Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 01:17 pm BST

PDB ID	:	5MWW
BMRB ID	:	34089
Title	:	Sigma1.1 domain of sigmaA from Bacillus subtilis
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Deposited on	:	2017-01-20

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:

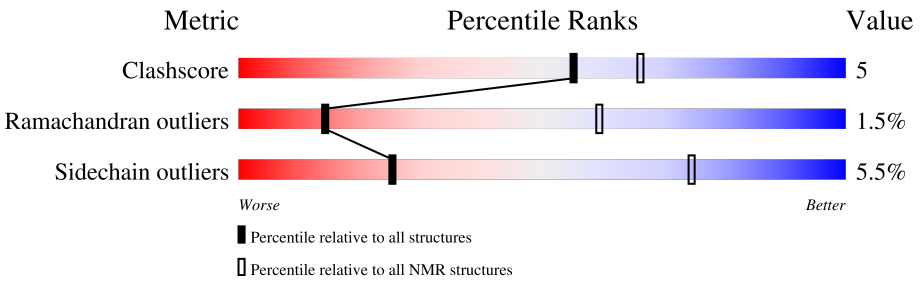
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 96%.

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	76	62% 8% • 29%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:10-A:63 (54)	0.33	1

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 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1199 atoms, of which 569 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	76	1199	385	569	100	143	2	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	LEU	-	expression tag	UNP A0A063XB56
A	73	GLU	-	expression tag	UNP A0A063XB56
A	74	HIS	-	expression tag	UNP A0A063XB56
A	75	HIS	-	expression tag	UNP A0A063XB56
A	76	HIS	-	expression tag	UNP A0A063XB56

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: RNA polymerase sigma factor SigA

Chain A: 62% 8% • 29%

A1 D2 K3 Q4 T5 H6 E7 T8 E9 L10 Q14 V15 Q18 M48 G59 L62 I63 S64 E65 N66 E67 E68 T69 E70 D71 L72 E73 H74 H75 H76

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 (medoid)

• Molecule 1: RNA polymerase sigma factor SigA

Chain A: 57% 13% • 29%

A1 D2 K3 Q4 T5 H6 E7 T8 E9 L10 Q14 V15 Q18 L19 T20 K24 M48 F54 Q58 G59 L62 I63 S64 E65 N66 E67 E68 T69 E70 D71 L72 E73 H74 H75 H76

4.2.2 Score per residue for model 2

• Molecule 1: RNA polymerase sigma factor SigA

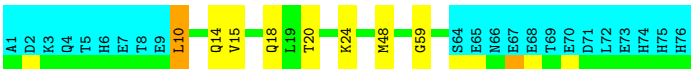
Chain A: 55% 14% • 29%

A1 D2 K3 Q4 T5 H6 E7 T8 E9 L10 T11 Q14 V15 Q18 L19 T20 K24 V28 E42 M48 G59 V60 E61 S64 E65 N66 E67 E68 T69 E70 D71 L72 E73 H74 H75 H76

4.2.3 Score per residue for model 3

- Molecule 1: RNA polymerase sigma factor SigA

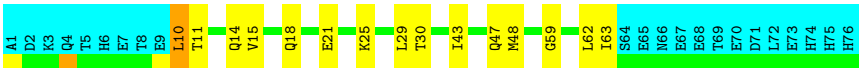
Chain A: 61% 9% • 29%



4.2.4 Score per residue for model 4

- Molecule 1: RNA polymerase sigma factor SigA

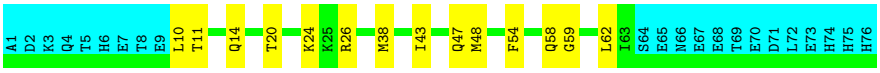
Chain A: 51% 18% • 29%



4.2.5 Score per residue for model 5

- Molecule 1: RNA polymerase sigma factor SigA

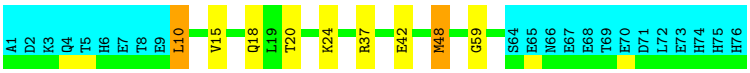
Chain A: 53% 18% 29%



4.2.6 Score per residue for model 6

- Molecule 1: RNA polymerase sigma factor SigA

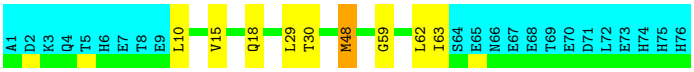
Chain A: 59% 9% • 29%



4.2.7 Score per residue for model 7

- Molecule 1: RNA polymerase sigma factor SigA

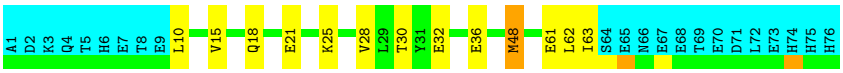
Chain A: 59% 11% • 29%



4.2.8 Score per residue for model 8

- Molecule 1: RNA polymerase sigma factor SigA

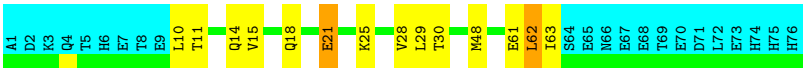
Chain A: 54% 16% • 29%



4.2.9 Score per residue for model 9

- Molecule 1: RNA polymerase sigma factor SigA

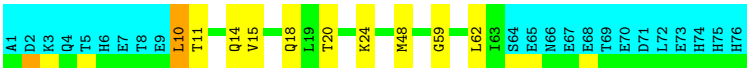
Chain A: 53% 16% • 29%



4.2.10 Score per residue for model 10

- Molecule 1: RNA polymerase sigma factor SigA

Chain A: 58% 12% • 29%



4.2.11 Score per residue for model 11

- Molecule 1: RNA polymerase sigma factor SigA

Chain A: 61% 9% • 29%

4.2.12 Score per residue for model 12

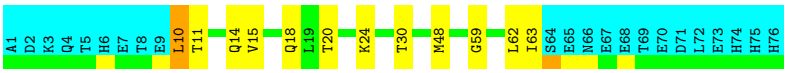
- Molecule 1: RNA polymerase sigma factor SigA

Chain A: 58% 12% • 29%

4.2.13 Score per residue for model 13

- Molecule 1: RNA polymerase sigma factor SigA

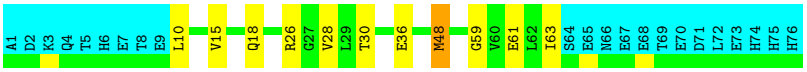
Chain A: 55% 14% • 29%



4.2.14 Score per residue for model 14

- Molecule 1: RNA polymerase sigma factor SigA

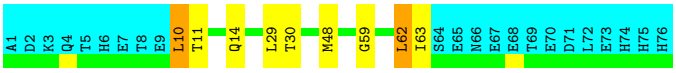
Chain A: 57% 13% • 29%



4.2.15 Score per residue for model 15

- Molecule 1: RNA polymerase sigma factor SigA

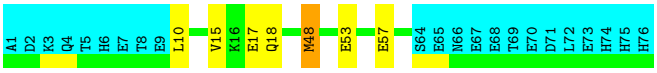
Chain A: 59% 9% • 29%



4.2.16 Score per residue for model 16

- Molecule 1: RNA polymerase sigma factor SigA

Chain A: 62% 8% • 29%



4.2.17 Score per residue for model 17

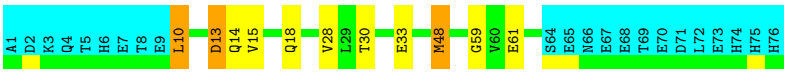
- Molecule 1: RNA polymerase sigma factor SigA

Chain A: 63% 7% • 29%

4.2.18 Score per residue for model 18

- Molecule 1: RNA polymerase sigma factor SigA

Chain A: 57% 11% • 29%



4.2.19 Score per residue for model 19

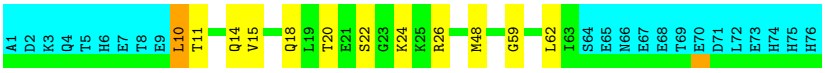
- Molecule 1: RNA polymerase sigma factor SigA

Chain A: 58% 12% • 29%

4.2.20 Score per residue for model 20

- Molecule 1: RNA polymerase sigma factor SigA

Chain A: 55% 14% • 29%



5 Refinement protocol and experimental data overview (i)

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

Of the 150 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	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	912
Number of shifts mapped to atoms	912
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	96%

6 Model quality (i)

6.1 Standard geometry (i)

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

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.4
All	All	0	3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	26	ARG	Sidechain	2
1	A	37	ARG	Sidechain	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	444	420	420	5±1
All	All	8880	8400	8400	91

