Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 01:40 AM EDT

PDB ID	:	2LFG
BMRB ID	:	17752
Title	:	Solution structure of the human prolactin receptor ecd domain d2
Authors	:	Dagil, R.; Knudsen, M.J.; Kragelund, B.B.; O'Shea, C.; Teilum, K.
Deposited on	:	2011-06-30

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

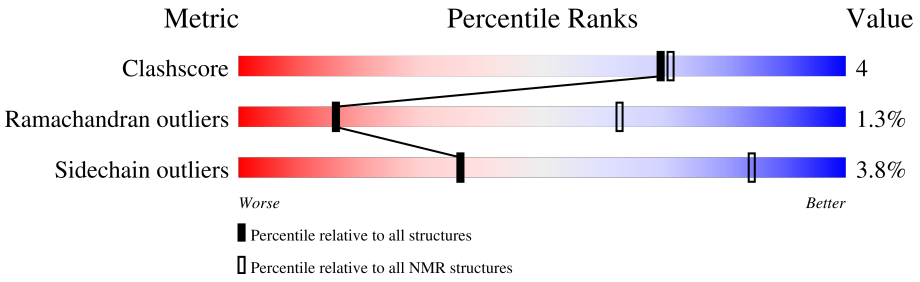
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 91%.

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	113	67% 5% 27%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 9 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:106-A:129, A:142-A:185, A:194-A:207 (82)	0.61	9

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1882 atoms, of which 936 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Prolactin receptor.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	113	1882	626	936	151	166	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	MET	-	initiating methionine	UNP P16471

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: Prolactin receptor

Chain A: 67% 5% 27%

M98 Y99 I100 V101 Q102 P103 D104 P105 P130 T131 L132 I133 D134 L135 K136 T137 G138 W139 F140 T141 L148 K168 L179 V180 Q181 C184 K185 P186 D187 H188 G189 Y190 W191 S192 A193 W194 S195 M208 N209 D210

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: Prolactin receptor

Chain A: 64% 8% • 27%

M98 Y99 I100 V101 Q102 P103 D104 P105 P106 L107 E108 L109 P130 T131 L132 I133 D134 L135 K136 T137 G138 W139 F140 T141 L148 K168 L179 V180 Q181 C184 K185 P186 D187 H188 G189 Y190 W191 S192 A193 W194 S195 M208 N209 D210

4.2.2 Score per residue for model 2

• Molecule 1: Prolactin receptor

Chain A: 60% 12% 27%

M98 Y99 I100 V101 Q102 P103 D104 P105 P106 L123 W124 P130 T131 L132 I133 D134 L135 K136 T137 G138 W139 F140 T141 R147 L148 F160 K168 L179 V180 Q181 V182 R183 C184 K185 P186 D187 H188 G189 Y190 W191 S192 A193 W194 S195 P196 A197 M208 N209 D210

4.2.3 Score per residue for model 3

- Molecule 1: Prolactin receptor

Chain A: 63% 9% • 27%

M98 Y99 I100 V101 Q102 P103 D104 P105 P106 L107 P130 T131 L132 I133 D134 L135 K136 T137 G138 W139 F140 T141 I146 R147 L148 A161 E166 L179 C184 K185 P186 D187 H188 G189 Y190 W191 S192 A193 W194 S195 I200 Q201 M208 N209 D210

4.2.4 Score per residue for model 4

- Molecule 1: Prolactin receptor

Chain A: 58% 15% 27%

M98 Y99 I100 V101 Q102 P103 D104 P105 K114 Y122 L123 W124 I125 K126 P130 T131 L132 I133 D134 L135 K136 T137 G138 W139 F140 T141 L142 L143 Y144 R147 L148 Q163 K168 Q181 C184 K185 P186 D187 H188 G189 Y190 W191 S192 A193 W194 S195 P196 M208 N209 D210

4.2.5 Score per residue for model 5

- Molecule 1: Prolactin receptor

Chain A: 65% 6% • 27%

M98 Y99 I100 V101 Q102 P103 D104 P105 E117 P130 T131 L132 I133 D134 L135 K136 T137 G138 W139 F140 T141 L148 K168 L179 V180 Q181 P186 D187 H188 G189 Y190 W191 S192 A193 W194 S195 P196 Q201 M208 N209 D210

4.2.6 Score per residue for model 6

- Molecule 1: Prolactin receptor

Chain A: 61% 12% 27%

M98 Y99 I100 V101 Q102 P103 D104 P105 P106 P116 E117 Y122 P130 T131 L132 I133 D134 L135 K136 T137 G138 W139 F140 T141 L148 Q163 K168 Q181 V182 R183 P186 D187 H188 G189 Y190 W191 S192 A193 W194 S195 P196 A197 M208 N209 D210

4.2.7 Score per residue for model 7

- Molecule 1: Prolactin receptor

Chain A: 63% 8% • 27%

M98 Y99 I100 V101 Q102 P103 D104 P105 P130 T131 L132 I133 D134 L135 K136 T137 G138 W139 F140 T141 L148 H159 F167 K168 Q176 L179 V180 Q181 V182 R183 P186 D187 H188 G189 Y190 W191 S192 A193 W194 S195 P196 M208 N209 D210

4.2.8 Score per residue for model 8

- Molecule 1: Prolactin receptor

Chain A: 58% 12% • 27%

M98 Y99 I100 V101 Q102 P103 D104 P105 P106 L107 P116 W124 P130 T131 L132 I133 D134 L135 K136 T137 G138 W139 F140 T141 L142 L143 Y144 L148 Q163 K168 L179 V180 Q181 C184 K185 P186 D187 H188 G189 Y190 W191 S192 A193 W194 S195 P196 A197 M208 N209 D210

4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Prolactin receptor

Chain A: 65% 8% 27%

M98 Y99 I100 V101 Q102 P103 D104 P105 P106 K114 L123 P130 T131 L132 I133 D134 L135 K136 T137 G138 W139 F140 T141 L142 L143 E155 K168 C184 K185 P186 D187 H188 G189 Y190 W191 S192 A193 W194 S195 M208 N209 D210

4.2.10 Score per residue for model 10

- Molecule 1: Prolactin receptor

Chain A: 69% • 27%

M98 Y99 I100 V101 Q102 P103 D104 P105 P130 T131 L132 I133 D134 L135 K136 T137 G138 W139 F140 T141 L148 K168 L179 P186 D187 H188 G189 Y190 W191 S192 A193 W194 S195 M208 N209 D210

4.2.11 Score per residue for model 11

- Molecule 1: Prolactin receptor

Chain A: 67% • • 27%

M98 Y99 I100 V101 Q102 P103 D104 P105 L123 P130 T131 L132 I133 D134 L135 K136 T137 G138 W139 F140 T141 R147 H159 F167 L172 Q181 P186 D187 H188 G189 Y190 W191 S192 A193 M208 N209 D210

4.2.12 Score per residue for model 12

- Molecule 1: Prolactin receptor

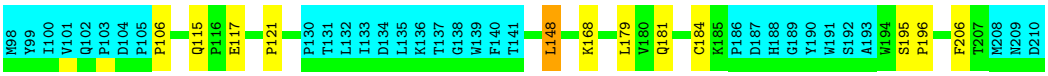
Chain A: 68% • • 27%

M98 Y99 I100 V101 Q102 P103 D104 P105 P130 T131 L132 I133 D134 L135 K136 T137 G138 W139 F140 T141 L148 Q163 L179 P186 D187 H188 G189 Y190 W191 S192 A193 W194 S195 P196 M208 N209 D210

4.2.13 Score per residue for model 13

- Molecule 1: Prolactin receptor

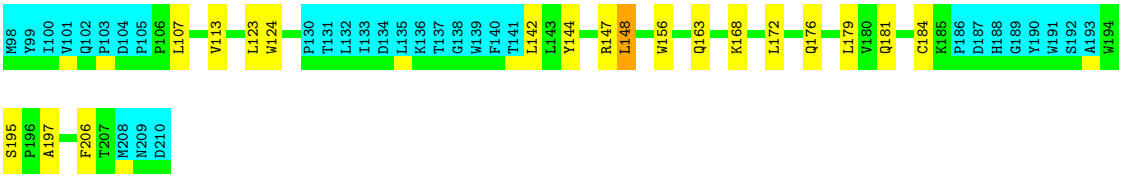
Chain A: 62% 10% • 27%



4.2.14 Score per residue for model 14

- Molecule 1: Prolactin receptor

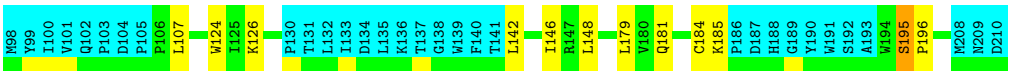
Chain A: 56% 16% • 27%



4.2.15 Score per residue for model 15

- Molecule 1: Prolactin receptor

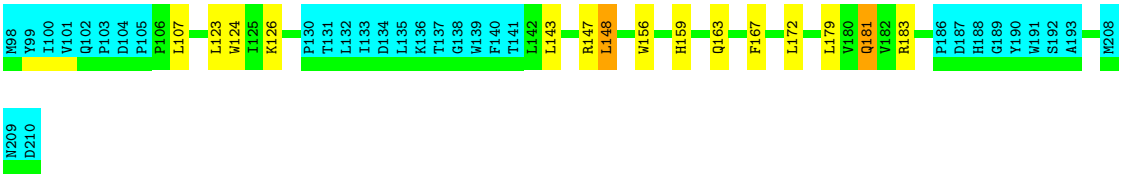
Chain A: 62% 10% • 27%



4.2.16 Score per residue for model 16

- Molecule 1: Prolactin receptor

Chain A: 59% 12% • 27%



4.2.17 Score per residue for model 17

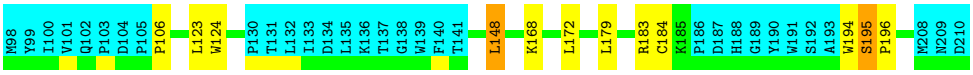
- Molecule 1: Prolactin receptor

Chain A: 65% 6% • 27%

4.2.18 Score per residue for model 18

- Molecule 1: Prolactin receptor

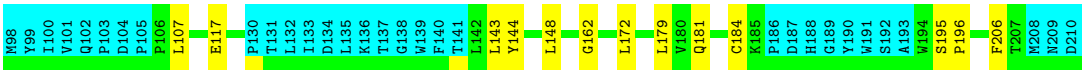
Chain A: 62% 9% • 27%



4.2.19 Score per residue for model 19

- Molecule 1: Prolactin receptor

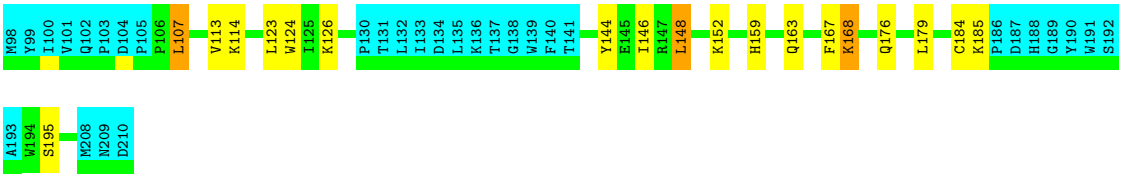
Chain A: 61% 12% 27%



4.2.20 Score per residue for model 20

- Molecule 1: Prolactin receptor

Chain A: 56% 14% • 27%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *?*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	**Classification**	**Version**
X-PLOR NIH	structure solution	2.25
TALOS	geometry optimization	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1470
Number of shifts mapped to atoms	1470
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	691	700	698	5±2
All	All	13820	14000	13960	102

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:LEU:HG	1:A:184:CYS:SG	0.91	2.06	15	1
1:A:106:PRO:HD3	1:A:184:CYS:SG	0.57	2.39	3	6
1:A:200:ILE:HG12	1:A:201:GLN:N	0.56	2.16	3	1
1:A:183:ARG:HG2	1:A:194:TRP:CZ3	0.54	2.37	6	2
1:A:183:ARG:HG3	1:A:194:TRP:CE3	0.53	2.39	2	1
1:A:183:ARG:HG2	1:A:194:TRP:CH2	0.53	2.39	6	1
1:A:181:GLN:OE1	1:A:194:TRP:HB3	0.52	2.04	1	4
1:A:143:LEU:HD11	1:A:163:GLN:HG2	0.52	1.81	8	1
1:A:148:LEU:HA	1:A:179:LEU:O	0.51	2.05	14	15
1:A:148:LEU:HD12	1:A:159:HIS:NE2	0.51	2.20	17	1
1:A:144:TYR:CE2	1:A:184:CYS:HB3	0.51	2.40	14	1
1:A:147:ARG:HB2	1:A:194:TRP:CZ2	0.50	2.41	2	2
1:A:168:LYS:N	1:A:168:LYS:HD2	0.50	2.21	20	1
1:A:124:TRP:CD1	1:A:168:LYS:HE3	0.50	2.41	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:195:SER:H	1:A:196:PRO:HD2	0.48	1.68	7	3
1:A:147:ARG:HG3	1:A:181:GLN:NE2	0.48	2.23	11	1
1:A:123:LEU:HB2	1:A:172:LEU:HD11	0.48	1.85	16	3
1:A:144:TYR:CD1	1:A:184:CYS:HB3	0.48	2.44	4	1
1:A:115:GLN:OE1	1:A:206:PHE:HA	0.48	2.08	13	1
1:A:181:GLN:NE2	1:A:181:GLN:HA	0.47	2.22	16	2
1:A:107:LEU:H	1:A:107:LEU:HD23	0.47	1.68	3	2
1:A:144:TYR:CD2	1:A:184:CYS:HB3	0.47	2.44	20	2
1:A:195:SER:OG	1:A:196:PRO:HD3	0.47	2.10	8	3
1:A:159:HIS:HB3	1:A:167:PHE:CZ	0.46	2.45	20	3
1:A:142:LEU:H	1:A:142:LEU:HD23	0.46	1.71	14	1
1:A:123:LEU:O	1:A:168:LYS:HA	0.46	2.11	4	3
1:A:124:TRP:CZ2	1:A:126:LYS:HD2	0.46	2.46	4	3
1:A:181:GLN:NE2	1:A:197:ALA:HB2	0.45	2.27	6	1
1:A:146:ILE:HA	1:A:181:GLN:O	0.45	2.11	15	1
1:A:181:GLN:HG2	1:A:196:PRO:O	0.45	2.12	13	4
1:A:121:PRO:HG3	1:A:206:PHE:O	0.44	2.12	13	1
1:A:172:LEU:HB2	1:A:206:PHE:CZ	0.44	2.48	19	2
1:A:143:LEU:CD1	1:A:163:GLN:HG2	0.44	2.43	17	1
1:A:148:LEU:HD12	1:A:159:HIS:CD2	0.44	2.48	17	1
1:A:181:GLN:HG2	1:A:197:ALA:HA	0.43	1.89	2	2
1:A:124:TRP:CZ2	1:A:126:LYS:HD3	0.43	2.49	16	1
1:A:124:TRP:CH2	1:A:126:LYS:HD2	0.42	2.48	15	1
1:A:146:ILE:HD12	1:A:146:ILE:N	0.42	2.29	20	1
1:A:142:LEU:HD21	1:A:184:CYS:SG	0.42	2.55	4	1
1:A:147:ARG:HG2	1:A:156:TRP:CE3	0.42	2.49	14	2
1:A:146:ILE:CD1	1:A:161:ALA:HB2	0.41	2.45	3	1
1:A:107:LEU:HD13	1:A:107:LEU:N	0.41	2.31	20	1
1:A:183:ARG:C	1:A:183:ARG:HD2	0.41	2.36	7	1
1:A:195:SER:HB2	1:A:196:PRO:HD3	0.41	1.91	18	1
1:A:122:TYR:CE1	1:A:168:LYS:HD2	0.41	2.51	4	1
1:A:143:LEU:HA	1:A:162:GLY:O	0.41	2.16	19	1
1:A:113:VAL:HG22	1:A:123:LEU:CD1	0.41	2.46	14	2
1:A:159:HIS:HB3	1:A:167:PHE:CE2	0.41	2.51	11	1
1:A:144:TYR:CE1	1:A:184:CYS:HB3	0.41	2.51	19	1
1:A:122:TYR:CE2	1:A:168:LYS:HD2	0.40	2.50	6	1
1:A:152:LYS:HE2	1:A:176:GLN:OE1	0.40	2.16	20	1
1:A:121:PRO:HB2	1:A:206:PHE:CE1	0.40	2.51	13	1
1:A:181:GLN:HE21	1:A:197:ALA:HB2	0.40	1.76	14	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	82/113 (73%)	77±2 (94±2%)	4±2 (4±2%)	1±1 (1±1%)	16 63
All	All	1640/2260 (73%)	1549 (94%)	70 (4%)	21 (1%)	16 63

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

Mol	Chain	Res	Type	Models (Total)
1	A	195	SER	16
1	A	163	GLN	2
1	A	106	PRO	1
1	A	116	PRO	1
1	A	117	GLU	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	75/103 (73%)	72±2 (96±2%)	3±2 (4±2%)	36 84
All	All	1500/2060 (73%)	1443 (96%)	57 (4%)	36 84

All 18 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	148	LEU	11
1	A	107	LEU	7
1	A	168	LYS	7
1	A	185	LYS	4
1	A	181	GLN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	163	GLN	4
1	A	114	LYS	3
1	A	117	GLU	3
1	A	201	GLN	2
1	A	176	GLN	2
1	A	143	LEU	2
1	A	183	ARG	2
1	A	109	LEU	1
1	A	160	PHE	1
1	A	166	GLU	1
1	A	200	ILE	1
1	A	116	PRO	1
1	A	155	GLU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1470
Number of shifts mapped to atoms	1470
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	15

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	110	0.29 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	107	-0.01 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	109	0.71 ± 0.14	Should be applied
^{15}N	98	0.94 ± 0.30	Should be applied

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 91%, i.e. 1095 atoms were assigned a chemical shift out of a possible 1208. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	390/396 (98%)	157/158 (99%)	160/164 (98%)	73/74 (99%)
Sidechain	593/681 (87%)	391/443 (88%)	195/215 (91%)	7/23 (30%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	112/131 (85%)	58/64 (91%)	50/59 (85%)	4/8 (50%)
Overall	1095/1208 (91%)	606/665 (91%)	405/438 (92%)	84/105 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1469 atoms were assigned a chemical shift out of a possible 1624. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	531/545 (97%)	214/218 (98%)	219/226 (97%)	98/101 (97%)
Sidechain	774/888 (87%)	510/579 (88%)	256/283 (90%)	8/26 (31%)
Aromatic	164/191 (86%)	84/93 (90%)	74/86 (86%)	6/12 (50%)
Overall	1469/1624 (90%)	808/890 (91%)	549/595 (92%)	112/139 (81%)

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.

