:A:THR:HG23	1:171:A:PRO:HG3	14	0.14
(1,942)	1:225:A:ILE:HD13	1:225:A:ILE:HG13	10	0.14
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	2	0.14
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	4	0.14
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	5	0.14
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	6	0.14
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	8	0.14
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	10	0.14
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	12	0.14
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	17	0.14
(1,250)	1:208:A:ARG:HB2	1:208:A:ARG:HB3	19	0.14
(1,149)	1:218:A:LEU:HA	1:218:A:LEU:HG	6	0.14
(1,149)	1:218:A:LEU:HA	1:218:A:LEU:HG	8	0.14
(1,143)	1:213:A:LYS:HA	1:213:A:LYS:HD2	9	0.14
(1,143)	1:213:A:LYS:HA	1:213:A:LYS:HD2	10	0.14
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD11	2	0.13
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD12	7	0.13
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD11	8	0.13
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD11	9	0.13
(1,3407)	1:164:A:LYS:HD2	1:164:A:LYS:HA	14	0.13
(1,3407)	1:164:A:LYS:HD3	1:164:A:LYS:HA	20	0.13
(1,3130)	1:197:A:PRO:HA	1:191:A:LYS:HD2	15	0.13
(1,2968)	1:225:A:ILE:H	1:225:A:ILE:HG21	19	0.13
(1,2292)	1:172:A:ASP:H	1:172:A:ASP:HA	18	0.13
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD21	5	0.13
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD21	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD23	13	0.13
(1,943)	1:225:A:ILE:HD13	1:225:A:ILE:HG12	2	0.13
(1,942)	1:225:A:ILE:HD12	1:225:A:ILE:HG13	5	0.13
(1,942)	1:225:A:ILE:HD12	1:225:A:ILE:HG13	6	0.13
(1,942)	1:225:A:ILE:HD11	1:225:A:ILE:HG13	7	0.13
(1,942)	1:225:A:ILE:HD11	1:225:A:ILE:HG13	12	0.13
(1,942)	1:225:A:ILE:HD13	1:225:A:ILE:HG13	14	0.13
(1,942)	1:225:A:ILE:HD11	1:225:A:ILE:HG13	15	0.13
(1,942)	1:225:A:ILE:HD13	1:225:A:ILE:HG13	17	0.13
(1,942)	1:225:A:ILE:HD13	1:225:A:ILE:HG13	18	0.13
(1,942)	1:225:A:ILE:HD11	1:225:A:ILE:HG13	20	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	1	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	2	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	3	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	4	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	5	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	6	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	7	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	8	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	9	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	10	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	11	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	13	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	14	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	15	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	16	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	18	0.13
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	20	0.13
(1,924)	1:211:A:LYS:HB3	1:211:A:LYS:HE3	19	0.13
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG21	7	0.13
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG22	16	0.13
(1,149)	1:218:A:LEU:HA	1:218:A:LEU:HG	1	0.13
(1,149)	1:218:A:LEU:HA	1:218:A:LEU:HG	5	0.13
(1,149)	1:218:A:LEU:HA	1:218:A:LEU:HG	13	0.13
(1,149)	1:218:A:LEU:HA	1:218:A:LEU:HG	15	0.13
(1,149)	1:218:A:LEU:HA	1:218:A:LEU:HG	17	0.13
(1,149)	1:218:A:LEU:HA	1:218:A:LEU:HG	20	0.13
(1,143)	1:213:A:LYS:HA	1:213:A:LYS:HD2	15	0.13
(1,143)	1:213:A:LYS:HA	1:213:A:LYS:HD2	20	0.13
(1,28)	1:230:A:LEU:HD22	1:230:A:LEU:HG	6	0.13
(1,28)	1:230:A:LEU:HD22	1:230:A:LEU:HG	12	0.13
(1,28)	1:230:A:LEU:HD22	1:230:A:LEU:HG	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:231:A:ILE:HB	1:231:A:ILE:HG22	18	0.13
(1,3713)	1:205:A:LYS:H	1:205:A:LYS:HD2	8	0.12
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD11	12	0.12
(1,3387)	1:211:A:LYS:HE3	1:216:A:GLU:HB2	18	0.12
(1,3145)	1:188:A:LYS:HB2	1:188:A:LYS:HE3	19	0.12
(1,2541)	1:189:A:GLU:H	1:215:A:LEU:HD12	5	0.12
(1,2451)	1:182:A:LEU:H	1:181:A:LEU:HD12	5	0.12
(1,1720)	1:151:A:SER:HA	2:577:B:LEU:HD21	4	0.12
(1,1488)	1:167:A:THR:HG23	1:171:A:PRO:HG3	13	0.12
(1,1459)	1:156:A:THR:HG23	1:156:A:THR:HA	1	0.12
(1,1445)	1:174:A:LEU:HD12	1:173:A:ASP:HB2	15	0.12