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:THR:HG22	1:A:63:ILE:HG13	0.55	1.79	15	8
1:A:11:THR:OG1	1:A:14:GLN:HG2	0.54	2.03	4	9
1:A:54:PHE:O	1:A:58:GLN:HG2	0.52	2.04	1	2
1:A:15:VAL:O	1:A:18:GLN:HG2	0.52	2.03	7	18
1:A:21:GLU:O	1:A:25:LYS:HG3	0.52	2.05	4	4
1:A:10:LEU:HB3	1:A:14:GLN:HB2	0.50	1.83	20	7
1:A:28:VAL:HA	1:A:61:GLU:O	0.50	2.06	2	5
1:A:20:THR:O	1:A:24:LYS:HG2	0.48	2.08	20	8
1:A:48:MET:HA	1:A:48:MET:CE	0.48	2.39	4	9
1:A:10:LEU:HD12	1:A:10:LEU:H	0.47	1.68	6	2
1:A:29:LEU:O	1:A:62:LEU:HA	0.45	2.12	7	6
1:A:48:MET:HA	1:A:48:MET:HE2	0.44	1.89	4	1
1:A:43:ILE:CG2	1:A:47:GLN:HB2	0.44	2.43	4	2
1:A:53:GLU:O	1:A:57:GLU:HG3	0.44	2.13	12	3
1:A:38:MET:SD	1:A:43:ILE:HD11	0.43	2.54	5	1
1:A:10:LEU:HB3	1:A:14:GLN:CB	0.43	2.43	1	3
1:A:22:SER:O	1:A:26:ARG:HG3	0.42	2.12	20	1
1:A:32:GLU:O	1:A:36:GLU:HB2	0.41	2.16	8	1
1:A:30:THR:O	1:A:33:GLU:HG2	0.41	2.16	18	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	54/76 (71%)	51±1 (94±2%)	2±1 (4±2%)	1±1 (1±1%)	14	59
All	All	1080/1520 (71%)	1019 (94%)	45 (4%)	16 (1%)	14	59

All 2 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	59	GLY	15
1	A	42	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	49/70 (70%)	46±1 (94±1%)	3±1 (6±1%)	25	74
All	All	980/1400 (70%)	926 (94%)	54 (6%)	25	74

All 8 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	10	LEU	20
1	A	48	MET	17
1	A	62	LEU	12
1	A	42	GLU	1
1	A	21	GLU	1
1	A	36	GLU	1
1	A	17	GLU	1
1	A	13	ASP	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (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 96% 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: *siga1.1_shifts.str*

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	912
Number of shifts mapped to atoms	912
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	72	-0.38 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	68	0.31 ± 0.15	None needed (< 0.5 ppm)
$^{13}C'$	72	-0.49 ± 0.13	None needed (< 0.5 ppm)
^{15}N	71	0.09 ± 0.25	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 96%, i.e. 709 atoms were assigned a chemical shift out of a possible 741. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	274/274 (100%)	112/112 (100%)	108/108 (100%)	54/54 (100%)
Sidechain	381/410 (93%)	254/262 (97%)	121/135 (90%)	6/13 (46%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	54/57 (95%)	27/27 (100%)	27/30 (90%)	0/0 (—%)
Overall	709/741 (96%)	393/401 (98%)	256/273 (94%)	60/67 (90%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 911 atoms were assigned a chemical shift out of a possible 1016. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	362/384 (94%)	147/156 (94%)	144/152 (95%)	71/76 (93%)
Sidechain	495/547 (90%)	329/346 (95%)	158/185 (85%)	8/16 (50%)
Aromatic	54/85 (64%)	27/43 (63%)	27/38 (71%)	0/4 (0%)
Overall	911/1016 (90%)	503/545 (92%)	329/375 (88%)	79/96 (82%)

7.1.4 Statistically unusual chemical shifts (i)

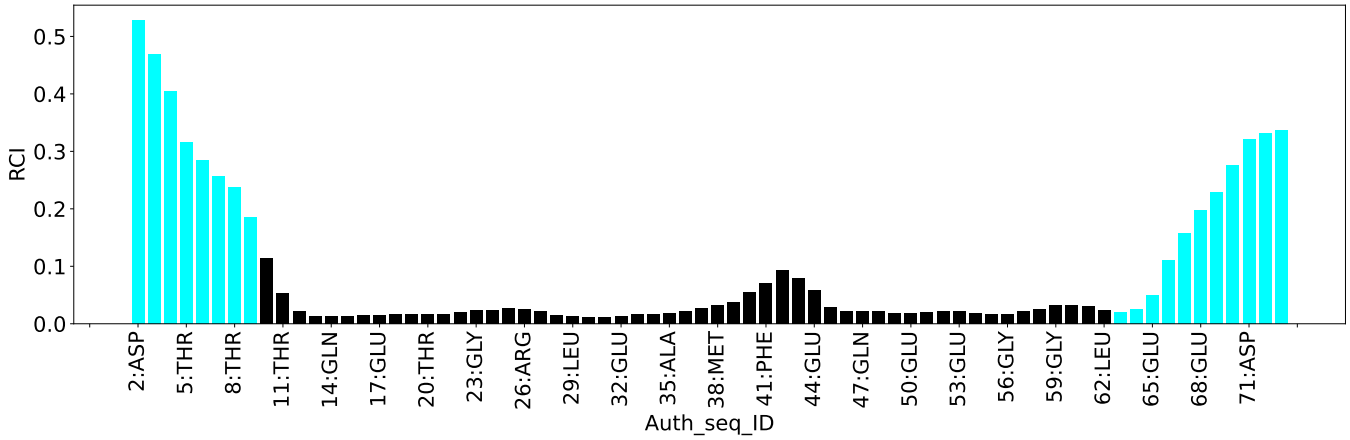
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	20	THR	HG1	5.90	0.08 – 2.19	22.6
1	A	16	LYS	HE3	1.73	1.92 – 3.89	-6.0
1	A	37	ARG	CZ	179.92	141.81 – 177.93	5.5
1	A	26	ARG	CZ	179.89	141.81 – 177.93	5.5

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:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
2:ASP
5:THR
8:THR
11:THR
14:GLN
17:GLU
20:THR
23:GLY
26:ARG
29:LEU
32:GLU
35:ALA
38:MET
41:PHE
44:GLU
47:GLN
50:GLU
53:GLU
56:GLY
59:GLY
62:LEU
65:GLU
68:GLU
71:ASP
Auth_seq_ID

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	1886
Intra-residue (|i-j|=0)	430
Sequential (|i-j|=1)	495
Medium range (|i-j|>1 and |i-j|<5)	475
Long range (|i-j|≥5)	486
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	24.8
Number of long range restraints per residue[1]	6.4

[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)	11.8	0.2
0.2-0.5 (Medium)	0.8	0.28
>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.There are no dihedral-angle violations

9 Distance violation analysis (i)

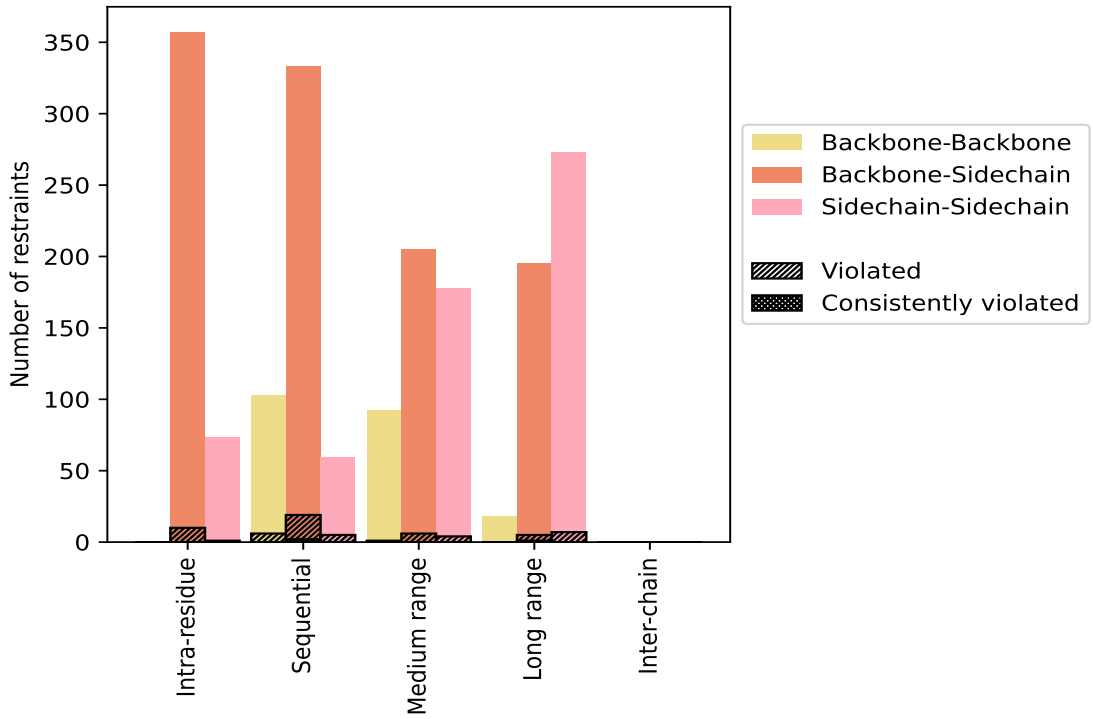
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	430	22.8	11	2.6	0.6	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	357	18.9	10	2.8	0.5	0	0.0	0.0
Sidechain-Sidechain	73	3.9	1	1.4	0.1	0	0.0	0.0
Sequential (|i-j|=1)	495	26.2	30	6.1	1.6	2	0.4	0.1
Backbone-Backbone	103	5.5	6	5.8	0.3	0	0.0	0.0
Backbone-Sidechain	333	17.7	19	5.7	1.0	2	0.6	0.1
Sidechain-Sidechain	59	3.1	5	8.5	0.3	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	475	25.2	11	2.3	0.6	0	0.0	0.0
Backbone-Backbone	92	4.9	1	1.1	0.1	0	0.0	0.0
Backbone-Sidechain	205	10.9	6	2.9	0.3	0	0.0	0.0
Sidechain-Sidechain	178	9.4	4	2.2	0.2	0	0.0	0.0
Long range (|i-j|≥5)	486	25.8	12	2.5	0.6	1	0.2	0.1
Backbone-Backbone	18	1.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	195	10.3	5	2.6	0.3	1	0.5	0.1
Sidechain-Sidechain	273	14.5	7	2.6	0.4	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	1886	100.0	64	3.4	3.4	3	0.2	0.2
Backbone-Backbone	213	11.3	7	3.3	0.4	0	0.0	0.0
Backbone-Sidechain	1090	57.8	40	3.7	2.1	3	0.3	0.2
Sidechain-Sidechain	583	30.9	17	2.9	0.9	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	1	6	3	4	0	14	0.15	0.23	0.04	0.13
2	1	3	2	2	0	8	0.14	0.2	0.03	0.14
3	0	7	2	3	0	12	0.14	0.2	0.03	0.12
4	1	6	2	3	0	12	0.15	0.2	0.03	0.15
5	3	5	2	4	0	14	0.15	0.28	0.05	0.14
6	1	9	2	2	0	14	0.15	0.25	0.04	0.14
7	1	10	3	2	0	16	0.15	0.22	0.03	0.15
8	2	8	4	1	0	15	0.15	0.19	0.03	0.15
9	3	6	4	2	0	15	0.15	0.22	0.03	0.16
10	2	6	3	1	0	12	0.15	0.2	0.03	0.14
11	1	4	2	3	0	10	0.16	0.2	0.03	0.16