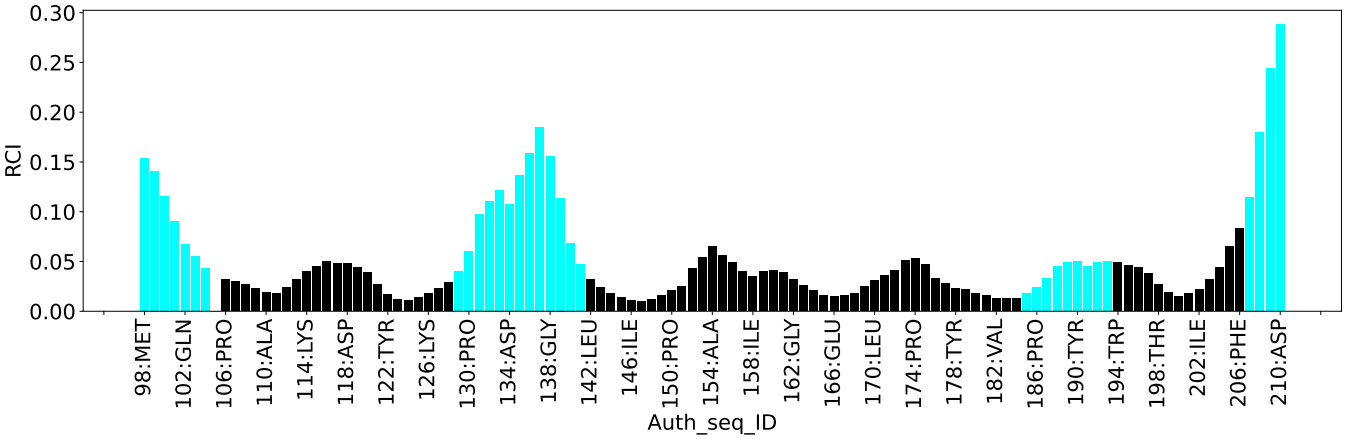
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	147	ARG	NH2	113.40	57.68 – 87.89	13.4
1	A	149	LYS	HD3	-0.77	0.54 – 2.65	-11.2
1	A	185	LYS	HD3	-0.25	0.54 – 2.65	-8.8
1	A	149	LYS	HD2	0.07	0.58 – 2.64	-7.5
1	A	185	LYS	HD2	0.09	0.58 – 2.64	-7.4
1	A	191	TRP	CE3	133.36	111.58 – 129.41	7.2
1	A	149	LYS	HE2	1.63	1.95 – 3.88	-6.6
1	A	127	TRP	HE1	5.84	6.88 – 13.28	-6.6
1	A	185	LYS	HG2	-0.20	0.13 – 2.61	-6.3
1	A	185	LYS	HB2	0.36	0.58 – 2.97	-5.9
1	A	149	LYS	HG2	-0.09	0.13 – 2.61	-5.9
1	A	191	TRP	HE3	5.10	5.27 – 9.37	-5.4
1	A	185	LYS	HB3	0.38	0.46 – 3.04	-5.3
1	A	149	LYS	HE3	1.87	1.92 – 3.89	-5.3
1	A	114	LYS	HB3	0.41	0.46 – 3.04	-5.2

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-

defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	2045
Intra-residue (|i-j|=0)	500
Sequential (|i-j|=1)	562
Medium range (|i-j|>1 and |i-j|<5)	214
Long range (|i-j|≥5)	769
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	105
Number of unmapped restraints	0
Number of restraints per residue	19.0
Number of long range restraints per residue[1]	6.8

[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 (i)

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 (i)

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)	13.6	0.2
0.2-0.5 (Medium)	3.4	0.44
>0.5 (Large)	None	None

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.2	3.1
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

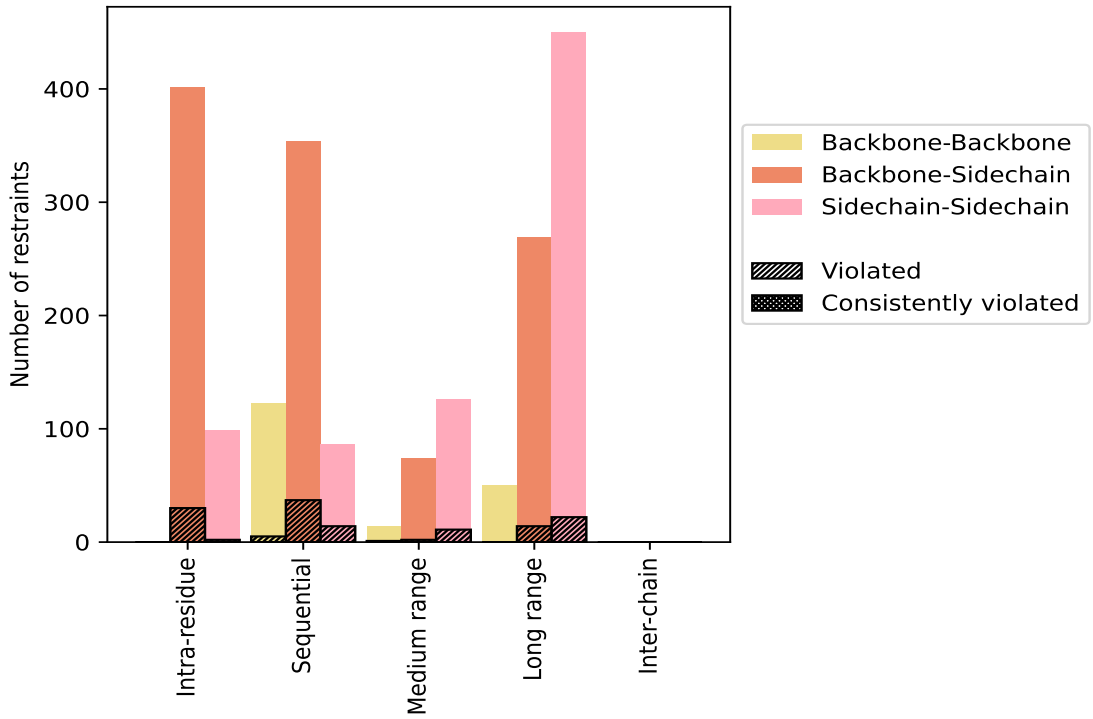
9.1 Summary of distance violations (i)

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)	500	24.4	32	6.4	1.6	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	401	19.6	30	7.5	1.5	0	0.0	0.0
Sidechain-Sidechain	99	4.8	2	2.0	0.1	0	0.0	0.0
Sequential (|i-j|=1)	562	27.5	56	10.0	2.7	0	0.0	0.0
Backbone-Backbone	122	6.0	5	4.1	0.2	0	0.0	0.0
Backbone-Sidechain	354	17.3	37	10.5	1.8	0	0.0	0.0
Sidechain-Sidechain	86	4.2	14	16.3	0.7	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	214	10.5	14	6.5	0.7	0	0.0	0.0
Backbone-Backbone	14	0.7	1	7.1	0.0	0	0.0	0.0
Backbone-Sidechain	74	3.6	2	2.7	0.1	0	0.0	0.0
Sidechain-Sidechain	126	6.2	11	8.7	0.5	0	0.0	0.0
Long range (|i-j|≥5)	769	37.6	36	4.7	1.8	0	0.0	0.0
Backbone-Backbone	50	2.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	269	13.2	14	5.2	0.7	0	0.0	0.0
Sidechain-Sidechain	450	22.0	22	4.9	1.1	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2045	100.0	138	6.7	6.7	0	0.0	0.0
Backbone-Backbone	186	9.1	6	3.2	0.3	0	0.0	0.0
Backbone-Sidechain	1098	53.7	83	7.6	4.1	0	0.0	0.0
Sidechain-Sidechain	761	37.2	49	6.4	2.4	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations (i)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	6	3	0	2	0	11	0.18	0.38	0.08	0.16
2	6	8	4	3	0	21	0.15	0.27	0.05	0.13
3	6	8	0	4	0	18	0.16	0.4	0.07	0.14
4	4	6	3	5	0	18	0.17	0.27	0.04	0.16
5	4	4	0	2	0	10	0.15	0.18	0.02	0.16
6	2	5	1	5	0	13	0.16	0.36	0.07	0.14
7	4	6	0	3	0	13	0.15	0.23	0.03	0.14
8	7	5	0	4	0	16	0.15	0.24	0.04	0.12
9	3	8	0	4	0	15	0.18	0.33	0.06	0.18
10	7	11	3	1	0	22	0.17	0.38	0.07	0.15
11	6	5	2	3	0	16	0.16	0.26	0.05	0.14

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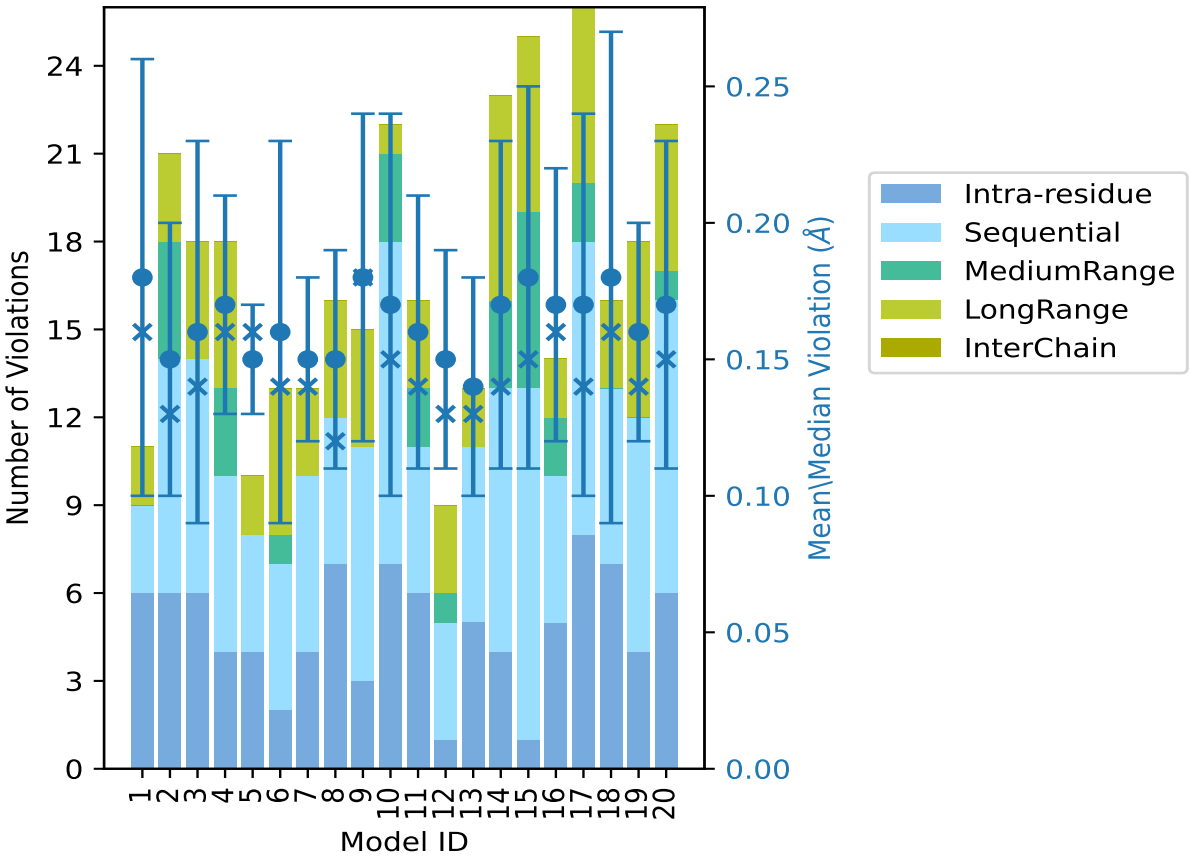
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	4	1	3	0	9	0.15	0.22	0.04	0.13
13	5	6	0	2	0	13	0.14	0.23	0.04	0.13
14	4	9	3	7	0	23	0.17	0.33	0.06	0.14
15	1	12	6	6	0	25	0.18	0.42	0.07	0.15
16	5	5	2	2	0	14	0.17	0.26	0.05	0.16
17	8	10	2	6	0	26	0.17	0.38	0.07	0.14
18	7	6	0	3	0	16	0.18	0.44	0.09	0.16
19	4	8	0	6	0	18	0.16	0.29	0.04	0.14
20	6	10	1	5	0	22	0.17	0.36	0.06	0.15

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

9.2.1 Bar graph : Distance Violation statistics for each model (i)



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

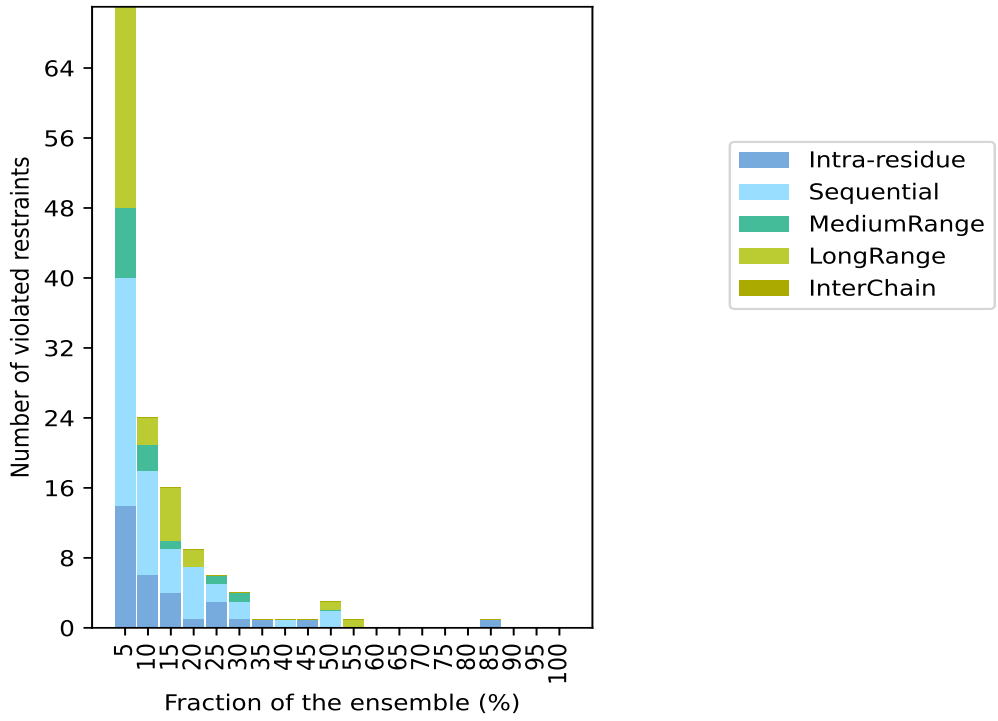
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1907(IR:468, SQ:506, MR:200, LR:733, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
14	26	8	23	0	71	1	5.0
6	12	3	3	0	24	2	10.0
4	5	1	6	0	16	3	15.0
1	6	0	2	0	9	4	20.0
3	2	1	0	0	6	5	25.0
1	2	1	0	0	4	6	30.0
1	0	0	0	0	1	7	35.0
0	1	0	0	0	1	8	40.0
1	0	0	0	0	1	9	45.0
0	2	0	1	0	3	10	50.0
0	0	0	1	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
1	0	0	0	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

