Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2MLE
BMRB ID	:	19816
Title	:	NMR structure of the C-domain of troponin C bound to the anchoring region of troponin I
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Deposited on	:	2014-02-26

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:

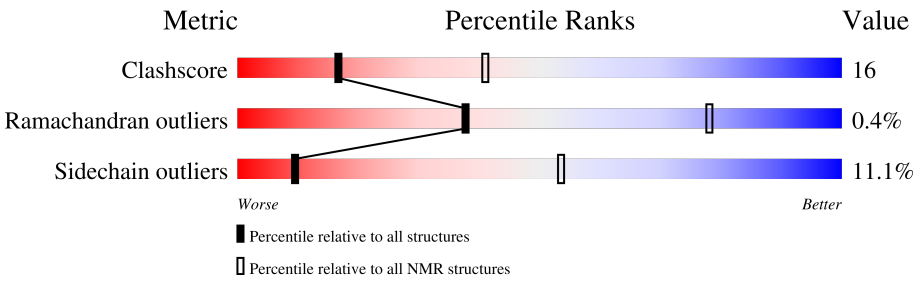
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 73%.

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	C	72	51% 35% • 11%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	C:94-C:157 (64)	1.19	14

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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1130 atoms, of which 545 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Troponin C, slow skeletal and cardiac muscles.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	C	72	1128	360	545	88	130	5	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	90	MET	-	initiating methionine	UNP P63316

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
2	C	2	2	2

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C:

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

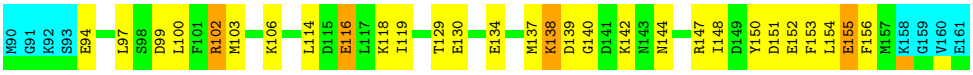
• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C:

4.2.2 Score per residue for model 2

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C:



4.2.3 Score per residue for model 3

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 47% 33% 7% • 11%

M90 G91 K92 S93 L97 S98 D99 L100 F101 R102 M103 F104 D105 K106 I112 D113 L114 D115 E116 L117 K118 I119 M120 L121 E126 T127 I128 D131 D132 I133 E134 E135 L136 M137 K138 D139 K142 R147 I148 E152 F153 L154 E155 F156 M157 K158 G159 V160 E161

4.2.4 Score per residue for model 4

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 51% 33% • 11%

M90 G91 K92 S93 E94 E95 D99 R102 M103 F104 D105 K106 N107 A108 I112 D113 L114 D115 E116 I119 M120 E126 T127 I128 D131 D132 I133 E134 E135 L136 M137 K142 R147 E152 E155 F156 M157 K158 G159 V160 E161

4.2.5 Score per residue for model 5

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 57% 25% 7% 11%

M90 G91 K92 S93 E94 E95 E96 L97 S98 D99 R102 M103 F104 I112 D113 L114 D115 E116 L117 T124 G125 E126 T129 E130 I133 M137 K142 R147 I148 E152 F153 L154 E155 K158 G159 V160 E161

4.2.6 Score per residue for model 6

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 49% 33% 6% • 11%

M90 G91 K92 S93 E94 E95 E96 L97 L100 F101 R102 M103 F104 D105 K106 I112 D113 L114 D115 E116 L117 K118 I119 E126 T127 I128 T129 E130 D131 D132 I133 M137 K138 D139 K142 D145 G146 R147 Y150 D151 E152 F153 L154 E155 K158 G159 V160 E161

4.2.7 Score per residue for model 7

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 54% 26% 7% • 11%

M90 G91 K92 S93 E94 L97 R102 K106 I112 E116 L117 K118 I119 M120 L121 E126 T127 I128 T129 E130 I133 E134 E135 K138 D139 K142 R147 I148 D149 E152 F153 L154 E155 K158 G159 V160 E161

4.2.8 Score per residue for model 8

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 58% 26% • 11%

M90 G91 K92 S93 E94 E95 E96 L97 R102 I112 D113 L114 D115 E116 L117 K118 L121 E126 T127 I128 I133 G140 D141 K142 R147 I148 E152 F153 L154 E155 F156 M157 K158 G159 V160 E161

4.2.9 Score per residue for model 9

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 47% 35% 7% 11%

M90 G91 K92 S93 E94 E95 E96 L97 R102 M103 F104 D105 K106 D109 I112 D113 L114 D115 E116 L117 K118 I119 I128 T129 E130 D131 D132 I133 E134 E135 L136 M137 K138 K142 N143 N144 R147 I148 D151 E152 E155 F156 M157 K158 G159 V160 E161

4.2.10 Score per residue for model 10

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 54% 31% • • 11%

M90 G91 K92 S93 E96 L97 M103 K106 I112 D113 L114 D115 E116 L117 K118 L121 T127 I128 T129 D132 I133 E134 E135 L136 M137 K138 D139 G140 D141 K142 R147 I148 E152 F153 L154 E155 K158 G159 V160 E161

4.2.11 Score per residue for model 11

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 57% 26% 6% 11%

M90 G91 K92 S93 E94 E95 E96 L97 R102 K106 Y111 I112 D113 L114 D115 E116 L117 K118 L121 T127 I128 T129 I133 E134 M137 K138 D139 K142 R147 I148 E152 F153 L154 E155 K158 G159 V160 E161

4.2.12 Score per residue for model 12

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 44% 39% • • 11%

M90 G91 K92 S93 E94 E95 E96 L97 F101 R102 M103 F104 Y111 I112 D113 L114 D115 E116 L117 K118 I119 M120 L121 E126 T127 I128 T129 E130 I133 E134 M137 R147 I148 D149 Y150 D151 E152 F153 L154 E155 F156 M157 K158 G159 V160 E161

4.2.13 Score per residue for model 13

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 53% 31% • • 11%

M90 G91 K92 S93 E94 L97 S98 D99 L100 F101 R102 K106 I112 D113 L114 D115 E116 L117 K118 I119 M120 L121 E126 T129 E134 M137 K138 D139 G140 D141 K142 R147 Y150 D151 E152 F153 L154 M157 K158 G159 V160 E161

4.2.14 Score per residue for model 14 (medoid)

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 40% 40% 8% 11%

M90 G91 K92 S93 E94 E95 E96 L97 S98 D99 L100 F101 R102 M103 F104 D105 K106 N107 A108 D109 G110 Y111 I112 D113 L114 D115 E116 L117 K118 L121 T127 I128 D131 E134 M137 K138 K142 R147 I148 D149 E152 F153 L154 E155 F156 M157 K158 G159 V160 E161

4.2.15 Score per residue for model 15

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 57% 26% 6% 11%

M90 G91 K92 S93 E94 E95 E96 L97 R102 M103 F104 D105 K106 I112 D113 E116 L117 K118 I119 M120 L121 T127 I128 D139 G140 D141 K142 R147 I148 E152 F153 L154 M157 K158 G159 V160 E161

4.2.16 Score per residue for model 16

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 47% 35% 7% 11%

M90 G91 K92 S93 E94 E95 E96 L97 R102 M103 F104 D105 K106 I112 D113 L114 D115 E116 L117 K118 I119 M120 L121 T124 G125 E126 T127 I128 I133 M137 D141 K142 R147 I148 E152 F153 L154 E155 F156 M157 K158 G159 V160 E161

4.2.17 Score per residue for model 17

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 46% 39% • 11%

M90 G91 K92 S93 E96 L97 S98 D99 L100 F101 R102 M103 F104 D105 K106 I112 D113 L114 D115 E116 L117 K118 I119 E126 T127 I128 T129 D132 I133 E134 E135 L136 M137 K138 K142 R147 I148 D149 Y150 D151 E152 F153 L154 E155 F156 M157 K158 G159 V160 E161

4.2.18 Score per residue for model 18

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 49% 33% 7% 11%

M90 G91 K92 S93 E94 L97 S98 D99 R102 M103 F104 D105 K106 N107 A108 I112 D113 L114 D115 E116 L117 K118 L121 T124 I128 D132 I133 E134 E135 L136 G140 D141 K142 R147 I148 E152 F153 L154 E155 F156 M157 K158 G159 V160 E161

4.2.19 Score per residue for model 19

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 54% 31% • 11%

M90 G91 K92 S93 E94 E95 E96 L97 F101 R102 M103 F104 D105 K106 Y111 I112 D113 L114 D115 E116 L117 K118 I119 T124 G125 E126 T127 I128 T129 I133 M137 R147 I148 D149 Y150 D151 E152 F153 L154 K158 G159 V160 E161

4.2.20 Score per residue for model 20

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 50% 29% 10% 11%

M90 G91 K92 S93 E94 E95 E96 L97 R102 D105 K106 I112 D113 L114 D115 E116 L117 K118 I119 M120 L121 Q122 E126 T127 I128 T129 I133 E134 E135 L136 M137 K138 D139 K142 R147 I148 E152 F153 L154 E155 K158 G159 V160 E161

5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	geometry optimization	
ProcheckNMR	refinement	
X-PLOR NIH	refinement	
X-PLOR NIH	geometry optimization	
CYANA	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	689
Number of shifts mapped to atoms	689
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	73%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	C	1.55±0.02	6±1/532 (1.2± 0.2%)	1.17±0.02	0±0/713 (0.0± 0.1%)
All	All	1.55	125/10640 (1.2%)	1.17	2/14260 (0.0%)

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	C	0.0±0.0	1.9±0.2
All	All	0	39

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	152	GLU	CD-OE2	-9.17	1.15	1.25	2	20
1	C	116	GLU	CD-OE1	-8.79	1.16	1.25	1	19
1	C	116	GLU	CD-OE2	-8.73	1.16	1.25	18	20
1	C	152	GLU	CD-OE1	-7.42	1.17	1.25	4	19
1	C	95	GLU	CD-OE2	-6.73	1.18	1.25	5	7
1	C	135	GLU	CD-OE2	-6.36	1.18	1.25	17	5
1	C	155	GLU	CD-OE2	-6.17	1.18	1.25	14	6
1	C	96	GLU	CD-OE1	-5.82	1.19	1.25	1	1
1	C	94	GLU	CD-OE2	-5.80	1.19	1.25	13	7
1	C	134	GLU	CD-OE1	-5.49	1.19	1.25	12	1
1	C	110	GLY	N-CA	5.48	1.54	1.46	14	1
1	C	155	GLU	CD-OE1	-5.48	1.19	1.25	7	1
1	C	126	GLU	CD-OE2	-5.44	1.19	1.25	7	9
1	C	96	GLU	CD-OE2	-5.38	1.19	1.25	14	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	130	GLU	CD-OE1	-5.29	1.19	1.25	2	1
1	C	134	GLU	CD-OE2	-5.19	1.20	1.25	14	1
1	C	130	GLU	CD-OE2	-5.11	1.20	1.25	9	1
1	C	109	ASP	CG-OD1	-5.03	1.13	1.25	9	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	C	126	GLU	N-CA-CB	-5.22	101.19	110.60	17	1
1	C	150	TYR	N-CA-CB	-5.05	101.50	110.60	17	1

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	C	147	ARG	Sidechain	20
1	C	102	ARG	Sidechain	19

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	C	526	482	482	16±3
All	All	10560	9640	9640	315