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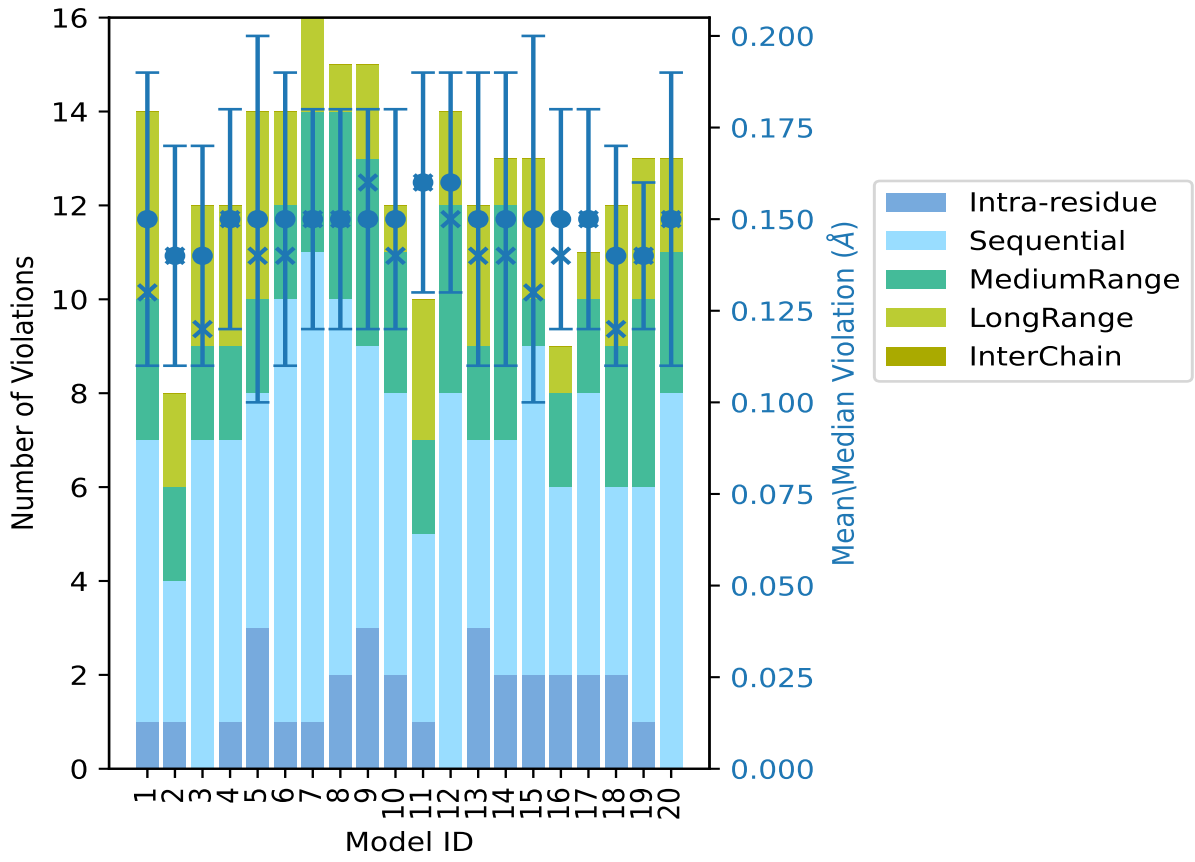
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	8	4	2	0	14	0.16	0.21	0.03	0.15
13	3	4	2	3	0	12	0.15	0.23	0.04	0.14
14	2	5	5	1	0	13	0.15	0.24	0.04	0.14
15	2	7	1	3	0	13	0.15	0.27	0.05	0.13
16	2	4	2	1	0	9	0.15	0.2	0.03	0.14
17	2	6	2	1	0	11	0.15	0.21	0.03	0.15
18	2	4	3	3	0	12	0.14	0.2	0.03	0.12
19	1	5	4	3	0	13	0.14	0.18	0.02	0.14
20	0	8	3	2	0	13	0.15	0.21	0.04	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

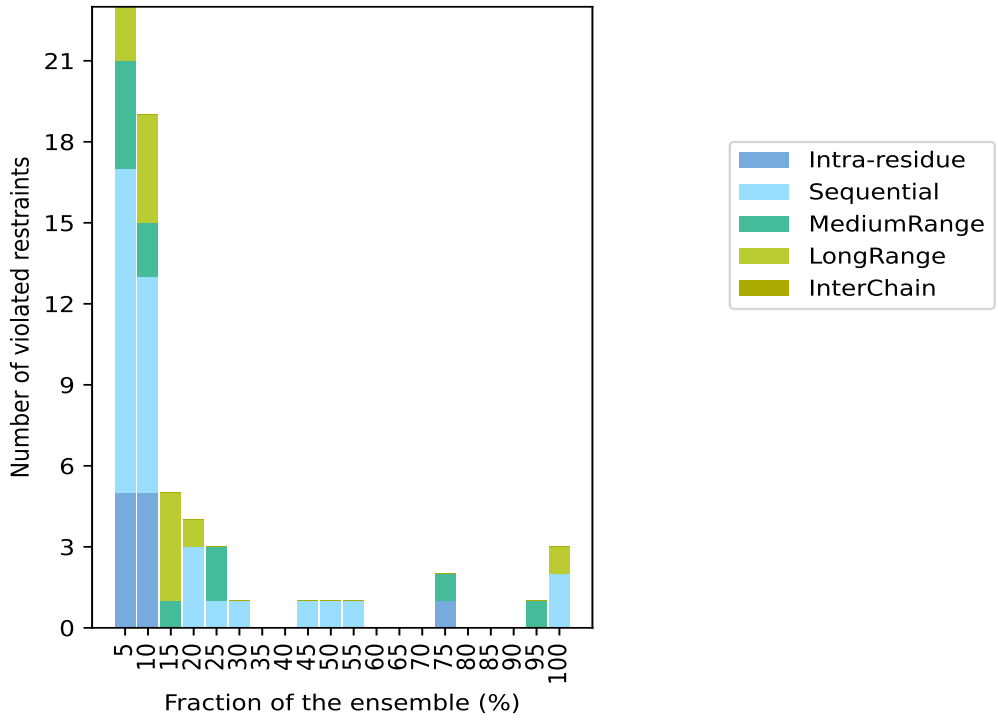
9.3 Distance violation statistics for the ensemble (i)

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, 1822(IR:419, SQ:465, MR:464, LR:474, 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]	%
5	12	4	2	0	23	1	5.0
5	8	2	4	0	19	2	10.0
0	0	1	4	0	5	3	15.0
0	3	0	1	0	4	4	20.0
0	1	2	0	0	3	5	25.0
0	1	0	0	0	1	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	1	0	0	0	1	9	45.0
0	1	0	0	0	1	10	50.0
0	1	0	0	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
1	0	1	0	0	2	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	1	0	0	1	19	95.0
0	2	0	1	0	3	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