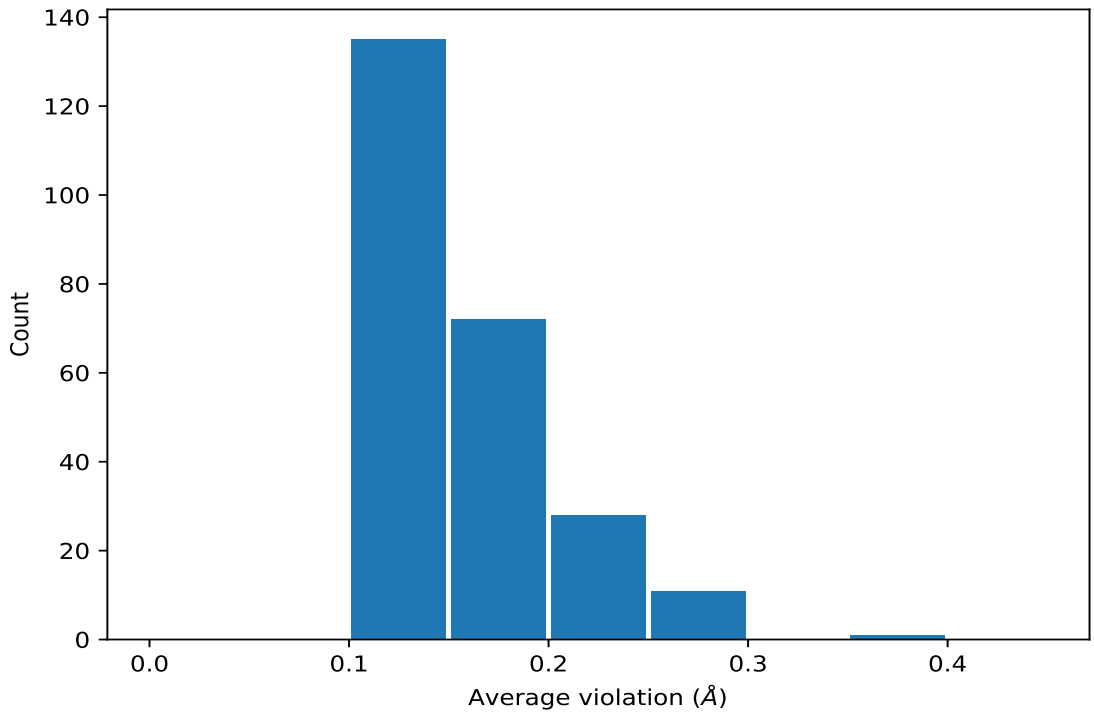
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of the 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)
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	17	0.21	0.06	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	17	0.21	0.06	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	17	0.21	0.06	0.2
(1,1450)	1:A:142:LEU:HB2	1:A:185:LYS:H	11	0.15	0.03	0.14
(1,1450)	1:A:142:LEU:HB3	1:A:185:LYS:H	11	0.15	0.03	0.14
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB1	10	0.17	0.03	0.17
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB2	10	0.17	0.03	0.17
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB3	10	0.17	0.03	0.17
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB1	10	0.17	0.03	0.17
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB2	10	0.17	0.03	0.17
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB3	10	0.17	0.03	0.17
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG21	10	0.13	0.02	0.12
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG22	10	0.13	0.02	0.12
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG23	10	0.13	0.02	0.12
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG21	10	0.13	0.02	0.12
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG22	10	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG23	10	0.13	0.02	0.12
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD11	10	0.12	0.01	0.12
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD12	10	0.12	0.01	0.12
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD13	10	0.12	0.01	0.12
(1,110)	1:A:135:LEU:HA	1:A:135:LEU:HG	9	0.15	0.04	0.14
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE2	8	0.14	0.03	0.12
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE3	8	0.14	0.03	0.12
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE2	8	0.14	0.03	0.12
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE3	8	0.14	0.03	0.12
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE2	7	0.18	0.05	0.2
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE3	7	0.18	0.05	0.2
(1,994)	1:A:100:ILE:HA	1:A:101:VAL:H	6	0.24	0.01	0.24
(1,179)	1:A:100:ILE:HD11	1:A:101:VAL:H	6	0.2	0.04	0.2
(1,179)	1:A:100:ILE:HD12	1:A:101:VAL:H	6	0.2	0.04	0.2
(1,179)	1:A:100:ILE:HD13	1:A:101:VAL:H	6	0.2	0.04	0.2
(1,806)	1:A:99:TYR:HE1	1:A:101:VAL:HA	6	0.17	0.04	0.17
(1,806)	1:A:99:TYR:HE2	1:A:101:VAL:HA	6	0.17	0.04	0.17
(1,857)	1:A:160:PHE:HA	1:A:160:PHE:HE1	6	0.12	0.01	0.12
(1,857)	1:A:160:PHE:HA	1:A:160:PHE:HE2	6	0.12	0.01	0.12
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD11	5	0.26	0.11	0.25
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD12	5	0.26	0.11	0.25
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD13	5	0.26	0.11	0.25
(1,1711)	1:A:136:LYS:HA	1:A:136:LYS:HE2	5	0.21	0.04	0.19
(1,1711)	1:A:136:LYS:HA	1:A:136:LYS:HE3	5	0.21	0.04	0.19
(1,1691)	1:A:132:LEU:HB2	1:A:133:ILE:H	5	0.19	0.06	0.19
(1,1691)	1:A:132:LEU:HB3	1:A:133:ILE:H	5	0.19	0.06	0.19
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD11	5	0.17	0.04	0.18
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD12	5	0.17	0.04	0.18
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD13	5	0.17	0.04	0.18
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB1	5	0.15	0.04	0.14
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB2	5	0.15	0.04	0.14
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB3	5	0.15	0.04	0.14
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB1	5	0.13	0.01	0.14
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB2	5	0.13	0.01	0.14
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB3	5	0.13	0.01	0.14
(1,797)	1:A:131:THR:HB	1:A:132:LEU:HD21	4	0.26	0.08	0.26
(1,797)	1:A:131:THR:HB	1:A:132:LEU:HD22	4	0.26	0.08	0.26
(1,797)	1:A:131:THR:HB	1:A:132:LEU:HD23	4	0.26	0.08	0.26
(1,445)	1:A:136:LYS:HA	1:A:137:THR:HG21	4	0.23	0.07	0.25
(1,445)	1:A:136:LYS:HA	1:A:137:THR:HG22	4	0.23	0.07	0.25
(1,445)	1:A:136:LYS:HA	1:A:137:THR:HG23	4	0.23	0.07	0.25
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG11	4	0.18	0.05	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG12	4	0.18	0.05	0.16
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG13	4	0.18	0.05	0.16
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG21	4	0.18	0.05	0.16
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG22	4	0.18	0.05	0.16
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG23	4	0.18	0.05	0.16
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG11	4	0.18	0.05	0.16
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG12	4	0.18	0.05	0.16
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG13	4	0.18	0.05	0.16
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG21	4	0.18	0.05	0.16
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG22	4	0.18	0.05	0.16
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG23	4	0.18	0.05	0.16
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG11	4	0.15	0.04	0.13
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG12	4	0.15	0.04	0.13
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG13	4	0.15	0.04	0.13
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG21	4	0.15	0.04	0.13
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG22	4	0.15	0.04	0.13
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG23	4	0.15	0.04	0.13
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG11	4	0.15	0.04	0.13
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG12	4	0.15	0.04	0.13
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG13	4	0.15	0.04	0.13
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG21	4	0.15	0.04	0.13
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG22	4	0.15	0.04	0.13
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG23	4	0.15	0.04	0.13
(1,1397)	1:A:106:PRO:HB2	1:A:107:LEU:H	4	0.14	0.01	0.15
(1,1397)	1:A:106:PRO:HB3	1:A:107:LEU:H	4	0.14	0.01	0.15
(1,673)	1:A:127:TRP:HE3	1:A:146:ILE:HG21	4	0.14	0.03	0.12
(1,673)	1:A:127:TRP:HE3	1:A:146:ILE:HG22	4	0.14	0.03	0.12
(1,673)	1:A:127:TRP:HE3	1:A:146:ILE:HG23	4	0.14	0.03	0.12
(1,1715)	1:A:136:LYS:HD2	1:A:137:THR:H	4	0.14	0.02	0.14
(1,1715)	1:A:136:LYS:HD3	1:A:137:THR:H	4	0.14	0.02	0.14
(1,1204)	1:A:164:GLN:H	1:A:165:THR:HG21	4	0.13	0.02	0.13
(1,1204)	1:A:164:GLN:H	1:A:165:THR:HG22	4	0.13	0.02	0.13
(1,1204)	1:A:164:GLN:H	1:A:165:THR:HG23	4	0.13	0.02	0.13
(1,1579)	1:A:114:LYS:HB2	1:A:114:LYS:HE2	4	0.12	0.01	0.12
(1,1579)	1:A:114:LYS:HB2	1:A:114:LYS:HE3	4	0.12	0.01	0.12
(1,1579)	1:A:114:LYS:HB3	1:A:114:LYS:HE2	4	0.12	0.01	0.12
(1,1579)	1:A:114:LYS:HB3	1:A:114:LYS:HE3	4	0.12	0.01	0.12
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG11	3	0.2	0.05	0.18
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG12	3	0.2	0.05	0.18
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG13	3	0.2	0.05	0.18
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG21	3	0.2	0.05	0.18
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG22	3	0.2	0.05	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG23	3	0.2	0.05	0.18
(1,1616)	1:A:119:ARG:HA	1:A:119:ARG:HD2	3	0.19	0.04	0.21
(1,1616)	1:A:119:ARG:HA	1:A:119:ARG:HD3	3	0.19	0.04	0.21
(1,1607)	1:A:117:GLU:HB2	1:A:118:ASP:HB2	3	0.18	0.02	0.19
(1,1607)	1:A:117:GLU:HB2	1:A:118:ASP:HB3	3	0.18	0.02	0.19
(1,1607)	1:A:117:GLU:HB3	1:A:118:ASP:HB2	3	0.18	0.02	0.19
(1,1607)	1:A:117:GLU:HB3	1:A:118:ASP:HB3	3	0.18	0.02	0.19
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD11	3	0.18	0.02	0.18
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD12	3	0.18	0.02	0.18
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD13	3	0.18	0.02	0.18
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD21	3	0.18	0.02	0.18
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD22	3	0.18	0.02	0.18
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD23	3	0.18	0.02	0.18
(1,1756)	1:A:143:LEU:HD11	1:A:163:GLN:HB2	3	0.18	0.04	0.19
(1,1756)	1:A:143:LEU:HD11	1:A:163:GLN:HB3	3	0.18	0.04	0.19
(1,1756)	1:A:143:LEU:HD12	1:A:163:GLN:HB2	3	0.18	0.04	0.19
(1,1756)	1:A:143:LEU:HD12	1:A:163:GLN:HB3	3	0.18	0.04	0.19
(1,1756)	1:A:143:LEU:HD13	1:A:163:GLN:HB2	3	0.18	0.04	0.19
(1,1756)	1:A:143:LEU:HD13	1:A:163:GLN:HB3	3	0.18	0.04	0.19
(1,1756)	1:A:143:LEU:HD21	1:A:163:GLN:HB2	3	0.18	0.04	0.19
(1,1756)	1:A:143:LEU:HD21	1:A:163:GLN:HB3	3	0.18	0.04	0.19
(1,1756)	1:A:143:LEU:HD22	1:A:163:GLN:HB2	3	0.18	0.04	0.19
(1,1756)	1:A:143:LEU:HD22	1:A:163:GLN:HB3	3	0.18	0.04	0.19
(1,1756)	1:A:143:LEU:HD23	1:A:163:GLN:HB2	3	0.18	0.04	0.19
(1,1756)	1:A:143:LEU:HD23	1:A:163:GLN:HB3	3	0.18	0.04	0.19
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG11	3	0.17	0.04	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG12	3	0.17	0.04	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG13	3	0.17	0.04	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG21	3	0.17	0.04	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG22	3	0.17	0.04	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG23	3	0.17	0.04	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG11	3	0.17	0.04	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG12	3	0.17	0.04	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG13	3	0.17	0.04	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG21	3	0.17	0.04	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG22	3	0.17	0.04	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG23	3	0.17	0.04	0.14
(1,2039)	1:A:191:TRP:HH2	1:A:160:PHE:HE1	3	0.15	0.02	0.14
(1,2039)	1:A:191:TRP:HH2	1:A:160:PHE:HE2	3	0.15	0.02	0.14
(1,1932)	1:A:177:LYS:H	1:A:177:LYS:HD2	3	0.15	0.02	0.14
(1,1932)	1:A:177:LYS:H	1:A:177:LYS:HD3	3	0.15	0.02	0.14
(1,531)	1:A:191:TRP:HE3	1:A:193:ALA:HB1	3	0.15	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,531)	1:A:191:TRP:HE3	1:A:193:ALA:HB2	3	0.15	0.02	0.14
(1,531)	1:A:191:TRP:HE3	1:A:193:ALA:HB3	3	0.15	0.02	0.14
(1,1070)	1:A:123:LEU:HG	1:A:124:TRP:H	3	0.14	0.03	0.13
(1,1985)	1:A:185:LYS:HA	1:A:185:LYS:HE2	3	0.14	0.02	0.15
(1,1985)	1:A:185:LYS:HA	1:A:185:LYS:HE3	3	0.14	0.02	0.15
(1,1366)	1:A:207:THR:HB	1:A:208:MET:H	3	0.14	0.03	0.13
(1,475)	1:A:127:TRP:HZ2	1:A:165:THR:HB	3	0.13	0.03	0.11
(1,394)	1:A:111:VAL:HB	1:A:112:GLU:H	3	0.13	0.01	0.12
(1,861)	1:A:143:LEU:HG	1:A:160:PHE:HZ	3	0.12	0.01	0.12
(1,1930)	1:A:176:GLN:HA	1:A:176:GLN:HE21	3	0.12	0.01	0.12
(1,1930)	1:A:176:GLN:HA	1:A:176:GLN:HE22	3	0.12	0.01	0.12
(1,1102)	1:A:133:ILE:HB	1:A:134:ASP:H	2	0.39	0.03	0.39
(1,537)	1:A:193:ALA:HB1	1:A:194:TRP:H	2	0.29	0.01	0.29
(1,537)	1:A:193:ALA:HB2	1:A:194:TRP:H	2	0.29	0.01	0.29
(1,537)	1:A:193:ALA:HB3	1:A:194:TRP:H	2	0.29	0.01	0.29
(1,1371)	1:A:209:ASN:HA	1:A:210:ASP:H	2	0.28	0.06	0.28
(1,798)	1:A:132:LEU:HA	1:A:133:ILE:HB	2	0.26	0.03	0.26
(1,1998)	1:A:190:TYR:HB2	1:A:191:TRP:H	2	0.21	0.07	0.21
(1,1998)	1:A:190:TYR:HB3	1:A:191:TRP:H	2	0.21	0.07	0.21
(1,530)	1:A:133:ILE:HG21	1:A:134:ASP:HB2	2	0.2	0.0	0.2
(1,530)	1:A:133:ILE:HG21	1:A:134:ASP:HB3	2	0.2	0.0	0.2
(1,530)	1:A:133:ILE:HG22	1:A:134:ASP:HB2	2	0.2	0.0	0.2
(1,530)	1:A:133:ILE:HG22	1:A:134:ASP:HB3	2	0.2	0.0	0.2
(1,530)	1:A:133:ILE:HG23	1:A:134:ASP:HB2	2	0.2	0.0	0.2
(1,530)	1:A:133:ILE:HG23	1:A:134:ASP:HB3	2	0.2	0.0	0.2
(1,1708)	1:A:136:LYS:H	1:A:136:LYS:HD2	2	0.2	0.02	0.2
(1,1708)	1:A:136:LYS:H	1:A:136:LYS:HD3	2	0.2	0.02	0.2
(1,833)	1:A:139:TRP:HA	1:A:139:TRP:HD1	2	0.18	0.06	0.18
(1,1399)	1:A:120:LYS:H	1:A:120:LYS:HG2	2	0.18	0.02	0.18
(1,1399)	1:A:120:LYS:H	1:A:120:LYS:HG3	2	0.18	0.02	0.18
(1,1759)	1:A:143:LEU:HD11	1:A:164:GLN:H	2	0.16	0.04	0.16
(1,1759)	1:A:143:LEU:HD12	1:A:164:GLN:H	2	0.16	0.04	0.16
(1,1759)	1:A:143:LEU:HD13	1:A:164:GLN:H	2	0.16	0.04	0.16
(1,1759)	1:A:143:LEU:HD21	1:A:164:GLN:H	2	0.16	0.04	0.16
(1,1759)	1:A:143:LEU:HD22	1:A:164:GLN:H	2	0.16	0.04	0.16
(1,1759)	1:A:143:LEU:HD23	1:A:164:GLN:H	2	0.16	0.04	0.16
(1,1099)	1:A:132:LEU:HA	1:A:134:ASP:H	2	0.14	0.02	0.14
(1,1746)	1:A:143:LEU:HD11	1:A:144:TYR:H	2	0.14	0.01	0.14
(1,1746)	1:A:143:LEU:HD12	1:A:144:TYR:H	2	0.14	0.01	0.14
(1,1746)	1:A:143:LEU:HD13	1:A:144:TYR:H	2	0.14	0.01	0.14
(1,1746)	1:A:143:LEU:HD21	1:A:144:TYR:H	2	0.14	0.01	0.14
(1,1746)	1:A:143:LEU:HD22	1:A:144:TYR:H	2	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1746)	1:A:143:LEU:HD23	1:A:144:TYR:H	2	0.14	0.01	0.14
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD11	2	0.14	0.02	0.14
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD12	2	0.14	0.02	0.14
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD13	2	0.14	0.02	0.14
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD21	2	0.14	0.02	0.14
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD22	2	0.14	0.02	0.14
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD23	2	0.14	0.02	0.14
(1,1587)	1:A:114:LYS:HE2	1:A:115:GLN:H	2	0.13	0.02	0.13
(1,1587)	1:A:114:LYS:HE3	1:A:115:GLN:H	2	0.13	0.02	0.13
(1,827)	1:A:112:GLU:HB2	1:A:124:TRP:HE3	2	0.12	0.02	0.12
(1,827)	1:A:112:GLU:HB3	1:A:124:TRP:HE3	2	0.12	0.02	0.12
(1,1800)	1:A:148:LEU:HD11	1:A:178:TYR:HB2	2	0.12	0.01	0.12
(1,1800)	1:A:148:LEU:HD11	1:A:178:TYR:HB3	2	0.12	0.01	0.12
(1,1800)	1:A:148:LEU:HD12	1:A:178:TYR:HB2	2	0.12	0.01	0.12
(1,1800)	1:A:148:LEU:HD12	1:A:178:TYR:HB3	2	0.12	0.01	0.12
(1,1800)	1:A:148:LEU:HD13	1:A:178:TYR:HB2	2	0.12	0.01	0.12
(1,1800)	1:A:148:LEU:HD13	1:A:178:TYR:HB3	2	0.12	0.01	0.12
(1,1800)	1:A:148:LEU:HD21	1:A:178:TYR:HB2	2	0.12	0.01	0.12
(1,1800)	1:A:148:LEU:HD21	1:A:178:TYR:HB3	2	0.12	0.01	0.12
(1,1800)	1:A:148:LEU:HD22	1:A:178:TYR:HB2	2	0.12	0.01	0.12
(1,1800)	1:A:148:LEU:HD22	1:A:178:TYR:HB3	2	0.12	0.01	0.12
(1,1800)	1:A:148:LEU:HD23	1:A:178:TYR:HB2	2	0.12	0.01	0.12
(1,1800)	1:A:148:LEU:HD23	1:A:178:TYR:HB3	2	0.12	0.01	0.12
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD11	2	0.12	0.01	0.12
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD12	2	0.12	0.01	0.12
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD13	2	0.12	0.01	0.12
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD21	2	0.12	0.01	0.12
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD22	2	0.12	0.01	0.12
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD23	2	0.12	0.01	0.12
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD11	2	0.12	0.01	0.12
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD12	2	0.12	0.01	0.12
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD13	2	0.12	0.01	0.12
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD21	2	0.12	0.01	0.12
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD22	2	0.12	0.01	0.12
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD23	2	0.12	0.01	0.12
(1,1575)	1:A:114:LYS:HA	1:A:114:LYS:HE2	2	0.12	0.01	0.12
(1,1575)	1:A:114:LYS:HA	1:A:114:LYS:HE3	2	0.12	0.01	0.12
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD11	2	0.12	0.01	0.12
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD12	2	0.12	0.01	0.12
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD13	2	0.12	0.01	0.12
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD21	2	0.12	0.01	0.12
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD22	2	0.12	0.01	0.12

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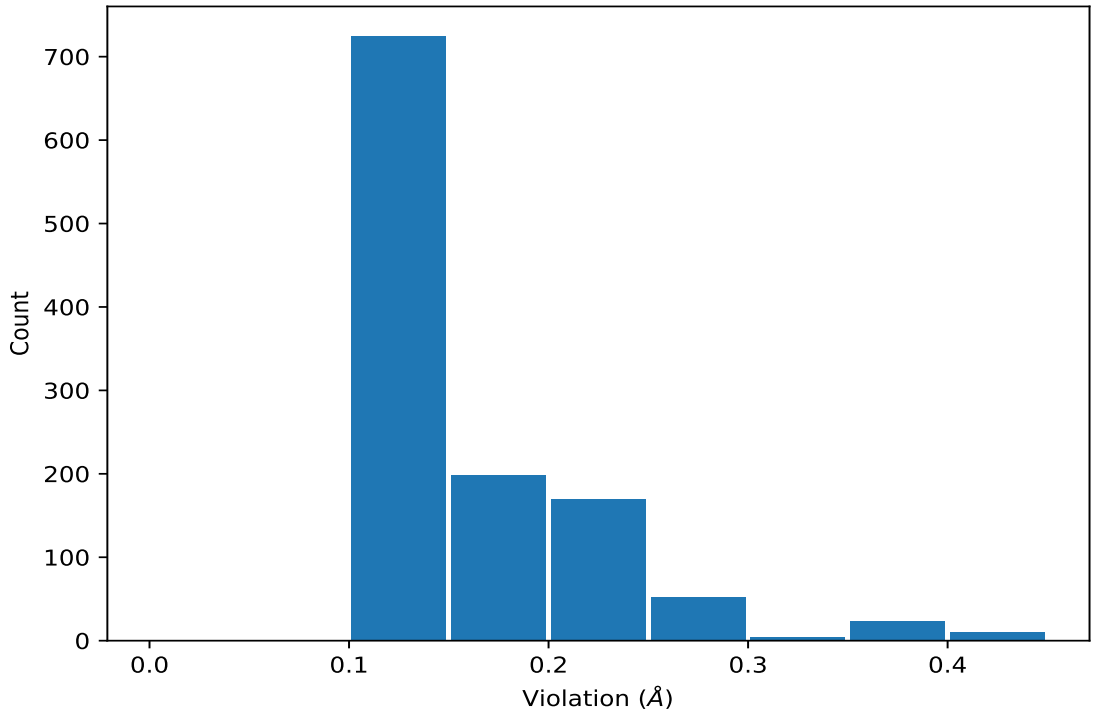
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD23	2	0.12	0.01	0.12
(1,1864)	1:A:156:TRP:HE3	1:A:157:GLU:HB2	2	0.12	0.01	0.12
(1,1864)	1:A:156:TRP:HE3	1:A:157:GLU:HB3	2	0.12	0.01	0.12
(1,2044)	1:A:191:TRP:HE3	1:A:192:SER:HA	2	0.12	0.01	0.12
(1,154)	1:A:208:MET:HA	1:A:208:MET:HE1	2	0.12	0.0	0.12
(1,154)	1:A:208:MET:HA	1:A:208:MET:HE2	2	0.12	0.0	0.12
(1,154)	1:A:208:MET:HA	1:A:208:MET:HE3	2	0.12	0.0	0.12
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG11	2	0.12	0.0	0.12
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG12	2	0.12	0.0	0.12
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG13	2	0.12	0.0	0.12
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG21	2	0.12	0.0	0.12
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG22	2	0.12	0.0	0.12
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG23	2	0.12	0.0	0.12
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG11	2	0.12	0.0	0.12
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG12	2	0.12	0.0	0.12
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG13	2	0.12	0.0	0.12
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG21	2	0.12	0.0	0.12
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG22	2	0.12	0.0	0.12
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG23	2	0.12	0.0	0.12
(1,1933)	1:A:177:LYS:HA	1:A:177:LYS:HD2	2	0.12	0.0	0.12
(1,1933)	1:A:177:LYS:HA	1:A:177:LYS:HD3	2	0.12	0.0	0.12