(1,942)	1:225:A:ILE:HD12	1:225:A:ILE:HG13	3	0.12
(1,942)	1:225:A:ILE:HD12	1:225:A:ILE:HG13	4	0.12
(1,942)	1:225:A:ILE:HD12	1:225:A:ILE:HG13	8	0.12
(1,942)	1:225:A:ILE:HD12	1:225:A:ILE:HG13	13	0.12
(1,942)	1:225:A:ILE:HD13	1:225:A:ILE:HG13	19	0.12
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	12	0.12
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	17	0.12
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG22	6	0.12
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG23	13	0.12
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG23	19	0.12
(1,149)	1:218:A:LEU:HA	1:218:A:LEU:HG	3	0.12
(1,149)	1:218:A:LEU:HA	1:218:A:LEU:HG	12	0.12
(1,143)	1:213:A:LYS:HA	1:213:A:LYS:HD2	1	0.12
(1,143)	1:213:A:LYS:HA	1:213:A:LYS:HD2	5	0.12
(1,28)	1:230:A:LEU:HD23	1:230:A:LEU:HG	1	0.12
(1,28)	1:230:A:LEU:HD23	1:230:A:LEU:HG	3	0.12
(1,28)	1:230:A:LEU:HD23	1:230:A:LEU:HG	7	0.12
(1,28)	1:230:A:LEU:HD22	1:230:A:LEU:HG	8	0.12
(1,28)	1:230:A:LEU:HD23	1:230:A:LEU:HG	10	0.12
(1,28)	1:230:A:LEU:HD23	1:230:A:LEU:HG	14	0.12
(1,28)	1:230:A:LEU:HD21	1:230:A:LEU:HG	19	0.12
(1,28)	1:230:A:LEU:HD23	1:230:A:LEU:HG	20	0.12
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD11	3	0.11
(1,3635)	1:182:A:LEU:H	1:182:A:LEU:HD13	10	0.11
(1,3407)	1:164:A:LYS:HD2	1:164:A:LYS:HA	4	0.11
(1,3407)	1:164:A:LYS:HD2	1:164:A:LYS:HA	9	0.11
(1,3290)	1:233:A:LYS:HG3	1:233:A:LYS:HE3	4	0.11
(1,2451)	1:182:A:LEU:H	1:181:A:LEU:HD13	3	0.11
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	1	0.11
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	2	0.11
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	4	0.11
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	7	0.11
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	9	0.11
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	11	0.11
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	14	0.11
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	15	0.11
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	20	0.11
(1,1581)	2:571:B:MET:HG3	2:571:B:MET:HA	18	0.11
(1,1488)	1:167:A:THR:HG22	1:171:A:PRO:HG3	5	0.11
(1,1488)	1:167:A:THR:HG23	1:171:A:PRO:HG3	16	0.11
(1,1488)	1:167:A:THR:HG22	1:171:A:PRO:HG3	19	0.11
(1,942)	1:225:A:ILE:HD12	1:225:A:ILE:HG13	1	0.11
(1,942)	1:225:A:ILE:HD12	1:225:A:ILE:HG13	9	0.11
(1,942)	1:225:A:ILE:HD11	1:225:A:ILE:HG13	11	0.11
(1,942)	1:225:A:ILE:HD13	1:225:A:ILE:HG13	16	0.11
(1,932)	1:211:A:LYS:HE2	1:211:A:LYS:HE3	19	0.11
(1,767)	1:144:A:SER:HB2	1:144:A:SER:HA	14	0.11
(1,215)	1:155:A:ARG:HB3	1:155:A:ARG:HD3	11	0.11
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG23	3	0.11
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG21	4	0.11
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG23	14	0.11
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG22	17	0.11
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG21	18	0.11
(1,28)	1:230:A:LEU:HD23	1:230:A:LEU:HG	4	0.11
(1,28)	1:230:A:LEU:HD23	1:230:A:LEU:HG	13	0.11
(1,28)	1:230:A:LEU:HD22	1:230:A:LEU:HG	15	0.11
(1,28)	1:230:A:LEU:HD21	1:230:A:LEU:HG	16	0.11
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD12	2	0.1
(1,3502)	1:151:A:SER:HB3	2:577:B:LEU:HD12	3	0.1
(1,3290)	1:233:A:LYS:HG2	1:233:A:LYS:HE3	9	0.1
(1,3290)	1:233:A:LYS:HG3	1:233:A:LYS:HE3	11	0.1
(1,2981)	1:231:A:ILE:H	1:230:A:LEU:HA	18	0.1
(1,2948)	1:223:A:ASN:H	1:222:A:GLN:HB2	20	0.1
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	5	0.1
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	6	0.1
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	8	0.1
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	10	0.1
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	12	0.1
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	13	0.1
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	16	0.1
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	17	0.1
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2411)	1:180:A:GLN:HE22	1:180:A:GLN:HE21	19	0.1
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG21	2	0.1
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG23	11	0.1
(1,162)	1:147:A:THR:HA	1:147:A:THR:HG23	12	0.1
(1,28)	1:230:A:LEU:HD22	1:230:A:LEU:HG	5	0.1
(1,28)	1:230:A:LEU:HD22	1:230:A:LEU:HG	9	0.1