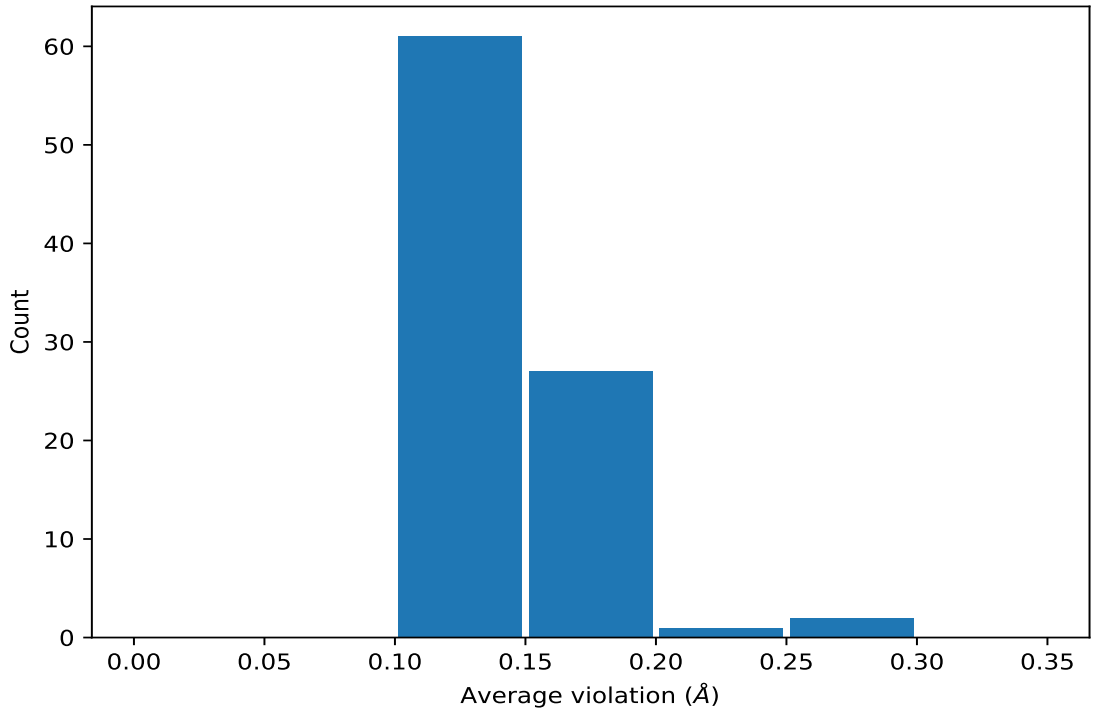
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	20	0.2	0.02	0.2
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	20	0.18	0.01	0.19
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	20	0.15	0.02	0.16
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	20	0.15	0.02	0.16
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	20	0.15	0.02	0.16
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	19	0.18	0.03	0.17
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	19	0.18	0.03	0.17
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	19	0.18	0.03	0.17
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	15	0.14	0.02	0.15
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	15	0.14	0.02	0.13
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB2	11	0.12	0.01	0.12
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB3	11	0.12	0.01	0.12
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB2	11	0.12	0.01	0.12
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB3	11	0.12	0.01	0.12
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB2	11	0.12	0.01	0.12
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB3	11	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,410)	1:A:43:ILE:HB	1:A:44:GLU:H	10	0.12	0.01	0.12
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG2	9	0.16	0.02	0.16
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG3	9	0.16	0.02	0.16
(1,164)	1:A:71:ASP:HA	1:A:72:LEU:H	6	0.13	0.02	0.14
(1,1367)	1:A:63:ILE:HG21	1:A:64:SER:HB3	5	0.16	0.02	0.16
(1,1367)	1:A:63:ILE:HG22	1:A:64:SER:HB3	5	0.16	0.02	0.16
(1,1367)	1:A:63:ILE:HG23	1:A:64:SER:HB3	5	0.16	0.02	0.16
(1,1550)	1:A:11:THR:HG21	1:A:14:GLN:HE21	5	0.14	0.02	0.15
(1,1550)	1:A:11:THR:HG21	1:A:14:GLN:HE22	5	0.14	0.02	0.15
(1,1550)	1:A:11:THR:HG22	1:A:14:GLN:HE21	5	0.14	0.02	0.15
(1,1550)	1:A:11:THR:HG22	1:A:14:GLN:HE22	5	0.14	0.02	0.15
(1,1550)	1:A:11:THR:HG23	1:A:14:GLN:HE21	5	0.14	0.02	0.15
(1,1550)	1:A:11:THR:HG23	1:A:14:GLN:HE22	5	0.14	0.02	0.15
(1,777)	1:A:11:THR:HA	1:A:15:VAL:HB	5	0.13	0.01	0.13
(1,1413)	1:A:67:GLU:HG2	1:A:68:GLU:HA	4	0.17	0.06	0.16
(1,1413)	1:A:67:GLU:HG3	1:A:68:GLU:HA	4	0.17	0.06	0.16
(1,1390)	1:A:70:GLU:HG2	1:A:71:ASP:HA	4	0.14	0.02	0.15
(1,1390)	1:A:70:GLU:HG3	1:A:71:ASP:HA	4	0.14	0.02	0.15
(1,645)	1:A:31:TYR:HD1	1:A:64:SER:HB2	4	0.12	0.01	0.12
(1,645)	1:A:31:TYR:HD2	1:A:64:SER:HB2	4	0.12	0.01	0.12
(1,1541)	1:A:8:THR:HA	1:A:9:GLU:HB2	4	0.12	0.01	0.12
(1,1541)	1:A:8:THR:HA	1:A:9:GLU:HB3	4	0.12	0.01	0.12
(1,1370)	1:A:30:THR:HG21	1:A:64:SER:HB2	3	0.17	0.01	0.18
(1,1370)	1:A:30:THR:HG22	1:A:64:SER:HB2	3	0.17	0.01	0.18
(1,1370)	1:A:30:THR:HG23	1:A:64:SER:HB2	3	0.17	0.01	0.18
(1,1461)	1:A:52:TYR:HE1	1:A:62:LEU:HD21	3	0.13	0.01	0.12
(1,1461)	1:A:52:TYR:HE1	1:A:62:LEU:HD22	3	0.13	0.01	0.12
(1,1461)	1:A:52:TYR:HE1	1:A:62:LEU:HD23	3	0.13	0.01	0.12
(1,1461)	1:A:52:TYR:HE2	1:A:62:LEU:HD21	3	0.13	0.01	0.12
(1,1461)	1:A:52:TYR:HE2	1:A:62:LEU:HD22	3	0.13	0.01	0.12
(1,1461)	1:A:52:TYR:HE2	1:A:62:LEU:HD23	3	0.13	0.01	0.12
(1,248)	1:A:16:LYS:H	1:A:18:GLN:HB2	3	0.11	0.0	0.11
(1,248)	1:A:16:LYS:H	1:A:18:GLN:HB3	3	0.11	0.0	0.11
(1,1662)	1:A:24:LYS:HE2	1:A:59:GLY:H	3	0.11	0.0	0.11
(1,1662)	1:A:24:LYS:HE3	1:A:59:GLY:H	3	0.11	0.0	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD11	3	0.11	0.0	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD12	3	0.11	0.0	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD13	3	0.11	0.0	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD21	3	0.11	0.0	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD22	3	0.11	0.0	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD23	3	0.11	0.0	0.11
(1,1598)	1:A:18:GLN:H	1:A:18:GLN:HG2	2	0.28	0.01	0.28