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:97:LEU:HD22	1:C:154:LEU:HD13	1.06	1.24	18	11
1:C:97:LEU:HD22	1:C:154:LEU:HD21	0.89	1.43	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:114:LEU:HD21	1:C:137:MET:HB2	0.88	1.42	1	3
1:C:117:LEU:HD23	1:C:133:ILE:HG23	0.87	1.46	8	2
1:C:114:LEU:HD22	1:C:133:ILE:HG22	0.87	1.46	1	1
1:C:117:LEU:HD22	1:C:133:ILE:HG23	0.83	1.50	16	2
1:C:106:LYS:HE2	1:C:119:ILE:HD12	0.76	1.56	20	4
1:C:106:LYS:HE3	1:C:119:ILE:HD12	0.75	1.56	2	3
1:C:114:LEU:HD11	1:C:137:MET:SD	0.71	2.25	2	1
1:C:121:LEU:HB3	1:C:128:ILE:HG21	0.70	1.63	11	1
1:C:128:ILE:CG2	1:C:133:ILE:HD11	0.68	2.18	8	1
1:C:97:LEU:HD22	1:C:154:LEU:CD2	0.66	2.18	17	1
1:C:104:PHE:CE1	1:C:117:LEU:HD23	0.66	2.25	3	1
1:C:97:LEU:HD13	1:C:154:LEU:HD12	0.65	1.67	8	2
1:C:114:LEU:CD1	1:C:133:ILE:HG22	0.65	2.22	8	1
1:C:97:LEU:CD2	1:C:154:LEU:HD13	0.65	2.21	11	3
1:C:129:THR:O	1:C:133:ILE:HD12	0.64	1.92	9	3
1:C:106:LYS:CE	1:C:119:ILE:HD12	0.63	2.23	20	5
1:C:114:LEU:HD13	1:C:137:MET:HG2	0.63	1.70	3	1
1:C:121:LEU:HB3	1:C:128:ILE:HD13	0.63	1.68	15	1
1:C:114:LEU:HD12	1:C:133:ILE:HG22	0.63	1.71	8	2
1:C:112:ILE:HB	1:C:148:ILE:HB	0.62	1.72	15	16
1:C:128:ILE:CD1	1:C:133:ILE:HD11	0.62	2.24	3	1
1:C:117:LEU:HD11	1:C:148:ILE:HD11	0.62	1.70	3	1
1:C:147:ARG:HB3	1:C:147:ARG:CZ	0.61	2.25	10	1
1:C:124:THR:HG22	1:C:126:GLU:HG2	0.61	1.70	16	1
1:C:106:LYS:HG2	1:C:116:GLU:HG2	0.59	1.73	17	5
1:C:114:LEU:CD2	1:C:134:GLU:HA	0.59	2.27	18	2
1:C:104:PHE:CE2	1:C:112:ILE:HG21	0.59	2.32	5	1
1:C:128:ILE:HB	1:C:133:ILE:HD11	0.58	1.75	20	1
1:C:141:ASP:N	1:C:148:ILE:HD12	0.58	2.13	15	1
1:C:100:LEU:HD23	1:C:157:MET:HE2	0.57	1.74	14	1
1:C:104:PHE:HB3	1:C:112:ILE:HD12	0.57	1.76	12	2
1:C:139:ASP:O	1:C:142:LYS:HE3	0.57	1.99	1	1
1:C:106:LYS:CE	1:C:116:GLU:HG2	0.57	2.30	14	1
1:C:121:LEU:HD23	1:C:128:ILE:HG13	0.57	1.74	18	1
1:C:121:LEU:HD12	1:C:133:ILE:HG12	0.57	1.76	10	2
1:C:135:GLU:HA	1:C:138:LYS:CE	0.57	2.29	7	1
1:C:127:THR:HG22	1:C:132:ASP:HB3	0.56	1.77	10	1
1:C:140:GLY:C	1:C:148:ILE:HD12	0.56	2.20	2	4
1:C:114:LEU:HD13	1:C:137:MET:CG	0.56	2.30	3	2
1:C:97:LEU:HD12	1:C:157:MET:SD	0.56	2.41	8	1
1:C:97:LEU:HD21	1:C:154:LEU:HD13	0.55	1.76	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:106:LYS:CG	1:C:116:GLU:HG2	0.54	2.32	18	2
1:C:142:LYS:HE3	1:C:155:GLU:CD	0.54	2.23	5	2
1:C:115:ASP:HA	1:C:118:LYS:HG2	0.54	1.79	8	2
1:C:128:ILE:HD11	1:C:133:ILE:HD11	0.53	1.79	18	1
1:C:97:LEU:HD22	1:C:154:LEU:CD1	0.53	2.17	18	2
1:C:128:ILE:CG1	1:C:133:ILE:HD11	0.53	2.32	6	1
1:C:97:LEU:HD13	1:C:154:LEU:CD2	0.53	2.33	20	1
1:C:97:LEU:HB3	1:C:157:MET:SD	0.52	2.43	1	1
1:C:140:GLY:HA2	1:C:156:PHE:CD1	0.52	2.39	2	2
1:C:106:LYS:HE3	1:C:116:GLU:HG2	0.52	1.82	14	2
1:C:107:ASN:O	1:C:108:ALA:HB3	0.52	2.04	4	2
1:C:121:LEU:HB3	1:C:128:ILE:HD12	0.52	1.82	12	3
1:C:97:LEU:HD11	1:C:153:PHE:CD2	0.52	2.40	15	2
1:C:97:LEU:CD2	1:C:154:LEU:HD21	0.52	2.29	17	1
1:C:104:PHE:CZ	1:C:117:LEU:HD23	0.51	2.40	3	2
1:C:97:LEU:HG	1:C:150:TYR:CE1	0.51	2.41	2	2
1:C:135:GLU:HA	1:C:138:LYS:HE3	0.51	1.82	3	1
1:C:106:LYS:CD	1:C:119:ILE:HD12	0.51	2.34	17	1
1:C:104:PHE:CE1	1:C:112:ILE:HG23	0.51	2.41	15	1
1:C:94:GLU:HA	1:C:97:LEU:HD21	0.51	1.83	20	2
1:C:117:LEU:HD11	1:C:148:ILE:CD1	0.50	2.36	3	1
1:C:112:ILE:CD1	1:C:153:PHE:CD1	0.50	2.94	15	1
1:C:114:LEU:HD21	1:C:134:GLU:HA	0.50	1.82	10	1
1:C:100:LEU:HD23	1:C:157:MET:CE	0.50	2.36	14	1
1:C:135:GLU:HA	1:C:138:LYS:HE2	0.50	1.81	7	1
1:C:142:LYS:HD2	1:C:155:GLU:CB	0.50	2.36	10	1
1:C:134:GLU:O	1:C:138:LYS:HG2	0.50	2.07	14	1
1:C:127:THR:O	1:C:128:ILE:HD13	0.50	2.06	16	1
1:C:114:LEU:CD2	1:C:133:ILE:HG22	0.50	2.31	1	2
1:C:134:GLU:O	1:C:138:LYS:HE2	0.50	2.07	1	1
1:C:153:PHE:HA	1:C:156:PHE:HB3	0.50	1.83	2	2
1:C:114:LEU:HD21	1:C:137:MET:SD	0.50	2.47	20	3
1:C:117:LEU:HD23	1:C:133:ILE:CG2	0.49	2.36	12	1
1:C:137:MET:HE1	1:C:147:ARG:CA	0.49	2.37	19	1
1:C:138:LYS:N	1:C:138:LYS:HD3	0.49	2.21	2	1
1:C:112:ILE:HD12	1:C:153:PHE:CD2	0.49	2.41	6	1
1:C:114:LEU:HD21	1:C:137:MET:HG2	0.49	1.84	19	2
1:C:154:LEU:HA	1:C:157:MET:HE2	0.49	1.84	18	2
1:C:130:GLU:HA	1:C:133:ILE:HD12	0.49	1.84	5	3
1:C:97:LEU:HD11	1:C:153:PHE:HD2	0.49	1.68	15	1
1:C:97:LEU:HD13	1:C:157:MET:SD	0.49	2.48	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:115:ASP:O	1:C:119:ILE:HG12	0.49	2.07	16	3
1:C:99:ASP:O	1:C:102:ARG:HG2	0.49	2.07	13	3
1:C:128:ILE:HG13	1:C:133:ILE:HD11	0.49	1.85	6	1
1:C:142:LYS:HD2	1:C:142:LYS:N	0.49	2.23	9	2
1:C:109:ASP:O	1:C:111:TYR:N	0.49	2.46	14	1
1:C:115:ASP:HA	1:C:118:LYS:CG	0.49	2.38	16	1
1:C:118:LYS:HA	1:C:133:ILE:HD13	0.49	1.84	7	1
1:C:101:PHE:CE1	1:C:112:ILE:CD1	0.48	2.97	17	1
1:C:112:ILE:HD13	1:C:153:PHE:CD1	0.48	2.43	17	1
1:C:114:LEU:HG	1:C:137:MET:SD	0.48	2.48	14	2
1:C:97:LEU:HB2	1:C:154:LEU:HD11	0.48	1.84	17	1
1:C:114:LEU:C	1:C:114:LEU:HD13	0.48	2.27	6	1
1:C:117:LEU:HD12	1:C:137:MET:SD	0.48	2.48	14	1
1:C:115:ASP:O	1:C:118:LYS:HG3	0.48	2.09	6	3
1:C:124:THR:HG22	1:C:126:GLU:HG3	0.48	1.85	1	2
1:C:135:GLU:CA	1:C:138:LYS:HE3	0.48	2.38	3	1
1:C:147:ARG:HB2	1:C:147:ARG:CZ	0.48	2.39	7	1
1:C:134:GLU:O	1:C:138:LYS:HE3	0.47	2.08	10	2
1:C:121:LEU:HD11	1:C:126:GLU:OE2	0.47	2.09	13	1
1:C:152:GLU:O	1:C:156:PHE:HB2	0.47	2.10	18	1
1:C:142:LYS:HE3	1:C:155:GLU:CG	0.47	2.39	20	1
1:C:134:GLU:HG3	1:C:138:LYS:CE	0.47	2.40	9	2
1:C:121:LEU:HD23	1:C:128:ILE:CG1	0.47	2.39	18	1
1:C:137:MET:SD	1:C:147:ARG:HA	0.47	2.49	11	1
1:C:121:LEU:HD23	1:C:128:ILE:HG21	0.47	1.87	20	1
1:C:107:ASN:O	1:C:108:ALA:CB	0.47	2.62	4	1
1:C:114:LEU:HD21	1:C:137:MET:CE	0.47	2.40	13	1
1:C:114:LEU:HD21	1:C:137:MET:CG	0.47	2.40	19	1
1:C:114:LEU:HD23	1:C:117:LEU:HD12	0.47	1.87	1	1
1:C:99:ASP:HA	1:C:102:ARG:NH2	0.46	2.26	14	2
1:C:106:LYS:HG3	1:C:116:GLU:HA	0.46	1.88	1	1
1:C:103:MET:O	1:C:106:LYS:NZ	0.46	2.47	1	1
1:C:139:ASP:O	1:C:142:LYS:HE2	0.46	2.11	2	2
1:C:115:ASP:HA	1:C:118:LYS:HG3	0.46	1.88	16	1
1:C:111:TYR:CB	1:C:147:ARG:HD2	0.46	2.41	19	1
1:C:106:LYS:HE3	1:C:119:ILE:CD1	0.46	2.40	6	1
1:C:142:LYS:HD2	1:C:155:GLU:CG	0.46	2.41	8	1
1:C:106:LYS:CE	1:C:116:GLU:HA	0.46	2.41	17	1
1:C:121:LEU:HB3	1:C:128:ILE:CD1	0.46	2.41	12	3
1:C:139:ASP:O	1:C:142:LYS:NZ	0.46	2.45	6	5
1:C:142:LYS:HD2	1:C:155:GLU:HB3	0.46	1.88	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:114:LEU:HD21	1:C:137:MET:CB	0.46	2.41	20	1
1:C:101:PHE:CE1	1:C:150:TYR:HA	0.45	2.46	19	2
1:C:97:LEU:HD22	1:C:154:LEU:HB2	0.45	1.89	3	1
1:C:118:LYS:HE2	1:C:119:ILE:CG1	0.45	2.41	6	1
1:C:145:ASP:O	1:C:147:ARG:NH2	0.45	2.50	6	1
1:C:106:LYS:HE3	1:C:119:ILE:HG13	0.45	1.89	3	2
1:C:114:LEU:CD2	1:C:137:MET:HB2	0.45	2.41	5	2
1:C:106:LYS:HG3	1:C:116:GLU:CG	0.45	2.41	15	1
1:C:106:LYS:HE2	1:C:119:ILE:CD1	0.45	2.42	17	1
1:C:97:LEU:HA	1:C:100:LEU:CD2	0.44	2.42	6	1
1:C:129:THR:O	1:C:133:ILE:HG12	0.44	2.12	6	1
1:C:117:LEU:CD2	1:C:133:ILE:HG23	0.44	2.32	16	1
1:C:101:PHE:CZ	1:C:112:ILE:HG13	0.44	2.48	3	1
1:C:140:GLY:HA3	1:C:148:ILE:CD1	0.44	2.42	10	1
1:C:106:LYS:HE3	1:C:116:GLU:HA	0.44	1.88	13	1
1:C:121:LEU:HD22	1:C:126:GLU:HG3	0.44	1.89	7	1
1:C:114:LEU:HB2	1:C:137:MET:CE	0.44	2.42	17	1
1:C:111:TYR:HB3	1:C:147:ARG:HG3	0.44	1.90	11	2
1:C:106:LYS:HB3	1:C:116:GLU:HG2	0.44	1.89	19	1
1:C:121:LEU:HD22	1:C:126:GLU:CB	0.44	2.43	7	1
1:C:153:PHE:CE2	1:C:157:MET:SD	0.44	3.11	16	1
1:C:132:ASP:O	1:C:136:LEU:HD13	0.44	2.13	9	1
1:C:147:ARG:CZ	1:C:147:ARG:CB	0.44	2.96	10	1
1:C:106:LYS:CE	1:C:116:GLU:HG3	0.44	2.43	15	1
1:C:103:MET:HG3	1:C:104:PHE:N	0.44	2.28	18	1
1:C:128:ILE:CB	1:C:133:ILE:HD11	0.44	2.42	20	1
1:C:142:LYS:NZ	1:C:155:GLU:HB2	0.43	2.28	1	2
1:C:134:GLU:HG2	1:C:138:LYS:HE2	0.43	1.90	3	1
1:C:121:LEU:HD12	1:C:128:ILE:HG21	0.43	1.88	15	1
1:C:137:MET:SD	1:C:148:ILE:HG12	0.43	2.53	5	1
1:C:139:ASP:O	1:C:142:LYS:CE	0.43	2.65	2	4
1:C:101:PHE:CE1	1:C:112:ILE:HG12	0.43	2.49	19	2
1:C:135:GLU:CA	1:C:138:LYS:HE2	0.43	2.42	7	1
1:C:97:LEU:HA	1:C:157:MET:HE3	0.43	1.88	14	1
1:C:97:LEU:HD13	1:C:154:LEU:HD13	0.43	1.89	17	1
1:C:118:LYS:HG3	1:C:133:ILE:HD13	0.43	1.90	18	1
1:C:142:LYS:HG3	1:C:155:GLU:HG2	0.43	1.91	4	1
1:C:153:PHE:O	1:C:157:MET:HG2	0.42	2.14	13	1
1:C:131:ASP:HA	1:C:134:GLU:HB3	0.42	1.91	3	1
1:C:114:LEU:HD23	1:C:137:MET:SD	0.42	2.54	6	1
1:C:142:LYS:HD3	1:C:152:GLU:HA	0.42	1.89	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:97:LEU:HD13	1:C:154:LEU:HA	0.42	1.91	12	1
1:C:132:ASP:O	1:C:136:LEU:HG	0.42	2.15	18	1
1:C:100:LEU:HA	1:C:103:MET:HG2	0.42	1.92	6	2
1:C:134:GLU:O	1:C:138:LYS:HG3	0.42	2.14	13	1
1:C:147:ARG:CZ	1:C:147:ARG:HB3	0.42	2.44	20	1
1:C:104:PHE:CB	1:C:112:ILE:HD12	0.42	2.44	16	1
1:C:112:ILE:HA	1:C:116:GLU:OE1	0.42	2.15	18	1
1:C:94:GLU:HA	1:C:97:LEU:CD2	0.42	2.44	20	1
1:C:118:LYS:HE2	1:C:119:ILE:HG13	0.42	1.92	6	1
1:C:113:ASP:HB3	1:C:116:GLU:HG3	0.42	1.90	14	1
1:C:115:ASP:O	1:C:118:LYS:CG	0.42	2.68	8	1
1:C:121:LEU:HG	1:C:133:ILE:CD1	0.42	2.45	16	1
1:C:121:LEU:HD12	1:C:133:ILE:HD11	0.42	1.91	11	1
1:C:105:ASP:O	1:C:106:LYS:NZ	0.41	2.53	4	1
1:C:141:ASP:HA	1:C:152:GLU:OE2	0.41	2.15	16	1
1:C:94:GLU:O	1:C:97:LEU:HB3	0.41	2.14	19	1
1:C:97:LEU:HD13	1:C:154:LEU:HD21	0.41	1.92	20	1
1:C:128:ILE:HB	1:C:133:ILE:CG1	0.41	2.44	17	1
1:C:126:GLU:O	1:C:128:ILE:N	0.41	2.53	4	1
1:C:142:LYS:HB2	1:C:152:GLU:HG2	0.41	1.92	20	1
1:C:142:LYS:HG3	1:C:155:GLU:CG	0.41	2.46	4	1
1:C:121:LEU:HB2	1:C:128:ILE:CD1	0.41	2.45	8	1
1:C:142:LYS:HD2	1:C:155:GLU:HG2	0.41	1.93	8	1
1:C:134:GLU:O	1:C:137:MET:HB3	0.41	2.15	3	2
1:C:106:LYS:HG3	1:C:116:GLU:HG2	0.41	1.92	2	1
1:C:132:ASP:O	1:C:136:LEU:HD22	0.41	2.15	17	1
1:C:106:LYS:HG2	1:C:116:GLU:HA	0.41	1.92	20	1
1:C:111:TYR:CG	1:C:147:ARG:HD2	0.41	2.50	12	1
1:C:104:PHE:HB3	1:C:112:ILE:HG12	0.41	1.92	17	1
1:C:130:GLU:CA	1:C:133:ILE:HD12	0.41	2.46	5	1
1:C:117:LEU:O	1:C:121:LEU:HG	0.41	2.16	7	1
1:C:106:LYS:HG2	1:C:119:ILE:HD12	0.41	1.93	15	1
1:C:112:ILE:O	1:C:148:ILE:N	0.41	2.48	19	1
1:C:106:LYS:HE2	1:C:116:GLU:O	0.41	2.16	11	1
1:C:106:LYS:HG3	1:C:116:GLU:HG3	0.41	1.92	15	1
1:C:142:LYS:CE	1:C:155:GLU:HG3	0.40	2.47	8	1
1:C:97:LEU:HA	1:C:157:MET:CE	0.40	2.46	14	1
1:C:106:LYS:HE3	1:C:116:GLU:HG3	0.40	1.93	15	1
1:C:97:LEU:CD1	1:C:154:LEU:HA	0.40	2.46	12	1
1:C:129:THR:O	1:C:130:GLU:HB2	0.40	2.16	5	1
1:C:104:PHE:HB3	1:C:112:ILE:HG23	0.40	1.93	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:137:MET:HE1	1:C:147:ARG:HA	0.40	1.93	19	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	C	64/72 (89%)	63±1 (98±2%)	1±1 (2±2%)	0±1 (0±1%)	38	78
All	All	1280/1440 (89%)	1253 (98%)	22 (2%)	5 (0%)	38	78

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	108	ALA	2
1	C	127	THR	1
1	C	128	ILE	1
1	C	110	GLY	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	C	58/64 (91%)	52±2 (89±3%)	6±2 (11±3%)	9	53
All	All	1160/1280 (91%)	1031 (89%)	129 (11%)	9	53

All 35 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	C	118	LYS	13
1	C	127	THR	10
1	C	147	ARG	9
1	C	129	THR	8
1	C	155	GLU	8
1	C	106	LYS	7
1	C	138	LYS	6
1	C	99	ASP	5
1	C	128	ILE	5
1	C	157	MET	4
1	C	103	MET	4
1	C	97	LEU	4
1	C	104	PHE	4
1	C	149	ASP	4
1	C	142	LYS	4
1	C	137	MET	3
1	C	120	MET	3
1	C	131	ASP	3
1	C	144	ASN	2
1	C	151	ASP	2
1	C	156	PHE	2
1	C	105	ASP	2
1	C	134	GLU	2
1	C	126	GLU	2
1	C	141	ASP	2
1	C	124	THR	2
1	C	94	GLU	1
1	C	135	GLU	1
1	C	117	LEU	1
1	C	95	GLU	1
1	C	150	TYR	1
1	C	107	ASN	1
1	C	113	ASP	1
1	C	136	LEU	1
1	C	122	GLN	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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 73% for the well-defined parts and 72% 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	689
Number of shifts mapped to atoms	689
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	71	-0.15 ± 0.22	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	65	0.03 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	70	0.32 ± 0.44	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 73%, i.e. 630 atoms were assigned a chemical shift out of a possible 862. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	258/324 (80%)	130/132 (98%)	64/128 (50%)	64/64 (100%)
Sidechain	362/480 (75%)	231/304 (76%)	131/162 (81%)	0/14 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	10/58 (17%)	10/28 (36%)	0/30 (0%)	0/0 (—%)
Overall	630/862 (73%)	371/464 (80%)	195/320 (61%)	64/78 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 689 atoms were assigned a chemical shift out of a possible 960. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	284/366 (78%)	143/150 (95%)	71/144 (49%)	70/72 (97%)
Sidechain	395/536 (74%)	250/340 (74%)	145/180 (81%)	0/16 (0%)
Aromatic	10/58 (17%)	10/28 (36%)	0/30 (0%)	0/0 (—%)
Overall	689/960 (72%)	403/518 (78%)	216/354 (61%)	70/88 (80%)