10 Dihedral-angle violation analysis

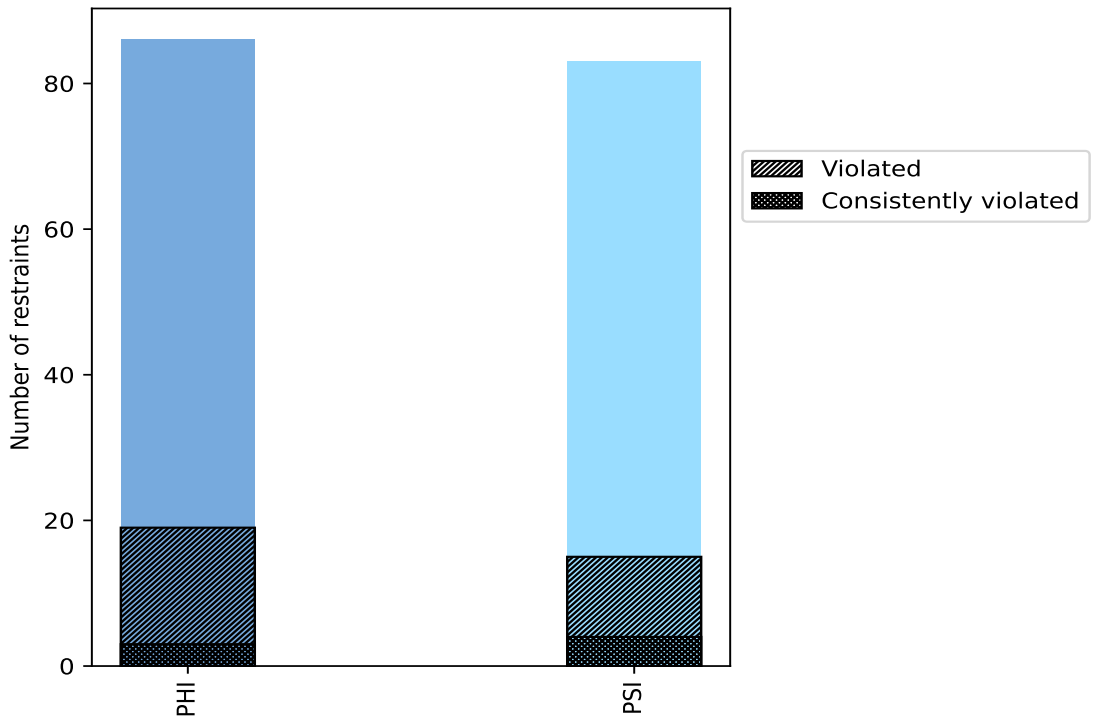
10.1 Summary of dihedral-angle violations

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	86	50.9	19	22.1	11.2	3	3.5	1.8
PSI	83	49.1	15	18.1	8.9	4	4.8	2.4
Total	169	100.0	34	20.1	20.1	7	4.1	4.1

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations



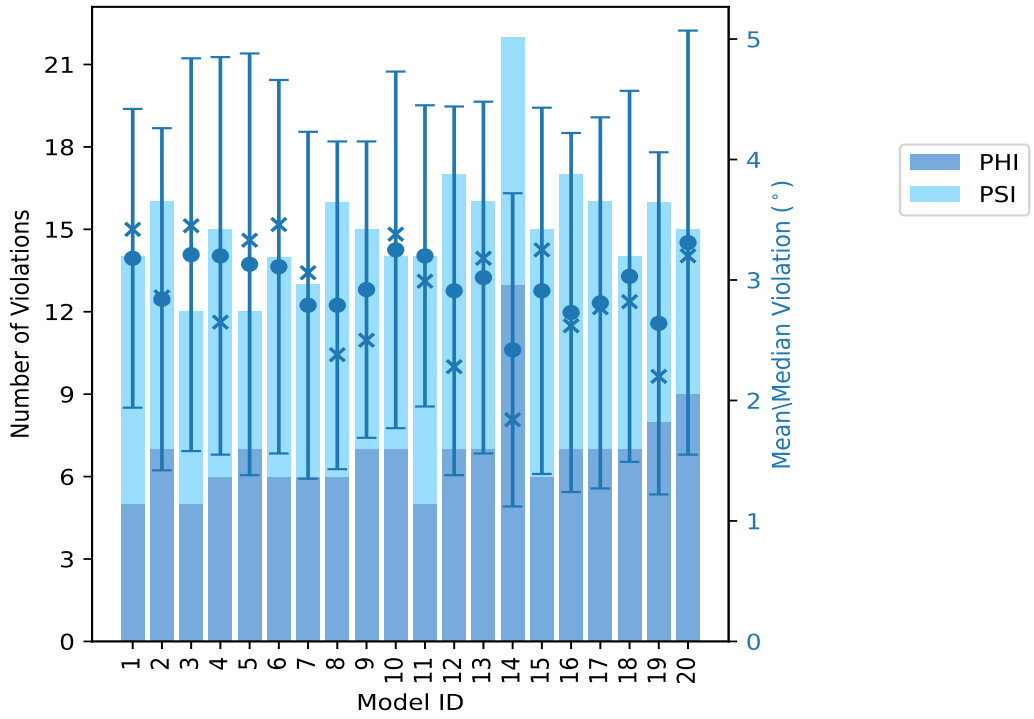
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	5	9	14	3.18	5.88	1.24	3.42
2	7	9	16	2.84	6.03	1.42	2.86
3	5	7	12	3.21	5.31	1.63	3.45
4	6	9	15	3.2	6.51	1.65	2.65
5	7	5	12	3.13	5.3	1.75	3.33
6	6	8	14	3.11	5.32	1.55	3.46
7	6	7	13	2.79	5.45	1.44	3.06
8	6	10	16	2.79	5.56	1.36	2.38
9	7	8	15	2.92	5.2	1.23	2.5
10	7	7	14	3.25	5.85	1.48	3.38
11	5	9	14	3.2	5.73	1.25	2.99
12	7	10	17	2.91	5.75	1.53	2.28
13	7	9	16	3.02	5.96	1.46	3.18
14	13	9	22	2.42	5.3	1.3	1.84
15	6	9	15	2.91	5.92	1.52	3.25
16	7	10	17	2.73	5.52	1.49	2.62
17	7	9	16	2.81	6.0	1.54	2.77
18	7	7	14	3.03	5.55	1.54	2.82
19	8	8	16	2.64	5.74	1.42	2.2
20	9	6	15	3.31	8.04	1.76	3.2