[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)
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	18	0.44
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	18	0.44
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	18	0.44
(1,1102)	1:A:133:ILE:HB	1:A:134:ASP:H	15	0.42
(1,752)	1:A:200:ILE:HD11	1:A:201:GLN:HB2	3	0.4
(1,752)	1:A:200:ILE:HD11	1:A:201:GLN:HB3	3	0.4
(1,752)	1:A:200:ILE:HD12	1:A:201:GLN:HB2	3	0.4
(1,752)	1:A:200:ILE:HD12	1:A:201:GLN:HB3	3	0.4
(1,752)	1:A:200:ILE:HD13	1:A:201:GLN:HB2	3	0.4
(1,752)	1:A:200:ILE:HD13	1:A:201:GLN:HB3	3	0.4
(1,925)	1:A:190:TYR:HA	1:A:191:TRP:HD1	10	0.38
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD11	1	0.38
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD12	1	0.38
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD13	1	0.38
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD11	17	0.38
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD12	17	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD13	17	0.38
(1,797)	1:A:131:THR:HB	1:A:132:LEU:HD21	17	0.36
(1,797)	1:A:131:THR:HB	1:A:132:LEU:HD22	17	0.36
(1,797)	1:A:131:THR:HB	1:A:132:LEU:HD23	17	0.36
(1,1500)	1:A:107:LEU:HD11	1:A:108:GLU:HB2	6	0.36
(1,1500)	1:A:107:LEU:HD11	1:A:108:GLU:HB3	6	0.36
(1,1500)	1:A:107:LEU:HD12	1:A:108:GLU:HB2	6	0.36
(1,1500)	1:A:107:LEU:HD12	1:A:108:GLU:HB3	6	0.36
(1,1500)	1:A:107:LEU:HD13	1:A:108:GLU:HB2	6	0.36
(1,1500)	1:A:107:LEU:HD13	1:A:108:GLU:HB3	6	0.36
(1,1500)	1:A:107:LEU:HD21	1:A:108:GLU:HB2	6	0.36
(1,1500)	1:A:107:LEU:HD21	1:A:108:GLU:HB3	6	0.36
(1,1500)	1:A:107:LEU:HD22	1:A:108:GLU:HB2	6	0.36
(1,1500)	1:A:107:LEU:HD22	1:A:108:GLU:HB3	6	0.36
(1,1500)	1:A:107:LEU:HD23	1:A:108:GLU:HB2	6	0.36
(1,1500)	1:A:107:LEU:HD23	1:A:108:GLU:HB3	6	0.36
(1,1102)	1:A:133:ILE:HB	1:A:134:ASP:H	20	0.36
(1,797)	1:A:131:THR:HB	1:A:132:LEU:HD21	14	0.33
(1,797)	1:A:131:THR:HB	1:A:132:LEU:HD22	14	0.33
(1,797)	1:A:131:THR:HB	1:A:132:LEU:HD23	14	0.33
(1,1371)	1:A:209:ASN:HA	1:A:210:ASP:H	9	0.33
(1,537)	1:A:193:ALA:HB1	1:A:194:TRP:H	18	0.3
(1,537)	1:A:193:ALA:HB2	1:A:194:TRP:H	18	0.3
(1,537)	1:A:193:ALA:HB3	1:A:194:TRP:H	18	0.3
(1,445)	1:A:136:LYS:HA	1:A:137:THR:HG21	10	0.3
(1,445)	1:A:136:LYS:HA	1:A:137:THR:HG22	10	0.3
(1,445)	1:A:136:LYS:HA	1:A:137:THR:HG23	10	0.3
(1,798)	1:A:132:LEU:HA	1:A:133:ILE:HB	19	0.29
(1,1998)	1:A:190:TYR:HB2	1:A:191:TRP:H	15	0.28
(1,1998)	1:A:190:TYR:HB3	1:A:191:TRP:H	15	0.28
(1,1309)	1:A:192:SER:HA	1:A:193:ALA:H	14	0.28
(1,537)	1:A:193:ALA:HB1	1:A:194:TRP:H	2	0.27
(1,537)	1:A:193:ALA:HB2	1:A:194:TRP:H	2	0.27
(1,537)	1:A:193:ALA:HB3	1:A:194:TRP:H	2	0.27
(1,445)	1:A:136:LYS:HA	1:A:137:THR:HG21	4	0.27
(1,445)	1:A:136:LYS:HA	1:A:137:THR:HG22	4	0.27
(1,445)	1:A:136:LYS:HA	1:A:137:THR:HG23	4	0.27
(1,994)	1:A:100:ILE:HA	1:A:101:VAL:H	14	0.26
(1,261)	1:A:164:GLN:HB2	1:A:165:THR:HA	20	0.26
(1,261)	1:A:164:GLN:HB3	1:A:165:THR:HA	20	0.26
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG11	15	0.26
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG12	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG13	15	0.26
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG21	15	0.26
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG22	15	0.26
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG23	15	0.26
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG11	15	0.26
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG12	15	0.26
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG13	15	0.26
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG21	15	0.26
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG22	15	0.26
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG23	15	0.26
(1,1711)	1:A:136:LYS:HA	1:A:136:LYS:HE2	11	0.26
(1,1711)	1:A:136:LYS:HA	1:A:136:LYS:HE3	11	0.26
(1,1711)	1:A:136:LYS:HA	1:A:136:LYS:HE2	16	0.26
(1,1711)	1:A:136:LYS:HA	1:A:136:LYS:HE3	16	0.26
(1,1691)	1:A:132:LEU:HB2	1:A:133:ILE:H	3	0.26
(1,1691)	1:A:132:LEU:HB3	1:A:133:ILE:H	3	0.26
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG11	10	0.26
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG12	10	0.26
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG13	10	0.26
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG21	10	0.26
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG22	10	0.26
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG23	10	0.26
(1,994)	1:A:100:ILE:HA	1:A:101:VAL:H	16	0.25
(1,179)	1:A:100:ILE:HD11	1:A:101:VAL:H	18	0.25
(1,179)	1:A:100:ILE:HD12	1:A:101:VAL:H	18	0.25
(1,179)	1:A:100:ILE:HD13	1:A:101:VAL:H	18	0.25
(1,1691)	1:A:132:LEU:HB2	1:A:133:ILE:H	17	0.25
(1,1691)	1:A:132:LEU:HB3	1:A:133:ILE:H	17	0.25
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD11	18	0.25
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD12	18	0.25
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD13	18	0.25
(1,994)	1:A:100:ILE:HA	1:A:101:VAL:H	2	0.24
(1,994)	1:A:100:ILE:HA	1:A:101:VAL:H	4	0.24
(1,833)	1:A:139:TRP:HA	1:A:139:TRP:HD1	1	0.24
(1,1710)	1:A:136:LYS:HA	1:A:136:LYS:HD2	8	0.24
(1,1710)	1:A:136:LYS:HA	1:A:136:LYS:HD3	8	0.24
(1,110)	1:A:135:LEU:HA	1:A:135:LEU:HG	17	0.24
(1,994)	1:A:100:ILE:HA	1:A:101:VAL:H	10	0.23
(1,994)	1:A:100:ILE:HA	1:A:101:VAL:H	15	0.23
(1,798)	1:A:132:LEU:HA	1:A:133:ILE:HB	9	0.23
(1,445)	1:A:136:LYS:HA	1:A:137:THR:HG21	6	0.23
(1,445)	1:A:136:LYS:HA	1:A:137:THR:HG22	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:A:136:LYS:HA	1:A:137:THR:HG23	6	0.23
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	11	0.23
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	11	0.23
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	11	0.23
(1,182)	1:A:103:PRO:HG2	1:A:104:ASP:HA	7	0.23
(1,182)	1:A:103:PRO:HG3	1:A:104:ASP:HA	7	0.23
(1,179)	1:A:100:ILE:HD11	1:A:101:VAL:H	8	0.23
(1,179)	1:A:100:ILE:HD12	1:A:101:VAL:H	8	0.23
(1,179)	1:A:100:ILE:HD13	1:A:101:VAL:H	8	0.23
(1,1697)	1:A:135:LEU:H	1:A:135:LEU:HB2	19	0.23
(1,1697)	1:A:135:LEU:H	1:A:135:LEU:HB3	19	0.23
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE2	13	0.23
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE3	13	0.23
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE2	20	0.23
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE3	20	0.23
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	1	0.22
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	1	0.22
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	1	0.22
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	14	0.22
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	14	0.22
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	14	0.22
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG11	15	0.22
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG12	15	0.22
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG13	15	0.22
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG21	15	0.22
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG22	15	0.22
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG23	15	0.22
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG11	15	0.22
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG12	15	0.22
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG13	15	0.22
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG21	15	0.22
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG22	15	0.22
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG23	15	0.22
(1,179)	1:A:100:ILE:HD11	1:A:101:VAL:H	11	0.22
(1,179)	1:A:100:ILE:HD12	1:A:101:VAL:H	11	0.22
(1,179)	1:A:100:ILE:HD13	1:A:101:VAL:H	11	0.22
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB1	6	0.22
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB2	6	0.22
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB3	6	0.22
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB1	6	0.22
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB2	6	0.22
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB3	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1756)	1:A:143:LEU:HD11	1:A:163:GLN:HB2	9	0.22
(1,1756)	1:A:143:LEU:HD11	1:A:163:GLN:HB3	9	0.22
(1,1756)	1:A:143:LEU:HD12	1:A:163:GLN:HB2	9	0.22
(1,1756)	1:A:143:LEU:HD12	1:A:163:GLN:HB3	9	0.22
(1,1756)	1:A:143:LEU:HD13	1:A:163:GLN:HB2	9	0.22
(1,1756)	1:A:143:LEU:HD13	1:A:163:GLN:HB3	9	0.22
(1,1756)	1:A:143:LEU:HD21	1:A:163:GLN:HB2	9	0.22
(1,1756)	1:A:143:LEU:HD21	1:A:163:GLN:HB3	9	0.22
(1,1756)	1:A:143:LEU:HD22	1:A:163:GLN:HB2	9	0.22
(1,1756)	1:A:143:LEU:HD22	1:A:163:GLN:HB3	9	0.22
(1,1756)	1:A:143:LEU:HD23	1:A:163:GLN:HB2	9	0.22
(1,1756)	1:A:143:LEU:HD23	1:A:163:GLN:HB3	9	0.22
(1,1708)	1:A:136:LYS:H	1:A:136:LYS:HD2	10	0.22
(1,1708)	1:A:136:LYS:H	1:A:136:LYS:HD3	10	0.22
(1,1616)	1:A:119:ARG:HA	1:A:119:ARG:HD2	11	0.22
(1,1616)	1:A:119:ARG:HA	1:A:119:ARG:HD3	11	0.22
(1,1371)	1:A:209:ASN:HA	1:A:210:ASP:H	20	0.22
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB1	12	0.22
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB2	12	0.22
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB3	12	0.22
(1,806)	1:A:99:TYR:HE1	1:A:101:VAL:HA	2	0.21
(1,806)	1:A:99:TYR:HE2	1:A:101:VAL:HA	2	0.21
(1,806)	1:A:99:TYR:HE1	1:A:101:VAL:HA	14	0.21
(1,806)	1:A:99:TYR:HE2	1:A:101:VAL:HA	14	0.21
(1,530)	1:A:133:ILE:HG21	1:A:134:ASP:HB2	15	0.21
(1,530)	1:A:133:ILE:HG21	1:A:134:ASP:HB3	15	0.21
(1,530)	1:A:133:ILE:HG22	1:A:134:ASP:HB2	15	0.21
(1,530)	1:A:133:ILE:HG22	1:A:134:ASP:HB3	15	0.21
(1,530)	1:A:133:ILE:HG23	1:A:134:ASP:HB2	15	0.21
(1,530)	1:A:133:ILE:HG23	1:A:134:ASP:HB3	15	0.21
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	16	0.21
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	16	0.21
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	16	0.21
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG11	2	0.21
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG12	2	0.21
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG13	2	0.21
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG21	2	0.21
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG22	2	0.21
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG23	2	0.21
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG11	2	0.21
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG12	2	0.21
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG13	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG21	2	0.21
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG22	2	0.21
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG23	2	0.21
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB1	9	0.21
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB2	9	0.21
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB3	9	0.21
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB1	9	0.21
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB2	9	0.21
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB3	9	0.21
(1,1759)	1:A:143:LEU:HD11	1:A:164:GLN:H	16	0.21
(1,1759)	1:A:143:LEU:HD12	1:A:164:GLN:H	16	0.21
(1,1759)	1:A:143:LEU:HD13	1:A:164:GLN:H	16	0.21
(1,1759)	1:A:143:LEU:HD21	1:A:164:GLN:H	16	0.21
(1,1759)	1:A:143:LEU:HD22	1:A:164:GLN:H	16	0.21
(1,1759)	1:A:143:LEU:HD23	1:A:164:GLN:H	16	0.21
(1,1712)	1:A:136:LYS:HB2	1:A:136:LYS:HE2	3	0.21
(1,1712)	1:A:136:LYS:HB2	1:A:136:LYS:HE3	3	0.21
(1,1712)	1:A:136:LYS:HB3	1:A:136:LYS:HE2	3	0.21
(1,1712)	1:A:136:LYS:HB3	1:A:136:LYS:HE3	3	0.21
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE2	16	0.21
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE3	16	0.21
(1,1616)	1:A:119:ARG:HA	1:A:119:ARG:HD2	17	0.21
(1,1616)	1:A:119:ARG:HA	1:A:119:ARG:HD3	17	0.21
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD11	20	0.21
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD12	20	0.21
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD13	20	0.21
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD21	20	0.21
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD22	20	0.21
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD23	20	0.21
(1,1450)	1:A:142:LEU:HB2	1:A:185:LYS:H	15	0.21
(1,1450)	1:A:142:LEU:HB3	1:A:185:LYS:H	15	0.21
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD11	1	0.21
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD12	1	0.21
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD13	1	0.21
(1,797)	1:A:131:THR:HB	1:A:132:LEU:HD21	4	0.2
(1,797)	1:A:131:THR:HB	1:A:132:LEU:HD22	4	0.2
(1,797)	1:A:131:THR:HB	1:A:132:LEU:HD23	4	0.2
(1,530)	1:A:133:ILE:HG21	1:A:134:ASP:HB2	20	0.2
(1,530)	1:A:133:ILE:HG21	1:A:134:ASP:HB3	20	0.2
(1,530)	1:A:133:ILE:HG22	1:A:134:ASP:HB2	20	0.2
(1,530)	1:A:133:ILE:HG22	1:A:134:ASP:HB3	20	0.2
(1,530)	1:A:133:ILE:HG23	1:A:134:ASP:HB2	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,530)	1:A:133:ILE:HG23	1:A:134:ASP:HB3	20	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	2	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	2	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	2	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	4	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	4	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	4	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	7	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	7	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	7	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	10	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	10	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	10	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	15	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	15	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	15	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	17	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	17	0.2
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	17	0.2
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE2	9	0.2
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE3	9	0.2
(1,1615)	1:A:119:ARG:HA	1:A:119:ARG:HG2	2	0.2
(1,1615)	1:A:119:ARG:HA	1:A:119:ARG:HG3	2	0.2
(1,1607)	1:A:117:GLU:HB2	1:A:118:ASP:HB2	8	0.2
(1,1607)	1:A:117:GLU:HB2	1:A:118:ASP:HB3	8	0.2
(1,1607)	1:A:117:GLU:HB3	1:A:118:ASP:HB2	8	0.2
(1,1607)	1:A:117:GLU:HB3	1:A:118:ASP:HB3	8	0.2
(1,1399)	1:A:120:LYS:H	1:A:120:LYS:HG2	10	0.2
(1,1399)	1:A:120:LYS:H	1:A:120:LYS:HG3	10	0.2
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD11	8	0.2
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD12	8	0.2
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD13	8	0.2
(1,1095)	1:A:131:THR:H	1:A:131:THR:HB	18	0.2
(1,806)	1:A:99:TYR:HE1	1:A:101:VAL:HA	4	0.19
(1,806)	1:A:99:TYR:HE2	1:A:101:VAL:HA	4	0.19
(1,801)	1:A:146:ILE:HG21	1:A:159:HIS:HB2	17	0.19
(1,801)	1:A:146:ILE:HG21	1:A:159:HIS:HB3	17	0.19
(1,801)	1:A:146:ILE:HG22	1:A:159:HIS:HB2	17	0.19
(1,801)	1:A:146:ILE:HG22	1:A:159:HIS:HB3	17	0.19
(1,801)	1:A:146:ILE:HG23	1:A:159:HIS:HB2	17	0.19
(1,801)	1:A:146:ILE:HG23	1:A:159:HIS:HB3	17	0.19
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	3	0.19
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	3	0.19
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	9	0.19
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	9	0.19
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	9	0.19
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	13	0.19
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	13	0.19
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	13	0.19
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	19	0.19
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	19	0.19
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	19	0.19
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	20	0.19
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	20	0.19
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	20	0.19
(1,2042)	1:A:191:TRP:HA	1:A:185:LYS:HB2	4	0.19
(1,2042)	1:A:191:TRP:HA	1:A:185:LYS:HB3	4	0.19
(1,1999)	1:A:191:TRP:HB2	1:A:193:ALA:HB1	14	0.19
(1,1999)	1:A:191:TRP:HB2	1:A:193:ALA:HB2	14	0.19
(1,1999)	1:A:191:TRP:HB2	1:A:193:ALA:HB3	14	0.19
(1,1999)	1:A:191:TRP:HB3	1:A:193:ALA:HB1	14	0.19
(1,1999)	1:A:191:TRP:HB3	1:A:193:ALA:HB2	14	0.19
(1,1999)	1:A:191:TRP:HB3	1:A:193:ALA:HB3	14	0.19
(1,179)	1:A:100:ILE:HD11	1:A:101:VAL:H	9	0.19
(1,179)	1:A:100:ILE:HD12	1:A:101:VAL:H	9	0.19
(1,179)	1:A:100:ILE:HD13	1:A:101:VAL:H	9	0.19
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB1	12	0.19
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB2	12	0.19
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB3	12	0.19
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB1	12	0.19