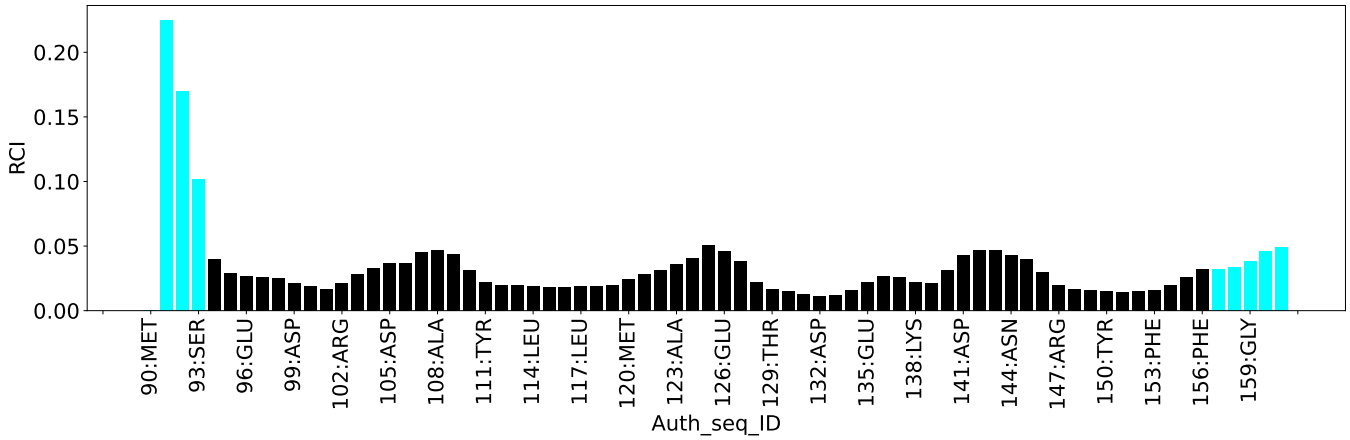
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

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 C:



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	957
Intra-residue (|i-j|=0)	303
Sequential (|i-j|=1)	258
Medium range (|i-j|>1 and |i-j|<5)	215
Long range (|i-j|≥5)	181
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	82
Number of unmapped restraints	0
Number of restraints per residue	14.4
Number of long range restraints per residue[1]	2.5

[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)	6.0	0.2
0.2-0.5 (Medium)	3.7	0.41
>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)	0.1	2.8
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

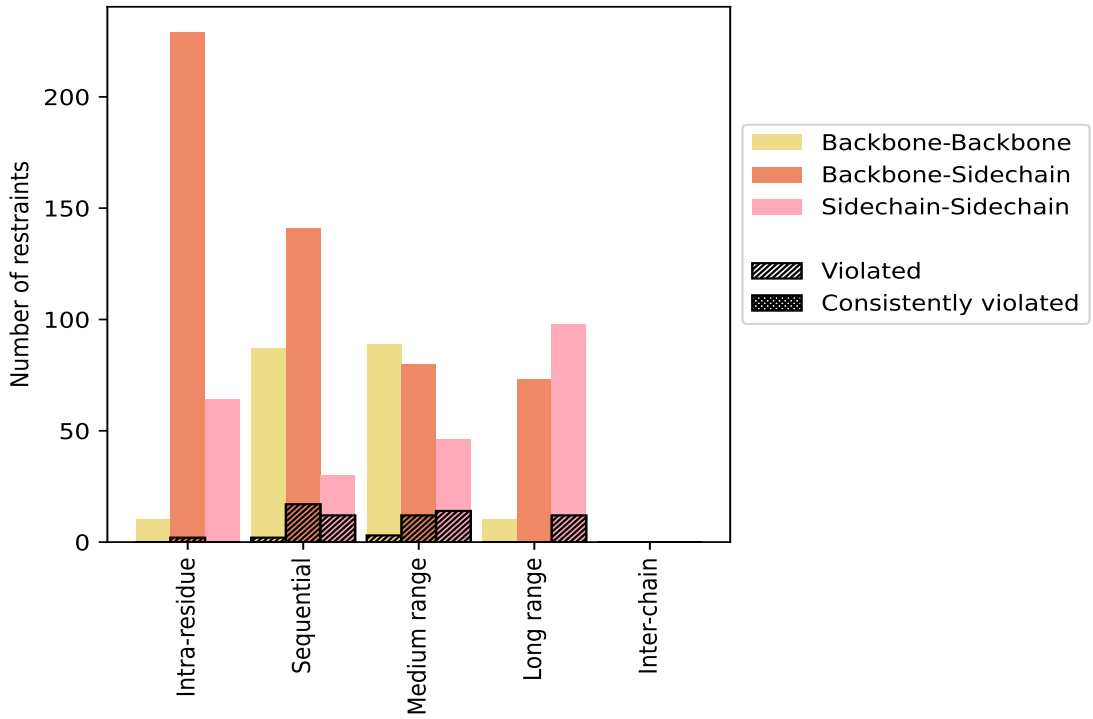
9.1 Summary of distance violations (i)

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)	303	31.7	2	0.7	0.2	0	0.0	0.0
Backbone-Backbone	10	1.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	229	23.9	2	0.9	0.2	0	0.0	0.0
Sidechain-Sidechain	64	6.7	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	258	27.0	31	12.0	3.2	0	0.0	0.0
Backbone-Backbone	87	9.1	2	2.3	0.2	0	0.0	0.0
Backbone-Sidechain	141	14.7	17	12.1	1.8	0	0.0	0.0
Sidechain-Sidechain	30	3.1	12	40.0	1.3	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	215	22.5	29	13.5	3.0	0	0.0	0.0
Backbone-Backbone	89	9.3	3	3.4	0.3	0	0.0	0.0
Backbone-Sidechain	80	8.4	12	15.0	1.3	0	0.0	0.0
Sidechain-Sidechain	46	4.8	14	30.4	1.5	0	0.0	0.0
Long range (|i-j|≥5)	181	18.9	12	6.6	1.3	0	0.0	0.0
Backbone-Backbone	10	1.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	73	7.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	98	10.2	12	12.2	1.3	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	957	100.0	74	7.7	7.7	0	0.0	0.0
Backbone-Backbone	196	20.5	5	2.6	0.5	0	0.0	0.0
Backbone-Sidechain	523	54.6	31	5.9	3.2	0	0.0	0.0
Sidechain-Sidechain	238	24.9	38	16.0	4.0	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	0	5	6	1	0	12	0.2	0.33	0.08	0.19
2	0	5	4	1	0	10	0.17	0.31	0.06	0.16
3	1	5	3	2	0	11	0.18	0.33	0.07	0.15
4	0	6	3	2	0	11	0.21	0.35	0.07	0.2
5	1	4	1	0	0	6	0.28	0.39	0.11	0.32
6	1	4	3	0	0	8	0.25	0.41	0.11	0.21
7	0	5	4	1	0	10	0.17	0.34	0.06	0.15
8	0	9	0	2	0	11	0.2	0.36	0.08	0.16
9	0	6	1	1	0	8	0.21	0.41	0.11	0.18
10	1	7	2	1	0	11	0.15	0.25	0.04	0.15
11	0	11	2	0	0	13	0.22	0.36	0.07	0.2

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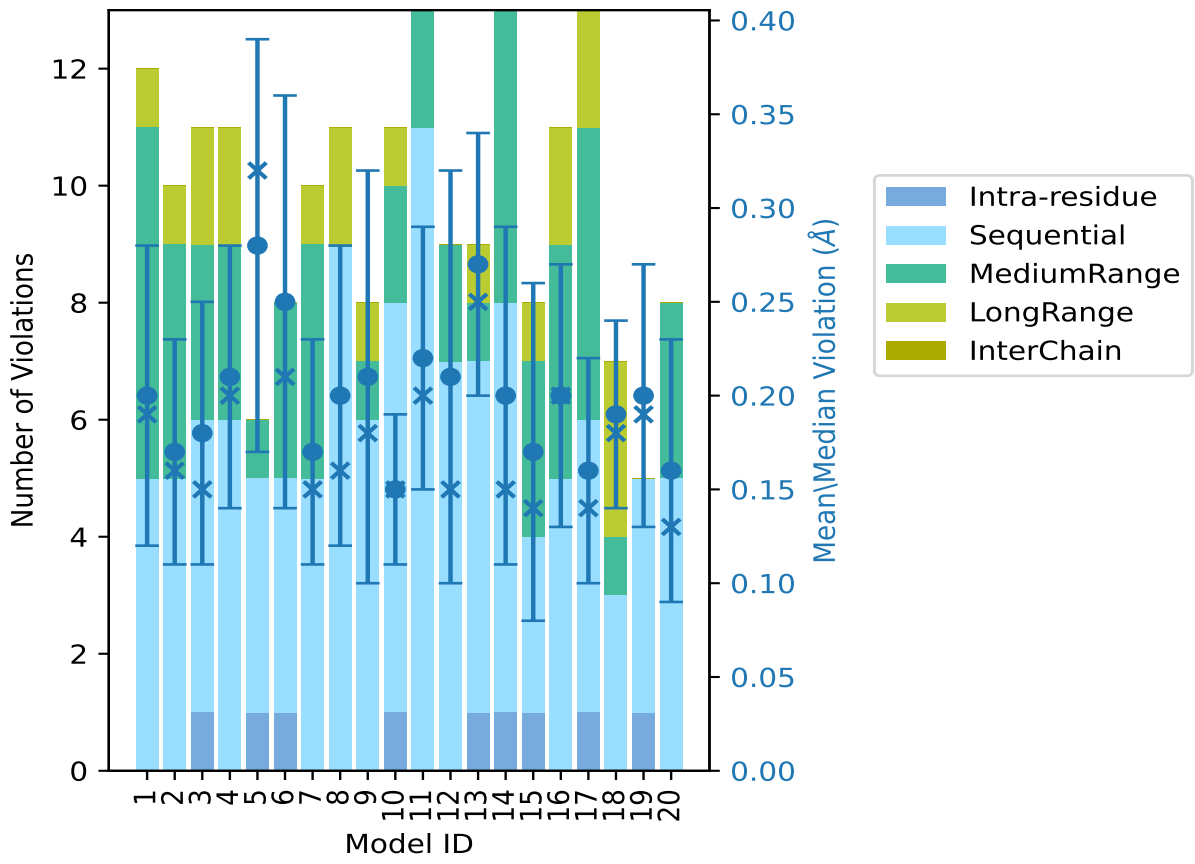
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	7	2	0	0	9	0.21	0.41	0.11	0.15
13	1	6	1	1	0	9	0.27	0.36	0.07	0.25
14	1	7	5	0	0	13	0.2	0.36	0.09	0.15
15	1	3	3	1	0	8	0.17	0.38	0.09	0.14
16	0	5	4	2	0	11	0.2	0.36	0.07	0.2
17	1	5	5	2	0	13	0.16	0.31	0.06	0.14
18	0	3	1	3	0	7	0.19	0.29	0.05	0.18
19	1	4	0	0	0	5	0.2	0.31	0.07	0.19
20	0	5	3	0	0	8	0.16	0.32	0.07	0.13

[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

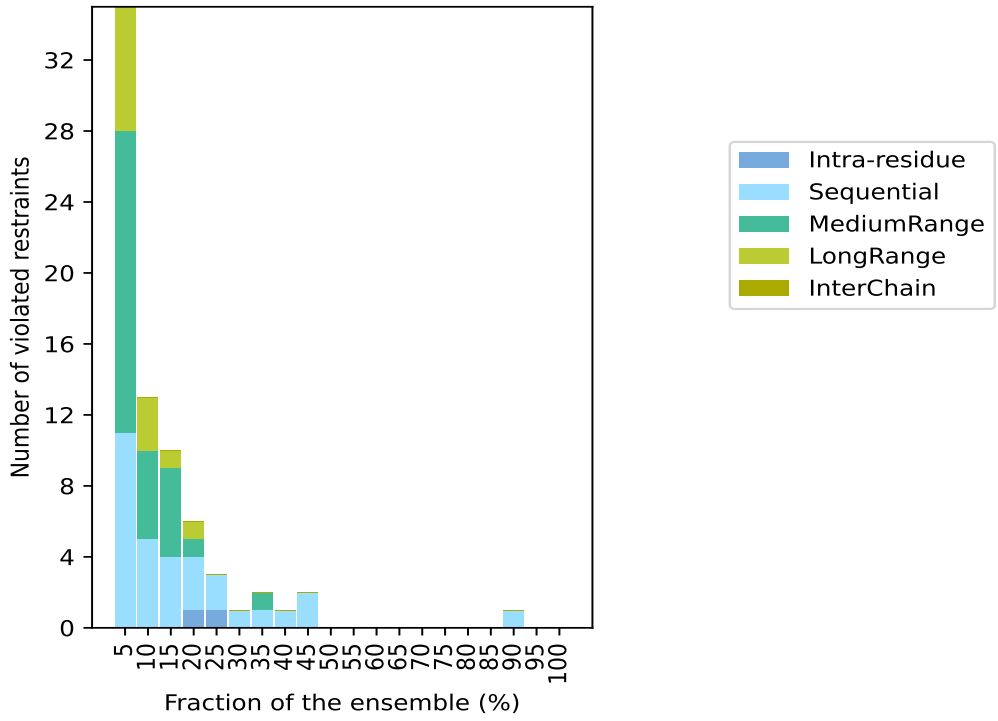
9.3 Distance violation statistics for the ensemble (i)

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, 883(IR:301, SQ:227, MR:186, LR:169, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	11	17	7	0	35	1	5.0
0	5	5	3	0	13	2	10.0
0	4	5	1	0	10	3	15.0
1	3	1	1	0	6	4	20.0
1	2	0	0	0	3	5	25.0
0	1	0	0	0	1	6	30.0
0	1	1	0	0	2	7	35.0
0	1	0	0	0	1	8	40.0
0	2	0	0	0	2	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	1	0	0	0	1	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