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
4	3	7	1	5.0
4	0	4	2	10.0
0	1	1	3	15.0
3	0	3	4	20.0
0	0	0	5	25.0
1	2	3	6	30.0
0	0	0	7	35.0
2	0	2	8	40.0
0	0	0	9	45.0
0	2	2	10	50.0
0	1	1	11	55.0

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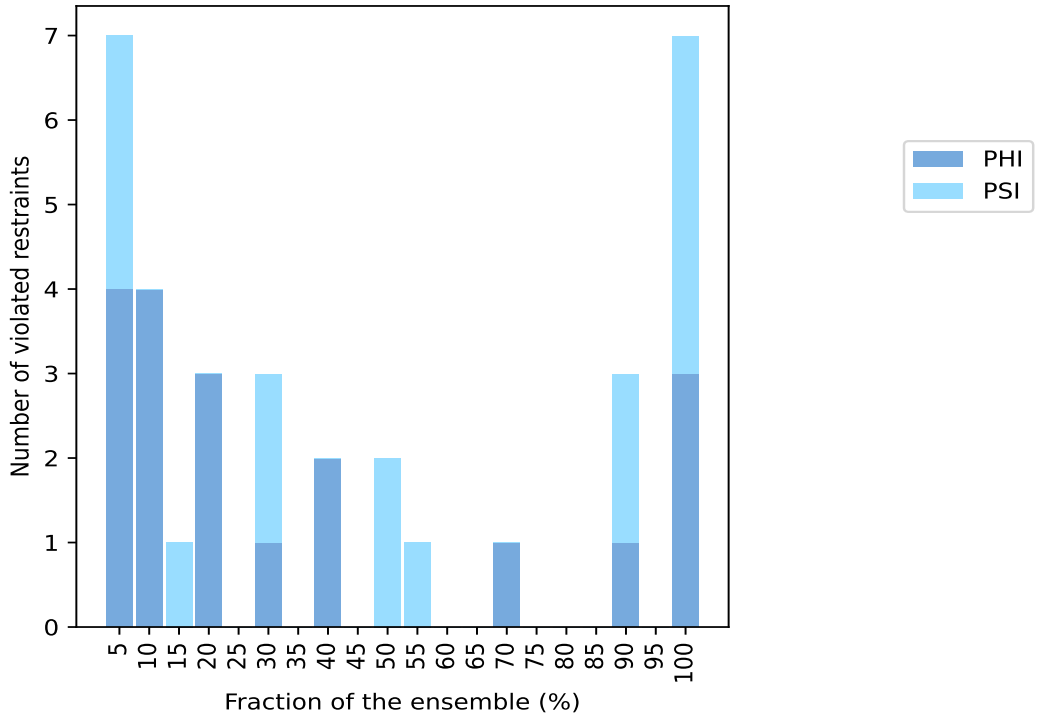
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
1	0	1	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
1	2	3	18	90.0
0	0	0	19	95.0
3	4	7	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble