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB2	12	0.19
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB3	12	0.19
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB1	14	0.19
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB2	14	0.19
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB3	14	0.19
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB1	14	0.19
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB2	14	0.19
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB3	14	0.19
(1,1756)	1:A:143:LEU:HD11	1:A:163:GLN:HB2	17	0.19
(1,1756)	1:A:143:LEU:HD11	1:A:163:GLN:HB3	17	0.19
(1,1756)	1:A:143:LEU:HD12	1:A:163:GLN:HB2	17	0.19
(1,1756)	1:A:143:LEU:HD12	1:A:163:GLN:HB3	17	0.19
(1,1756)	1:A:143:LEU:HD13	1:A:163:GLN:HB2	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1756)	1:A:143:LEU:HD13	1:A:163:GLN:HB3	17	0.19
(1,1756)	1:A:143:LEU:HD21	1:A:163:GLN:HB2	17	0.19
(1,1756)	1:A:143:LEU:HD21	1:A:163:GLN:HB3	17	0.19
(1,1756)	1:A:143:LEU:HD22	1:A:163:GLN:HB2	17	0.19
(1,1756)	1:A:143:LEU:HD22	1:A:163:GLN:HB3	17	0.19
(1,1756)	1:A:143:LEU:HD23	1:A:163:GLN:HB2	17	0.19
(1,1756)	1:A:143:LEU:HD23	1:A:163:GLN:HB3	17	0.19
(1,1711)	1:A:136:LYS:HA	1:A:136:LYS:HE2	4	0.19
(1,1711)	1:A:136:LYS:HA	1:A:136:LYS:HE3	4	0.19
(1,1691)	1:A:132:LEU:HB2	1:A:133:ILE:H	19	0.19
(1,1691)	1:A:132:LEU:HB3	1:A:133:ILE:H	19	0.19
(1,1652)	1:A:124:TRP:HZ3	1:A:126:LYS:HE2	15	0.19
(1,1652)	1:A:124:TRP:HZ3	1:A:126:LYS:HE3	15	0.19
(1,1607)	1:A:117:GLU:HB2	1:A:118:ASP:HB2	17	0.19
(1,1607)	1:A:117:GLU:HB2	1:A:118:ASP:HB3	17	0.19
(1,1607)	1:A:117:GLU:HB3	1:A:118:ASP:HB2	17	0.19
(1,1607)	1:A:117:GLU:HB3	1:A:118:ASP:HB3	17	0.19
(1,1450)	1:A:142:LEU:HB2	1:A:185:LYS:H	18	0.19
(1,1450)	1:A:142:LEU:HB3	1:A:185:LYS:H	18	0.19
(1,1328)	1:A:200:ILE:H	1:A:200:ILE:HD11	3	0.19
(1,1328)	1:A:200:ILE:H	1:A:200:ILE:HD12	3	0.19
(1,1328)	1:A:200:ILE:H	1:A:200:ILE:HD13	3	0.19
(1,673)	1:A:127:TRP:HE3	1:A:146:ILE:HG21	20	0.18
(1,673)	1:A:127:TRP:HE3	1:A:146:ILE:HG22	20	0.18
(1,673)	1:A:127:TRP:HE3	1:A:146:ILE:HG23	20	0.18
(1,531)	1:A:191:TRP:HE3	1:A:193:ALA:HB1	10	0.18
(1,531)	1:A:191:TRP:HE3	1:A:193:ALA:HB2	10	0.18
(1,531)	1:A:191:TRP:HE3	1:A:193:ALA:HB3	10	0.18
(1,2039)	1:A:191:TRP:HH2	1:A:160:PHE:HE1	9	0.18
(1,2039)	1:A:191:TRP:HH2	1:A:160:PHE:HE2	9	0.18
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE2	17	0.18
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE3	17	0.18
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE2	17	0.18
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE3	17	0.18
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE2	19	0.18
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE3	19	0.18
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE2	19	0.18
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE3	19	0.18
(1,1711)	1:A:136:LYS:HA	1:A:136:LYS:HE2	5	0.18
(1,1711)	1:A:136:LYS:HA	1:A:136:LYS:HE3	5	0.18
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD11	18	0.18
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD12	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD13	18	0.18
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD21	18	0.18
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD22	18	0.18
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD23	18	0.18
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG11	16	0.18
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG12	16	0.18
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG13	16	0.18
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG21	16	0.18
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG22	16	0.18
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG23	16	0.18
(1,1450)	1:A:142:LEU:HB2	1:A:185:LYS:H	4	0.18
(1,1450)	1:A:142:LEU:HB3	1:A:185:LYS:H	4	0.18
(1,1366)	1:A:207:THR:HB	1:A:208:MET:H	5	0.18
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD11	5	0.18
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD12	5	0.18
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD13	5	0.18
(1,1070)	1:A:123:LEU:HG	1:A:124:TRP:H	19	0.18
(1,797)	1:A:131:THR:HB	1:A:132:LEU:HD21	1	0.17
(1,797)	1:A:131:THR:HB	1:A:132:LEU:HD22	1	0.17
(1,797)	1:A:131:THR:HB	1:A:132:LEU:HD23	1	0.17
(1,475)	1:A:127:TRP:HZ2	1:A:165:THR:HB	19	0.17
(1,1932)	1:A:177:LYS:H	1:A:177:LYS:HD2	7	0.17
(1,1932)	1:A:177:LYS:H	1:A:177:LYS:HD3	7	0.17
(1,1832)	1:A:150:PRO:HA	1:A:151:GLU:HG2	14	0.17
(1,1832)	1:A:150:PRO:HA	1:A:151:GLU:HG3	14	0.17
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB1	10	0.17
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB2	10	0.17
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB3	10	0.17
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB1	10	0.17
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB2	10	0.17
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB3	10	0.17
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB1	15	0.17
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB2	15	0.17
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB3	15	0.17
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB1	15	0.17
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB2	15	0.17
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB3	15	0.17
(1,1722)	1:A:141:THR:HB	1:A:163:GLN:HG2	5	0.17
(1,1722)	1:A:141:THR:HB	1:A:163:GLN:HG3	5	0.17
(1,1708)	1:A:136:LYS:H	1:A:136:LYS:HD2	13	0.17
(1,1708)	1:A:136:LYS:H	1:A:136:LYS:HD3	13	0.17
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD11	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD12	7	0.17
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD13	7	0.17
(1,110)	1:A:135:LEU:HA	1:A:135:LEU:HG	14	0.17
(1,569)	1:A:201:GLN:HE21	1:A:202:ILE:HD11	4	0.16
(1,569)	1:A:201:GLN:HE21	1:A:202:ILE:HD12	4	0.16
(1,569)	1:A:201:GLN:HE21	1:A:202:ILE:HD13	4	0.16
(1,569)	1:A:201:GLN:HE22	1:A:202:ILE:HD11	4	0.16
(1,569)	1:A:201:GLN:HE22	1:A:202:ILE:HD12	4	0.16
(1,569)	1:A:201:GLN:HE22	1:A:202:ILE:HD13	4	0.16
(1,536)	1:A:193:ALA:HB1	1:A:194:TRP:HD1	10	0.16
(1,536)	1:A:193:ALA:HB2	1:A:194:TRP:HD1	10	0.16
(1,536)	1:A:193:ALA:HB3	1:A:194:TRP:HD1	10	0.16
(1,378)	1:A:99:TYR:HA	1:A:100:ILE:HB	15	0.16
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG21	3	0.16
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG22	3	0.16
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG23	3	0.16
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG21	3	0.16
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG22	3	0.16
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG23	3	0.16
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG21	5	0.16
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG22	5	0.16
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG23	5	0.16
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG21	5	0.16
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG22	5	0.16
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG23	5	0.16
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG11	12	0.16
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG12	12	0.16
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG13	12	0.16
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG21	12	0.16
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG22	12	0.16
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG23	12	0.16
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG11	12	0.16
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG12	12	0.16
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG13	12	0.16
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG21	12	0.16
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG22	12	0.16
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG23	12	0.16
(1,1985)	1:A:185:LYS:HA	1:A:185:LYS:HE2	18	0.16
(1,1985)	1:A:185:LYS:HA	1:A:185:LYS:HE3	18	0.16
(1,1715)	1:A:136:LYS:HD2	1:A:137:THR:H	15	0.16
(1,1715)	1:A:136:LYS:HD3	1:A:137:THR:H	15	0.16
(1,1620)	1:A:120:LYS:H	1:A:120:LYS:HE2	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1620)	1:A:120:LYS:H	1:A:120:LYS:HE3	9	0.16
(1,1606)	1:A:117:GLU:HB2	1:A:118:ASP:H	20	0.16
(1,1606)	1:A:117:GLU:HB3	1:A:118:ASP:H	20	0.16
(1,1499)	1:A:107:LEU:HD11	1:A:108:GLU:HA	6	0.16
(1,1499)	1:A:107:LEU:HD12	1:A:108:GLU:HA	6	0.16
(1,1499)	1:A:107:LEU:HD13	1:A:108:GLU:HA	6	0.16
(1,1499)	1:A:107:LEU:HD21	1:A:108:GLU:HA	6	0.16
(1,1499)	1:A:107:LEU:HD22	1:A:108:GLU:HA	6	0.16
(1,1499)	1:A:107:LEU:HD23	1:A:108:GLU:HA	6	0.16
(1,1450)	1:A:142:LEU:HB2	1:A:185:LYS:H	13	0.16
(1,1450)	1:A:142:LEU:HB3	1:A:185:LYS:H	13	0.16
(1,1399)	1:A:120:LYS:H	1:A:120:LYS:HG2	4	0.16
(1,1399)	1:A:120:LYS:H	1:A:120:LYS:HG3	4	0.16
(1,1397)	1:A:106:PRO:HB2	1:A:107:LEU:H	1	0.16
(1,1397)	1:A:106:PRO:HB3	1:A:107:LEU:H	1	0.16
(1,1310)	1:A:145:GLU:H	1:A:146:ILE:HD11	17	0.16
(1,1310)	1:A:145:GLU:H	1:A:146:ILE:HD12	17	0.16
(1,1310)	1:A:145:GLU:H	1:A:146:ILE:HD13	17	0.16
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD11	16	0.16
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD12	16	0.16
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD13	16	0.16
(1,806)	1:A:99:TYR:HE1	1:A:101:VAL:HA	15	0.15
(1,806)	1:A:99:TYR:HE2	1:A:101:VAL:HA	15	0.15
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB1	11	0.15
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB2	11	0.15
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB3	11	0.15
(1,390)	1:A:100:ILE:HG21	1:A:190:TYR:H	4	0.15
(1,390)	1:A:100:ILE:HG22	1:A:190:TYR:H	4	0.15
(1,390)	1:A:100:ILE:HG23	1:A:190:TYR:H	4	0.15
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG21	6	0.15
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG22	6	0.15
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG23	6	0.15
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG21	6	0.15
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG22	6	0.15
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG23	6	0.15
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG11	10	0.15
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG12	10	0.15
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG13	10	0.15
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG21	10	0.15
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG22	10	0.15
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG23	10	0.15
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG11	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG12	10	0.15
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG13	10	0.15
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG21	10	0.15
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG22	10	0.15
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG23	10	0.15
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG11	16	0.15
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG12	16	0.15
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG13	16	0.15
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG21	16	0.15
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG22	16	0.15
(1,2030)	1:A:183:ARG:HG2	1:A:182:VAL:HG23	16	0.15
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG11	16	0.15
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG12	16	0.15
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG13	16	0.15
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG21	16	0.15
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG22	16	0.15
(1,2030)	1:A:183:ARG:HG3	1:A:182:VAL:HG23	16	0.15
(1,1985)	1:A:185:LYS:HA	1:A:185:LYS:HE2	2	0.15
(1,1985)	1:A:185:LYS:HA	1:A:185:LYS:HE3	2	0.15
(1,179)	1:A:100:ILE:HD11	1:A:101:VAL:H	7	0.15
(1,179)	1:A:100:ILE:HD12	1:A:101:VAL:H	7	0.15
(1,179)	1:A:100:ILE:HD13	1:A:101:VAL:H	7	0.15
(1,179)	1:A:100:ILE:HD11	1:A:101:VAL:H	17	0.15
(1,179)	1:A:100:ILE:HD12	1:A:101:VAL:H	17	0.15
(1,179)	1:A:100:ILE:HD13	1:A:101:VAL:H	17	0.15
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD11	9	0.15
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD12	9	0.15
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD13	9	0.15
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD21	9	0.15
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD22	9	0.15
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD23	9	0.15
(1,1715)	1:A:136:LYS:HD2	1:A:137:THR:H	20	0.15
(1,1715)	1:A:136:LYS:HD3	1:A:137:THR:H	20	0.15
(1,1711)	1:A:136:LYS:HA	1:A:136:LYS:HE2	18	0.15
(1,1711)	1:A:136:LYS:HA	1:A:136:LYS:HE3	18	0.15
(1,1691)	1:A:132:LEU:HB2	1:A:133:ILE:H	13	0.15
(1,1691)	1:A:132:LEU:HB3	1:A:133:ILE:H	13	0.15
(1,1607)	1:A:117:GLU:HB2	1:A:118:ASP:HB2	7	0.15
(1,1607)	1:A:117:GLU:HB2	1:A:118:ASP:HB3	7	0.15
(1,1607)	1:A:117:GLU:HB3	1:A:118:ASP:HB2	7	0.15
(1,1607)	1:A:117:GLU:HB3	1:A:118:ASP:HB3	7	0.15
(1,1587)	1:A:114:LYS:HE2	1:A:115:GLN:H	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1587)	1:A:114:LYS:HE3	1:A:115:GLN:H	5	0.15
(1,1571)	1:A:114:LYS:H	1:A:114:LYS:HE2	20	0.15
(1,1571)	1:A:114:LYS:H	1:A:114:LYS:HE3	20	0.15
(1,1569)	1:A:114:LYS:H	1:A:114:LYS:HG2	4	0.15
(1,1569)	1:A:114:LYS:H	1:A:114:LYS:HG3	4	0.15
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD11	14	0.15
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD12	14	0.15
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD13	14	0.15
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD21	14	0.15
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD22	14	0.15
(1,1552)	1:A:113:VAL:HB	1:A:123:LEU:HD23	14	0.15
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG11	15	0.15
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG12	15	0.15
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG13	15	0.15
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG21	15	0.15
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG22	15	0.15
(1,1474)	1:A:100:ILE:HA	1:A:101:VAL:HG23	15	0.15
(1,1397)	1:A:106:PRO:HB2	1:A:107:LEU:H	3	0.15
(1,1397)	1:A:106:PRO:HB3	1:A:107:LEU:H	3	0.15
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB1	10	0.15
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB2	10	0.15
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB3	10	0.15
(1,1204)	1:A:164:GLN:H	1:A:165:THR:HG21	16	0.15
(1,1204)	1:A:164:GLN:H	1:A:165:THR:HG22	16	0.15
(1,1204)	1:A:164:GLN:H	1:A:165:THR:HG23	16	0.15
(1,110)	1:A:135:LEU:HA	1:A:135:LEU:HG	10	0.15
(1,110)	1:A:135:LEU:HA	1:A:135:LEU:HG	16	0.15
(1,1099)	1:A:132:LEU:HA	1:A:134:ASP:H	15	0.15
(1,966)	1:A:99:TYR:HE1	1:A:100:ILE:HB	11	0.14
(1,966)	1:A:99:TYR:HE2	1:A:100:ILE:HB	11	0.14
(1,861)	1:A:143:LEU:HG	1:A:160:PHE:HZ	14	0.14
(1,857)	1:A:160:PHE:HA	1:A:160:PHE:HE1	10	0.14
(1,857)	1:A:160:PHE:HA	1:A:160:PHE:HE2	10	0.14
(1,827)	1:A:112:GLU:HB2	1:A:124:TRP:HE3	20	0.14
(1,827)	1:A:112:GLU:HB3	1:A:124:TRP:HE3	20	0.14
(1,820)	1:A:122:TYR:HD1	1:A:168:LYS:HG2	4	0.14
(1,820)	1:A:122:TYR:HD1	1:A:168:LYS:HG3	4	0.14
(1,820)	1:A:122:TYR:HD2	1:A:168:LYS:HG2	4	0.14
(1,820)	1:A:122:TYR:HD2	1:A:168:LYS:HG3	4	0.14
(1,806)	1:A:99:TYR:HE1	1:A:101:VAL:HA	16	0.14
(1,806)	1:A:99:TYR:HE2	1:A:101:VAL:HA	16	0.14
(1,673)	1:A:127:TRP:HE3	1:A:146:ILE:HG21	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:A:127:TRP:HE3	1:A:146:ILE:HG22	3	0.14
(1,673)	1:A:127:TRP:HE3	1:A:146:ILE:HG23	3	0.14
(1,531)	1:A:191:TRP:HE3	1:A:193:ALA:HB1	15	0.14
(1,531)	1:A:191:TRP:HE3	1:A:193:ALA:HB2	15	0.14
(1,531)	1:A:191:TRP:HE3	1:A:193:ALA:HB3	15	0.14
(1,469)	1:A:164:GLN:HB2	1:A:165:THR:H	20	0.14
(1,469)	1:A:164:GLN:HB3	1:A:165:THR:H	20	0.14
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB1	12	0.14
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB2	12	0.14
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB3	12	0.14
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB1	17	0.14
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB2	17	0.14
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB3	17	0.14
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD11	5	0.14
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD12	5	0.14
(1,44)	1:A:132:LEU:HA	1:A:132:LEU:HD13	5	0.14
(1,394)	1:A:111:VAL:HB	1:A:112:GLU:H	19	0.14
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD11	2	0.14
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD12	2	0.14
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD13	2	0.14
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD11	11	0.14
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD12	11	0.14
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD13	11	0.14
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD11	15	0.14
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD12	15	0.14