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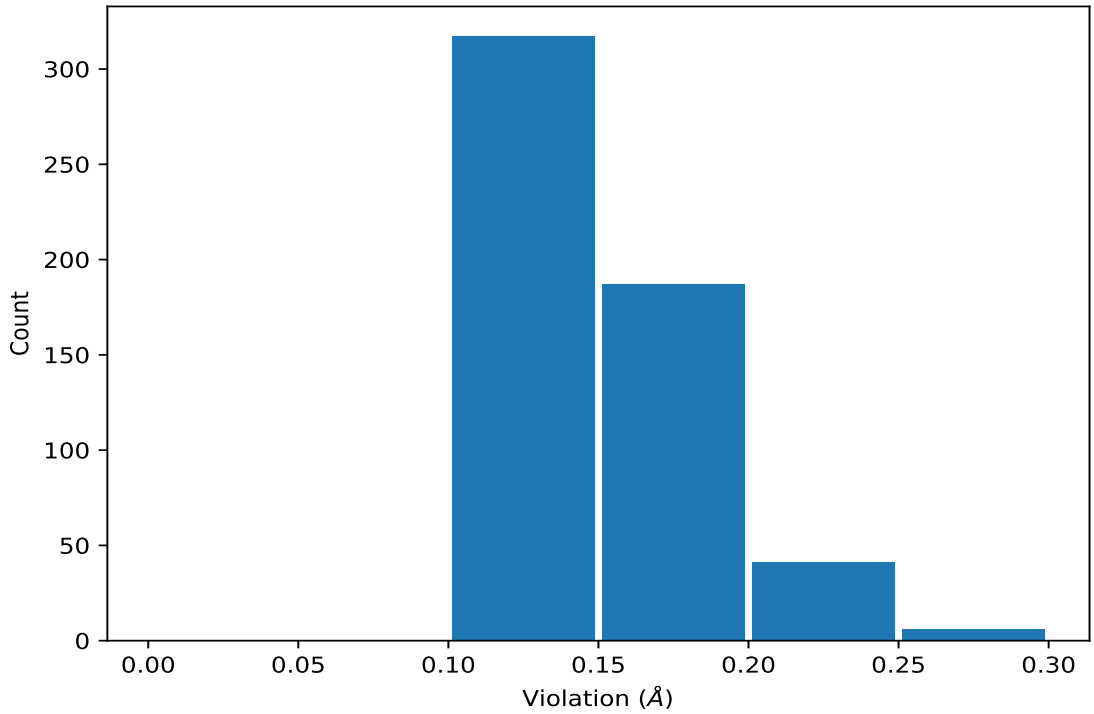
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1598)	1:A:18:GLN:H	1:A:18:GLN:HG3	2	0.28	0.01	0.28
(1,337)	1:A:47:GLN:HA	1:A:47:GLN:HE22	2	0.18	0.05	0.18
(1,1363)	1:A:64:SER:HA	1:A:67:GLU:HG2	2	0.18	0.0	0.18
(1,1363)	1:A:64:SER:HA	1:A:67:GLU:HG3	2	0.18	0.0	0.18
(1,726)	1:A:4:GLN:HA	1:A:5:THR:HG21	2	0.15	0.01	0.15
(1,726)	1:A:4:GLN:HA	1:A:5:THR:HG22	2	0.15	0.01	0.15
(1,726)	1:A:4:GLN:HA	1:A:5:THR:HG23	2	0.15	0.01	0.15
(1,718)	1:A:7:GLU:HA	1:A:7:GLU:HG2	2	0.15	0.03	0.15
(1,718)	1:A:7:GLU:HA	1:A:7:GLU:HG3	2	0.15	0.03	0.15
(1,1454)	1:A:52:TYR:HD1	1:A:62:LEU:HG	2	0.15	0.02	0.15
(1,1454)	1:A:52:TYR:HD2	1:A:62:LEU:HG	2	0.15	0.02	0.15
(1,450)	1:A:69:THR:HA	1:A:71:ASP:H	2	0.14	0.02	0.14
(1,34)	1:A:69:THR:HA	1:A:70:GLU:H	2	0.13	0.01	0.13
(1,196)	1:A:14:GLN:HB2	1:A:14:GLN:HE22	2	0.12	0.01	0.12
(1,196)	1:A:14:GLN:HB3	1:A:14:GLN:HE22	2	0.12	0.01	0.12
(1,417)	1:A:46:ASP:HA	1:A:46:ASP:HB3	2	0.12	0.01	0.12
(1,1349)	1:A:63:ILE:HB	1:A:64:SER:HB3	2	0.12	0.02	0.12
(1,780)	1:A:10:LEU:HD11	1:A:11:THR:HA	2	0.12	0.0	0.12
(1,780)	1:A:10:LEU:HD12	1:A:11:THR:HA	2	0.12	0.0	0.12
(1,780)	1:A:10:LEU:HD13	1:A:11:THR:HA	2	0.12	0.0	0.12
(1,1369)	1:A:30:THR:HG21	1:A:64:SER:HB3	2	0.12	0.01	0.12
(1,1369)	1:A:30:THR:HG22	1:A:64:SER:HB3	2	0.12	0.01	0.12
(1,1369)	1:A:30:THR:HG23	1:A:64:SER:HB3	2	0.12	0.01	0.12
(1,1869)	1:A:68:GLU:HB2	1:A:69:THR:H	2	0.12	0.0	0.12
(1,1869)	1:A:68:GLU:HB3	1:A:69:THR:H	2	0.12	0.0	0.12
(1,708)	1:A:67:GLU:HB3	1:A:68:GLU:H	2	0.12	0.0	0.12
(1,728)	1:A:43:ILE:HD11	1:A:48:MET:HA	2	0.12	0.0	0.12
(1,728)	1:A:43:ILE:HD12	1:A:48:MET:HA	2	0.12	0.0	0.12
(1,728)	1:A:43:ILE:HD13	1:A:48:MET:HA	2	0.12	0.0	0.12
(1,340)	1:A:64:SER:HA	1:A:65:GLU:H	2	0.11	0.0	0.11
(1,1051)	1:A:28:VAL:HB	1:A:29:LEU:HA	2	0.11	0.0	0.11
(1,1103)	1:A:35:ALA:HA	1:A:52:TYR:HE1	2	0.11	0.0	0.11
(1,1103)	1:A:35:ALA:HA	1:A:52:TYR:HE2	2	0.11	0.0	0.11