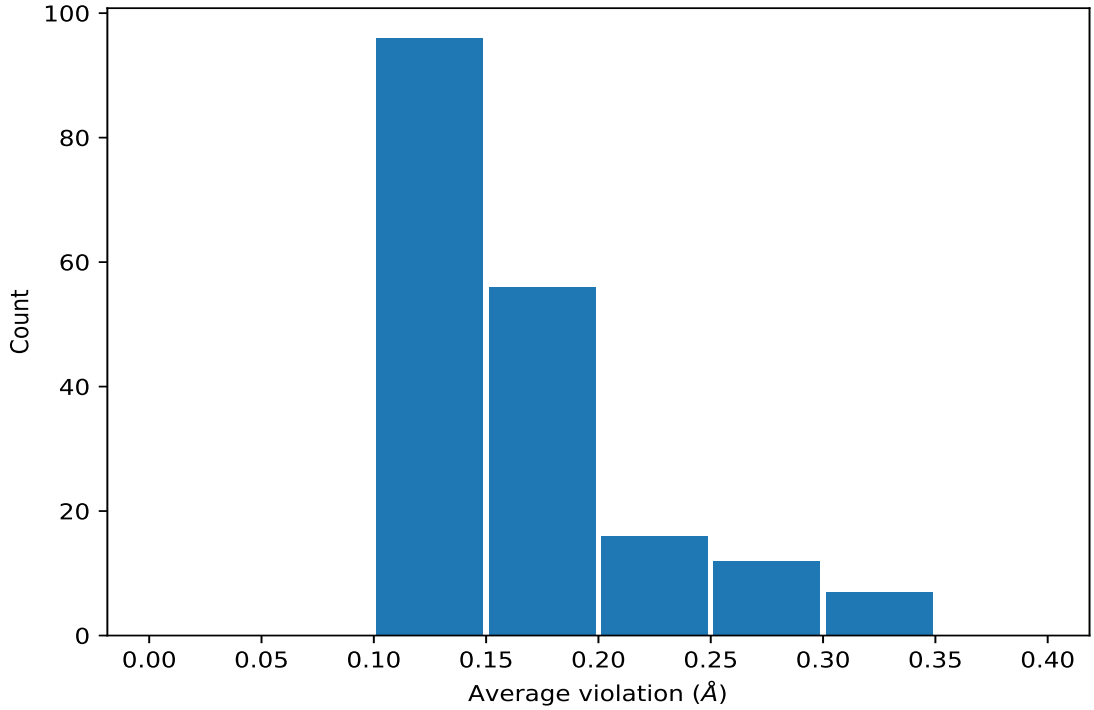
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	18	0.33	0.05	0.34
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	18	0.33	0.05	0.34
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	18	0.33	0.05	0.34
(1,805)	1:C:97:LEU:HD11	1:C:98:SER:HA	9	0.16	0.03	0.15
(1,805)	1:C:97:LEU:HD12	1:C:98:SER:HA	9	0.16	0.03	0.15
(1,805)	1:C:97:LEU:HD13	1:C:98:SER:HA	9	0.16	0.03	0.15
(1,805)	1:C:97:LEU:HD21	1:C:98:SER:HA	9	0.16	0.03	0.15
(1,805)	1:C:97:LEU:HD22	1:C:98:SER:HA	9	0.16	0.03	0.15
(1,805)	1:C:97:LEU:HD23	1:C:98:SER:HA	9	0.16	0.03	0.15
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE2	9	0.16	0.04	0.15
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE3	9	0.16	0.04	0.15
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE2	9	0.16	0.04	0.15
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE3	9	0.16	0.04	0.15
(1,899)	1:C:135:GLU:HG2	1:C:136:LEU:HA	8	0.33	0.04	0.32
(1,899)	1:C:135:GLU:HG3	1:C:136:LEU:HA	8	0.33	0.04	0.32
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB2	7	0.17	0.04	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB3	7	0.17	0.04	0.16
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB2	7	0.17	0.04	0.16
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB3	7	0.17	0.04	0.16
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB2	7	0.17	0.04	0.16
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB3	7	0.17	0.04	0.16
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG21	7	0.15	0.04	0.14
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG22	7	0.15	0.04	0.14
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG23	7	0.15	0.04	0.14
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG21	7	0.15	0.04	0.14
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG22	7	0.15	0.04	0.14
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG23	7	0.15	0.04	0.14
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG21	7	0.15	0.04	0.14
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG22	7	0.15	0.04	0.14
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG23	7	0.15	0.04	0.14
(1,362)	1:C:148:ILE:HD11	1:C:149:ASP:H	6	0.16	0.04	0.15
(1,362)	1:C:148:ILE:HD12	1:C:149:ASP:H	6	0.16	0.04	0.15
(1,362)	1:C:148:ILE:HD13	1:C:149:ASP:H	6	0.16	0.04	0.15
(1,827)	1:C:106:LYS:HG2	1:C:107:ASN:HA	5	0.33	0.04	0.32
(1,827)	1:C:106:LYS:HG3	1:C:107:ASN:HA	5	0.33	0.04	0.32
(1,262)	1:C:158:LYS:HA	1:C:158:LYS:HD2	5	0.29	0.06	0.26
(1,262)	1:C:158:LYS:HA	1:C:158:LYS:HD3	5	0.29	0.06	0.26
(1,96)	1:C:137:MET:HA	1:C:138:LYS:HE2	5	0.2	0.03	0.21
(1,96)	1:C:137:MET:HA	1:C:138:LYS:HE3	5	0.2	0.03	0.21
(1,848)	1:C:113:ASP:HB2	1:C:114:LEU:HG	4	0.2	0.12	0.14
(1,848)	1:C:113:ASP:HB3	1:C:114:LEU:HG	4	0.2	0.12	0.14
(1,516)	1:C:141:ASP:H	1:C:142:LYS:HE2	4	0.2	0.07	0.18
(1,516)	1:C:141:ASP:H	1:C:142:LYS:HE3	4	0.2	0.07	0.18
(1,98)	1:C:128:ILE:HA	1:C:128:ILE:HD11	4	0.19	0.05	0.2
(1,98)	1:C:128:ILE:HA	1:C:128:ILE:HD12	4	0.19	0.05	0.2
(1,98)	1:C:128:ILE:HA	1:C:128:ILE:HD13	4	0.19	0.05	0.2
(1,349)	1:C:157:MET:HA	1:C:161:GLU:H	4	0.18	0.04	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD11	4	0.17	0.03	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD12	4	0.17	0.03	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD13	4	0.17	0.03	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD21	4	0.17	0.03	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD22	4	0.17	0.03	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD23	4	0.17	0.03	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD11	4	0.17	0.03	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD12	4	0.17	0.03	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD13	4	0.17	0.03	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD21	4	0.17	0.03	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD22	4	0.17	0.03	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD23	4	0.17	0.03	0.18
(1,829)	1:C:106:LYS:HG2	1:C:116:GLU:HG2	4	0.13	0.02	0.12
(1,829)	1:C:106:LYS:HG2	1:C:116:GLU:HG3	4	0.13	0.02	0.12
(1,829)	1:C:106:LYS:HG3	1:C:116:GLU:HG2	4	0.13	0.02	0.12
(1,829)	1:C:106:LYS:HG3	1:C:116:GLU:HG3	4	0.13	0.02	0.12
(1,895)	1:C:132:ASP:HB2	1:C:133:ILE:HD11	3	0.27	0.01	0.27
(1,895)	1:C:132:ASP:HB2	1:C:133:ILE:HD12	3	0.27	0.01	0.27
(1,895)	1:C:132:ASP:HB2	1:C:133:ILE:HD13	3	0.27	0.01	0.27
(1,895)	1:C:132:ASP:HB3	1:C:133:ILE:HD11	3	0.27	0.01	0.27
(1,895)	1:C:132:ASP:HB3	1:C:133:ILE:HD12	3	0.27	0.01	0.27
(1,895)	1:C:132:ASP:HB3	1:C:133:ILE:HD13	3	0.27	0.01	0.27
(1,30)	1:C:90:MET:HE1	1:C:92:LYS:HD2	3	0.2	0.11	0.13
(1,30)	1:C:90:MET:HE1	1:C:92:LYS:HD3	3	0.2	0.11	0.13
(1,30)	1:C:90:MET:HE2	1:C:92:LYS:HD2	3	0.2	0.11	0.13
(1,30)	1:C:90:MET:HE2	1:C:92:LYS:HD3	3	0.2	0.11	0.13
(1,30)	1:C:90:MET:HE3	1:C:92:LYS:HD2	3	0.2	0.11	0.13
(1,30)	1:C:90:MET:HE3	1:C:92:LYS:HD3	3	0.2	0.11	0.13
(1,82)	1:C:147:ARG:HG2	1:C:148:ILE:HD11	3	0.17	0.05	0.14
(1,82)	1:C:147:ARG:HG2	1:C:148:ILE:HD12	3	0.17	0.05	0.14
(1,82)	1:C:147:ARG:HG2	1:C:148:ILE:HD13	3	0.17	0.05	0.14
(1,82)	1:C:147:ARG:HG3	1:C:148:ILE:HD11	3	0.17	0.05	0.14
(1,82)	1:C:147:ARG:HG3	1:C:148:ILE:HD12	3	0.17	0.05	0.14
(1,82)	1:C:147:ARG:HG3	1:C:148:ILE:HD13	3	0.17	0.05	0.14
(1,125)	1:C:115:ASP:HB3	1:C:118:LYS:HD2	3	0.16	0.05	0.15
(1,125)	1:C:115:ASP:HB3	1:C:118:LYS:HD3	3	0.16	0.05	0.15
(1,272)	1:C:92:LYS:HD2	1:C:95:GLU:HB2	3	0.16	0.04	0.16
(1,272)	1:C:92:LYS:HD2	1:C:95:GLU:HB3	3	0.16	0.04	0.16
(1,272)	1:C:92:LYS:HD3	1:C:95:GLU:HB2	3	0.16	0.04	0.16
(1,272)	1:C:92:LYS:HD3	1:C:95:GLU:HB3	3	0.16	0.04	0.16
(1,7)	1:C:120:MET:HE1	1:C:121:LEU:HA	3	0.16	0.01	0.16
(1,7)	1:C:120:MET:HE2	1:C:121:LEU:HA	3	0.16	0.01	0.16
(1,7)	1:C:120:MET:HE3	1:C:121:LEU:HA	3	0.16	0.01	0.16
(1,85)	1:C:128:ILE:HD11	1:C:129:THR:H	3	0.15	0.04	0.13
(1,85)	1:C:128:ILE:HD12	1:C:129:THR:H	3	0.15	0.04	0.13
(1,85)	1:C:128:ILE:HD13	1:C:129:THR:H	3	0.15	0.04	0.13
(1,933)	1:C:147:ARG:HG2	1:C:149:ASP:HB2	3	0.15	0.05	0.12
(1,933)	1:C:147:ARG:HG2	1:C:149:ASP:HB3	3	0.15	0.05	0.12
(1,933)	1:C:147:ARG:HG3	1:C:149:ASP:HB2	3	0.15	0.05	0.12
(1,933)	1:C:147:ARG:HG3	1:C:149:ASP:HB3	3	0.15	0.05	0.12
(1,766)	1:C:148:ILE:HB	1:C:156:PHE:HE1	3	0.14	0.02	0.16
(1,766)	1:C:148:ILE:HB	1:C:156:PHE:HE2	3	0.14	0.02	0.16
(1,74)	1:C:116:GLU:HB2	1:C:119:ILE:HD11	3	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,74)	1:C:116:GLU:HB2	1:C:119:ILE:HD12	3	0.12	0.01	0.12
(1,74)	1:C:116:GLU:HB2	1:C:119:ILE:HD13	3	0.12	0.01	0.12
(1,74)	1:C:116:GLU:HB3	1:C:119:ILE:HD11	3	0.12	0.01	0.12
(1,74)	1:C:116:GLU:HB3	1:C:119:ILE:HD12	3	0.12	0.01	0.12
(1,74)	1:C:116:GLU:HB3	1:C:119:ILE:HD13	3	0.12	0.01	0.12
(1,156)	1:C:154:LEU:HB2	1:C:155:GLU:HG2	2	0.29	0.02	0.29
(1,156)	1:C:154:LEU:HB2	1:C:155:GLU:HG3	2	0.29	0.02	0.29
(1,156)	1:C:154:LEU:HB3	1:C:155:GLU:HG2	2	0.29	0.02	0.29
(1,156)	1:C:154:LEU:HB3	1:C:155:GLU:HG3	2	0.29	0.02	0.29
(1,259)	1:C:134:GLU:HG2	1:C:138:LYS:HD2	2	0.24	0.03	0.24
(1,259)	1:C:134:GLU:HG2	1:C:138:LYS:HD3	2	0.24	0.03	0.24
(1,259)	1:C:134:GLU:HG3	1:C:138:LYS:HD2	2	0.24	0.03	0.24
(1,259)	1:C:134:GLU:HG3	1:C:138:LYS:HD3	2	0.24	0.03	0.24
(1,29)	1:C:90:MET:HE1	1:C:92:LYS:HB2	2	0.16	0.02	0.16
(1,29)	1:C:90:MET:HE1	1:C:92:LYS:HB3	2	0.16	0.02	0.16
(1,29)	1:C:90:MET:HE2	1:C:92:LYS:HB2	2	0.16	0.02	0.16
(1,29)	1:C:90:MET:HE2	1:C:92:LYS:HB3	2	0.16	0.02	0.16
(1,29)	1:C:90:MET:HE3	1:C:92:LYS:HB2	2	0.16	0.02	0.16
(1,29)	1:C:90:MET:HE3	1:C:92:LYS:HB3	2	0.16	0.02	0.16
(1,111)	1:C:97:LEU:HB3	1:C:154:LEU:HB2	2	0.14	0.03	0.14
(1,111)	1:C:97:LEU:HB3	1:C:154:LEU:HB3	2	0.14	0.03	0.14
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD11	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD12	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD13	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD21	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD22	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD23	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD11	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD12	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD13	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD21	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD22	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD23	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD11	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD12	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD13	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD21	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD22	2	0.14	0.01	0.14
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD23	2	0.14	0.01	0.14
(1,311)	1:C:142:LYS:HG3	1:C:152:GLU:HB3	2	0.14	0.02	0.14
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD11	2	0.14	0.02	0.14
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD12	2	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD13	2	0.14	0.02	0.14
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD21	2	0.14	0.02	0.14
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD22	2	0.14	0.02	0.14
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD23	2	0.14	0.02	0.14
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD11	2	0.14	0.02	0.14
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD12	2	0.14	0.02	0.14
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD13	2	0.14	0.02	0.14
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD21	2	0.14	0.02	0.14
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD22	2	0.14	0.02	0.14
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD23	2	0.14	0.02	0.14
(1,941)	1:C:154:LEU:HD11	1:C:155:GLU:HA	2	0.14	0.02	0.14
(1,941)	1:C:154:LEU:HD12	1:C:155:GLU:HA	2	0.14	0.02	0.14
(1,941)	1:C:154:LEU:HD13	1:C:155:GLU:HA	2	0.14	0.02	0.14
(1,941)	1:C:154:LEU:HD21	1:C:155:GLU:HA	2	0.14	0.02	0.14
(1,941)	1:C:154:LEU:HD22	1:C:155:GLU:HA	2	0.14	0.02	0.14
(1,941)	1:C:154:LEU:HD23	1:C:155:GLU:HA	2	0.14	0.02	0.14
(1,75)	1:C:118:LYS:HD2	1:C:119:ILE:HD11	2	0.13	0.01	0.13
(1,75)	1:C:118:LYS:HD2	1:C:119:ILE:HD12	2	0.13	0.01	0.13
(1,75)	1:C:118:LYS:HD2	1:C:119:ILE:HD13	2	0.13	0.01	0.13
(1,75)	1:C:118:LYS:HD3	1:C:119:ILE:HD11	2	0.13	0.01	0.13
(1,75)	1:C:118:LYS:HD3	1:C:119:ILE:HD12	2	0.13	0.01	0.13
(1,75)	1:C:118:LYS:HD3	1:C:119:ILE:HD13	2	0.13	0.01	0.13
(1,885)	1:C:121:LEU:HD11	1:C:124:THR:HG21	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD11	1:C:124:THR:HG22	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD11	1:C:124:THR:HG23	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD12	1:C:124:THR:HG21	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD12	1:C:124:THR:HG22	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD12	1:C:124:THR:HG23	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD13	1:C:124:THR:HG21	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD13	1:C:124:THR:HG22	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD13	1:C:124:THR:HG23	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD21	1:C:124:THR:HG21	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD21	1:C:124:THR:HG22	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD21	1:C:124:THR:HG23	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD22	1:C:124:THR:HG21	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD22	1:C:124:THR:HG22	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD22	1:C:124:THR:HG23	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD23	1:C:124:THR:HG21	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD23	1:C:124:THR:HG22	2	0.12	0.02	0.12
(1,885)	1:C:121:LEU:HD23	1:C:124:THR:HG23	2	0.12	0.02	0.12
(1,168)	1:C:118:LYS:HD2	1:C:119:ILE:HA	2	0.12	0.0	0.12
(1,168)	1:C:118:LYS:HD3	1:C:119:ILE:HA	2	0.12	0.0	0.12

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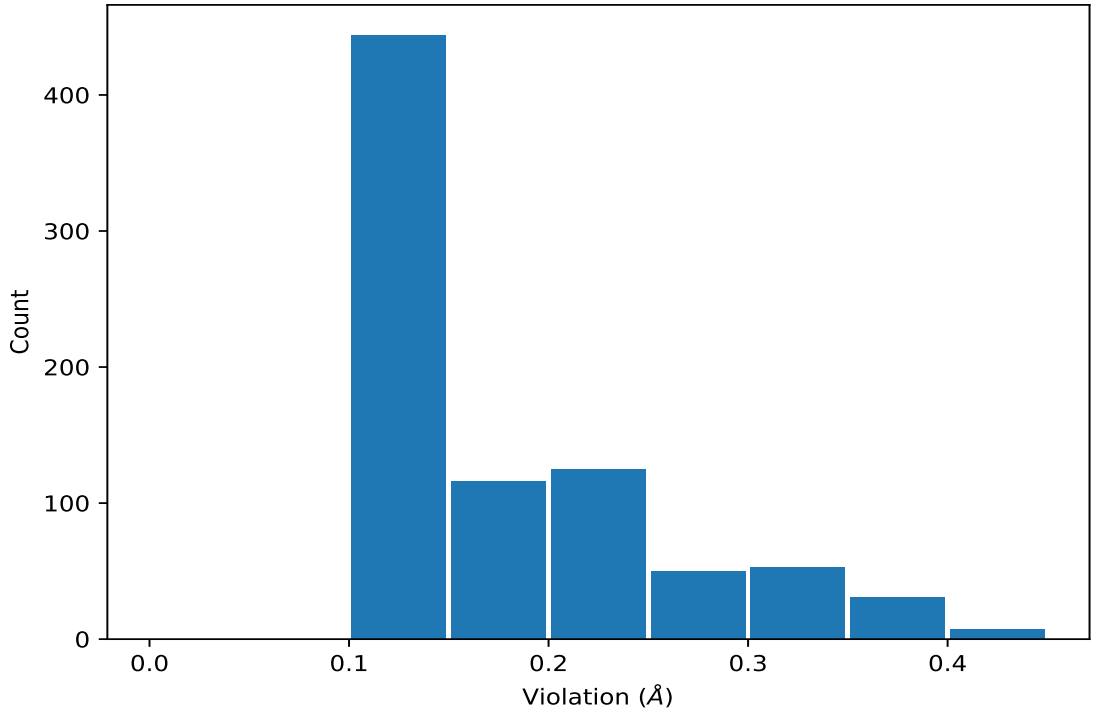
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,192)	1:C:153:PHE:HA	1:C:155:GLU:HG2	2	0.12	0.0	0.12
(1,192)	1:C:153:PHE:HA	1:C:155:GLU:HG3	2	0.12	0.0	0.12
(1,446)	1:C:136:LEU:H	1:C:139:ASP:HB2	2	0.12	0.0	0.12