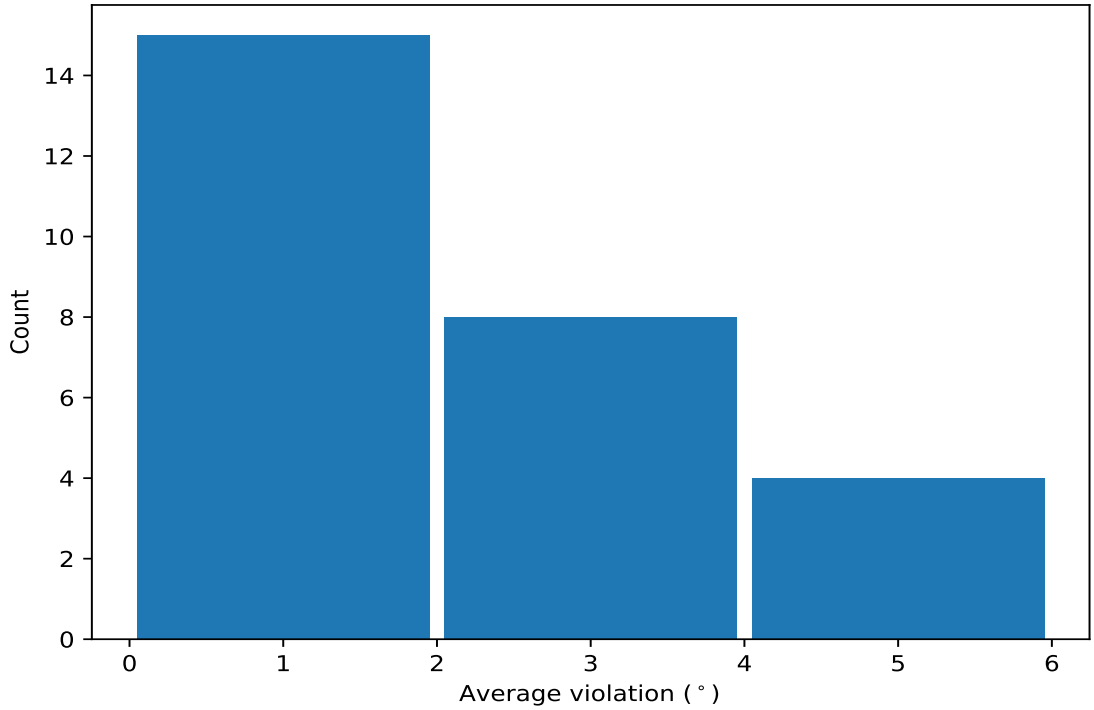


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle restraints

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	20	5.62	0.27	5.64
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	20	4.49	0.59	4.45
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	20	4.32	0.52	4.29
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	20	4.14	0.71	3.94
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	20	3.68	0.41	3.66
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	20	3.38	0.73	3.58
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	20	3.13	0.85	3.15
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	18	3.22	1.28	2.94
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	18	2.24	0.42	2.3
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	18	2.24	0.87	2.09
(1,26)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	14	1.26	0.21	1.3
(1,3)	1:147:A:THR:N	1:147:A:THR:CA	1:147:A:THR:C	1:148:A:GLU:N	11	1.22	0.2	1.18
(1,159)	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	2:587:B:PRO:N	10	3.51	2.08	2.8
(1,157)	2:582:B:PRO:N	2:582:B:PRO:CA	2:582:B:PRO:C	2:583:B:PRO:N	10	1.96	0.52	1.84
(1,160)	2:585:B:PRO:C	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	8	1.73	0.72	1.39
(1,42)	1:166:A:SER:C	1:167:A:THR:N	1:167:A:THR:CA	1:167:A:THR:C	8	1.23	0.18	1.23
(1,167)	2:590:B:PRO:N	2:590:B:PRO:CA	2:590:B:PRO:C	2:591:B:SER:N	6	1.47	0.42	1.4
(1,110)	1:201:A:ASN:C	1:202:A:SER:N	1:202:A:SER:CA	1:202:A:SER:C	6	1.23	0.15	1.23
(1,25)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:ASN:N	6	1.16	0.16	1.12
(1,69)	1:180:A:GLN:C	1:181:A:LEU:N	1:181:A:LEU:CA	1:181:A:LEU:C	4	1.47	0.46	1.42

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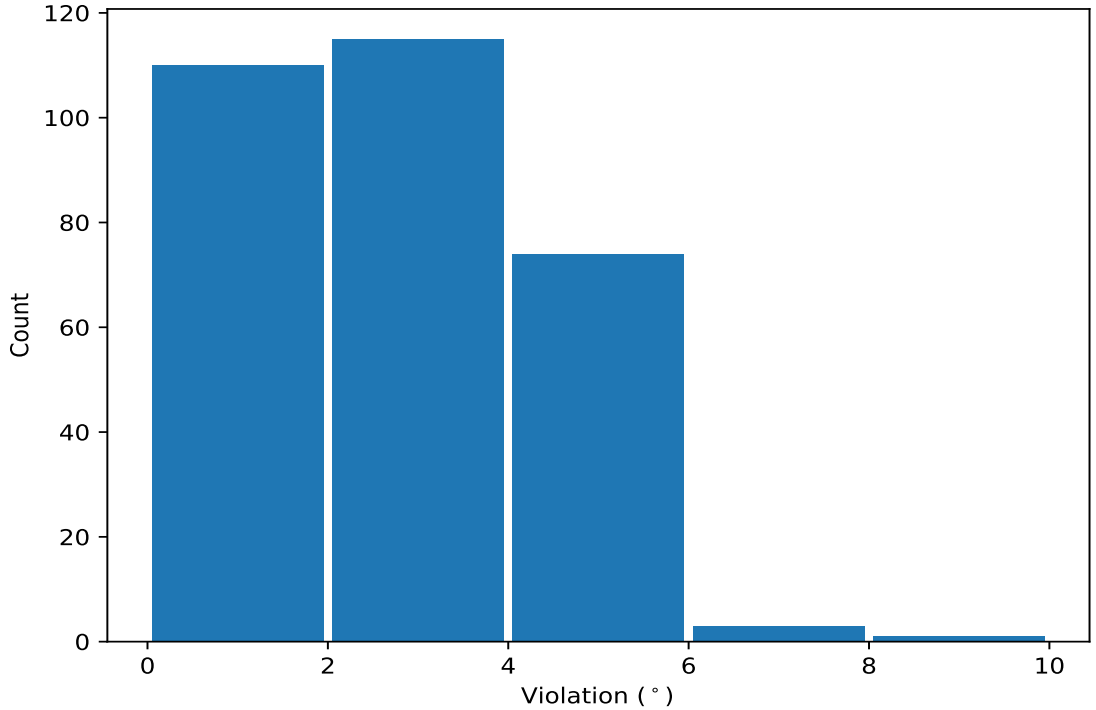
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,92)	1:192:A:SER:C	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	4	1.42	0.4	1.25
(1,128)	1:211:A:LYS:C	1:212:A:PRO:N	1:212:A:PRO:CA	1:212:A:PRO:C	4	1.25	0.19	1.26
(1,29)	1:161:A:THR:N	1:161:A:THR:CA	1:161:A:THR:C	1:162:A:GLU:N	3	1.36	0.25	1.29
(1,162)	2:586:B:PRO:C	2:587:B:PRO:N	2:587:B:PRO:CA	2:587:B:PRO:C	2	2.59	0.61	2.59
(1,158)	2:581:B:ALA:C	2:582:B:PRO:N	2:582:B:PRO:CA	2:582:B:PRO:C	2	1.98	0.68	1.98
(1,142)	1:218:A:LEU:C	1:219:A:GLU:N	1:219:A:GLU:CA	1:219:A:GLU:C	2	1.65	0.23	1.65
(1,138)	1:216:A:GLU:C	1:217:A:ASP:N	1:217:A:ASP:CA	1:217:A:ASP:C	2	1.5	0.4	1.5

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,159)	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	2:587:B:PRO:N	20	8.04