[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)
(1,1598)	1:A:18:GLN:H	1:A:18:GLN:HG2	5	0.28
(1,1598)	1:A:18:GLN:H	1:A:18:GLN:HG3	5	0.28
(1,1598)	1:A:18:GLN:H	1:A:18:GLN:HG2	15	0.27
(1,1598)	1:A:18:GLN:H	1:A:18:GLN:HG3	15	0.27
(1,1413)	1:A:67:GLU:HG2	1:A:68:GLU:HA	6	0.25
(1,1413)	1:A:67:GLU:HG3	1:A:68:GLU:HA	6	0.25
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	14	0.24
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	1	0.23
(1,337)	1:A:47:GLN:HA	1:A:47:GLN:HE22	13	0.23
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	9	0.22
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	1	0.22
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	1	0.22
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	1	0.22
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	7	0.22
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	7	0.22
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	14	0.22
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	14	0.22
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	14	0.22
(1,673)	1:A:8:THR:HA	1:A:8:THR:HG21	9	0.22
(1,673)	1:A:8:THR:HA	1:A:8:THR:HG22	9	0.22
(1,673)	1:A:8:THR:HA	1:A:8:THR:HG23	9	0.22
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	5	0.21
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	12	0.21
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	15	0.21
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	17	0.21
(1,1413)	1:A:67:GLU:HG2	1:A:68:GLU:HA	20	0.21
(1,1413)	1:A:67:GLU:HG3	1:A:68:GLU:HA	20	0.21
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	2	0.2
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	3	0.2
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	4	0.2
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	6	0.2
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	7	0.2
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	10	0.2
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	16	0.2
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	18	0.2
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	7	0.2
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	11	0.2
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	12	0.2
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	16	0.2
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	16	0.2
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	16	0.2
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	20	0.2
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	20	0.2
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	20	0.2
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG2	5	0.2
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG3	5	0.2
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	13	0.19
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	1	0.19
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	3	0.19
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	9	0.19
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	10	0.19
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	14	0.19
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	15	0.19
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	17	0.19
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	20	0.19
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	8	0.19
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	8	0.19
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	18	0.19
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	18	0.19
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	18	0.19
(1,1539)	1:A:4:GLN:HB2	1:A:14:GLN:HE21	1	0.19
(1,1539)	1:A:4:GLN:HB2	1:A:14:GLN:HE22	1	0.19
(1,1539)	1:A:4:GLN:HB3	1:A:14:GLN:HE21	1	0.19
(1,1539)	1:A:4:GLN:HB3	1:A:14:GLN:HE22	1	0.19
(1,1367)	1:A:63:ILE:HG21	1:A:64:SER:HB3	12	0.19
(1,1367)	1:A:63:ILE:HG22	1:A:64:SER:HB3	12	0.19
(1,1367)	1:A:63:ILE:HG23	1:A:64:SER:HB3	12	0.19
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	13	0.19
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	13	0.19
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	13	0.19
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	11	0.18
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	20	0.18
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	4	0.18
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	6	0.18
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	13	0.18
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	18	0.18
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	3	0.18
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	3	0.18
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	3	0.18
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	9	0.18
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	9	0.18
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	9	0.18
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG2	11	0.18
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG3	11	0.18
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG2	19	0.18
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG3	19	0.18
(1,718)	1:A:7:GLU:HA	1:A:7:GLU:HG2	6	0.18
(1,718)	1:A:7:GLU:HA	1:A:7:GLU:HG3	6	0.18
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	16	0.18
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	8	0.18
(1,1370)	1:A:30:THR:HG21	1:A:64:SER:HB2	11	0.18
(1,1370)	1:A:30:THR:HG22	1:A:64:SER:HB2	11	0.18
(1,1370)	1:A:30:THR:HG23	1:A:64:SER:HB2	11	0.18
(1,1370)	1:A:30:THR:HG21	1:A:64:SER:HB2	15	0.18
(1,1370)	1:A:30:THR:HG22	1:A:64:SER:HB2	15	0.18
(1,1370)	1:A:30:THR:HG23	1:A:64:SER:HB2	15	0.18
(1,1367)	1:A:63:ILE:HG21	1:A:64:SER:HB3	20	0.18
(1,1367)	1:A:63:ILE:HG22	1:A:64:SER:HB3	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1367)	1:A:63:ILE:HG23	1:A:64:SER:HB3	20	0.18
(1,1363)	1:A:64:SER:HA	1:A:67:GLU:HG2	3	0.18
(1,1363)	1:A:64:SER:HA	1:A:67:GLU:HG3	3	0.18
(1,1363)	1:A:64:SER:HA	1:A:67:GLU:HG2	8	0.18
(1,1363)	1:A:64:SER:HA	1:A:67:GLU:HG3	8	0.18
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	1	0.18
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	1	0.18
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	1	0.18
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	8	0.17
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	2	0.17
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	5	0.17
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	8	0.17
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	6	0.17
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	6	0.17
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	6	0.17
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	12	0.17
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	12	0.17
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	12	0.17
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	17	0.17
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	17	0.17
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	17	0.17
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	19	0.17
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	19	0.17
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	19	0.17
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG2	9	0.17
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG3	9	0.17
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	7	0.17
(1,1550)	1:A:11:THR:HG21	1:A:14:GLN:HE21	19	0.17
(1,1550)	1:A:11:THR:HG21	1:A:14:GLN:HE22	19	0.17
(1,1550)	1:A:11:THR:HG22	1:A:14:GLN:HE21	19	0.17
(1,1550)	1:A:11:THR:HG22	1:A:14:GLN:HE22	19	0.17
(1,1550)	1:A:11:THR:HG23	1:A:14:GLN:HE21	19	0.17
(1,1550)	1:A:11:THR:HG23	1:A:14:GLN:HE22	19	0.17
(1,148)	1:A:61:GLU:HG2	1:A:62:LEU:H	4	0.17
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	8	0.17
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	8	0.17
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	8	0.17
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	10	0.17
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	10	0.17
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	10	0.17
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	14	0.17
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	14	0.17
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	17	0.17
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	17	0.17
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	17	0.17
(1,887)	1:A:18:GLN:H	1:A:19:LEU:HB3	19	0.16
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	16	0.16
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	11	0.16
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	11	0.16
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	11	0.16
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	13	0.16
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	13	0.16
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	13	0.16
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG2	10	0.16
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG3	10	0.16
(1,726)	1:A:4:GLN:HA	1:A:5:THR:HG21	7	0.16
(1,726)	1:A:4:GLN:HA	1:A:5:THR:HG22	7	0.16
(1,726)	1:A:4:GLN:HA	1:A:5:THR:HG23	7	0.16
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	9	0.16
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	11	0.16
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	14	0.16
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	13	0.16
(1,1454)	1:A:52:TYR:HD1	1:A:62:LEU:HG	3	0.16
(1,1454)	1:A:52:TYR:HD2	1:A:62:LEU:HG	3	0.16
(1,1370)	1:A:30:THR:HG21	1:A:64:SER:HB2	4	0.16
(1,1370)	1:A:30:THR:HG22	1:A:64:SER:HB2	4	0.16
(1,1370)	1:A:30:THR:HG23	1:A:64:SER:HB2	4	0.16
(1,1367)	1:A:63:ILE:HG21	1:A:64:SER:HB3	9	0.16
(1,1367)	1:A:63:ILE:HG22	1:A:64:SER:HB3	9	0.16
(1,1367)	1:A:63:ILE:HG23	1:A:64:SER:HB3	9	0.16
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	4	0.16
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	4	0.16
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	4	0.16
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	9	0.16