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD13	15	0.14
(1,2039)	1:A:191:TRP:HH2	1:A:160:PHE:HE1	14	0.14
(1,2039)	1:A:191:TRP:HH2	1:A:160:PHE:HE2	14	0.14
(1,2039)	1:A:191:TRP:HH2	1:A:160:PHE:HE1	15	0.14
(1,2039)	1:A:191:TRP:HH2	1:A:160:PHE:HE2	15	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG11	1	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG12	1	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG13	1	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG21	1	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG22	1	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG23	1	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG11	1	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG12	1	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG13	1	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG21	1	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG22	1	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG23	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG11	6	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG12	6	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG13	6	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG21	6	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG22	6	0.14
(1,2027)	1:A:188:HIS:HB2	1:A:101:VAL:HG23	6	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG11	6	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG12	6	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG13	6	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG21	6	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG22	6	0.14
(1,2027)	1:A:188:HIS:HB3	1:A:101:VAL:HG23	6	0.14
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG11	14	0.14
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG12	14	0.14
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG13	14	0.14
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG21	14	0.14
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG22	14	0.14
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG23	14	0.14
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG11	14	0.14
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG12	14	0.14
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG13	14	0.14
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG21	14	0.14
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG22	14	0.14
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG23	14	0.14
(1,2020)	1:A:176:GLN:HE21	1:A:152:LYS:HD2	8	0.14
(1,2020)	1:A:176:GLN:HE21	1:A:152:LYS:HD3	8	0.14
(1,2020)	1:A:176:GLN:HE22	1:A:152:LYS:HD2	8	0.14
(1,2020)	1:A:176:GLN:HE22	1:A:152:LYS:HD3	8	0.14
(1,1998)	1:A:190:TYR:HB2	1:A:191:TRP:H	10	0.14
(1,1998)	1:A:190:TYR:HB3	1:A:191:TRP:H	10	0.14
(1,1966)	1:A:181:GLN:HG2	1:A:198:THR:H	11	0.14
(1,1966)	1:A:181:GLN:HG3	1:A:198:THR:H	11	0.14
(1,1932)	1:A:177:LYS:H	1:A:177:LYS:HD2	19	0.14
(1,1932)	1:A:177:LYS:H	1:A:177:LYS:HD3	19	0.14
(1,1930)	1:A:176:GLN:HA	1:A:176:GLN:HE21	14	0.14
(1,1930)	1:A:176:GLN:HA	1:A:176:GLN:HE22	14	0.14
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE2	7	0.14
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE3	7	0.14
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE2	7	0.14
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE3	7	0.14
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB1	3	0.14
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB2	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB3	3	0.14
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB1	3	0.14
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB2	3	0.14
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB3	3	0.14
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB1	7	0.14
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB2	7	0.14
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB3	7	0.14
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB1	7	0.14
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB2	7	0.14
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB3	7	0.14
(1,1746)	1:A:143:LEU:HD11	1:A:144:TYR:H	3	0.14
(1,1746)	1:A:143:LEU:HD12	1:A:144:TYR:H	3	0.14
(1,1746)	1:A:143:LEU:HD13	1:A:144:TYR:H	3	0.14
(1,1746)	1:A:143:LEU:HD21	1:A:144:TYR:H	3	0.14
(1,1746)	1:A:143:LEU:HD22	1:A:144:TYR:H	3	0.14
(1,1746)	1:A:143:LEU:HD23	1:A:144:TYR:H	3	0.14
(1,1579)	1:A:114:LYS:HB2	1:A:114:LYS:HE2	11	0.14
(1,1579)	1:A:114:LYS:HB2	1:A:114:LYS:HE3	11	0.14
(1,1579)	1:A:114:LYS:HB3	1:A:114:LYS:HE2	11	0.14
(1,1579)	1:A:114:LYS:HB3	1:A:114:LYS:HE3	11	0.14
(1,1558)	1:A:113:VAL:HG11	1:A:124:TRP:H	19	0.14
(1,1558)	1:A:113:VAL:HG12	1:A:124:TRP:H	19	0.14
(1,1558)	1:A:113:VAL:HG13	1:A:124:TRP:H	19	0.14
(1,1558)	1:A:113:VAL:HG21	1:A:124:TRP:H	19	0.14
(1,1558)	1:A:113:VAL:HG22	1:A:124:TRP:H	19	0.14
(1,1558)	1:A:113:VAL:HG23	1:A:124:TRP:H	19	0.14
(1,1541)	1:A:112:GLU:HG2	1:A:113:VAL:H	19	0.14
(1,1541)	1:A:112:GLU:HG3	1:A:113:VAL:H	19	0.14
(1,1503)	1:A:107:LEU:HD11	1:A:130:PRO:HA	19	0.14
(1,1503)	1:A:107:LEU:HD12	1:A:130:PRO:HA	19	0.14
(1,1503)	1:A:107:LEU:HD13	1:A:130:PRO:HA	19	0.14
(1,1503)	1:A:107:LEU:HD21	1:A:130:PRO:HA	19	0.14
(1,1503)	1:A:107:LEU:HD22	1:A:130:PRO:HA	19	0.14
(1,1503)	1:A:107:LEU:HD23	1:A:130:PRO:HA	19	0.14
(1,1450)	1:A:142:LEU:HB2	1:A:185:LYS:H	6	0.14
(1,1450)	1:A:142:LEU:HB3	1:A:185:LYS:H	6	0.14
(1,1450)	1:A:142:LEU:HB2	1:A:185:LYS:H	11	0.14
(1,1450)	1:A:142:LEU:HB3	1:A:185:LYS:H	11	0.14
(1,1397)	1:A:106:PRO:HB2	1:A:107:LEU:H	13	0.14
(1,1397)	1:A:106:PRO:HB3	1:A:107:LEU:H	13	0.14
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB1	7	0.14
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB2	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB3	7	0.14
(1,1204)	1:A:164:GLN:H	1:A:165:THR:HG21	2	0.14
(1,1204)	1:A:164:GLN:H	1:A:165:THR:HG22	2	0.14
(1,1204)	1:A:164:GLN:H	1:A:165:THR:HG23	2	0.14
(1,110)	1:A:135:LEU:HA	1:A:135:LEU:HG	11	0.14
(1,94)	1:A:119:ARG:HA	1:A:119:ARG:HD2	2	0.13
(1,94)	1:A:119:ARG:HA	1:A:119:ARG:HD3	2	0.13
(1,93)	1:A:119:ARG:HA	1:A:119:ARG:HD2	2	0.13
(1,93)	1:A:119:ARG:HA	1:A:119:ARG:HD3	2	0.13
(1,917)	1:A:99:TYR:HE1	1:A:101:VAL:HB	14	0.13
(1,917)	1:A:99:TYR:HE2	1:A:101:VAL:HB	14	0.13
(1,552)	1:A:111:VAL:H	1:A:200:ILE:HD11	3	0.13
(1,552)	1:A:111:VAL:H	1:A:200:ILE:HD12	3	0.13
(1,552)	1:A:111:VAL:H	1:A:200:ILE:HD13	3	0.13
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD11	16	0.13
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD12	16	0.13
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD13	16	0.13
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG21	12	0.13
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG22	12	0.13
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG23	12	0.13
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG21	12	0.13
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG22	12	0.13
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG23	12	0.13
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG21	20	0.13
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG22	20	0.13
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG23	20	0.13
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG21	20	0.13
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG22	20	0.13
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG23	20	0.13
(1,2044)	1:A:191:TRP:HE3	1:A:192:SER:HA	15	0.13
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD11	17	0.13
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD12	17	0.13
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD13	17	0.13
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD21	17	0.13
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD22	17	0.13
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD23	17	0.13
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD11	17	0.13
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD12	17	0.13
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD13	17	0.13
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD21	17	0.13
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD22	17	0.13
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD23	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1970)	1:A:182:VAL:HG11	1:A:184:CYS:HB2	4	0.13
(1,1970)	1:A:182:VAL:HG11	1:A:184:CYS:HB3	4	0.13
(1,1970)	1:A:182:VAL:HG12	1:A:184:CYS:HB2	4	0.13
(1,1970)	1:A:182:VAL:HG12	1:A:184:CYS:HB3	4	0.13
(1,1970)	1:A:182:VAL:HG13	1:A:184:CYS:HB2	4	0.13
(1,1970)	1:A:182:VAL:HG13	1:A:184:CYS:HB3	4	0.13
(1,1970)	1:A:182:VAL:HG21	1:A:184:CYS:HB2	4	0.13
(1,1970)	1:A:182:VAL:HG21	1:A:184:CYS:HB3	4	0.13
(1,1970)	1:A:182:VAL:HG22	1:A:184:CYS:HB2	4	0.13
(1,1970)	1:A:182:VAL:HG22	1:A:184:CYS:HB3	4	0.13
(1,1970)	1:A:182:VAL:HG23	1:A:184:CYS:HB2	4	0.13
(1,1970)	1:A:182:VAL:HG23	1:A:184:CYS:HB3	4	0.13
(1,1932)	1:A:177:LYS:H	1:A:177:LYS:HD2	3	0.13
(1,1932)	1:A:177:LYS:H	1:A:177:LYS:HD3	3	0.13
(1,189)	1:A:110:ALA:HB1	1:A:111:VAL:H	13	0.13
(1,189)	1:A:110:ALA:HB2	1:A:111:VAL:H	13	0.13
(1,189)	1:A:110:ALA:HB3	1:A:111:VAL:H	13	0.13
(1,1864)	1:A:156:TRP:HE3	1:A:157:GLU:HB2	12	0.13
(1,1864)	1:A:156:TRP:HE3	1:A:157:GLU:HB3	12	0.13
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE2	18	0.13
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE3	18	0.13
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE2	18	0.13
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE3	18	0.13
(1,1800)	1:A:148:LEU:HD11	1:A:178:TYR:HB2	9	0.13
(1,1800)	1:A:148:LEU:HD11	1:A:178:TYR:HB3	9	0.13
(1,1800)	1:A:148:LEU:HD12	1:A:178:TYR:HB2	9	0.13
(1,1800)	1:A:148:LEU:HD12	1:A:178:TYR:HB3	9	0.13
(1,1800)	1:A:148:LEU:HD13	1:A:178:TYR:HB2	9	0.13
(1,1800)	1:A:148:LEU:HD13	1:A:178:TYR:HB3	9	0.13
(1,1800)	1:A:148:LEU:HD21	1:A:178:TYR:HB2	9	0.13
(1,1800)	1:A:148:LEU:HD21	1:A:178:TYR:HB3	9	0.13
(1,1800)	1:A:148:LEU:HD22	1:A:178:TYR:HB2	9	0.13
(1,1800)	1:A:148:LEU:HD22	1:A:178:TYR:HB3	9	0.13
(1,1800)	1:A:148:LEU:HD23	1:A:178:TYR:HB2	9	0.13
(1,1800)	1:A:148:LEU:HD23	1:A:178:TYR:HB3	9	0.13
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB1	19	0.13
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB2	19	0.13
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB3	19	0.13
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB1	19	0.13
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB2	19	0.13
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB3	19	0.13
(1,1746)	1:A:143:LEU:HD11	1:A:144:TYR:H	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1746)	1:A:143:LEU:HD12	1:A:144:TYR:H	8	0.13
(1,1746)	1:A:143:LEU:HD13	1:A:144:TYR:H	8	0.13
(1,1746)	1:A:143:LEU:HD21	1:A:144:TYR:H	8	0.13
(1,1746)	1:A:143:LEU:HD22	1:A:144:TYR:H	8	0.13
(1,1746)	1:A:143:LEU:HD23	1:A:144:TYR:H	8	0.13
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD11	2	0.13
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD12	2	0.13
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD13	2	0.13
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD21	2	0.13
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD22	2	0.13
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD23	2	0.13
(1,1648)	1:A:124:TRP:HE1	1:A:126:LYS:HD2	15	0.13
(1,1648)	1:A:124:TRP:HE1	1:A:126:LYS:HD3	15	0.13
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE2	1	0.13
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE3	1	0.13
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE2	11	0.13
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE3	11	0.13
(1,1616)	1:A:119:ARG:HA	1:A:119:ARG:HD2	8	0.13
(1,1616)	1:A:119:ARG:HA	1:A:119:ARG:HD3	8	0.13
(1,1575)	1:A:114:LYS:HA	1:A:114:LYS:HE2	18	0.13
(1,1575)	1:A:114:LYS:HA	1:A:114:LYS:HE3	18	0.13
(1,1450)	1:A:142:LEU:HB2	1:A:185:LYS:H	5	0.13
(1,1450)	1:A:142:LEU:HB3	1:A:185:LYS:H	5	0.13
(1,1450)	1:A:142:LEU:HB2	1:A:185:LYS:H	8	0.13
(1,1450)	1:A:142:LEU:HB3	1:A:185:LYS:H	8	0.13
(1,1450)	1:A:142:LEU:HB2	1:A:185:LYS:H	19	0.13
(1,1450)	1:A:142:LEU:HB3	1:A:185:LYS:H	19	0.13
(1,1366)	1:A:207:THR:HB	1:A:208:MET:H	14	0.13
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB1	17	0.13
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB2	17	0.13
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB3	17	0.13
(1,1190)	1:A:145:GLU:HG2	1:A:159:HIS:H	18	0.13
(1,1190)	1:A:145:GLU:HG3	1:A:159:HIS:H	18	0.13
(1,110)	1:A:135:LEU:HA	1:A:135:LEU:HG	5	0.13
(1,1073)	1:A:113:VAL:HB	1:A:124:TRP:H	14	0.13
(1,1070)	1:A:123:LEU:HG	1:A:124:TRP:H	15	0.13
(1,861)	1:A:143:LEU:HG	1:A:160:PHE:HZ	20	0.12
(1,857)	1:A:160:PHE:HA	1:A:160:PHE:HE1	14	0.12
(1,857)	1:A:160:PHE:HA	1:A:160:PHE:HE2	14	0.12
(1,857)	1:A:160:PHE:HA	1:A:160:PHE:HE1	20	0.12
(1,857)	1:A:160:PHE:HA	1:A:160:PHE:HE2	20	0.12
(1,852)	1:A:159:HIS:HE1	1:A:169:ILE:HG21	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,852)	1:A:159:HIS:HE1	1:A:169:ILE:HG22	17	0.12
(1,852)	1:A:159:HIS:HE1	1:A:169:ILE:HG23	17	0.12
(1,837)	1:A:135:LEU:HG	1:A:140:PHE:HD1	17	0.12
(1,837)	1:A:135:LEU:HG	1:A:140:PHE:HD2	17	0.12
(1,833)	1:A:139:TRP:HA	1:A:139:TRP:HD1	6	0.12
(1,830)	1:A:124:TRP:HD1	1:A:168:LYS:HG2	6	0.12
(1,830)	1:A:124:TRP:HD1	1:A:168:LYS:HG3	6	0.12
(1,531)	1:A:191:TRP:HE3	1:A:193:ALA:HB1	2	0.12
(1,531)	1:A:191:TRP:HE3	1:A:193:ALA:HB2	2	0.12
(1,531)	1:A:191:TRP:HE3	1:A:193:ALA:HB3	2	0.12
(1,460)	1:A:158:ILE:HD11	1:A:194:TRP:HZ2	17	0.12
(1,460)	1:A:158:ILE:HD12	1:A:194:TRP:HZ2	17	0.12
(1,460)	1:A:158:ILE:HD13	1:A:194:TRP:HZ2	17	0.12
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB1	2	0.12
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB2	2	0.12
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB3	2	0.12
(1,394)	1:A:111:VAL:HB	1:A:112:GLU:H	2	0.12
(1,394)	1:A:111:VAL:HB	1:A:112:GLU:H	11	0.12
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD11	6	0.12
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD12	6	0.12
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD13	6	0.12
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD11	17	0.12
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD12	17	0.12
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD13	17	0.12
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG21	7	0.12
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG22	7	0.12
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG23	7	0.12
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG21	7	0.12
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG22	7	0.12
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG23	7	0.12
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG21	9	0.12
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG22	9	0.12
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG23	9	0.12
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG21	9	0.12
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG22	9	0.12
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG23	9	0.12
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG21	13	0.12
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG22	13	0.12
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG23	13	0.12
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG21	13	0.12
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG22	13	0.12
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG23	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2034)	1:A:185:LYS:HD2	1:A:143:LEU:HD11	2	0.12
(1,2034)	1:A:185:LYS:HD2	1:A:143:LEU:HD12	2	0.12
(1,2034)	1:A:185:LYS:HD2	1:A:143:LEU:HD13	2	0.12
(1,2034)	1:A:185:LYS:HD2	1:A:143:LEU:HD21	2	0.12
(1,2034)	1:A:185:LYS:HD2	1:A:143:LEU:HD22	2	0.12
(1,2034)	1:A:185:LYS:HD2	1:A:143:LEU:HD23	2	0.12
(1,2034)	1:A:185:LYS:HD3	1:A:143:LEU:HD11	2	0.12
(1,2034)	1:A:185:LYS:HD3	1:A:143:LEU:HD12	2	0.12
(1,2034)	1:A:185:LYS:HD3	1:A:143:LEU:HD13	2	0.12
(1,2034)	1:A:185:LYS:HD3	1:A:143:LEU:HD21	2	0.12
(1,2034)	1:A:185:LYS:HD3	1:A:143:LEU:HD22	2	0.12
(1,2034)	1:A:185:LYS:HD3	1:A:143:LEU:HD23	2	0.12
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG11	6	0.12
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG12	6	0.12
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG13	6	0.12
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG21	6	0.12
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG22	6	0.12
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG23	6	0.12
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG11	6	0.12
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG12	6	0.12
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG13	6	0.12
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG21	6	0.12
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG22	6	0.12