[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)
(1,899)	1:C:135:GLU:HG2	1:C:136:LEU:HA	9	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:C:135:GLU:HG3	1:C:136:LEU:HA	9	0.41
(1,848)	1:C:113:ASP:HB2	1:C:114:LEU:HG	6	0.41
(1,848)	1:C:113:ASP:HB3	1:C:114:LEU:HG	6	0.41
(1,722)	1:C:124:THR:H	1:C:125:GLY:H	12	0.41
(1,262)	1:C:158:LYS:HA	1:C:158:LYS:HD2	6	0.4
(1,262)	1:C:158:LYS:HA	1:C:158:LYS:HD3	6	0.4
(1,899)	1:C:135:GLU:HG2	1:C:136:LEU:HA	5	0.39
(1,899)	1:C:135:GLU:HG3	1:C:136:LEU:HA	5	0.39
(1,827)	1:C:106:LYS:HG2	1:C:107:ASN:HA	5	0.38
(1,827)	1:C:106:LYS:HG3	1:C:107:ASN:HA	5	0.38
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	15	0.38
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	15	0.38
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	15	0.38
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	5	0.37
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	5	0.37
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	5	0.37
(1,827)	1:C:106:LYS:HG2	1:C:107:ASN:HA	11	0.36
(1,827)	1:C:106:LYS:HG3	1:C:107:ASN:HA	11	0.36
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	6	0.36
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	6	0.36
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	6	0.36
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	8	0.36
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	8	0.36
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	8	0.36
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	14	0.36
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	14	0.36
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	14	0.36
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	16	0.36
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	16	0.36
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	16	0.36
(1,420)	1:C:108:ALA:H	1:C:110:GLY:H	14	0.36
(1,30)	1:C:90:MET:HE1	1:C:92:LYS:HD2	13	0.36
(1,30)	1:C:90:MET:HE1	1:C:92:LYS:HD3	13	0.36
(1,30)	1:C:90:MET:HE2	1:C:92:LYS:HD2	13	0.36
(1,30)	1:C:90:MET:HE2	1:C:92:LYS:HD3	13	0.36
(1,30)	1:C:90:MET:HE3	1:C:92:LYS:HD2	13	0.36
(1,30)	1:C:90:MET:HE3	1:C:92:LYS:HD3	13	0.36
(1,899)	1:C:135:GLU:HG2	1:C:136:LEU:HA	13	0.35
(1,899)	1:C:135:GLU:HG3	1:C:136:LEU:HA	13	0.35
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	4	0.35
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	4	0.35
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	4	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	13	0.35
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	13	0.35
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	13	0.35
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	7	0.34
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	7	0.34
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	7	0.34
(1,899)	1:C:135:GLU:HG2	1:C:136:LEU:HA	1	0.33
(1,899)	1:C:135:GLU:HG3	1:C:136:LEU:HA	1	0.33
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	1	0.33
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	1	0.33
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	1	0.33
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	3	0.33
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	3	0.33
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	3	0.33
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	9	0.33
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	9	0.33
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	9	0.33
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	11	0.33
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	11	0.33
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	11	0.33
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	12	0.33
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	12	0.33
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	12	0.33
(1,123)	1:C:150:TYR:HB3	1:C:151:ASP:HB2	13	0.33
(1,123)	1:C:150:TYR:HB3	1:C:151:ASP:HB3	13	0.33
(1,899)	1:C:135:GLU:HG2	1:C:136:LEU:HA	11	0.32
(1,899)	1:C:135:GLU:HG3	1:C:136:LEU:HA	11	0.32
(1,827)	1:C:106:LYS:HG2	1:C:107:ASN:HA	1	0.32
(1,827)	1:C:106:LYS:HG3	1:C:107:ASN:HA	1	0.32
(1,827)	1:C:106:LYS:HG2	1:C:107:ASN:HA	8	0.32
(1,827)	1:C:106:LYS:HG3	1:C:107:ASN:HA	8	0.32
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	20	0.32
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	20	0.32
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	20	0.32
(1,824)	1:C:105:ASP:HA	1:C:106:LYS:HG2	19	0.31
(1,824)	1:C:105:ASP:HA	1:C:106:LYS:HG3	19	0.31
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	2	0.31
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	2	0.31
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	2	0.31
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	17	0.31
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	17	0.31
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	17	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,262)	1:C:158:LYS:HA	1:C:158:LYS:HD2	14	0.31
(1,262)	1:C:158:LYS:HA	1:C:158:LYS:HD3	14	0.31
(1,156)	1:C:154:LEU:HB2	1:C:155:GLU:HG2	4	0.31
(1,156)	1:C:154:LEU:HB2	1:C:155:GLU:HG3	4	0.31
(1,156)	1:C:154:LEU:HB3	1:C:155:GLU:HG2	4	0.31
(1,156)	1:C:154:LEU:HB3	1:C:155:GLU:HG3	4	0.31
(1,516)	1:C:141:ASP:H	1:C:142:LYS:HE2	14	0.3
(1,516)	1:C:141:ASP:H	1:C:142:LYS:HE3	14	0.3
(1,899)	1:C:135:GLU:HG2	1:C:136:LEU:HA	12	0.29
(1,899)	1:C:135:GLU:HG3	1:C:136:LEU:HA	12	0.29
(1,899)	1:C:135:GLU:HG2	1:C:136:LEU:HA	18	0.29
(1,899)	1:C:135:GLU:HG3	1:C:136:LEU:HA	18	0.29
(1,899)	1:C:135:GLU:HG2	1:C:136:LEU:HA	4	0.28
(1,899)	1:C:135:GLU:HG3	1:C:136:LEU:HA	4	0.28
(1,895)	1:C:132:ASP:HB2	1:C:133:ILE:HD11	11	0.28
(1,895)	1:C:132:ASP:HB2	1:C:133:ILE:HD12	11	0.28
(1,895)	1:C:132:ASP:HB2	1:C:133:ILE:HD13	11	0.28
(1,895)	1:C:132:ASP:HB3	1:C:133:ILE:HD11	11	0.28
(1,895)	1:C:132:ASP:HB3	1:C:133:ILE:HD12	11	0.28
(1,895)	1:C:132:ASP:HB3	1:C:133:ILE:HD13	11	0.28
(1,895)	1:C:132:ASP:HB2	1:C:133:ILE:HD11	9	0.27
(1,895)	1:C:132:ASP:HB2	1:C:133:ILE:HD12	9	0.27
(1,895)	1:C:132:ASP:HB2	1:C:133:ILE:HD13	9	0.27
(1,895)	1:C:132:ASP:HB3	1:C:133:ILE:HD11	9	0.27
(1,895)	1:C:132:ASP:HB3	1:C:133:ILE:HD12	9	0.27
(1,895)	1:C:132:ASP:HB3	1:C:133:ILE:HD13	9	0.27
(1,156)	1:C:154:LEU:HB2	1:C:155:GLU:HG2	8	0.27
(1,156)	1:C:154:LEU:HB2	1:C:155:GLU:HG3	8	0.27
(1,156)	1:C:154:LEU:HB3	1:C:155:GLU:HG2	8	0.27
(1,156)	1:C:154:LEU:HB3	1:C:155:GLU:HG3	8	0.27
(1,915)	1:C:137:MET:HG2	1:C:141:ASP:HB2	16	0.26
(1,915)	1:C:137:MET:HG3	1:C:141:ASP:HB2	16	0.26
(1,262)	1:C:158:LYS:HA	1:C:158:LYS:HD2	5	0.26
(1,262)	1:C:158:LYS:HA	1:C:158:LYS:HD3	5	0.26
(1,259)	1:C:134:GLU:HG2	1:C:138:LYS:HD2	16	0.26
(1,259)	1:C:134:GLU:HG2	1:C:138:LYS:HD3	16	0.26
(1,259)	1:C:134:GLU:HG3	1:C:138:LYS:HD2	16	0.26
(1,259)	1:C:134:GLU:HG3	1:C:138:LYS:HD3	16	0.26
(1,98)	1:C:128:ILE:HA	1:C:128:ILE:HD11	17	0.25
(1,98)	1:C:128:ILE:HA	1:C:128:ILE:HD12	17	0.25
(1,98)	1:C:128:ILE:HA	1:C:128:ILE:HD13	17	0.25
(1,96)	1:C:137:MET:HA	1:C:138:LYS:HE2	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:C:137:MET:HA	1:C:138:LYS:HE3	13	0.25
(1,895)	1:C:132:ASP:HB2	1:C:133:ILE:HD11	19	0.25
(1,895)	1:C:132:ASP:HB2	1:C:133:ILE:HD12	19	0.25
(1,895)	1:C:132:ASP:HB2	1:C:133:ILE:HD13	19	0.25
(1,895)	1:C:132:ASP:HB3	1:C:133:ILE:HD11	19	0.25
(1,895)	1:C:132:ASP:HB3	1:C:133:ILE:HD12	19	0.25
(1,895)	1:C:132:ASP:HB3	1:C:133:ILE:HD13	19	0.25
(1,827)	1:C:106:LYS:HG2	1:C:107:ASN:HA	12	0.25
(1,827)	1:C:106:LYS:HG3	1:C:107:ASN:HA	12	0.25
(1,362)	1:C:148:ILE:HD11	1:C:149:ASP:H	9	0.25
(1,362)	1:C:148:ILE:HD12	1:C:149:ASP:H	9	0.25
(1,362)	1:C:148:ILE:HD13	1:C:149:ASP:H	9	0.25
(1,262)	1:C:158:LYS:HA	1:C:158:LYS:HD2	10	0.25
(1,262)	1:C:158:LYS:HA	1:C:158:LYS:HD3	10	0.25
(1,82)	1:C:147:ARG:HG2	1:C:148:ILE:HD11	4	0.24
(1,82)	1:C:147:ARG:HG2	1:C:148:ILE:HD12	4	0.24
(1,82)	1:C:147:ARG:HG2	1:C:148:ILE:HD13	4	0.24
(1,82)	1:C:147:ARG:HG3	1:C:148:ILE:HD11	4	0.24
(1,82)	1:C:147:ARG:HG3	1:C:148:ILE:HD12	4	0.24
(1,82)	1:C:147:ARG:HG3	1:C:148:ILE:HD13	4	0.24
(1,933)	1:C:147:ARG:HG2	1:C:149:ASP:HB2	2	0.23
(1,933)	1:C:147:ARG:HG2	1:C:149:ASP:HB3	2	0.23
(1,933)	1:C:147:ARG:HG3	1:C:149:ASP:HB2	2	0.23
(1,933)	1:C:147:ARG:HG3	1:C:149:ASP:HB3	2	0.23
(1,780)	1:C:155:GLU:H	1:C:157:MET:HE1	3	0.23
(1,780)	1:C:155:GLU:H	1:C:157:MET:HE2	3	0.23
(1,780)	1:C:155:GLU:H	1:C:157:MET:HE3	3	0.23
(1,750)	1:C:101:PHE:HB2	1:C:150:TYR:HE1	13	0.23
(1,750)	1:C:101:PHE:HB2	1:C:150:TYR:HE2	13	0.23
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG21	3	0.23
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG22	3	0.23
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG23	3	0.23
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG21	3	0.23
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG22	3	0.23
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG23	3	0.23
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG21	3	0.23
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG22	3	0.23
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG23	3	0.23
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB2	8	0.23
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB3	8	0.23
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB2	8	0.23
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB3	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB2	8	0.23
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB3	8	0.23
(1,262)	1:C:158:LYS:HA	1:C:158:LYS:HD2	13	0.23
(1,262)	1:C:158:LYS:HA	1:C:158:LYS:HD3	13	0.23
(1,125)	1:C:115:ASP:HB3	1:C:118:LYS:HD2	6	0.23
(1,125)	1:C:115:ASP:HB3	1:C:118:LYS:HD3	6	0.23
(1,98)	1:C:128:ILE:HA	1:C:128:ILE:HD11	3	0.22
(1,98)	1:C:128:ILE:HA	1:C:128:ILE:HD12	3	0.22
(1,98)	1:C:128:ILE:HA	1:C:128:ILE:HD13	3	0.22
(1,96)	1:C:137:MET:HA	1:C:138:LYS:HE2	18	0.22
(1,96)	1:C:137:MET:HA	1:C:138:LYS:HE3	18	0.22
(1,891)	1:C:129:THR:H	1:C:132:ASP:HB2	16	0.22
(1,891)	1:C:129:THR:H	1:C:132:ASP:HB3	16	0.22
(1,805)	1:C:97:LEU:HD11	1:C:98:SER:HA	11	0.22
(1,805)	1:C:97:LEU:HD12	1:C:98:SER:HA	11	0.22
(1,805)	1:C:97:LEU:HD13	1:C:98:SER:HA	11	0.22
(1,805)	1:C:97:LEU:HD21	1:C:98:SER:HA	11	0.22
(1,805)	1:C:97:LEU:HD22	1:C:98:SER:HA	11	0.22
(1,805)	1:C:97:LEU:HD23	1:C:98:SER:HA	11	0.22
(1,516)	1:C:141:ASP:H	1:C:142:LYS:HE2	15	0.22
(1,516)	1:C:141:ASP:H	1:C:142:LYS:HE3	15	0.22
(1,349)	1:C:157:MET:HA	1:C:161:GLU:H	7	0.22
(1,272)	1:C:92:LYS:HD2	1:C:95:GLU:HB2	1	0.22
(1,272)	1:C:92:LYS:HD2	1:C:95:GLU:HB3	1	0.22
(1,272)	1:C:92:LYS:HD3	1:C:95:GLU:HB2	1	0.22
(1,272)	1:C:92:LYS:HD3	1:C:95:GLU:HB3	1	0.22
(1,96)	1:C:137:MET:HA	1:C:138:LYS:HE2	20	0.21
(1,96)	1:C:137:MET:HA	1:C:138:LYS:HE3	20	0.21
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE2	3	0.21
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE3	3	0.21
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE2	3	0.21
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE3	3	0.21
(1,85)	1:C:128:ILE:HD11	1:C:129:THR:H	4	0.21
(1,85)	1:C:128:ILE:HD12	1:C:129:THR:H	4	0.21
(1,85)	1:C:128:ILE:HD13	1:C:129:THR:H	4	0.21
(1,83)	1:C:106:LYS:HE2	1:C:119:ILE:HG21	18	0.21
(1,83)	1:C:106:LYS:HE2	1:C:119:ILE:HG22	18	0.21
(1,83)	1:C:106:LYS:HE2	1:C:119:ILE:HG23	18	0.21
(1,83)	1:C:106:LYS:HE3	1:C:119:ILE:HG21	18	0.21
(1,83)	1:C:106:LYS:HE3	1:C:119:ILE:HG22	18	0.21
(1,83)	1:C:106:LYS:HE3	1:C:119:ILE:HG23	18	0.21
(1,805)	1:C:97:LEU:HD11	1:C:98:SER:HA	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,805)	1:C:97:LEU:HD12	1:C:98:SER:HA	16	0.21
(1,805)	1:C:97:LEU:HD13	1:C:98:SER:HA	16	0.21
(1,805)	1:C:97:LEU:HD21	1:C:98:SER:HA	16	0.21
(1,805)	1:C:97:LEU:HD22	1:C:98:SER:HA	16	0.21
(1,805)	1:C:97:LEU:HD23	1:C:98:SER:HA	16	0.21
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG21	2	0.21
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG22	2	0.21
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG23	2	0.21
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG21	2	0.21
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG22	2	0.21
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG23	2	0.21
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG21	2	0.21
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG22	2	0.21
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG23	2	0.21
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB2	11	0.21
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB3	11	0.21
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB2	11	0.21
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB3	11	0.21
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB2	11	0.21
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB3	11	0.21
(1,259)	1:C:134:GLU:HG2	1:C:138:LYS:HD2	14	0.21
(1,259)	1:C:134:GLU:HG2	1:C:138:LYS:HD3	14	0.21
(1,259)	1:C:134:GLU:HG3	1:C:138:LYS:HD2	14	0.21
(1,259)	1:C:134:GLU:HG3	1:C:138:LYS:HD3	14	0.21
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE2	11	0.2
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE3	11	0.2
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE2	11	0.2
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE3	11	0.2
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE2	16	0.2
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE3	16	0.2
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE2	16	0.2
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE3	16	0.2
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD11	11	0.2
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD12	11	0.2
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD13	11	0.2
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD21	11	0.2
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD22	11	0.2
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD23	11	0.2
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD11	11	0.2
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD12	11	0.2
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD13	11	0.2
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD21	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD22	11	0.2
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD23	11	0.2
(1,805)	1:C:97:LEU:HD11	1:C:98:SER:HA	2	0.2
(1,805)	1:C:97:LEU:HD12	1:C:98:SER:HA	2	0.2
(1,805)	1:C:97:LEU:HD13	1:C:98:SER:HA	2	0.2
(1,805)	1:C:97:LEU:HD21	1:C:98:SER:HA	2	0.2
(1,805)	1:C:97:LEU:HD22	1:C:98:SER:HA	2	0.2
(1,805)	1:C:97:LEU:HD23	1:C:98:SER:HA	2	0.2
(1,614)	1:C:100:LEU:H	1:C:103:MET:HG2	1	0.2
(1,614)	1:C:100:LEU:H	1:C:103:MET:HG3	1	0.2
(1,349)	1:C:157:MET:HA	1:C:161:GLU:H	4	0.2
(1,184)	1:C:103:MET:HG2	1:C:104:PHE:HA	1	0.2
(1,184)	1:C:103:MET:HG3	1:C:104:PHE:HA	1	0.2
(1,98)	1:C:128:ILE:HA	1:C:128:ILE:HD11	19	0.19
(1,98)	1:C:128:ILE:HA	1:C:128:ILE:HD12	19	0.19
(1,98)	1:C:128:ILE:HA	1:C:128:ILE:HD13	19	0.19
(1,96)	1:C:137:MET:HA	1:C:138:LYS:HE2	11	0.19
(1,96)	1:C:137:MET:HA	1:C:138:LYS:HE3	11	0.19
(1,58)	1:C:130:GLU:HA	1:C:133:ILE:HD11	6	0.19
(1,58)	1:C:130:GLU:HA	1:C:133:ILE:HD12	6	0.19
(1,58)	1:C:130:GLU:HA	1:C:133:ILE:HD13	6	0.19