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	9	0.16
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	9	0.16
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	12	0.16
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	12	0.16
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	12	0.16
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	20	0.16
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	20	0.16
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	20	0.16
(1,838)	1:A:15:VAL:H	1:A:16:LYS:HB3	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	4	0.15
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	4	0.15
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	4	0.15
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	10	0.15
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	10	0.15
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	10	0.15
(1,777)	1:A:11:THR:HA	1:A:15:VAL:HB	1	0.15
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG2	8	0.15
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG3	8	0.15
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG2	12	0.15
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG3	12	0.15
(1,710)	1:A:7:GLU:HA	1:A:8:THR:H	8	0.15
(1,450)	1:A:69:THR:HA	1:A:71:ASP:H	19	0.15
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	12	0.15
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	15	0.15
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	17	0.15
(1,164)	1:A:71:ASP:HA	1:A:72:LEU:H	20	0.15
(1,1550)	1:A:11:THR:HG21	1:A:14:GLN:HE21	12	0.15
(1,1550)	1:A:11:THR:HG21	1:A:14:GLN:HE22	12	0.15
(1,1550)	1:A:11:THR:HG22	1:A:14:GLN:HE21	12	0.15
(1,1550)	1:A:11:THR:HG22	1:A:14:GLN:HE22	12	0.15
(1,1550)	1:A:11:THR:HG23	1:A:14:GLN:HE21	12	0.15
(1,1550)	1:A:11:THR:HG23	1:A:14:GLN:HE22	12	0.15
(1,1550)	1:A:11:THR:HG21	1:A:14:GLN:HE21	14	0.15
(1,1550)	1:A:11:THR:HG21	1:A:14:GLN:HE22	14	0.15
(1,1550)	1:A:11:THR:HG22	1:A:14:GLN:HE21	14	0.15
(1,1550)	1:A:11:THR:HG22	1:A:14:GLN:HE22	14	0.15
(1,1550)	1:A:11:THR:HG23	1:A:14:GLN:HE21	14	0.15
(1,1550)	1:A:11:THR:HG23	1:A:14:GLN:HE22	14	0.15
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	2	0.15
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	5	0.15
(1,1390)	1:A:70:GLU:HG2	1:A:71:ASP:HA	7	0.15
(1,1390)	1:A:70:GLU:HG3	1:A:71:ASP:HA	7	0.15
(1,1390)	1:A:70:GLU:HG2	1:A:71:ASP:HA	17	0.15
(1,1390)	1:A:70:GLU:HG3	1:A:71:ASP:HA	17	0.15
(1,1367)	1:A:63:ILE:HG21	1:A:64:SER:HB3	7	0.15
(1,1367)	1:A:63:ILE:HG22	1:A:64:SER:HB3	7	0.15
(1,1367)	1:A:63:ILE:HG23	1:A:64:SER:HB3	7	0.15
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	6	0.15
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	6	0.15
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	6	0.15
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	7	0.15
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	7	0.15
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	15	0.15
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	15	0.15
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	15	0.15
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	18	0.15
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	18	0.15
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	18	0.15
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG2	1	0.14
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG3	1	0.14
(1,726)	1:A:4:GLN:HA	1:A:5:THR:HG21	10	0.14
(1,726)	1:A:4:GLN:HA	1:A:5:THR:HG22	10	0.14
(1,726)	1:A:4:GLN:HA	1:A:5:THR:HG23	10	0.14
(1,645)	1:A:31:TYR:HD1	1:A:64:SER:HB2	9	0.14
(1,645)	1:A:31:TYR:HD2	1:A:64:SER:HB2	9	0.14
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB2	5	0.14
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB3	5	0.14
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB2	5	0.14
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB3	5	0.14
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB2	5	0.14
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB3	5	0.14
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB2	19	0.14
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB3	19	0.14
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB2	19	0.14
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB3	19	0.14
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB2	19	0.14
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB3	19	0.14
(1,410)	1:A:43:ILE:HB	1:A:44:GLU:H	12	0.14
(1,34)	1:A:69:THR:HA	1:A:70:GLU:H	12	0.14
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	10	0.14
(1,164)	1:A:71:ASP:HA	1:A:72:LEU:H	4	0.14
(1,164)	1:A:71:ASP:HA	1:A:72:LEU:H	6	0.14
(1,164)	1:A:71:ASP:HA	1:A:72:LEU:H	7	0.14
(1,1541)	1:A:8:THR:HA	1:A:9:GLU:HB2	6	0.14
(1,1541)	1:A:8:THR:HA	1:A:9:GLU:HB3	6	0.14
(1,1461)	1:A:52:TYR:HE1	1:A:62:LEU:HD21	11	0.14
(1,1461)	1:A:52:TYR:HE1	1:A:62:LEU:HD22	11	0.14
(1,1461)	1:A:52:TYR:HE1	1:A:62:LEU:HD23	11	0.14
(1,1461)	1:A:52:TYR:HE2	1:A:62:LEU:HD21	11	0.14
(1,1461)	1:A:52:TYR:HE2	1:A:62:LEU:HD22	11	0.14
(1,1461)	1:A:52:TYR:HE2	1:A:62:LEU:HD23	11	0.14
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	10	0.14
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	17	0.14
(1,1390)	1:A:70:GLU:HG2	1:A:71:ASP:HA	12	0.14
(1,1390)	1:A:70:GLU:HG3	1:A:71:ASP:HA	12	0.14
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	2	0.14
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	2	0.14
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	2	0.14
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	16	0.14
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	16	0.14
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	16	0.14
(1,1349)	1:A:63:ILE:HB	1:A:64:SER:HB3	14	0.14
(1,1219)	1:A:43:ILE:HD11	1:A:47:GLN:HG2	5	0.14
(1,1219)	1:A:43:ILE:HD12	1:A:47:GLN:HG2	5	0.14
(1,1219)	1:A:43:ILE:HD13	1:A:47:GLN:HG2	5	0.14
(1,972)	1:A:25:LYS:HE2	1:A:26:ARG:H	12	0.13
(1,972)	1:A:25:LYS:HE3	1:A:26:ARG:H	12	0.13
(1,777)	1:A:11:THR:HA	1:A:15:VAL:HB	12	0.13
(1,777)	1:A:11:THR:HA	1:A:15:VAL:HB	14	0.13
(1,645)	1:A:31:TYR:HD1	1:A:64:SER:HB2	12	0.13
(1,645)	1:A:31:TYR:HD2	1:A:64:SER:HB2	12	0.13
(1,417)	1:A:46:ASP:HA	1:A:46:ASP:HB3	15	0.13
(1,410)	1:A:43:ILE:HB	1:A:44:GLU:H	9	0.13
(1,410)	1:A:43:ILE:HB	1:A:44:GLU:H	15	0.13
(1,351)	1:A:8:THR:HA	1:A:9:GLU:H	7	0.13
(1,337)	1:A:47:GLN:HA	1:A:47:GLN:HE22	5	0.13
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	2	0.13
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	4	0.13
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	8	0.13
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	18	0.13
(1,196)	1:A:14:GLN:HB2	1:A:14:GLN:HE22	10	0.13
(1,196)	1:A:14:GLN:HB3	1:A:14:GLN:HE22	10	0.13
(1,1885)	1:A:73:GLU:H	1:A:73:GLU:HB2	16	0.13
(1,1885)	1:A:73:GLU:H	1:A:73:GLU:HB3	16	0.13
(1,1860)	1:A:65:GLU:HB2	1:A:66:ASN:HB2	8	0.13
(1,1860)	1:A:65:GLU:HB2	1:A:66:ASN:HB3	8	0.13
(1,1860)	1:A:65:GLU:HB3	1:A:66:ASN:HB2	8	0.13
(1,1860)	1:A:65:GLU:HB3	1:A:66:ASN:HB3	8	0.13
(1,181)	1:A:8:THR:H	1:A:9:GLU:H	15	0.13
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	14	0.13
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	16	0.13
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	18	0.13
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1454)	1:A:52:TYR:HD1	1:A:62:LEU:HG	6	0.13
(1,1454)	1:A:52:TYR:HD2	1:A:62:LEU:HG	6	0.13
(1,1389)	1:A:70:GLU:HA	1:A:71:ASP:HB2	6	0.13
(1,1369)	1:A:30:THR:HG21	1:A:64:SER:HB3	5	0.13
(1,1369)	1:A:30:THR:HG22	1:A:64:SER:HB3	5	0.13
(1,1369)	1:A:30:THR:HG23	1:A:64:SER:HB3	5	0.13
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	3	0.13
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	3	0.13
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	3	0.13
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	5	0.13
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	5	0.13
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	5	0.13
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	19	0.13
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	19	0.13
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	19	0.13
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	5	0.12
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	5	0.12
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	5	0.12
(1,780)	1:A:10:LEU:HD11	1:A:11:THR:HA	15	0.12
(1,780)	1:A:10:LEU:HD12	1:A:11:THR:HA	15	0.12
(1,780)	1:A:10:LEU:HD13	1:A:11:THR:HA	15	0.12
(1,780)	1:A:10:LEU:HD11	1:A:11:THR:HA	18	0.12
(1,780)	1:A:10:LEU:HD12	1:A:11:THR:HA	18	0.12
(1,780)	1:A:10:LEU:HD13	1:A:11:THR:HA	18	0.12
(1,777)	1:A:11:THR:HA	1:A:15:VAL:HB	7	0.12
(1,777)	1:A:11:THR:HA	1:A:15:VAL:HB	18	0.12
(1,728)	1:A:43:ILE:HD11	1:A:48:MET:HA	18	0.12
(1,728)	1:A:43:ILE:HD12	1:A:48:MET:HA	18	0.12
(1,728)	1:A:43:ILE:HD13	1:A:48:MET:HA	18	0.12
(1,718)	1:A:7:GLU:HA	1:A:7:GLU:HG2	14	0.12
(1,718)	1:A:7:GLU:HA	1:A:7:GLU:HG3	14	0.12
(1,708)	1:A:67:GLU:HB3	1:A:68:GLU:H	7	0.12
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB2	9	0.12
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB3	9	0.12
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB2	9	0.12
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB3	9	0.12
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB2	9	0.12
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB3	9	0.12
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB2	11	0.12
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB3	11	0.12
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB2	11	0.12
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB3	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB2	11	0.12
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB3	11	0.12
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB2	13	0.12
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB3	13	0.12
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB2	13	0.12
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB3	13	0.12
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB2	13	0.12