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG23	6	0.12
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG11	15	0.12
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG12	15	0.12
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG13	15	0.12
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG21	15	0.12
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG22	15	0.12
(1,2021)	1:A:189:GLY:HA2	1:A:101:VAL:HG23	15	0.12
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG11	15	0.12
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG12	15	0.12
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG13	15	0.12
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG21	15	0.12
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG22	15	0.12
(1,2021)	1:A:189:GLY:HA3	1:A:101:VAL:HG23	15	0.12
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD11	16	0.12
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD12	16	0.12
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD13	16	0.12
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD21	16	0.12
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD22	16	0.12
(1,2016)	1:A:181:GLN:HE21	1:A:179:LEU:HD23	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD11	16	0.12
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD12	16	0.12
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD13	16	0.12
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD21	16	0.12
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD22	16	0.12
(1,2016)	1:A:181:GLN:HE22	1:A:179:LEU:HD23	16	0.12
(1,1992)	1:A:186:PRO:HG2	1:A:187:ASP:H	14	0.12
(1,1992)	1:A:186:PRO:HG3	1:A:187:ASP:H	14	0.12
(1,1933)	1:A:177:LYS:HA	1:A:177:LYS:HD2	6	0.12
(1,1933)	1:A:177:LYS:HA	1:A:177:LYS:HD3	6	0.12
(1,1930)	1:A:176:GLN:HA	1:A:176:GLN:HE21	8	0.12
(1,1930)	1:A:176:GLN:HA	1:A:176:GLN:HE22	8	0.12
(1,1873)	1:A:157:GLU:HG2	1:A:158:ILE:H	20	0.12
(1,1873)	1:A:157:GLU:HG3	1:A:158:ILE:H	20	0.12
(1,1858)	1:A:154:ALA:HB1	1:A:155:GLU:HB2	5	0.12
(1,1858)	1:A:154:ALA:HB1	1:A:155:GLU:HB3	5	0.12
(1,1858)	1:A:154:ALA:HB2	1:A:155:GLU:HB2	5	0.12
(1,1858)	1:A:154:ALA:HB2	1:A:155:GLU:HB3	5	0.12
(1,1858)	1:A:154:ALA:HB3	1:A:155:GLU:HB2	5	0.12
(1,1858)	1:A:154:ALA:HB3	1:A:155:GLU:HB3	5	0.12
(1,1850)	1:A:152:LYS:H	1:A:152:LYS:HD2	8	0.12
(1,1850)	1:A:152:LYS:H	1:A:152:LYS:HD3	8	0.12
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE2	9	0.12
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE3	9	0.12
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE2	9	0.12
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE3	9	0.12
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE2	11	0.12
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE3	11	0.12
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE2	11	0.12
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE3	11	0.12
(1,1800)	1:A:148:LEU:HD11	1:A:178:TYR:HB2	15	0.12
(1,1800)	1:A:148:LEU:HD11	1:A:178:TYR:HB3	15	0.12
(1,1800)	1:A:148:LEU:HD12	1:A:178:TYR:HB2	15	0.12
(1,1800)	1:A:148:LEU:HD12	1:A:178:TYR:HB3	15	0.12
(1,1800)	1:A:148:LEU:HD13	1:A:178:TYR:HB2	15	0.12
(1,1800)	1:A:148:LEU:HD13	1:A:178:TYR:HB3	15	0.12
(1,1800)	1:A:148:LEU:HD21	1:A:178:TYR:HB2	15	0.12
(1,1800)	1:A:148:LEU:HD21	1:A:178:TYR:HB3	15	0.12
(1,1800)	1:A:148:LEU:HD22	1:A:178:TYR:HB2	15	0.12
(1,1800)	1:A:148:LEU:HD22	1:A:178:TYR:HB3	15	0.12
(1,1800)	1:A:148:LEU:HD23	1:A:178:TYR:HB2	15	0.12
(1,1800)	1:A:148:LEU:HD23	1:A:178:TYR:HB3	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1783)	1:A:147:ARG:HH21	1:A:181:GLN:HB2	11	0.12
(1,1783)	1:A:147:ARG:HH21	1:A:181:GLN:HB3	11	0.12
(1,1783)	1:A:147:ARG:HH22	1:A:181:GLN:HB2	11	0.12
(1,1783)	1:A:147:ARG:HH22	1:A:181:GLN:HB3	11	0.12
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD11	15	0.12
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD12	15	0.12
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD13	15	0.12
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD21	15	0.12
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD22	15	0.12
(1,1776)	1:A:147:ARG:HA	1:A:148:LEU:HD23	15	0.12
(1,1759)	1:A:143:LEU:HD11	1:A:164:GLN:H	4	0.12
(1,1759)	1:A:143:LEU:HD12	1:A:164:GLN:H	4	0.12
(1,1759)	1:A:143:LEU:HD13	1:A:164:GLN:H	4	0.12
(1,1759)	1:A:143:LEU:HD21	1:A:164:GLN:H	4	0.12
(1,1759)	1:A:143:LEU:HD22	1:A:164:GLN:H	4	0.12
(1,1759)	1:A:143:LEU:HD23	1:A:164:GLN:H	4	0.12
(1,1756)	1:A:143:LEU:HD11	1:A:163:GLN:HB2	8	0.12
(1,1756)	1:A:143:LEU:HD11	1:A:163:GLN:HB3	8	0.12
(1,1756)	1:A:143:LEU:HD12	1:A:163:GLN:HB2	8	0.12
(1,1756)	1:A:143:LEU:HD12	1:A:163:GLN:HB3	8	0.12
(1,1756)	1:A:143:LEU:HD13	1:A:163:GLN:HB2	8	0.12
(1,1756)	1:A:143:LEU:HD13	1:A:163:GLN:HB3	8	0.12
(1,1756)	1:A:143:LEU:HD21	1:A:163:GLN:HB2	8	0.12
(1,1756)	1:A:143:LEU:HD21	1:A:163:GLN:HB3	8	0.12
(1,1756)	1:A:143:LEU:HD22	1:A:163:GLN:HB2	8	0.12
(1,1756)	1:A:143:LEU:HD22	1:A:163:GLN:HB3	8	0.12
(1,1756)	1:A:143:LEU:HD23	1:A:163:GLN:HB2	8	0.12
(1,1756)	1:A:143:LEU:HD23	1:A:163:GLN:HB3	8	0.12
(1,1715)	1:A:136:LYS:HD2	1:A:137:THR:H	14	0.12
(1,1715)	1:A:136:LYS:HD3	1:A:137:THR:H	14	0.12
(1,1579)	1:A:114:LYS:HB2	1:A:114:LYS:HE2	8	0.12
(1,1579)	1:A:114:LYS:HB2	1:A:114:LYS:HE3	8	0.12
(1,1579)	1:A:114:LYS:HB3	1:A:114:LYS:HE2	8	0.12
(1,1579)	1:A:114:LYS:HB3	1:A:114:LYS:HE3	8	0.12
(1,1579)	1:A:114:LYS:HB2	1:A:114:LYS:HE2	10	0.12
(1,1579)	1:A:114:LYS:HB2	1:A:114:LYS:HE3	10	0.12
(1,1579)	1:A:114:LYS:HB3	1:A:114:LYS:HE2	10	0.12
(1,1579)	1:A:114:LYS:HB3	1:A:114:LYS:HE3	10	0.12
(1,1579)	1:A:114:LYS:HB2	1:A:114:LYS:HE2	17	0.12
(1,1579)	1:A:114:LYS:HB2	1:A:114:LYS:HE3	17	0.12
(1,1579)	1:A:114:LYS:HB3	1:A:114:LYS:HE2	17	0.12
(1,1579)	1:A:114:LYS:HB3	1:A:114:LYS:HE3	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,154)	1:A:208:MET:HA	1:A:208:MET:HE1	8	0.12
(1,154)	1:A:208:MET:HA	1:A:208:MET:HE2	8	0.12
(1,154)	1:A:208:MET:HA	1:A:208:MET:HE3	8	0.12
(1,1493)	1:A:107:LEU:H	1:A:128:SER:HB2	19	0.12
(1,1493)	1:A:107:LEU:H	1:A:128:SER:HB3	19	0.12
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG11	2	0.12
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG12	2	0.12
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG13	2	0.12
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG21	2	0.12
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG22	2	0.12
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG23	2	0.12
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG11	2	0.12
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG12	2	0.12
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG13	2	0.12
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG21	2	0.12
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG22	2	0.12
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG23	2	0.12
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD11	2	0.12
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD12	2	0.12
(1,1458)	1:A:132:LEU:H	1:A:132:LEU:HD13	2	0.12
(1,1450)	1:A:142:LEU:HB2	1:A:185:LYS:H	12	0.12
(1,1450)	1:A:142:LEU:HB3	1:A:185:LYS:H	12	0.12
(1,1397)	1:A:106:PRO:HB2	1:A:107:LEU:H	14	0.12
(1,1397)	1:A:106:PRO:HB3	1:A:107:LEU:H	14	0.12
(1,1363)	1:A:207:THR:HG21	1:A:208:MET:H	17	0.12
(1,1363)	1:A:207:THR:HG22	1:A:208:MET:H	17	0.12
(1,1363)	1:A:207:THR:HG23	1:A:208:MET:H	17	0.12
(1,1204)	1:A:164:GLN:H	1:A:165:THR:HG21	4	0.12
(1,1204)	1:A:164:GLN:H	1:A:165:THR:HG22	4	0.12
(1,1204)	1:A:164:GLN:H	1:A:165:THR:HG23	4	0.12
(1,110)	1:A:135:LEU:HA	1:A:135:LEU:HG	19	0.12
(1,110)	1:A:135:LEU:HA	1:A:135:LEU:HG	20	0.12
(1,1099)	1:A:132:LEU:HA	1:A:134:ASP:H	20	0.12
(1,1070)	1:A:123:LEU:HG	1:A:124:TRP:H	4	0.12
(1,909)	1:A:191:TRP:H	1:A:191:TRP:HD1	10	0.11
(1,861)	1:A:143:LEU:HG	1:A:160:PHE:HZ	1	0.11
(1,857)	1:A:160:PHE:HA	1:A:160:PHE:HE1	7	0.11
(1,857)	1:A:160:PHE:HA	1:A:160:PHE:HE2	7	0.11
(1,857)	1:A:160:PHE:HA	1:A:160:PHE:HE1	12	0.11
(1,857)	1:A:160:PHE:HA	1:A:160:PHE:HE2	12	0.11
(1,857)	1:A:160:PHE:HA	1:A:160:PHE:HE1	17	0.11
(1,857)	1:A:160:PHE:HA	1:A:160:PHE:HE2	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:A:112:GLU:HB2	1:A:124:TRP:HE3	7	0.11
(1,827)	1:A:112:GLU:HB3	1:A:124:TRP:HE3	7	0.11
(1,806)	1:A:99:TYR:HE1	1:A:101:VAL:HA	10	0.11
(1,806)	1:A:99:TYR:HE2	1:A:101:VAL:HA	10	0.11
(1,674)	1:A:146:ILE:HG21	1:A:167:PHE:HE1	17	0.11
(1,674)	1:A:146:ILE:HG21	1:A:167:PHE:HE2	17	0.11
(1,674)	1:A:146:ILE:HG22	1:A:167:PHE:HE1	17	0.11
(1,674)	1:A:146:ILE:HG22	1:A:167:PHE:HE2	17	0.11
(1,674)	1:A:146:ILE:HG23	1:A:167:PHE:HE1	17	0.11
(1,674)	1:A:146:ILE:HG23	1:A:167:PHE:HE2	17	0.11
(1,673)	1:A:127:TRP:HE3	1:A:146:ILE:HG21	8	0.11
(1,673)	1:A:127:TRP:HE3	1:A:146:ILE:HG22	8	0.11
(1,673)	1:A:127:TRP:HE3	1:A:146:ILE:HG23	8	0.11
(1,673)	1:A:127:TRP:HE3	1:A:146:ILE:HG21	14	0.11
(1,673)	1:A:127:TRP:HE3	1:A:146:ILE:HG22	14	0.11
(1,673)	1:A:127:TRP:HE3	1:A:146:ILE:HG23	14	0.11
(1,475)	1:A:127:TRP:HZ2	1:A:165:THR:HB	7	0.11
(1,475)	1:A:127:TRP:HZ2	1:A:165:THR:HB	12	0.11
(1,470)	1:A:164:GLN:HA	1:A:165:THR:H	20	0.11
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB1	10	0.11
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB2	10	0.11
(1,458)	1:A:151:GLU:HA	1:A:153:ALA:HB3	10	0.11
(1,445)	1:A:136:LYS:HA	1:A:137:THR:HG21	17	0.11
(1,445)	1:A:136:LYS:HA	1:A:137:THR:HG22	17	0.11
(1,445)	1:A:136:LYS:HA	1:A:137:THR:HG23	17	0.11
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD11	9	0.11
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD12	9	0.11
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD13	9	0.11
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD11	10	0.11
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD12	10	0.11
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD13	10	0.11
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD11	14	0.11
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD12	14	0.11
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD13	14	0.11
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD11	18	0.11
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD12	18	0.11
(1,377)	1:A:99:TYR:HA	1:A:100:ILE:HD13	18	0.11
(1,37)	1:A:113:VAL:HA	1:A:123:LEU:HG	13	0.11
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG21	8	0.11
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG22	8	0.11
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG23	8	0.11
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG21	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG22	8	0.11
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG23	8	0.11
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG21	18	0.11
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG22	18	0.11
(1,337)	1:A:99:TYR:HE1	1:A:100:ILE:HG23	18	0.11
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG21	18	0.11
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG22	18	0.11
(1,337)	1:A:99:TYR:HE2	1:A:100:ILE:HG23	18	0.11
(1,2044)	1:A:191:TRP:HE3	1:A:192:SER:HA	3	0.11
(1,2032)	1:A:185:LYS:HB2	1:A:190:TYR:H	16	0.11
(1,2032)	1:A:185:LYS:HB3	1:A:190:TYR:H	16	0.11
(1,2026)	1:A:186:PRO:HD2	1:A:185:LYS:HD2	19	0.11
(1,2026)	1:A:186:PRO:HD2	1:A:185:LYS:HD3	19	0.11
(1,2026)	1:A:186:PRO:HD3	1:A:185:LYS:HD2	19	0.11
(1,2026)	1:A:186:PRO:HD3	1:A:185:LYS:HD3	19	0.11
(1,2017)	1:A:181:GLN:HE21	1:A:179:LEU:HB2	11	0.11
(1,2017)	1:A:181:GLN:HE21	1:A:179:LEU:HB3	11	0.11
(1,2017)	1:A:181:GLN:HE22	1:A:179:LEU:HB2	11	0.11
(1,2017)	1:A:181:GLN:HE22	1:A:179:LEU:HB3	11	0.11
(1,1985)	1:A:185:LYS:HA	1:A:185:LYS:HE2	13	0.11
(1,1985)	1:A:185:LYS:HA	1:A:185:LYS:HE3	13	0.11
(1,1933)	1:A:177:LYS:HA	1:A:177:LYS:HD2	20	0.11
(1,1933)	1:A:177:LYS:HA	1:A:177:LYS:HD3	20	0.11
(1,1930)	1:A:176:GLN:HA	1:A:176:GLN:HE21	3	0.11
(1,1930)	1:A:176:GLN:HA	1:A:176:GLN:HE22	3	0.11
(1,1864)	1:A:156:TRP:HE3	1:A:157:GLU:HB2	9	0.11
(1,1864)	1:A:156:TRP:HE3	1:A:157:GLU:HB3	9	0.11
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE2	8	0.11
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE3	8	0.11
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE2	8	0.11
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE3	8	0.11
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE2	10	0.11
(1,1841)	1:A:151:GLU:HB2	1:A:152:LYS:HE3	10	0.11
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE2	10	0.11
(1,1841)	1:A:151:GLU:HB3	1:A:152:LYS:HE3	10	0.11
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB1	20	0.11
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB2	20	0.11
(1,1787)	1:A:147:ARG:HH21	1:A:197:ALA:HB3	20	0.11
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB1	20	0.11
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB2	20	0.11
(1,1787)	1:A:147:ARG:HH22	1:A:197:ALA:HB3	20	0.11
(1,1717)	1:A:140:PHE:HD1	1:A:142:LEU:HD11	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1717)	1:A:140:PHE:HD1	1:A:142:LEU:HD12	15	0.11
(1,1717)	1:A:140:PHE:HD1	1:A:142:LEU:HD13	15	0.11
(1,1717)	1:A:140:PHE:HD1	1:A:142:LEU:HD21	15	0.11
(1,1717)	1:A:140:PHE:HD1	1:A:142:LEU:HD22	15	0.11
(1,1717)	1:A:140:PHE:HD1	1:A:142:LEU:HD23	15	0.11
(1,1717)	1:A:140:PHE:HD2	1:A:142:LEU:HD11	15	0.11
(1,1717)	1:A:140:PHE:HD2	1:A:142:LEU:HD12	15	0.11
(1,1717)	1:A:140:PHE:HD2	1:A:142:LEU:HD13	15	0.11
(1,1717)	1:A:140:PHE:HD2	1:A:142:LEU:HD21	15	0.11
(1,1717)	1:A:140:PHE:HD2	1:A:142:LEU:HD22	15	0.11
(1,1717)	1:A:140:PHE:HD2	1:A:142:LEU:HD23	15	0.11
(1,1715)	1:A:136:LYS:HD2	1:A:137:THR:H	2	0.11
(1,1715)	1:A:136:LYS:HD3	1:A:137:THR:H	2	0.11
(1,1705)	1:A:135:LEU:HD11	1:A:140:PHE:HZ	2	0.11
(1,1705)	1:A:135:LEU:HD12	1:A:140:PHE:HZ	2	0.11
(1,1705)	1:A:135:LEU:HD13	1:A:140:PHE:HZ	2	0.11
(1,1705)	1:A:135:LEU:HD21	1:A:140:PHE:HZ	2	0.11
(1,1705)	1:A:135:LEU:HD22	1:A:140:PHE:HZ	2	0.11
(1,1705)	1:A:135:LEU:HD23	1:A:140:PHE:HZ	2	0.11
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD11	13	0.11
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD12	13	0.11
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD13	13	0.11
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD21	13	0.11
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD22	13	0.11
(1,1696)	1:A:134:ASP:HA	1:A:135:LEU:HD23	13	0.11
(1,1694)	1:A:133:ILE:HG21	1:A:135:LEU:HB2	6	0.11
(1,1694)	1:A:133:ILE:HG21	1:A:135:LEU:HB3	6	0.11
(1,1694)	1:A:133:ILE:HG22	1:A:135:LEU:HB2	6	0.11
(1,1694)	1:A:133:ILE:HG22	1:A:135:LEU:HB3	6	0.11
(1,1694)	1:A:133:ILE:HG23	1:A:135:LEU:HB2	6	0.11
(1,1694)	1:A:133:ILE:HG23	1:A:135:LEU:HB3	6	0.11
(1,1691)	1:A:132:LEU:HB2	1:A:133:ILE:H	10	0.11
(1,1691)	1:A:132:LEU:HB3	1:A:133:ILE:H	10	0.11
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE2	3	0.11
(1,1621)	1:A:120:LYS:HA	1:A:120:LYS:HE3	3	0.11
(1,1587)	1:A:114:LYS:HE2	1:A:115:GLN:H	13	0.11
(1,1587)	1:A:114:LYS:HE3	1:A:115:GLN:H	13	0.11
(1,1575)	1:A:114:LYS:HA	1:A:114:LYS:HE2	13	0.11
(1,1575)	1:A:114:LYS:HA	1:A:114:LYS:HE3	13	0.11
(1,154)	1:A:208:MET:HA	1:A:208:MET:HE1	1	0.11
(1,154)	1:A:208:MET:HA	1:A:208:MET:HE2	1	0.11
(1,154)	1:A:208:MET:HA	1:A:208:MET:HE3	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG11	4	0.11
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG12	4	0.11
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG13	4	0.11
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG21	4	0.11
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG22	4	0.11
(1,1469)	1:A:99:TYR:HB2	1:A:101:VAL:HG23	4	0.11
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG11	4	0.11
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG12	4	0.11
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG13	4	0.11
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG21	4	0.11
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG22	4	0.11
(1,1469)	1:A:99:TYR:HB3	1:A:101:VAL:HG23	4	0.11
(1,1450)	1:A:142:LEU:HB2	1:A:185:LYS:H	3	0.11
(1,1450)	1:A:142:LEU:HB3	1:A:185:LYS:H	3	0.11
(1,1423)	1:A:172:LEU:H	1:A:172:LEU:HG	17	0.11
(1,1366)	1:A:207:THR:HB	1:A:208:MET:H	19	0.11
(1,1333)	1:A:200:ILE:HG12	1:A:201:GLN:H	3	0.11
(1,1333)	1:A:200:ILE:HG13	1:A:201:GLN:H	3	0.11
(1,1311)	1:A:193:ALA:HA	1:A:194:TRP:H	2	0.11
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB1	3	0.11
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB2	3	0.11
(1,1306)	1:A:192:SER:H	1:A:193:ALA:HB3	3	0.11
(1,1261)	1:A:176:GLN:HB2	1:A:177:LYS:H	18	0.11
(1,1261)	1:A:176:GLN:HB3	1:A:177:LYS:H	18	0.11
(1,1204)	1:A:164:GLN:H	1:A:165:THR:HG21	1	0.11
(1,1204)	1:A:164:GLN:H	1:A:165:THR:HG22	1	0.11
(1,1204)	1:A:164:GLN:H	1:A:165:THR:HG23	1	0.11
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD11	17	0.11
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD12	17	0.11
(1,1106)	1:A:133:ILE:H	1:A:133:ILE:HD13	17	0.11
(1,110)	1:A:135:LEU:HA	1:A:135:LEU:HG	18	0.11