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB2	13	0.19
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB3	13	0.19
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB2	13	0.19
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB3	13	0.19
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB2	13	0.19
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB3	13	0.19
(1,29)	1:C:90:MET:HE1	1:C:92:LYS:HB2	15	0.19
(1,29)	1:C:90:MET:HE1	1:C:92:LYS:HB3	15	0.19
(1,29)	1:C:90:MET:HE2	1:C:92:LYS:HB2	15	0.19
(1,29)	1:C:90:MET:HE2	1:C:92:LYS:HB3	15	0.19
(1,29)	1:C:90:MET:HE3	1:C:92:LYS:HB2	15	0.19
(1,29)	1:C:90:MET:HE3	1:C:92:LYS:HB3	15	0.19
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD11	6	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD12	6	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD13	6	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD21	6	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD22	6	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD23	6	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD11	6	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD12	6	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD13	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD21	6	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD22	6	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD23	6	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD11	18	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD12	18	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD13	18	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD21	18	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD22	18	0.18
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD23	18	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD11	18	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD12	18	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD13	18	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD21	18	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD22	18	0.18
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD23	18	0.18
(1,813)	1:C:99:ASP:HB2	1:C:100:LEU:HD11	11	0.18
(1,813)	1:C:99:ASP:HB2	1:C:100:LEU:HD12	11	0.18
(1,813)	1:C:99:ASP:HB2	1:C:100:LEU:HD13	11	0.18
(1,813)	1:C:99:ASP:HB2	1:C:100:LEU:HD21	11	0.18
(1,813)	1:C:99:ASP:HB2	1:C:100:LEU:HD22	11	0.18
(1,813)	1:C:99:ASP:HB2	1:C:100:LEU:HD23	11	0.18
(1,813)	1:C:99:ASP:HB3	1:C:100:LEU:HD11	11	0.18
(1,813)	1:C:99:ASP:HB3	1:C:100:LEU:HD12	11	0.18
(1,813)	1:C:99:ASP:HB3	1:C:100:LEU:HD13	11	0.18
(1,813)	1:C:99:ASP:HB3	1:C:100:LEU:HD21	11	0.18
(1,813)	1:C:99:ASP:HB3	1:C:100:LEU:HD22	11	0.18
(1,813)	1:C:99:ASP:HB3	1:C:100:LEU:HD23	11	0.18
(1,621)	1:C:103:MET:HG2	1:C:105:ASP:H	1	0.18
(1,621)	1:C:103:MET:HG3	1:C:105:ASP:H	1	0.18
(1,62)	1:C:130:GLU:HG2	1:C:133:ILE:HD11	4	0.18
(1,62)	1:C:130:GLU:HG2	1:C:133:ILE:HD12	4	0.18
(1,62)	1:C:130:GLU:HG2	1:C:133:ILE:HD13	4	0.18
(1,62)	1:C:130:GLU:HG3	1:C:133:ILE:HD11	4	0.18
(1,62)	1:C:130:GLU:HG3	1:C:133:ILE:HD12	4	0.18
(1,62)	1:C:130:GLU:HG3	1:C:133:ILE:HD13	4	0.18
(1,111)	1:C:97:LEU:HB3	1:C:154:LEU:HB2	17	0.18
(1,111)	1:C:97:LEU:HB3	1:C:154:LEU:HB3	17	0.18
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE2	4	0.17
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE3	4	0.17
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE2	4	0.17
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE3	4	0.17
(1,7)	1:C:120:MET:HE1	1:C:121:LEU:HA	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:C:120:MET:HE2	1:C:121:LEU:HA	17	0.17
(1,7)	1:C:120:MET:HE3	1:C:121:LEU:HA	17	0.17
(1,67)	1:C:141:ASP:HB2	1:C:148:ILE:HD11	10	0.17
(1,67)	1:C:141:ASP:HB2	1:C:148:ILE:HD12	10	0.17
(1,67)	1:C:141:ASP:HB2	1:C:148:ILE:HD13	10	0.17
(1,362)	1:C:148:ILE:HD11	1:C:149:ASP:H	14	0.17
(1,362)	1:C:148:ILE:HD12	1:C:149:ASP:H	14	0.17
(1,362)	1:C:148:ILE:HD13	1:C:149:ASP:H	14	0.17
(1,349)	1:C:157:MET:HA	1:C:161:GLU:H	17	0.17
(1,348)	1:C:127:THR:HB	1:C:128:ILE:H	10	0.17
(1,848)	1:C:113:ASP:HB2	1:C:114:LEU:HG	8	0.16
(1,848)	1:C:113:ASP:HB3	1:C:114:LEU:HG	8	0.16
(1,829)	1:C:106:LYS:HG2	1:C:116:GLU:HG2	18	0.16
(1,829)	1:C:106:LYS:HG2	1:C:116:GLU:HG3	18	0.16
(1,829)	1:C:106:LYS:HG3	1:C:116:GLU:HG2	18	0.16
(1,829)	1:C:106:LYS:HG3	1:C:116:GLU:HG3	18	0.16
(1,805)	1:C:97:LEU:HD11	1:C:98:SER:HA	13	0.16
(1,805)	1:C:97:LEU:HD12	1:C:98:SER:HA	13	0.16
(1,805)	1:C:97:LEU:HD13	1:C:98:SER:HA	13	0.16
(1,805)	1:C:97:LEU:HD21	1:C:98:SER:HA	13	0.16
(1,805)	1:C:97:LEU:HD22	1:C:98:SER:HA	13	0.16
(1,805)	1:C:97:LEU:HD23	1:C:98:SER:HA	13	0.16
(1,766)	1:C:148:ILE:HB	1:C:156:PHE:HE1	8	0.16
(1,766)	1:C:148:ILE:HB	1:C:156:PHE:HE2	8	0.16
(1,766)	1:C:148:ILE:HB	1:C:156:PHE:HE1	16	0.16
(1,766)	1:C:148:ILE:HB	1:C:156:PHE:HE2	16	0.16
(1,7)	1:C:120:MET:HE1	1:C:121:LEU:HA	2	0.16
(1,7)	1:C:120:MET:HE2	1:C:121:LEU:HA	2	0.16
(1,7)	1:C:120:MET:HE3	1:C:121:LEU:HA	2	0.16
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG21	19	0.16
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG22	19	0.16
(1,457)	1:C:123:ALA:H	1:C:124:THR:HG23	19	0.16
(1,362)	1:C:148:ILE:HD11	1:C:149:ASP:H	10	0.16
(1,362)	1:C:148:ILE:HD12	1:C:149:ASP:H	10	0.16
(1,362)	1:C:148:ILE:HD13	1:C:149:ASP:H	10	0.16
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB2	10	0.16
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB3	10	0.16
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB2	10	0.16
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB3	10	0.16
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB2	10	0.16
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB3	10	0.16
(1,272)	1:C:92:LYS:HD2	1:C:95:GLU:HB2	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:C:92:LYS:HD2	1:C:95:GLU:HB3	11	0.16
(1,272)	1:C:92:LYS:HD3	1:C:95:GLU:HB2	11	0.16
(1,272)	1:C:92:LYS:HD3	1:C:95:GLU:HB3	11	0.16
(1,96)	1:C:137:MET:HA	1:C:138:LYS:HE2	2	0.15
(1,96)	1:C:137:MET:HA	1:C:138:LYS:HE3	2	0.15
(1,941)	1:C:154:LEU:HD11	1:C:155:GLU:HA	20	0.15
(1,941)	1:C:154:LEU:HD12	1:C:155:GLU:HA	20	0.15
(1,941)	1:C:154:LEU:HD13	1:C:155:GLU:HA	20	0.15
(1,941)	1:C:154:LEU:HD21	1:C:155:GLU:HA	20	0.15
(1,941)	1:C:154:LEU:HD22	1:C:155:GLU:HA	20	0.15
(1,941)	1:C:154:LEU:HD23	1:C:155:GLU:HA	20	0.15
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE2	8	0.15
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE3	8	0.15
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE2	8	0.15
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE3	8	0.15
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE2	10	0.15
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE3	10	0.15
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE2	10	0.15
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE3	10	0.15
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD11	3	0.15
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD12	3	0.15
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD13	3	0.15
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD21	3	0.15
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD22	3	0.15
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD23	3	0.15
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD11	3	0.15
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD12	3	0.15
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD13	3	0.15
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD21	3	0.15
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD22	3	0.15
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD23	3	0.15
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD11	3	0.15
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD12	3	0.15
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD13	3	0.15
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD21	3	0.15
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD22	3	0.15
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD23	3	0.15
(1,805)	1:C:97:LEU:HD11	1:C:98:SER:HA	7	0.15
(1,805)	1:C:97:LEU:HD12	1:C:98:SER:HA	7	0.15
(1,805)	1:C:97:LEU:HD13	1:C:98:SER:HA	7	0.15
(1,805)	1:C:97:LEU:HD21	1:C:98:SER:HA	7	0.15
(1,805)	1:C:97:LEU:HD22	1:C:98:SER:HA	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,805)	1:C:97:LEU:HD23	1:C:98:SER:HA	7	0.15
(1,805)	1:C:97:LEU:HD11	1:C:98:SER:HA	15	0.15
(1,805)	1:C:97:LEU:HD12	1:C:98:SER:HA	15	0.15
(1,805)	1:C:97:LEU:HD13	1:C:98:SER:HA	15	0.15
(1,805)	1:C:97:LEU:HD21	1:C:98:SER:HA	15	0.15
(1,805)	1:C:97:LEU:HD22	1:C:98:SER:HA	15	0.15
(1,805)	1:C:97:LEU:HD23	1:C:98:SER:HA	15	0.15
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD11	18	0.15
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD12	18	0.15
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD13	18	0.15
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD21	18	0.15
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD22	18	0.15
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD23	18	0.15
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD11	18	0.15
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD12	18	0.15
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD13	18	0.15
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD21	18	0.15
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD22	18	0.15
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD23	18	0.15
(1,795)	1:C:94:GLU:HG2	1:C:97:LEU:HD11	12	0.15
(1,795)	1:C:94:GLU:HG2	1:C:97:LEU:HD12	12	0.15
(1,795)	1:C:94:GLU:HG2	1:C:97:LEU:HD13	12	0.15
(1,795)	1:C:94:GLU:HG2	1:C:97:LEU:HD21	12	0.15
(1,795)	1:C:94:GLU:HG2	1:C:97:LEU:HD22	12	0.15
(1,795)	1:C:94:GLU:HG2	1:C:97:LEU:HD23	12	0.15
(1,795)	1:C:94:GLU:HG3	1:C:97:LEU:HD11	12	0.15
(1,795)	1:C:94:GLU:HG3	1:C:97:LEU:HD12	12	0.15
(1,795)	1:C:94:GLU:HG3	1:C:97:LEU:HD13	12	0.15
(1,795)	1:C:94:GLU:HG3	1:C:97:LEU:HD21	12	0.15
(1,795)	1:C:94:GLU:HG3	1:C:97:LEU:HD22	12	0.15
(1,795)	1:C:94:GLU:HG3	1:C:97:LEU:HD23	12	0.15
(1,631)	1:C:138:LYS:HE2	1:C:139:ASP:H	14	0.15
(1,631)	1:C:138:LYS:HE3	1:C:139:ASP:H	14	0.15
(1,467)	1:C:93:SER:H	1:C:95:GLU:H	7	0.15
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG21	7	0.15
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG22	7	0.15
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG23	7	0.15
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG21	7	0.15
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG22	7	0.15
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG23	7	0.15
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG21	7	0.15
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG22	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG23	7	0.15
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB2	7	0.15
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB3	7	0.15
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB2	7	0.15
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB3	7	0.15
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB2	7	0.15
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB3	7	0.15
(1,311)	1:C:142:LYS:HG3	1:C:152:GLU:HB3	4	0.15
(1,125)	1:C:115:ASP:HB3	1:C:118:LYS:HD2	14	0.15
(1,125)	1:C:115:ASP:HB3	1:C:118:LYS:HD3	14	0.15
(1,912)	1:C:137:MET:HG2	1:C:138:LYS:HB2	16	0.14
(1,912)	1:C:137:MET:HG2	1:C:138:LYS:HB3	16	0.14
(1,912)	1:C:137:MET:HG3	1:C:138:LYS:HB2	16	0.14
(1,912)	1:C:137:MET:HG3	1:C:138:LYS:HB3	16	0.14
(1,885)	1:C:121:LEU:HD11	1:C:124:THR:HG21	17	0.14
(1,885)	1:C:121:LEU:HD11	1:C:124:THR:HG22	17	0.14
(1,885)	1:C:121:LEU:HD11	1:C:124:THR:HG23	17	0.14
(1,885)	1:C:121:LEU:HD12	1:C:124:THR:HG21	17	0.14
(1,885)	1:C:121:LEU:HD12	1:C:124:THR:HG22	17	0.14
(1,885)	1:C:121:LEU:HD12	1:C:124:THR:HG23	17	0.14
(1,885)	1:C:121:LEU:HD13	1:C:124:THR:HG21	17	0.14
(1,885)	1:C:121:LEU:HD13	1:C:124:THR:HG22	17	0.14
(1,885)	1:C:121:LEU:HD13	1:C:124:THR:HG23	17	0.14
(1,885)	1:C:121:LEU:HD21	1:C:124:THR:HG21	17	0.14
(1,885)	1:C:121:LEU:HD21	1:C:124:THR:HG22	17	0.14
(1,885)	1:C:121:LEU:HD21	1:C:124:THR:HG23	17	0.14
(1,885)	1:C:121:LEU:HD22	1:C:124:THR:HG21	17	0.14
(1,885)	1:C:121:LEU:HD22	1:C:124:THR:HG22	17	0.14
(1,885)	1:C:121:LEU:HD22	1:C:124:THR:HG23	17	0.14
(1,885)	1:C:121:LEU:HD23	1:C:124:THR:HG21	17	0.14
(1,885)	1:C:121:LEU:HD23	1:C:124:THR:HG22	17	0.14
(1,885)	1:C:121:LEU:HD23	1:C:124:THR:HG23	17	0.14
(1,82)	1:C:147:ARG:HG2	1:C:148:ILE:HD11	10	0.14
(1,82)	1:C:147:ARG:HG2	1:C:148:ILE:HD12	10	0.14
(1,82)	1:C:147:ARG:HG2	1:C:148:ILE:HD13	10	0.14
(1,82)	1:C:147:ARG:HG3	1:C:148:ILE:HD11	10	0.14
(1,82)	1:C:147:ARG:HG3	1:C:148:ILE:HD12	10	0.14
(1,82)	1:C:147:ARG:HG3	1:C:148:ILE:HD13	10	0.14
(1,82)	1:C:147:ARG:HG2	1:C:148:ILE:HD11	14	0.14
(1,82)	1:C:147:ARG:HG2	1:C:148:ILE:HD12	14	0.14
(1,82)	1:C:147:ARG:HG2	1:C:148:ILE:HD13	14	0.14
(1,82)	1:C:147:ARG:HG3	1:C:148:ILE:HD11	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:C:147:ARG:HG3	1:C:148:ILE:HD12	14	0.14
(1,82)	1:C:147:ARG:HG3	1:C:148:ILE:HD13	14	0.14
(1,805)	1:C:97:LEU:HD11	1:C:98:SER:HA	6	0.14
(1,805)	1:C:97:LEU:HD12	1:C:98:SER:HA	6	0.14
(1,805)	1:C:97:LEU:HD13	1:C:98:SER:HA	6	0.14
(1,805)	1:C:97:LEU:HD21	1:C:98:SER:HA	6	0.14
(1,805)	1:C:97:LEU:HD22	1:C:98:SER:HA	6	0.14
(1,805)	1:C:97:LEU:HD23	1:C:98:SER:HA	6	0.14
(1,805)	1:C:97:LEU:HD11	1:C:98:SER:HA	14	0.14
(1,805)	1:C:97:LEU:HD12	1:C:98:SER:HA	14	0.14
(1,805)	1:C:97:LEU:HD13	1:C:98:SER:HA	14	0.14
(1,805)	1:C:97:LEU:HD21	1:C:98:SER:HA	14	0.14
(1,805)	1:C:97:LEU:HD22	1:C:98:SER:HA	14	0.14
(1,805)	1:C:97:LEU:HD23	1:C:98:SER:HA	14	0.14
(1,75)	1:C:118:LYS:HD2	1:C:119:ILE:HD11	10	0.14
(1,75)	1:C:118:LYS:HD2	1:C:119:ILE:HD12	10	0.14
(1,75)	1:C:118:LYS:HD2	1:C:119:ILE:HD13	10	0.14
(1,75)	1:C:118:LYS:HD3	1:C:119:ILE:HD11	10	0.14
(1,75)	1:C:118:LYS:HD3	1:C:119:ILE:HD12	10	0.14
(1,75)	1:C:118:LYS:HD3	1:C:119:ILE:HD13	10	0.14
(1,74)	1:C:116:GLU:HB2	1:C:119:ILE:HD11	4	0.14
(1,74)	1:C:116:GLU:HB2	1:C:119:ILE:HD12	4	0.14
(1,74)	1:C:116:GLU:HB2	1:C:119:ILE:HD13	4	0.14
(1,74)	1:C:116:GLU:HB3	1:C:119:ILE:HD11	4	0.14
(1,74)	1:C:116:GLU:HB3	1:C:119:ILE:HD12	4	0.14
(1,74)	1:C:116:GLU:HB3	1:C:119:ILE:HD13	4	0.14
(1,7)	1:C:120:MET:HE1	1:C:121:LEU:HA	20	0.14
(1,7)	1:C:120:MET:HE2	1:C:121:LEU:HA	20	0.14
(1,7)	1:C:120:MET:HE3	1:C:121:LEU:HA	20	0.14
(1,654)	1:C:154:LEU:HG	1:C:155:GLU:H	17	0.14
(1,516)	1:C:141:ASP:H	1:C:142:LYS:HE2	10	0.14
(1,516)	1:C:141:ASP:H	1:C:142:LYS:HE3	10	0.14
(1,362)	1:C:148:ILE:HD11	1:C:149:ASP:H	11	0.14
(1,362)	1:C:148:ILE:HD12	1:C:149:ASP:H	11	0.14
(1,362)	1:C:148:ILE:HD13	1:C:149:ASP:H	11	0.14
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG21	17	0.14
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG22	17	0.14
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG23	17	0.14
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG21	17	0.14
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG22	17	0.14
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG23	17	0.14
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG21	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG22	17	0.14