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,159)	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	2:587:B:PRO:N	4	6.51
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	2	6.03
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	17	6.0
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	13	5.96
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	15	5.92
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	1	5.88
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	10	5.85
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	20	5.77
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	12	5.75
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	4	5.75
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	19	5.74
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	11	5.73
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	8	5.56
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	18	5.55
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	16	5.52
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	19	5.48
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	7	5.45
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	12	5.45
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	6	5.32
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	3	5.31
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	6	5.3
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	5	5.3
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	14	5.3
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	3	5.3
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	17	5.28
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	15	5.26
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	18	5.25
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	14	5.24
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	5	5.22
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	10	5.21
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	9	5.2
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	18	5.19
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	3	5.16
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	5	5.09
(1,106)	1:199:A:TYR:C	1:200:A:TYR:N	1:200:A:TYR:CA	1:200:A:TYR:C	9	5.04
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	11	5.04
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	16	4.98
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	5	4.95
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	4	4.9
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	7	4.89
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	10	4.87
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	11	4.87
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	8	4.73
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	12	4.73
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	13	4.68
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	6	4.67
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	10	4.63
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	4	4.57
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	6	4.54
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	18	4.49
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	3	4.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	2	4.46
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	12	4.43
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	15	4.42
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	9	4.41
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	9	4.35
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	5	4.34
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	20	4.33
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	3	4.3
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	1	4.28
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	2	4.28
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	2	4.27
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	4	4.25
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	8	4.24
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	16	4.21
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	13	4.21
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	16	4.19
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	17	4.18
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	10	4.11
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	13	4.09
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	12	4.09
(1,159)	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	2:587:B:PRO:N	14	4.06
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	6	4.04
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	4	4.03
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	14	4.03
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	13	4.02
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	1	4.0
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	13	3.98
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	13	3.95
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	20	3.94
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	7	3.93
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	13	3.93
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	1	3.93
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	7	3.89
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	8	3.87
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	17	3.86
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	19	3.86
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	17	3.84
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	16	3.84
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	11	3.81
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	12	3.8
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	8	3.8
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	16	3.77
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	6	3.76
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	3	3.76
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	1	3.75
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	2	3.74
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	18	3.74
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	15	3.73
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	8	3.7
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	19	3.7
(1,159)	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	2:587:B:PRO:N	16	3.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	1	3.68
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	6	3.67
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	20	3.67
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	1	3.65
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	15	3.64
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	11	3.62
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	7	3.61
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	10	3.58
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	17	3.55
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	5	3.54
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	12	3.54
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	15	3.52
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	14	3.5
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	20	3.49
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	14	3.48
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	8	3.46
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	15	3.45
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	10	3.44
(1,17)	1:155:A:ARG:N	1:155:A:ARG:CA	1:155:A:ARG:C	1:156:A:THR:N	17	3.41
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	12	3.37
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	2	3.35
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	19	3.34
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	18	3.32
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	10	3.31
(1,96)	1:194:A:SER:C	1:195:A:GLY:N	1:195:A:GLY:CA	1:195:A:GLY:C	19	3.28
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	15	3.25
(1,160)	2:585:B:PRO:C	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	20	3.24
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	6	3.24
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	2	3.24
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	17	3.24
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	2	3.21
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	16	3.21
(1,162)	2:586:B:PRO:C	2:587:B:PRO:N	2:587:B:PRO:CA	2:587:B:PRO:C	20	3.2
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	1	3.2
(1,159)	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	2:587:B:PRO:N	9	3.17
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	18	3.16
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	4	3.16
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	3	3.14
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	11	3.14
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	5	3.12
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	14	3.11
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	1	3.09
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	7	3.09
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	7	3.06
(1,157)	2:582:B:PRO:N	2:582:B:PRO:CA	2:582:B:PRO:C	2:583:B:PRO:N	11	3.0
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	20	3.0
(1,11)	1:152:A:PRO:N	1:152:A:PRO:CA	1:152:A:PRO:C	1:153:A:ASP:N	9	2.98
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	11	2.97
(1,91)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:SER:N	9	2.91
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	20	2.9
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	8	2.79