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB3	13	0.12
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB2	14	0.12
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB3	14	0.12
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB2	14	0.12
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB3	14	0.12
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB2	14	0.12
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB3	14	0.12
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB2	17	0.12
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB3	17	0.12
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB2	17	0.12
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB3	17	0.12
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB2	17	0.12
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB3	17	0.12
(1,450)	1:A:69:THR:HA	1:A:71:ASP:H	10	0.12
(1,439)	1:A:66:ASN:H	1:A:66:ASN:HB2	9	0.12
(1,417)	1:A:46:ASP:HA	1:A:46:ASP:HB3	17	0.12
(1,410)	1:A:43:ILE:HB	1:A:44:GLU:H	1	0.12
(1,410)	1:A:43:ILE:HB	1:A:44:GLU:H	3	0.12
(1,410)	1:A:43:ILE:HB	1:A:44:GLU:H	20	0.12
(1,34)	1:A:69:THR:HA	1:A:70:GLU:H	7	0.12
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	19	0.12
(1,248)	1:A:16:LYS:H	1:A:18:GLN:HB2	9	0.12
(1,248)	1:A:16:LYS:H	1:A:18:GLN:HB3	9	0.12
(1,196)	1:A:14:GLN:HB2	1:A:14:GLN:HE22	13	0.12
(1,196)	1:A:14:GLN:HB3	1:A:14:GLN:HE22	13	0.12
(1,1869)	1:A:68:GLU:HB2	1:A:69:THR:H	1	0.12
(1,1869)	1:A:68:GLU:HB3	1:A:69:THR:H	1	0.12
(1,1869)	1:A:68:GLU:HB2	1:A:69:THR:H	14	0.12
(1,1869)	1:A:68:GLU:HB3	1:A:69:THR:H	14	0.12
(1,1760)	1:A:41:PHE:HA	1:A:42:GLU:HG2	6	0.12
(1,1760)	1:A:41:PHE:HA	1:A:42:GLU:HG3	6	0.12
(1,1662)	1:A:24:LYS:HE2	1:A:59:GLY:H	1	0.12
(1,1662)	1:A:24:LYS:HE3	1:A:59:GLY:H	1	0.12
(1,1550)	1:A:11:THR:HG21	1:A:14:GLN:HE21	9	0.12
(1,1550)	1:A:11:THR:HG21	1:A:14:GLN:HE22	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1550)	1:A:11:THR:HG22	1:A:14:GLN:HE21	9	0.12
(1,1550)	1:A:11:THR:HG22	1:A:14:GLN:HE22	9	0.12
(1,1550)	1:A:11:THR:HG23	1:A:14:GLN:HE21	9	0.12
(1,1550)	1:A:11:THR:HG23	1:A:14:GLN:HE22	9	0.12
(1,1541)	1:A:8:THR:HA	1:A:9:GLU:HB2	19	0.12
(1,1541)	1:A:8:THR:HA	1:A:9:GLU:HB3	19	0.12
(1,1541)	1:A:8:THR:HA	1:A:9:GLU:HB2	20	0.12
(1,1541)	1:A:8:THR:HA	1:A:9:GLU:HB3	20	0.12
(1,1538)	1:A:4:GLN:HB2	1:A:14:GLN:HB2	4	0.12
(1,1538)	1:A:4:GLN:HB2	1:A:14:GLN:HB3	4	0.12
(1,1538)	1:A:4:GLN:HB3	1:A:14:GLN:HB2	4	0.12
(1,1538)	1:A:4:GLN:HB3	1:A:14:GLN:HB3	4	0.12
(1,1461)	1:A:52:TYR:HE1	1:A:62:LEU:HD21	13	0.12
(1,1461)	1:A:52:TYR:HE1	1:A:62:LEU:HD22	13	0.12
(1,1461)	1:A:52:TYR:HE1	1:A:62:LEU:HD23	13	0.12
(1,1461)	1:A:52:TYR:HE2	1:A:62:LEU:HD21	13	0.12
(1,1461)	1:A:52:TYR:HE2	1:A:62:LEU:HD22	13	0.12
(1,1461)	1:A:52:TYR:HE2	1:A:62:LEU:HD23	13	0.12
(1,1461)	1:A:52:TYR:HE1	1:A:62:LEU:HD21	19	0.12
(1,1461)	1:A:52:TYR:HE1	1:A:62:LEU:HD22	19	0.12
(1,1461)	1:A:52:TYR:HE1	1:A:62:LEU:HD23	19	0.12
(1,1461)	1:A:52:TYR:HE2	1:A:62:LEU:HD21	19	0.12
(1,1461)	1:A:52:TYR:HE2	1:A:62:LEU:HD22	19	0.12
(1,1461)	1:A:52:TYR:HE2	1:A:62:LEU:HD23	19	0.12
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	1	0.12
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	4	0.12
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	11	0.12
(1,1413)	1:A:67:GLU:HG2	1:A:68:GLU:HA	8	0.12
(1,1413)	1:A:67:GLU:HG3	1:A:68:GLU:HA	8	0.12
(1,1404)	1:A:63:ILE:HG21	1:A:67:GLU:HB2	6	0.12
(1,1404)	1:A:63:ILE:HG22	1:A:67:GLU:HB2	6	0.12
(1,1404)	1:A:63:ILE:HG23	1:A:67:GLU:HB2	6	0.12
(1,1367)	1:A:63:ILE:HG21	1:A:64:SER:HB3	5	0.12
(1,1367)	1:A:63:ILE:HG22	1:A:64:SER:HB3	5	0.12
(1,1367)	1:A:63:ILE:HG23	1:A:64:SER:HB3	5	0.12
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG21	11	0.12
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG22	11	0.12
(1,1353)	1:A:30:THR:H	1:A:63:ILE:HG23	11	0.12
(1,814)	1:A:15:VAL:HG11	1:A:18:GLN:HA	2	0.11
(1,814)	1:A:15:VAL:HG12	1:A:18:GLN:HA	2	0.11
(1,814)	1:A:15:VAL:HG13	1:A:18:GLN:HA	2	0.11
(1,791)	1:A:13:ASP:HB2	1:A:14:GLN:HA	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG2	16	0.11
(1,744)	1:A:69:THR:HA	1:A:70:GLU:HG3	16	0.11
(1,728)	1:A:43:ILE:HD11	1:A:48:MET:HA	2	0.11
(1,728)	1:A:43:ILE:HD12	1:A:48:MET:HA	2	0.11
(1,728)	1:A:43:ILE:HD13	1:A:48:MET:HA	2	0.11
(1,708)	1:A:67:GLU:HB3	1:A:68:GLU:H	15	0.11
(1,645)	1:A:31:TYR:HD1	1:A:64:SER:HB2	5	0.11
(1,645)	1:A:31:TYR:HD2	1:A:64:SER:HB2	5	0.11
(1,645)	1:A:31:TYR:HD1	1:A:64:SER:HB2	7	0.11
(1,645)	1:A:31:TYR:HD2	1:A:64:SER:HB2	7	0.11
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB2	2	0.11
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB3	2	0.11
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB2	2	0.11
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB3	2	0.11
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB2	2	0.11
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB3	2	0.11
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB2	4	0.11
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB3	4	0.11
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB2	4	0.11
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB3	4	0.11
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB2	4	0.11
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB3	4	0.11
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB2	6	0.11
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB3	6	0.11
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB2	6	0.11
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB3	6	0.11
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB2	6	0.11
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB3	6	0.11
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB2	10	0.11
(1,505)	1:A:20:THR:HG21	1:A:21:GLU:HB3	10	0.11
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB2	10	0.11
(1,505)	1:A:20:THR:HG22	1:A:21:GLU:HB3	10	0.11
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB2	10	0.11
(1,505)	1:A:20:THR:HG23	1:A:21:GLU:HB3	10	0.11
(1,442)	1:A:5:THR:HA	1:A:5:THR:HG21	18	0.11
(1,442)	1:A:5:THR:HA	1:A:5:THR:HG22	18	0.11
(1,442)	1:A:5:THR:HA	1:A:5:THR:HG23	18	0.11
(1,410)	1:A:43:ILE:HB	1:A:44:GLU:H	7	0.11
(1,410)	1:A:43:ILE:HB	1:A:44:GLU:H	10	0.11
(1,410)	1:A:43:ILE:HB	1:A:44:GLU:H	16	0.11
(1,410)	1:A:43:ILE:HB	1:A:44:GLU:H	17	0.11
(1,340)	1:A:64:SER:HA	1:A:65:GLU:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:A:64:SER:HA	1:A:65:GLU:H	8	0.11
(1,273)	1:A:22:SER:H	1:A:24:LYS:HG3	13	0.11
(1,248)	1:A:16:LYS:H	1:A:18:GLN:HB2	1	0.11
(1,248)	1:A:16:LYS:H	1:A:18:GLN:HB3	1	0.11
(1,248)	1:A:16:LYS:H	1:A:18:GLN:HB2	14	0.11
(1,248)	1:A:16:LYS:H	1:A:18:GLN:HB3	14	0.11
(1,1872)	1:A:69:THR:HA	1:A:72:LEU:HD11	20	0.11
(1,1872)	1:A:69:THR:HA	1:A:72:LEU:HD12	20	0.11
(1,1872)	1:A:69:THR:HA	1:A:72:LEU:HD13	20	0.11
(1,1872)	1:A:69:THR:HA	1:A:72:LEU:HD21	20	0.11
(1,1872)	1:A:69:THR:HA	1:A:72:LEU:HD22	20	0.11
(1,1872)	1:A:69:THR:HA	1:A:72:LEU:HD23	20	0.11
(1,1850)	1:A:61:GLU:HG2	1:A:62:LEU:HD11	3	0.11
(1,1850)	1:A:61:GLU:HG2	1:A:62:LEU:HD12	3	0.11
(1,1850)	1:A:61:GLU:HG2	1:A:62:LEU:HD13	3	0.11
(1,1850)	1:A:61:GLU:HG2	1:A:62:LEU:HD21	3	0.11
(1,1850)	1:A:61:GLU:HG2	1:A:62:LEU:HD22	3	0.11
(1,1850)	1:A:61:GLU:HG2	1:A:62:LEU:HD23	3	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD11	1	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD12	1	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD13	1	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD21	1	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD22	1	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD23	1	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD11	5	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD12	5	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD13	5	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD21	5	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD22	5	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD23	5	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD11	15	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD12	15	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD13	15	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD21	15	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD22	15	0.11
(1,1792)	1:A:49:ASP:HA	1:A:62:LEU:HD23	15	0.11
(1,1662)	1:A:24:LYS:HE2	1:A:59:GLY:H	3	0.11
(1,1662)	1:A:24:LYS:HE3	1:A:59:GLY:H	3	0.11
(1,1662)	1:A:24:LYS:HE2	1:A:59:GLY:H	19	0.11
(1,1662)	1:A:24:LYS:HE3	1:A:59:GLY:H	19	0.11
(1,164)	1:A:71:ASP:HA	1:A:72:LEU:H	3	0.11
(1,164)	1:A:71:ASP:HA	1:A:72:LEU:H	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1550)	1:A:11:THR:HG21	1:A:14:GLN:HE21	20	0.11
(1,1550)	1:A:11:THR:HG21	1:A:14:GLN:HE22	20	0.11
(1,1550)	1:A:11:THR:HG22	1:A:14:GLN:HE21	20	0.11
(1,1550)	1:A:11:THR:HG22	1:A:14:GLN:HE22	20	0.11
(1,1550)	1:A:11:THR:HG23	1:A:14:GLN:HE21	20	0.11
(1,1550)	1:A:11:THR:HG23	1:A:14:GLN:HE22	20	0.11
(1,1541)	1:A:8:THR:HA	1:A:9:GLU:HB2	8	0.11
(1,1541)	1:A:8:THR:HA	1:A:9:GLU:HB3	8	0.11
(1,1488)	1:A:41:PHE:H	1:A:41:PHE:HZ	8	0.11
(1,146)	1:A:62:LEU:H	1:A:62:LEU:HG	9	0.11
(1,1413)	1:A:67:GLU:HG2	1:A:68:GLU:HA	4	0.11
(1,1413)	1:A:67:GLU:HG3	1:A:68:GLU:HA	4	0.11
(1,1390)	1:A:70:GLU:HG2	1:A:71:ASP:HA	15	0.11
(1,1390)	1:A:70:GLU:HG3	1:A:71:ASP:HA	15	0.11
(1,1372)	1:A:64:SER:HB2	1:A:67:GLU:HG2	8	0.11
(1,1372)	1:A:64:SER:HB2	1:A:67:GLU:HG3	8	0.11
(1,1369)	1:A:30:THR:HG21	1:A:64:SER:HB3	20	0.11
(1,1369)	1:A:30:THR:HG22	1:A:64:SER:HB3	20	0.11
(1,1369)	1:A:30:THR:HG23	1:A:64:SER:HB3	20	0.11
(1,1349)	1:A:63:ILE:HB	1:A:64:SER:HB3	20	0.11
(1,1203)	1:A:44:GLU:HA	1:A:45:SER:HB2	3	0.11
(1,1203)	1:A:44:GLU:HA	1:A:45:SER:HB3	3	0.11
(1,1103)	1:A:35:ALA:HA	1:A:52:TYR:HE1	13	0.11
(1,1103)	1:A:35:ALA:HA	1:A:52:TYR:HE2	13	0.11
(1,1103)	1:A:35:ALA:HA	1:A:52:TYR:HE1	18	0.11
(1,1103)	1:A:35:ALA:HA	1:A:52:TYR:HE2	18	0.11
(1,1051)	1:A:28:VAL:HB	1:A:29:LEU:HA	6	0.11
(1,1051)	1:A:28:VAL:HB	1:A:29:LEU:HA	17	0.11
(1,1009)	1:A:27:GLY:HA2	1:A:28:VAL:HG21	13	0.11
(1,1009)	1:A:27:GLY:HA2	1:A:28:VAL:HG22	13	0.11
(1,1009)	1:A:27:GLY:HA2	1:A:28:VAL:HG23	13	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found