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG23	17	0.14
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB2	16	0.14
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB3	16	0.14
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB2	16	0.14
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB3	16	0.14
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB2	16	0.14
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB3	16	0.14
(1,29)	1:C:90:MET:HE1	1:C:92:LYS:HB2	5	0.14
(1,29)	1:C:90:MET:HE1	1:C:92:LYS:HB3	5	0.14
(1,29)	1:C:90:MET:HE2	1:C:92:LYS:HB2	5	0.14
(1,29)	1:C:90:MET:HE2	1:C:92:LYS:HB3	5	0.14
(1,29)	1:C:90:MET:HE3	1:C:92:LYS:HB2	5	0.14
(1,29)	1:C:90:MET:HE3	1:C:92:LYS:HB3	5	0.14
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE2	7	0.13
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE3	7	0.13
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE2	7	0.13
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE3	7	0.13
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD11	12	0.13
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD12	12	0.13
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD13	12	0.13
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD21	12	0.13
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD22	12	0.13
(1,900)	1:C:135:GLU:HG2	1:C:136:LEU:HD23	12	0.13
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD11	12	0.13
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD12	12	0.13
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD13	12	0.13
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD21	12	0.13
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD22	12	0.13
(1,900)	1:C:135:GLU:HG3	1:C:136:LEU:HD23	12	0.13
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD11	1	0.13
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD12	1	0.13
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD13	1	0.13
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD21	1	0.13
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD22	1	0.13
(1,877)	1:C:120:MET:HE1	1:C:121:LEU:HD23	1	0.13
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD11	1	0.13
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD12	1	0.13
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD13	1	0.13
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD21	1	0.13
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD22	1	0.13
(1,877)	1:C:120:MET:HE2	1:C:121:LEU:HD23	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD11	1	0.13
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD12	1	0.13
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD13	1	0.13
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD21	1	0.13
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD22	1	0.13
(1,877)	1:C:120:MET:HE3	1:C:121:LEU:HD23	1	0.13
(1,858)	1:C:114:LEU:HD11	1:C:137:MET:HE1	3	0.13
(1,858)	1:C:114:LEU:HD11	1:C:137:MET:HE2	3	0.13
(1,858)	1:C:114:LEU:HD11	1:C:137:MET:HE3	3	0.13
(1,858)	1:C:114:LEU:HD12	1:C:137:MET:HE1	3	0.13
(1,858)	1:C:114:LEU:HD12	1:C:137:MET:HE2	3	0.13
(1,858)	1:C:114:LEU:HD12	1:C:137:MET:HE3	3	0.13
(1,858)	1:C:114:LEU:HD13	1:C:137:MET:HE1	3	0.13
(1,858)	1:C:114:LEU:HD13	1:C:137:MET:HE2	3	0.13
(1,858)	1:C:114:LEU:HD13	1:C:137:MET:HE3	3	0.13
(1,858)	1:C:114:LEU:HD21	1:C:137:MET:HE1	3	0.13
(1,858)	1:C:114:LEU:HD21	1:C:137:MET:HE2	3	0.13
(1,858)	1:C:114:LEU:HD21	1:C:137:MET:HE3	3	0.13
(1,858)	1:C:114:LEU:HD22	1:C:137:MET:HE1	3	0.13
(1,858)	1:C:114:LEU:HD22	1:C:137:MET:HE2	3	0.13
(1,858)	1:C:114:LEU:HD22	1:C:137:MET:HE3	3	0.13
(1,858)	1:C:114:LEU:HD23	1:C:137:MET:HE1	3	0.13
(1,858)	1:C:114:LEU:HD23	1:C:137:MET:HE2	3	0.13
(1,858)	1:C:114:LEU:HD23	1:C:137:MET:HE3	3	0.13
(1,85)	1:C:128:ILE:HD11	1:C:129:THR:H	8	0.13
(1,85)	1:C:128:ILE:HD12	1:C:129:THR:H	8	0.13
(1,85)	1:C:128:ILE:HD13	1:C:129:THR:H	8	0.13
(1,844)	1:C:111:TYR:HE1	1:C:147:ARG:HD2	7	0.13
(1,844)	1:C:111:TYR:HE1	1:C:147:ARG:HD3	7	0.13
(1,844)	1:C:111:TYR:HE2	1:C:147:ARG:HD2	7	0.13
(1,844)	1:C:111:TYR:HE2	1:C:147:ARG:HD3	7	0.13
(1,829)	1:C:106:LYS:HG2	1:C:116:GLU:HG2	17	0.13
(1,829)	1:C:106:LYS:HG2	1:C:116:GLU:HG3	17	0.13
(1,829)	1:C:106:LYS:HG3	1:C:116:GLU:HG2	17	0.13
(1,829)	1:C:106:LYS:HG3	1:C:116:GLU:HG3	17	0.13
(1,516)	1:C:141:ASP:H	1:C:142:LYS:HE2	8	0.13
(1,516)	1:C:141:ASP:H	1:C:142:LYS:HE3	8	0.13
(1,463)	1:C:109:ASP:H	1:C:110:GLY:H	14	0.13
(1,362)	1:C:148:ILE:HD11	1:C:149:ASP:H	3	0.13
(1,362)	1:C:148:ILE:HD12	1:C:149:ASP:H	3	0.13
(1,362)	1:C:148:ILE:HD13	1:C:149:ASP:H	3	0.13
(1,312)	1:C:142:LYS:HG2	1:C:152:GLU:HB3	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:C:90:MET:HE1	1:C:92:LYS:HD2	1	0.13
(1,30)	1:C:90:MET:HE1	1:C:92:LYS:HD3	1	0.13
(1,30)	1:C:90:MET:HE2	1:C:92:LYS:HD2	1	0.13
(1,30)	1:C:90:MET:HE2	1:C:92:LYS:HD3	1	0.13
(1,30)	1:C:90:MET:HE3	1:C:92:LYS:HD2	1	0.13
(1,30)	1:C:90:MET:HE3	1:C:92:LYS:HD3	1	0.13
(1,105)	1:C:140:GLY:HA3	1:C:142:LYS:HE2	11	0.13
(1,105)	1:C:140:GLY:HA3	1:C:142:LYS:HE3	11	0.13
(1,941)	1:C:154:LEU:HD11	1:C:155:GLU:HA	17	0.12
(1,941)	1:C:154:LEU:HD12	1:C:155:GLU:HA	17	0.12
(1,941)	1:C:154:LEU:HD13	1:C:155:GLU:HA	17	0.12
(1,941)	1:C:154:LEU:HD21	1:C:155:GLU:HA	17	0.12
(1,941)	1:C:154:LEU:HD22	1:C:155:GLU:HA	17	0.12
(1,941)	1:C:154:LEU:HD23	1:C:155:GLU:HA	17	0.12
(1,933)	1:C:147:ARG:HG2	1:C:149:ASP:HB2	7	0.12
(1,933)	1:C:147:ARG:HG2	1:C:149:ASP:HB3	7	0.12
(1,933)	1:C:147:ARG:HG3	1:C:149:ASP:HB2	7	0.12
(1,933)	1:C:147:ARG:HG3	1:C:149:ASP:HB3	7	0.12
(1,855)	1:C:114:LEU:HD11	1:C:137:MET:HB2	1	0.12
(1,855)	1:C:114:LEU:HD12	1:C:137:MET:HB2	1	0.12
(1,855)	1:C:114:LEU:HD13	1:C:137:MET:HB2	1	0.12
(1,855)	1:C:114:LEU:HD21	1:C:137:MET:HB2	1	0.12
(1,855)	1:C:114:LEU:HD22	1:C:137:MET:HB2	1	0.12
(1,855)	1:C:114:LEU:HD23	1:C:137:MET:HB2	1	0.12
(1,85)	1:C:128:ILE:HD11	1:C:129:THR:H	9	0.12
(1,85)	1:C:128:ILE:HD12	1:C:129:THR:H	9	0.12
(1,85)	1:C:128:ILE:HD13	1:C:129:THR:H	9	0.12
(1,848)	1:C:113:ASP:HB2	1:C:114:LEU:HG	7	0.12
(1,848)	1:C:113:ASP:HB3	1:C:114:LEU:HG	7	0.12
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD11	4	0.12
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD12	4	0.12
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD13	4	0.12
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD21	4	0.12
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD22	4	0.12
(1,796)	1:C:94:GLU:HG2	1:C:154:LEU:HD23	4	0.12
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD11	4	0.12
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD12	4	0.12
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD13	4	0.12
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD21	4	0.12
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD22	4	0.12
(1,796)	1:C:94:GLU:HG3	1:C:154:LEU:HD23	4	0.12
(1,774)	1:C:101:PHE:HE1	1:C:104:PHE:HB3	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:C:101:PHE:HE2	1:C:104:PHE:HB3	17	0.12
(1,75)	1:C:118:LYS:HD2	1:C:119:ILE:HD11	5	0.12
(1,75)	1:C:118:LYS:HD2	1:C:119:ILE:HD12	5	0.12
(1,75)	1:C:118:LYS:HD2	1:C:119:ILE:HD13	5	0.12
(1,75)	1:C:118:LYS:HD3	1:C:119:ILE:HD11	5	0.12
(1,75)	1:C:118:LYS:HD3	1:C:119:ILE:HD12	5	0.12
(1,75)	1:C:118:LYS:HD3	1:C:119:ILE:HD13	5	0.12
(1,74)	1:C:116:GLU:HB2	1:C:119:ILE:HD11	16	0.12
(1,74)	1:C:116:GLU:HB2	1:C:119:ILE:HD12	16	0.12
(1,74)	1:C:116:GLU:HB2	1:C:119:ILE:HD13	16	0.12
(1,74)	1:C:116:GLU:HB3	1:C:119:ILE:HD11	16	0.12
(1,74)	1:C:116:GLU:HB3	1:C:119:ILE:HD12	16	0.12
(1,74)	1:C:116:GLU:HB3	1:C:119:ILE:HD13	16	0.12
(1,660)	1:C:131:ASP:H	1:C:133:ILE:HD11	20	0.12
(1,660)	1:C:131:ASP:H	1:C:133:ILE:HD12	20	0.12
(1,660)	1:C:131:ASP:H	1:C:133:ILE:HD13	20	0.12
(1,66)	1:C:148:ILE:HD11	1:C:152:GLU:HB2	3	0.12
(1,66)	1:C:148:ILE:HD12	1:C:152:GLU:HB2	3	0.12
(1,66)	1:C:148:ILE:HD13	1:C:152:GLU:HB2	3	0.12
(1,446)	1:C:136:LEU:H	1:C:139:ASP:HB2	20	0.12
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG21	14	0.12
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG22	14	0.12
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG23	14	0.12
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG21	14	0.12
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG22	14	0.12
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG23	14	0.12
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG21	14	0.12
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG22	14	0.12
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG23	14	0.12
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB2	2	0.12
(1,322)	1:C:97:LEU:HD11	1:C:98:SER:HB3	2	0.12
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB2	2	0.12
(1,322)	1:C:97:LEU:HD12	1:C:98:SER:HB3	2	0.12
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB2	2	0.12
(1,322)	1:C:97:LEU:HD13	1:C:98:SER:HB3	2	0.12
(1,311)	1:C:142:LYS:HG3	1:C:152:GLU:HB3	16	0.12
(1,192)	1:C:153:PHE:HA	1:C:155:GLU:HG2	15	0.12
(1,192)	1:C:153:PHE:HA	1:C:155:GLU:HG3	15	0.12
(1,168)	1:C:118:LYS:HD2	1:C:119:ILE:HA	3	0.12
(1,168)	1:C:118:LYS:HD3	1:C:119:ILE:HA	3	0.12
(1,168)	1:C:118:LYS:HD2	1:C:119:ILE:HA	8	0.12
(1,168)	1:C:118:LYS:HD3	1:C:119:ILE:HA	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	1:C:128:ILE:HA	1:C:128:ILE:HD11	15	0.11
(1,98)	1:C:128:ILE:HA	1:C:128:ILE:HD12	15	0.11
(1,98)	1:C:128:ILE:HA	1:C:128:ILE:HD13	15	0.11
(1,933)	1:C:147:ARG:HG2	1:C:149:ASP:HB2	9	0.11
(1,933)	1:C:147:ARG:HG2	1:C:149:ASP:HB3	9	0.11
(1,933)	1:C:147:ARG:HG3	1:C:149:ASP:HB2	9	0.11
(1,933)	1:C:147:ARG:HG3	1:C:149:ASP:HB3	9	0.11
(1,92)	1:C:126:GLU:H	1:C:128:ILE:HD11	6	0.11
(1,92)	1:C:126:GLU:H	1:C:128:ILE:HD12	6	0.11
(1,92)	1:C:126:GLU:H	1:C:128:ILE:HD13	6	0.11
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE2	9	0.11
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE3	9	0.11
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE2	9	0.11
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE3	9	0.11
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE2	12	0.11
(1,914)	1:C:137:MET:HG2	1:C:138:LYS:HE3	12	0.11
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE2	12	0.11
(1,914)	1:C:137:MET:HG3	1:C:138:LYS:HE3	12	0.11
(1,886)	1:C:121:LEU:HD11	1:C:125:GLY:H	12	0.11
(1,886)	1:C:121:LEU:HD12	1:C:125:GLY:H	12	0.11
(1,886)	1:C:121:LEU:HD13	1:C:125:GLY:H	12	0.11
(1,886)	1:C:121:LEU:HD21	1:C:125:GLY:H	12	0.11
(1,886)	1:C:121:LEU:HD22	1:C:125:GLY:H	12	0.11
(1,886)	1:C:121:LEU:HD23	1:C:125:GLY:H	12	0.11
(1,885)	1:C:121:LEU:HD11	1:C:124:THR:HG21	2	0.11
(1,885)	1:C:121:LEU:HD11	1:C:124:THR:HG22	2	0.11
(1,885)	1:C:121:LEU:HD11	1:C:124:THR:HG23	2	0.11
(1,885)	1:C:121:LEU:HD12	1:C:124:THR:HG21	2	0.11
(1,885)	1:C:121:LEU:HD12	1:C:124:THR:HG22	2	0.11
(1,885)	1:C:121:LEU:HD12	1:C:124:THR:HG23	2	0.11
(1,885)	1:C:121:LEU:HD13	1:C:124:THR:HG21	2	0.11
(1,885)	1:C:121:LEU:HD13	1:C:124:THR:HG22	2	0.11
(1,885)	1:C:121:LEU:HD13	1:C:124:THR:HG23	2	0.11
(1,885)	1:C:121:LEU:HD21	1:C:124:THR:HG21	2	0.11
(1,885)	1:C:121:LEU:HD21	1:C:124:THR:HG22	2	0.11
(1,885)	1:C:121:LEU:HD21	1:C:124:THR:HG23	2	0.11
(1,885)	1:C:121:LEU:HD22	1:C:124:THR:HG21	2	0.11
(1,885)	1:C:121:LEU:HD22	1:C:124:THR:HG22	2	0.11
(1,885)	1:C:121:LEU:HD22	1:C:124:THR:HG23	2	0.11
(1,885)	1:C:121:LEU:HD23	1:C:124:THR:HG21	2	0.11
(1,885)	1:C:121:LEU:HD23	1:C:124:THR:HG22	2	0.11
(1,885)	1:C:121:LEU:HD23	1:C:124:THR:HG23	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:C:113:ASP:HB2	1:C:114:LEU:HG	17	0.11
(1,848)	1:C:113:ASP:HB3	1:C:114:LEU:HG	17	0.11
(1,829)	1:C:106:LYS:HG2	1:C:116:GLU:HG2	2	0.11
(1,829)	1:C:106:LYS:HG2	1:C:116:GLU:HG3	2	0.11
(1,829)	1:C:106:LYS:HG3	1:C:116:GLU:HG2	2	0.11
(1,829)	1:C:106:LYS:HG3	1:C:116:GLU:HG3	2	0.11
(1,829)	1:C:106:LYS:HG2	1:C:116:GLU:HG2	15	0.11
(1,829)	1:C:106:LYS:HG2	1:C:116:GLU:HG3	15	0.11
(1,829)	1:C:106:LYS:HG3	1:C:116:GLU:HG2	15	0.11
(1,829)	1:C:106:LYS:HG3	1:C:116:GLU:HG3	15	0.11
(1,805)	1:C:97:LEU:HD11	1:C:98:SER:HA	19	0.11
(1,805)	1:C:97:LEU:HD12	1:C:98:SER:HA	19	0.11
(1,805)	1:C:97:LEU:HD13	1:C:98:SER:HA	19	0.11
(1,805)	1:C:97:LEU:HD21	1:C:98:SER:HA	19	0.11
(1,805)	1:C:97:LEU:HD22	1:C:98:SER:HA	19	0.11
(1,805)	1:C:97:LEU:HD23	1:C:98:SER:HA	19	0.11
(1,766)	1:C:148:ILE:HB	1:C:156:PHE:HE1	3	0.11
(1,766)	1:C:148:ILE:HB	1:C:156:PHE:HE2	3	0.11
(1,74)	1:C:116:GLU:HB2	1:C:119:ILE:HD11	14	0.11
(1,74)	1:C:116:GLU:HB2	1:C:119:ILE:HD12	14	0.11
(1,74)	1:C:116:GLU:HB2	1:C:119:ILE:HD13	14	0.11
(1,74)	1:C:116:GLU:HB3	1:C:119:ILE:HD11	14	0.11
(1,74)	1:C:116:GLU:HB3	1:C:119:ILE:HD12	14	0.11
(1,74)	1:C:116:GLU:HB3	1:C:119:ILE:HD13	14	0.11
(1,446)	1:C:136:LEU:H	1:C:139:ASP:HB2	2	0.11
(1,362)	1:C:148:ILE:HD11	1:C:149:ASP:H	12	0.11
(1,362)	1:C:148:ILE:HD12	1:C:149:ASP:H	12	0.11
(1,362)	1:C:148:ILE:HD13	1:C:149:ASP:H	12	0.11
(1,349)	1:C:157:MET:HA	1:C:161:GLU:H	10	0.11
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG21	1	0.11
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG22	1	0.11
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG23	1	0.11
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG21	1	0.11
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG22	1	0.11
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG23	1	0.11
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG21	1	0.11
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG22	1	0.11
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG23	1	0.11
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG21	15	0.11
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG22	15	0.11
(1,339)	1:C:120:MET:HE1	1:C:124:THR:HG23	15	0.11
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG21	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG22	15	0.11
(1,339)	1:C:120:MET:HE2	1:C:124:THR:HG23	15	0.11
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG21	15	0.11
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG22	15	0.11
(1,339)	1:C:120:MET:HE3	1:C:124:THR:HG23	15	0.11
(1,336)	1:C:121:LEU:HA	1:C:124:THR:HG21	18	0.11
(1,336)	1:C:121:LEU:HA	1:C:124:THR:HG22	18	0.11
(1,336)	1:C:121:LEU:HA	1:C:124:THR:HG23	18	0.11
(1,323)	1:C:154:LEU:HD11	1:C:155:GLU:HA	20	0.11
(1,323)	1:C:154:LEU:HD12	1:C:155:GLU:HA	20	0.11
(1,323)	1:C:154:LEU:HD13	1:C:155:GLU:HA	20	0.11
(1,30)	1:C:90:MET:HE1	1:C:92:LYS:HD2	20	0.11
(1,30)	1:C:90:MET:HE1	1:C:92:LYS:HD3	20	0.11
(1,30)	1:C:90:MET:HE2	1:C:92:LYS:HD2	20	0.11
(1,30)	1:C:90:MET:HE2	1:C:92:LYS:HD3	20	0.11
(1,30)	1:C:90:MET:HE3	1:C:92:LYS:HD2	20	0.11
(1,30)	1:C:90:MET:HE3	1:C:92:LYS:HD3	20	0.11
(1,272)	1:C:92:LYS:HD2	1:C:95:GLU:HB2	17	0.11
(1,272)	1:C:92:LYS:HD2	1:C:95:GLU:HB3	17	0.11
(1,272)	1:C:92:LYS:HD3	1:C:95:GLU:HB2	17	0.11
(1,272)	1:C:92:LYS:HD3	1:C:95:GLU:HB3	17	0.11
(1,192)	1:C:153:PHE:HA	1:C:155:GLU:HG2	10	0.11
(1,192)	1:C:153:PHE:HA	1:C:155:GLU:HG3	10	0.11
(1,125)	1:C:115:ASP:HB3	1:C:118:LYS:HD2	1	0.11
(1,125)	1:C:115:ASP:HB3	1:C:118:LYS:HD3	1	0.11
(1,111)	1:C:97:LEU:HB3	1:C:154:LEU:HB2	9	0.11
(1,111)	1:C:97:LEU:HB3	1:C:154:LEU:HB3	9	0.11