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	20	2.77
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	14	2.72
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	15	2.71
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	1	2.69
(1,160)	2:585:B:PRO:C	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	4	2.65
(1,158)	2:581:B:ALA:C	2:582:B:PRO:N	2:582:B:PRO:CA	2:582:B:PRO:C	11	2.65
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	16	2.62
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	6	2.61
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	4	2.52
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	2	2.51
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	9	2.5
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	14	2.49
(1,157)	2:582:B:PRO:N	2:582:B:PRO:CA	2:582:B:PRO:C	2:583:B:PRO:N	18	2.47
(1,159)	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	2:587:B:PRO:N	11	2.43
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	13	2.42
(1,157)	2:582:B:PRO:N	2:582:B:PRO:CA	2:582:B:PRO:C	2:583:B:PRO:N	1	2.35
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	9	2.35
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	11	2.31
(1,157)	2:582:B:PRO:N	2:582:B:PRO:CA	2:582:B:PRO:C	2:583:B:PRO:N	13	2.3
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	17	2.3
(1,167)	2:590:B:PRO:N	2:590:B:PRO:CA	2:590:B:PRO:C	2:591:B:SER:N	12	2.28
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	9	2.26
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	18	2.25
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	19	2.25
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	19	2.24
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	10	2.24
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	4	2.2
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	19	2.17
(1,159)	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	2:587:B:PRO:N	10	2.17
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	19	2.16
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	11	2.12
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	13	2.1
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	4	2.09
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	11	2.09
(1,92)	1:192:A:SER:C	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	9	2.09
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	12	2.07
(1,69)	1:180:A:GLN:C	1:181:A:LEU:N	1:181:A:LEU:CA	1:181:A:LEU:C	9	2.04
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	6	2.04
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	17	2.02
(1,162)	2:586:B:PRO:C	2:587:B:PRO:N	2:587:B:PRO:CA	2:587:B:PRO:C	10	1.98
(1,159)	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	2:587:B:PRO:N	8	1.98
(1,169)	2:590:B:PRO:C	2:591:B:SER:N	2:591:B:SER:CA	2:591:B:SER:C	14	1.95
(1,159)	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	2:587:B:PRO:N	12	1.95
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	2	1.94
(1,157)	2:582:B:PRO:N	2:582:B:PRO:CA	2:582:B:PRO:C	2:583:B:PRO:N	2	1.91
(1,138)	1:216:A:GLU:C	1:217:A:ASP:N	1:217:A:ASP:CA	1:217:A:ASP:C	7	1.9
(1,142)	1:218:A:LEU:C	1:219:A:GLU:N	1:219:A:GLU:CA	1:219:A:GLU:C	13	1.88
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	14	1.88
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	10	1.86
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	8	1.84
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	8	1.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,69)	1:180:A:GLN:C	1:181:A:LEU:N	1:181:A:LEU:CA	1:181:A:LEU:C	14	1.8
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	16	1.8
(1,157)	2:582:B:PRO:N	2:582:B:PRO:CA	2:582:B:PRO:C	2:583:B:PRO:N	14	1.76
(1,89)	1:192:A:SER:N	1:192:A:SER:CA	1:192:A:SER:C	1:193:A:ASP:N	9	1.75
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	15	1.74
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	3	1.72
(1,26)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	13	1.72
(1,29)	1:161:A:THR:N	1:161:A:THR:CA	1:161:A:THR:C	1:162:A:GLU:N	16	1.7
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	4	1.69
(1,32)	1:161:A:THR:C	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	12	1.68
(1,167)	2:590:B:PRO:N	2:590:B:PRO:CA	2:590:B:PRO:C	2:591:B:SER:N	14	1.67
(1,163)	2:588:B:PRO:N	2:588:B:PRO:CA	2:588:B:PRO:C	2:589:B:PRO:N	7	1.67
(1,3)	1:147:A:THR:N	1:147:A:THR:CA	1:147:A:THR:C	1:148:A:GLU:N	2	1.63
(1,153)	2:579:B:PRO:N	2:579:B:PRO:CA	2:579:B:PRO:C	2:580:B:GLY:N	8	1.61
(1,3)	1:147:A:THR:N	1:147:A:THR:CA	1:147:A:THR:C	1:148:A:GLU:N	3	1.59
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	18	1.58
(1,65)	1:178:A:ALA:C	1:179:A:GLU:N	1:179:A:GLU:CA	1:179:A:GLU:C	2	1.57
(1,42)	1:166:A:SER:C	1:167:A:THR:N	1:167:A:THR:CA	1:167:A:THR:C	15	1.57
(1,157)	2:582:B:PRO:N	2:582:B:PRO:CA	2:582:B:PRO:C	2:583:B:PRO:N	17	1.51
(1,83)	1:189:A:GLU:N	1:189:A:GLU:CA	1:189:A:GLU:C	1:190:A:TYR:N	4	1.51
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	20	1.5
(1,157)	2:582:B:PRO:N	2:582:B:PRO:CA	2:582:B:PRO:C	2:583:B:PRO:N	8	1.49
(1,110)	1:201:A:ASN:C	1:202:A:SER:N	1:202:A:SER:CA	1:202:A:SER:C	19	1.49
(1,26)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	18	1.49
(1,25)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:ASN:N	3	1.48
(1,160)	2:585:B:PRO:C	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	12	1.47
(1,128)	1:211:A:LYS:C	1:212:A:PRO:N	1:212:A:PRO:CA	1:212:A:PRO:C	20	1.46
(1,160)	2:585:B:PRO:C	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	16	1.45
(1,167)	2:590:B:PRO:N	2:590:B:PRO:CA	2:590:B:PRO:C	2:591:B:SER:N	1	1.44
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	14	1.44
(1,157)	2:582:B:PRO:N	2:582:B:PRO:CA	2:582:B:PRO:C	2:583:B:PRO:N	9	1.43
(1,128)	1:211:A:LYS:C	1:212:A:PRO:N	1:212:A:PRO:CA	1:212:A:PRO:C	14	1.43
(1,142)	1:218:A:LEU:C	1:219:A:GLU:N	1:219:A:GLU:CA	1:219:A:GLU:C	19	1.42
(1,26)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1	1.42
(1,26)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	19	1.42
(1,26)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	7	1.37
(1,167)	2:590:B:PRO:N	2:590:B:PRO:CA	2:590:B:PRO:C	2:591:B:SER:N	8	1.36
(1,56)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:THR:N	7	1.36
(1,42)	1:166:A:SER:C	1:167:A:THR:N	1:167:A:THR:CA	1:167:A:THR:C	18	1.36
(1,157)	2:582:B:PRO:N	2:582:B:PRO:CA	2:582:B:PRO:C	2:583:B:PRO:N	12	1.35
(1,160)	2:585:B:PRO:C	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	14	1.33
(1,154)	2:578:B:PRO:C	2:579:B:PRO:N	2:579:B:PRO:CA	2:579:B:PRO:C	12	1.33
(1,42)	1:166:A:SER:C	1:167:A:THR:N	1:167:A:THR:CA	1:167:A:THR:C	19	1.33
(1,26)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	3	1.33
(1,110)	1:201:A:ASN:C	1:202:A:SER:N	1:202:A:SER:CA	1:202:A:SER:C	5	1.32
(1,160)	2:585:B:PRO:C	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	17	1.31
(1,92)	1:192:A:SER:C	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	18	1.31
(1,158)	2:581:B:ALA:C	2:582:B:PRO:N	2:582:B:PRO:CA	2:582:B:PRO:C	14	1.3
(1,26)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	8	1.3
(1,26)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	17	1.3
(1,29)	1:161:A:THR:N	1:161:A:THR:CA	1:161:A:THR:C	1:162:A:GLU:N	19	1.29