10 Dihedral-angle violation analysis (i)

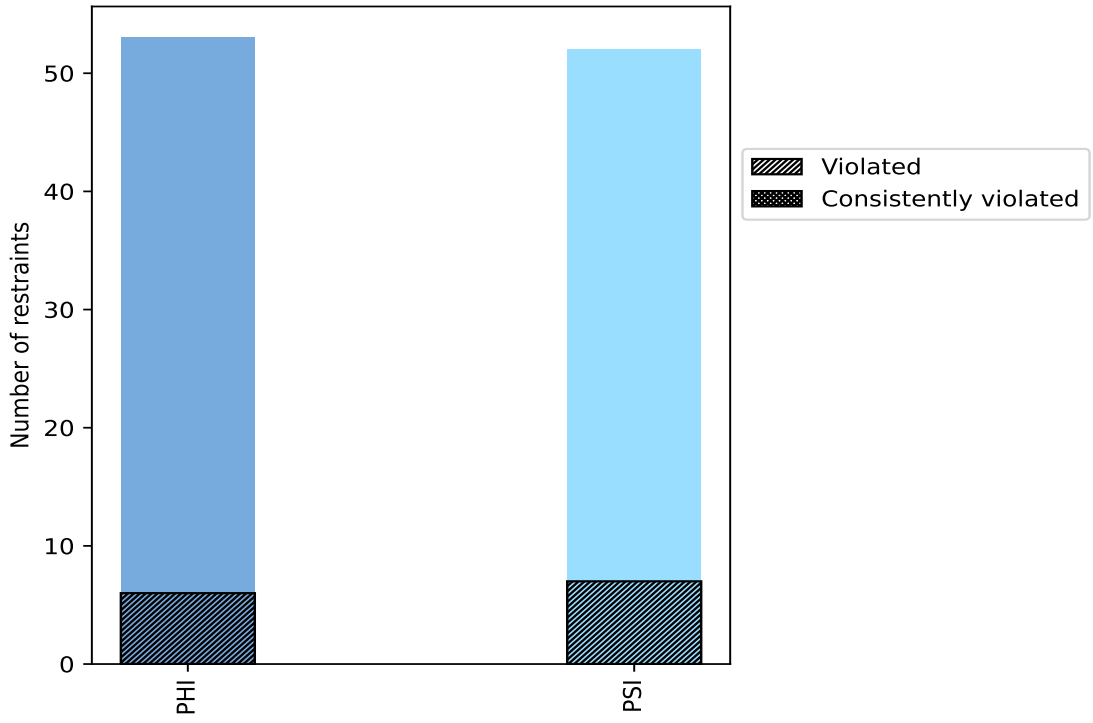
10.1 Summary of dihedral-angle violations (i)

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	53	50.5	6	11.3	5.7	0	0.0	0.0
PSI	52	49.5	7	13.5	6.7	0	0.0	0.0
Total	105	100.0	13	12.4	12.4	0	0.0	0.0

[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 (i)



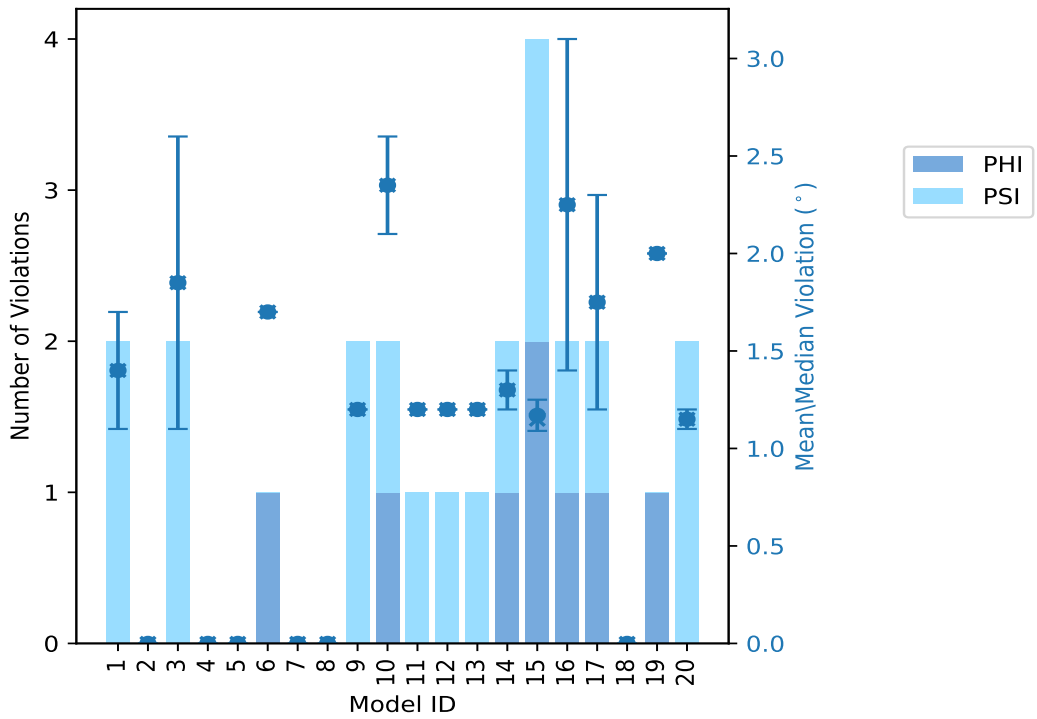
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	0	2	2	1.4	1.7	0.3	1.4
2	0	0	0	0.0	0.0	0.0	0.0
3	0	2	2	1.85	2.6	0.75	1.85
4	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0.0	0.0	0.0	0.0
6	1	0	1	1.7	1.7	0.0	1.7
7	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0.0	0.0	0.0	0.0
9	0	2	2	1.2	1.2	0.0	1.2
10	1	1	2	2.35	2.6	0.25	2.35
11	0	1	1	1.2	1.2	0.0	1.2
12	0	1	1	1.2	1.2	0.0	1.2
13	0	1	1	1.2	1.2	0.0	1.2
14	1	1	2	1.3	1.4	0.1	1.3
15	2	2	4	1.17	1.3	0.08	1.15
16	1	1	2	2.25	3.1	0.85	2.25
17	1	1	2	1.75	2.3	0.55	1.75
18	0	0	0	0.0	0.0	0.0	0.0
19	1	0	1	2.0	2.0	0.0	2.0
20	0	2	2	1.15	1.2	0.05	1.15

10.2.1 Bar graph : Dihedral violation statistics for each model (i)



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

10.3 Dihedral-angle violation statistics for the ensemble (i)

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
2	1	3	2	10.0
0	2	2	3	15.0
0	0	0	4	20.0
0	0	0	5	25.0
0	1	1	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

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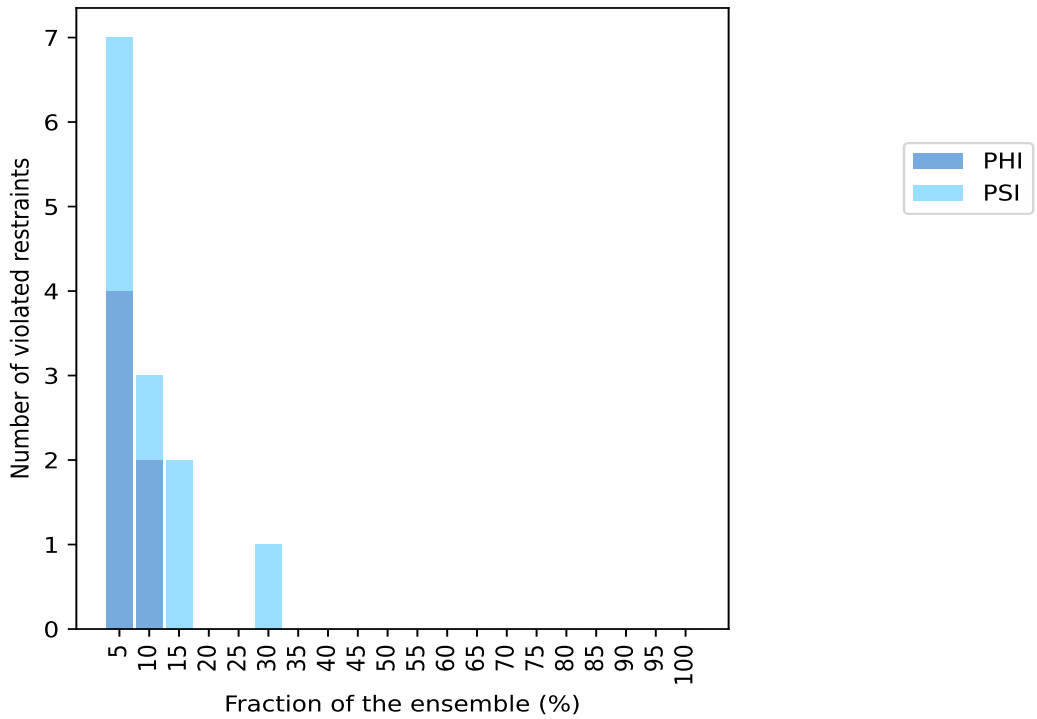
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

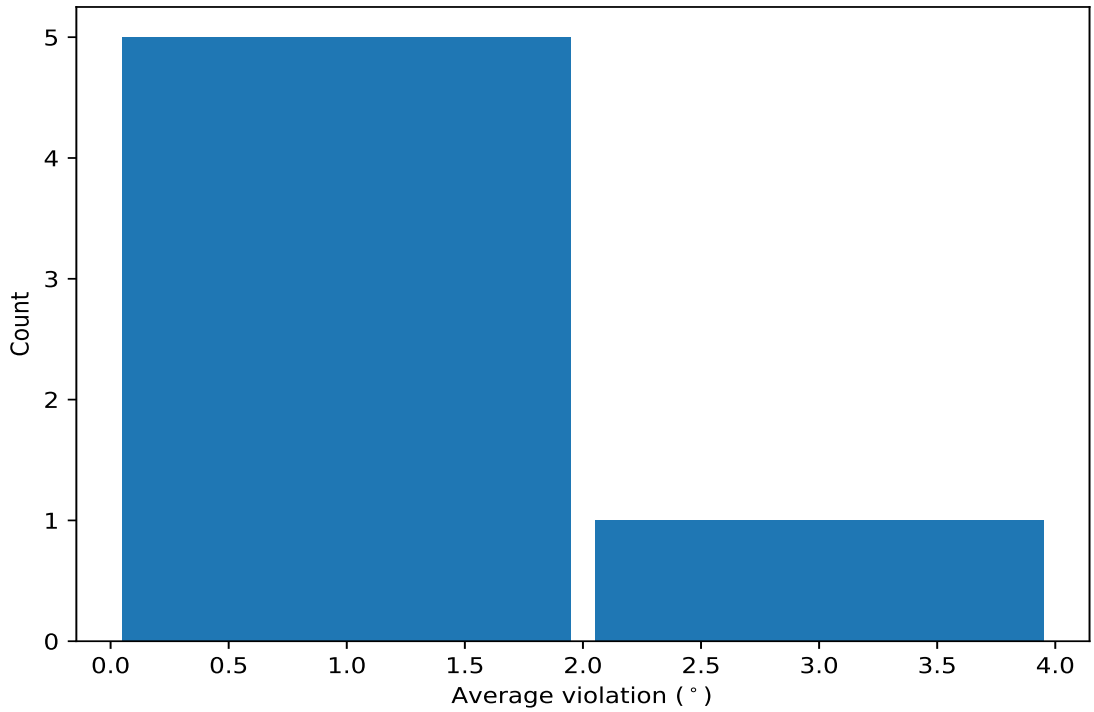


10.4 Most violated dihedral-angle restraints in the ensemble (i)

10.4.1 Histogram : Distribution of mean dihedral-angle violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



10.4.2 Table: Most violated dihedral-angle 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.

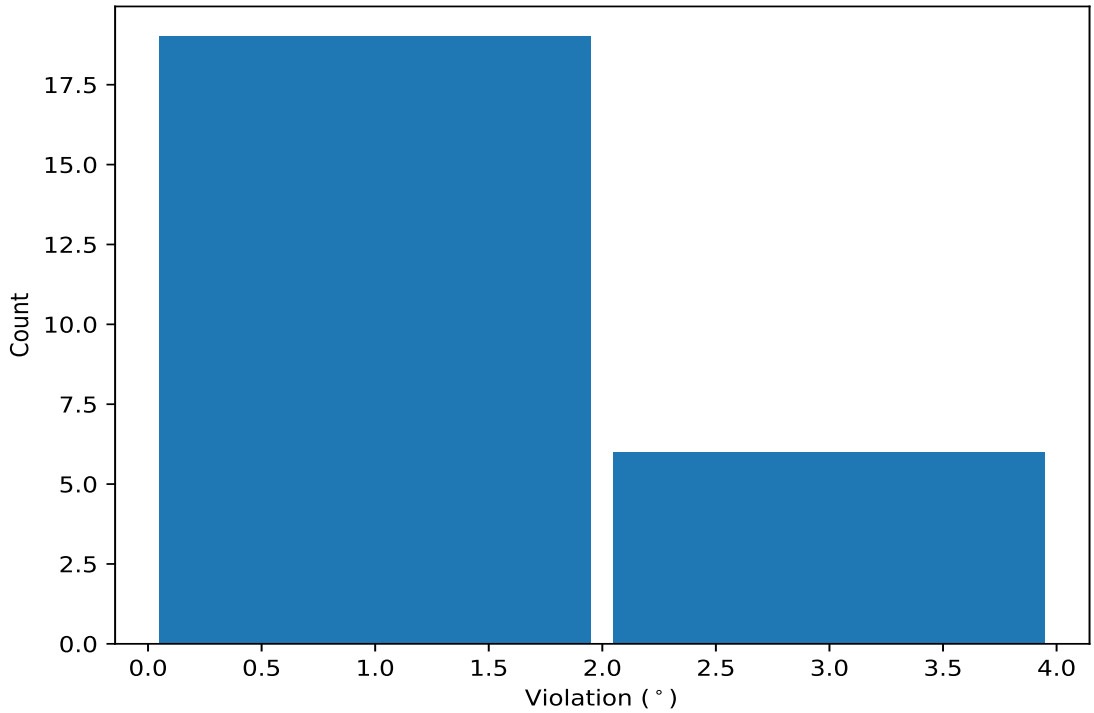
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,31)	1:A:142:LEU:N	1:A:142:LEU:CA	1:A:142:LEU:C	1:A:143:LEU:N	6	1.38	0.55	1.15
(1,2)	1:A:101:VAL:N	1:A:101:VAL:CA	1:A:101:VAL:C	1:A:102:GLN:N	3	1.83	0.58	1.7
(1,27)	1:A:126:LYS:N	1:A:126:LYS:CA	1:A:126:LYS:C	1:A:127:TRP:N	3	1.2	0.0	1.2
(1,94)	1:A:196:PRO:C	1:A:197:ALA:N	1:A:197:ALA:CA	1:A:197:ALA:C	2	2.7	0.4	2.7
(1,30)	1:A:141:THR:C	1:A:142:LEU:N	1:A:142:LEU:CA	1:A:142:LEU:C	2	1.9	0.2	1.9
(1,93)	1:A:188:HIS:N	1:A:188:HIS:CA	1:A:188:HIS:C	1:A:189:GLY:N	2	1.3	0.1	1.3

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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 (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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,94)	1:A:196:PRO:C	1:A:197:ALA:N	1:A:197:ALA:CA	1:A:197:ALA:C	16	3.1
(1,31)	1:A:142:LEU:N	1:A:142:LEU:CA	1:A:142:LEU:C	1:A:143:LEU:N	10	2.6
(1,2)	1:A:101:VAL:N	1:A:101:VAL:CA	1:A:101:VAL:C	1:A:102:GLN:N	3	2.6
(1,94)	1:A:196:PRO:C	1:A:197:ALA:N	1:A:197:ALA:CA	1:A:197:ALA:C	17	2.3
(1,30)	1:A:141:THR:C	1:A:142:LEU:N	1:A:142:LEU:CA	1:A:142:LEU:C	10	2.1
(1,1)	1:A:100:ILE:C	1:A:101:VAL:N	1:A:101:VAL:CA	1:A:101:VAL:C	19	2.0
(1,30)	1:A:141:THR:C	1:A:142:LEU:N	1:A:142:LEU:CA	1:A:142:LEU:C	6	1.7
(1,2)	1:A:101:VAL:N	1:A:101:VAL:CA	1:A:101:VAL:C	1:A:102:GLN:N	1	1.7
(1,93)	1:A:188:HIS:N	1:A:188:HIS:CA	1:A:188:HIS:C	1:A:189:GLY:N	16	1.4
(1,86)	1:A:183:ARG:C	1:A:184:CYS:N	1:A:184:CYS:CA	1:A:184:CYS:C	14	1.4
(1,34)	1:A:143:LEU:C	1:A:144:TYR:N	1:A:144:TYR:CA	1:A:144:TYR:C	15	1.3
(1,93)	1:A:188:HIS:N	1:A:188:HIS:CA	1:A:188:HIS:C	1:A:189:GLY:N	9	1.2
(1,7)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:ALA:N	17	1.2
(1,31)	1:A:142:LEU:N	1:A:142:LEU:CA	1:A:142:LEU:C	1:A:143:LEU:N	12	1.2
(1,31)	1:A:142:LEU:N	1:A:142:LEU:CA	1:A:142:LEU:C	1:A:143:LEU:N	13	1.2
(1,27)	1:A:126:LYS:N	1:A:126:LYS:CA	1:A:126:LYS:C	1:A:127:TRP:N	9	1.2
(1,27)	1:A:126:LYS:N	1:A:126:LYS:CA	1:A:126:LYS:C	1:A:127:TRP:N	15	1.2
(1,27)	1:A:126:LYS:N	1:A:126:LYS:CA	1:A:126:LYS:C	1:A:127:TRP:N	20	1.2
(1,2)	1:A:101:VAL:N	1:A:101:VAL:CA	1:A:101:VAL:C	1:A:102:GLN:N	14	1.2
(1,11)	1:A:111:VAL:N	1:A:111:VAL:CA	1:A:111:VAL:C	1:A:112:GLU:N	11	1.2
(1,89)	1:A:185:LYS:N	1:A:185:LYS:CA	1:A:185:LYS:C	1:A:186:PRO:N	3	1.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,88)	1:A:184:CYS:C	1:A:185:LYS:N	1:A:185:LYS:CA	1:A:185:LYS:C	15	1.1
(1,31)	1:A:142:LEU:N	1:A:142:LEU:CA	1:A:142:LEU:C	1:A:143:LEU:N	1	1.1
(1,31)	1:A:142:LEU:N	1:A:142:LEU:CA	1:A:142:LEU:C	1:A:143:LEU:N	15	1.1
(1,31)	1:A:142:LEU:N	1:A:142:LEU:CA	1:A:142:LEU:C	1:A:143:LEU:N	20	1.1