10 Dihedral-angle violation analysis (i)

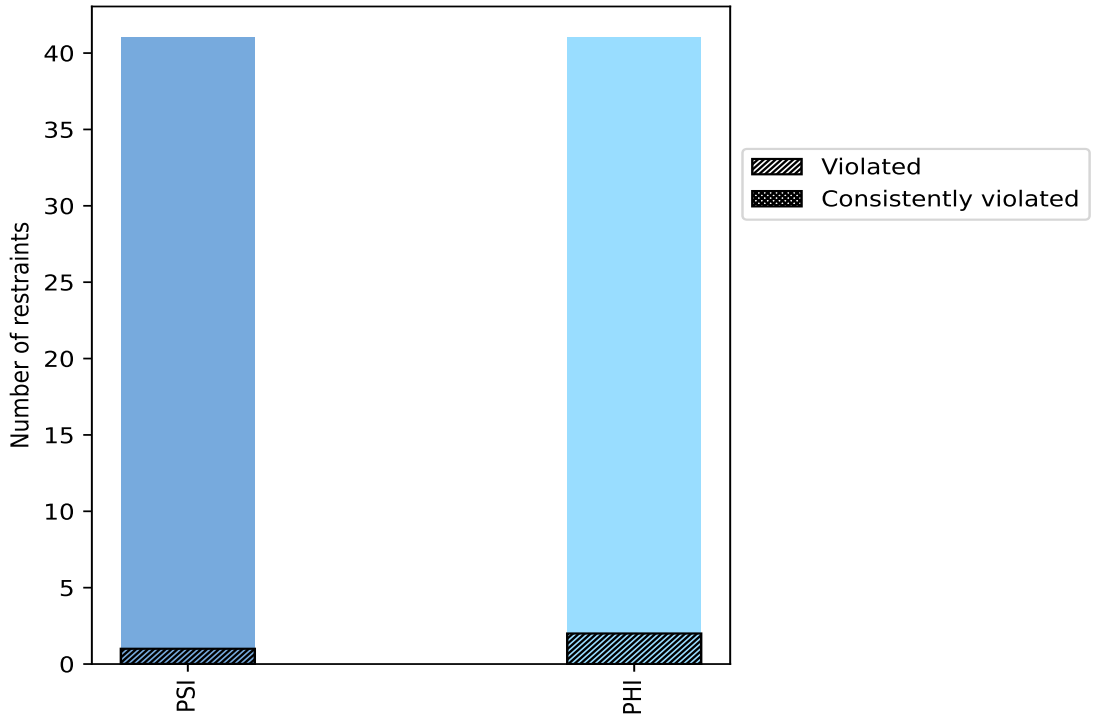
10.1 Summary of dihedral-angle violations (i)

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]
PSI	41	50.0	1	2.4	1.2	0	0.0	0.0
PHI	41	50.0	2	4.9	2.4	0	0.0	0.0
Total	82	100.0	3	3.7	3.7	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)



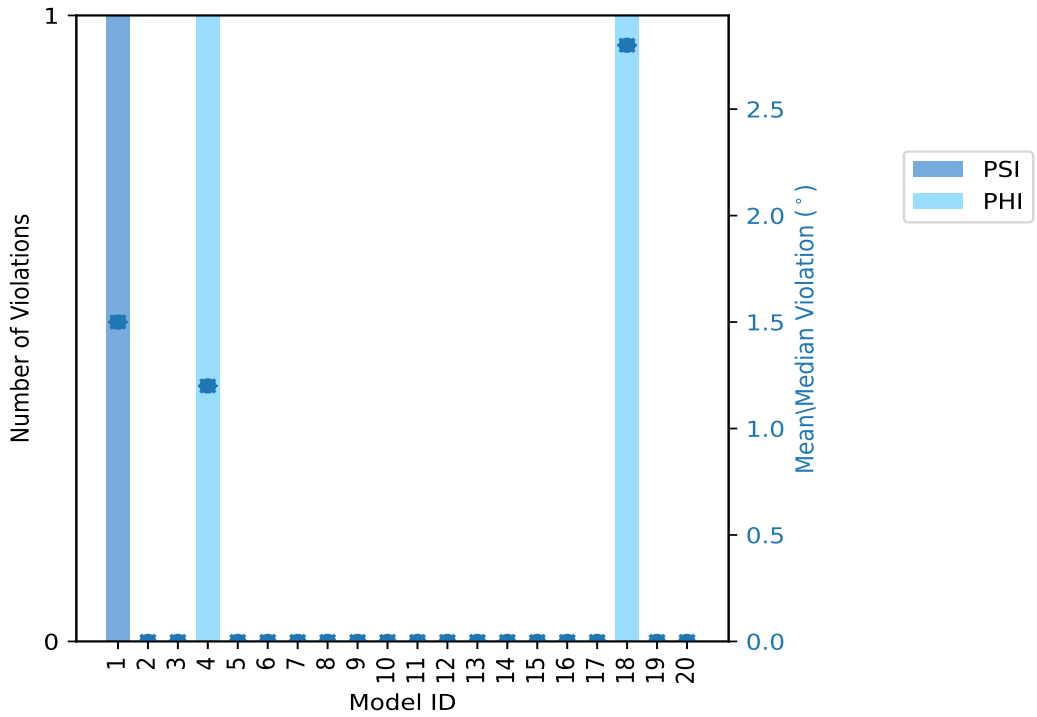
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PSI	PHI	Total				
1	1	0	1	1.5	1.5	0.0	1.5
2	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0.0	0.0	0.0	0.0
4	0	1	1	1.2	1.2	0.0	1.2
5	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0.0	0.0	0.0	0.0
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	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0.0	0.0	0.0	0.0
18	0	1	1	2.8	2.8	0.0	2.8
19	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0.0	0.0	0.0	0.0

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	
PSI	PHI	Total	Count[1]	%
1	2	3	1	5.0
0	0	0	2	10.0
0	0	0	3	15.0
0	0	0	4	20.0
0	0	0	5	25.0
0	0	0	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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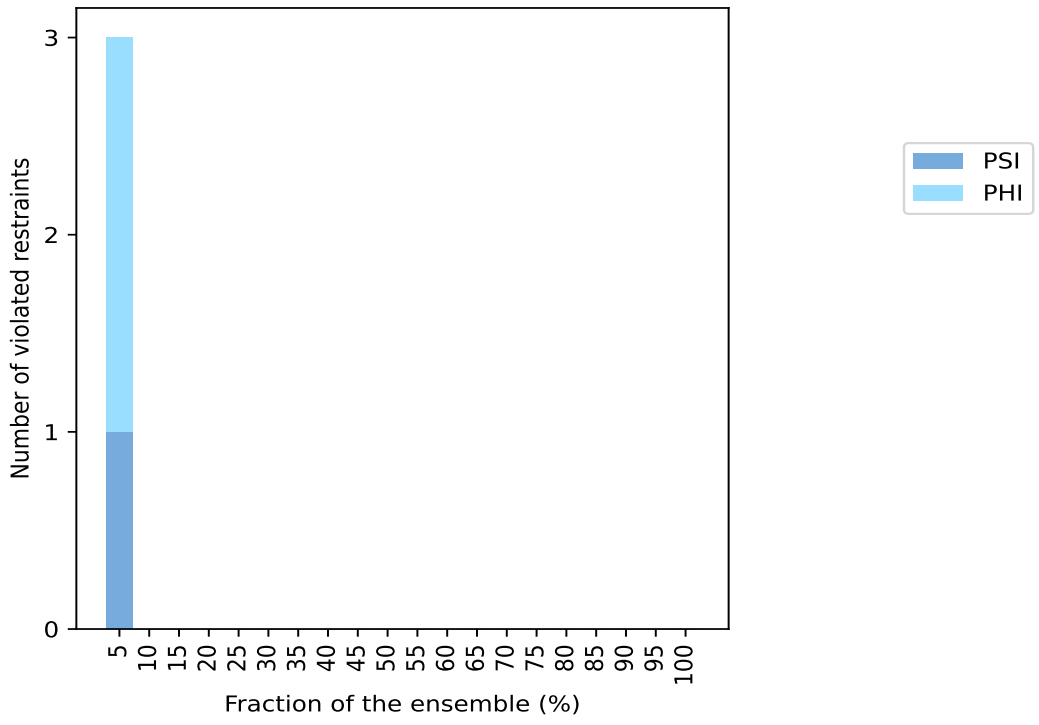
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[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)

No violations found

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.
Data insufficient to plot histogram

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 (°)
(1,65)	1:C:147:ARG:C	1:C:148:ILE:N	1:C:148:ILE:CA	1:C:148:ILE:C	18	2.8
(1,2)	1:C:94:GLU:N	1:C:94:GLU:CA	1:C:94:GLU:C	1:C:95:GLU:N	1	1.5
(1,23)	1:C:111:TYR:C	1:C:112:ILE:N	1:C:112:ILE:CA	1:C:112:ILE:C	4	1.2