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,110)	1:201:A:ASN:C	1:202:A:SER:N	1:202:A:SER:CA	1:202:A:SER:C	20	1.28
(1,160)	2:585:B:PRO:C	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	9	1.27
(1,3)	1:147:A:THR:N	1:147:A:THR:CA	1:147:A:THR:C	1:148:A:GLU:N	12	1.25
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	18	1.24
(1,3)	1:147:A:THR:N	1:147:A:THR:CA	1:147:A:THR:C	1:148:A:GLU:N	5	1.24
(1,3)	1:147:A:THR:N	1:147:A:THR:CA	1:147:A:THR:C	1:148:A:GLU:N	16	1.24
(1,42)	1:166:A:SER:C	1:167:A:THR:N	1:167:A:THR:CA	1:167:A:THR:C	5	1.23
(1,42)	1:166:A:SER:C	1:167:A:THR:N	1:167:A:THR:CA	1:167:A:THR:C	14	1.23
(1,79)	1:187:A:TRP:N	1:187:A:TRP:CA	1:187:A:TRP:C	1:188:A:LYS:N	15	1.22
(1,92)	1:192:A:SER:C	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	14	1.2
(1,25)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:ASN:N	15	1.2
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	5	1.19
(1,25)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:ASN:N	1	1.18
(1,3)	1:147:A:THR:N	1:147:A:THR:CA	1:147:A:THR:C	1:148:A:GLU:N	6	1.18
(1,110)	1:201:A:ASN:C	1:202:A:SER:N	1:202:A:SER:CA	1:202:A:SER:C	10	1.17
(1,159)	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	2:587:B:PRO:N	6	1.13
(1,110)	1:201:A:ASN:C	1:202:A:SER:N	1:202:A:SER:CA	1:202:A:SER:C	4	1.13
(1,160)	2:585:B:PRO:C	2:586:B:PRO:N	2:586:B:PRO:CA	2:586:B:PRO:C	8	1.12
(1,73)	1:182:A:LEU:C	1:183:A:SER:N	1:183:A:SER:CA	1:183:A:SER:C	14	1.12
(1,42)	1:166:A:SER:C	1:167:A:THR:N	1:167:A:THR:CA	1:167:A:THR:C	2	1.12
(1,26)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	14	1.12
(1,3)	1:147:A:THR:N	1:147:A:THR:CA	1:147:A:THR:C	1:148:A:GLU:N	4	1.11
(1,138)	1:216:A:GLU:C	1:217:A:ASP:N	1:217:A:ASP:CA	1:217:A:ASP:C	10	1.1
(1,26)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	2	1.1
(1,128)	1:211:A:LYS:C	1:212:A:PRO:N	1:212:A:PRO:CA	1:212:A:PRO:C	7	1.09
(1,29)	1:161:A:THR:N	1:161:A:THR:CA	1:161:A:THR:C	1:162:A:GLU:N	11	1.09
(1,92)	1:192:A:SER:C	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	16	1.08
(1,26)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	20	1.08
(1,3)	1:147:A:THR:N	1:147:A:THR:CA	1:147:A:THR:C	1:148:A:GLU:N	19	1.08
(1,25)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:ASN:N	13	1.07
(1,3)	1:147:A:THR:N	1:147:A:THR:CA	1:147:A:THR:C	1:148:A:GLU:N	17	1.06
(1,167)	2:590:B:PRO:N	2:590:B:PRO:CA	2:590:B:PRO:C	2:591:B:SER:N	15	1.04
(1,167)	2:590:B:PRO:N	2:590:B:PRO:CA	2:590:B:PRO:C	2:591:B:SER:N	16	1.04
(1,128)	1:211:A:LYS:C	1:212:A:PRO:N	1:212:A:PRO:CA	1:212:A:PRO:C	17	1.04
(1,69)	1:180:A:GLN:C	1:181:A:LEU:N	1:181:A:LEU:CA	1:181:A:LEU:C	16	1.04
(1,166)	2:588:B:PRO:C	2:589:B:PRO:N	2:589:B:PRO:CA	2:589:B:PRO:C	16	1.03
(1,42)	1:166:A:SER:C	1:167:A:THR:N	1:167:A:THR:CA	1:167:A:THR:C	6	1.03
(1,26)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	15	1.03
(1,25)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:ASN:N	2	1.02
(1,3)	1:147:A:THR:N	1:147:A:THR:CA	1:147:A:THR:C	1:148:A:GLU:N	13	1.02
(1,110)	1:201:A:ASN:C	1:202:A:SER:N	1:202:A:SER:CA	1:202:A:SER:C	3	1.01
(1,26)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	5	1.01
(1,25)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:ASN:N	17	1.01
(1,3)	1:147:A:THR:N	1:147:A:THR:CA	1:147:A:THR:C	1:148:A:GLU:N	7	1.01
(1,69)	1:180:A:GLN:C	1:181:A:LEU:N	1:181:A:LEU:CA	1:181:A:LEU:C	12	1.0
(1,42)	1:166:A:SER:C	1:167:A:THR:N	1:167:A:THR:CA	1:167:A:THR:C	13	1.0
(1,26)	1:158:A:TYR:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	6	1.0