Full wwPDB NMR Structure Validation Report (i)

Jun 5, 2023 – 06:01 PM EDT

PDB ID	:	2M0R
BMRB ID	:	18818
Title	:	Solution structure and dynamics of human S100A14
Authors	:	Bertini, I.; Borsi, V.; Cerofolini, L.; Das Gupta, S.; Fragai, M.; Luchinat, C.
Deposited on	:	2012-11-05

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:

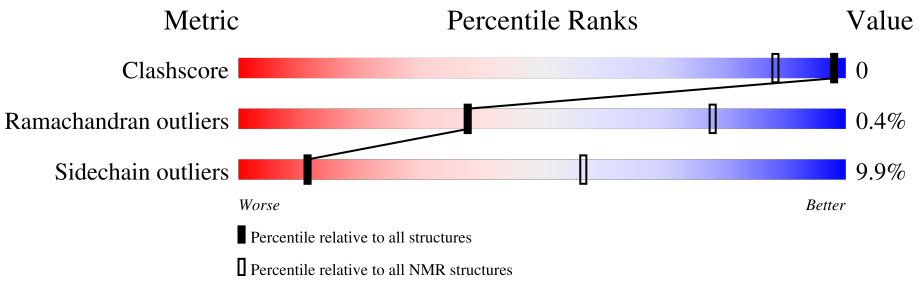
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 41%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	104	62% 8% 30%
1	B	104	63% 6% 31%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:14-A:60, A:64-A:71, A:79-A:96, B:118-B:163, B:168-B:175, B:183-B:200 (145)	1.01	16

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 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 6, 7, 9, 10, 11, 12, 13, 14, 15, 16, 18, 20, 22, 23, 24, 25, 29
2	5, 8, 27
3	4, 30
4	19, 28
Single-model clusters	17; 21; 26

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3230 atoms, of which 1596 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein S100-A14.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	104	1615	504	798	145	163	5	0
1	B	104	1615	504	798	145	163	5	0

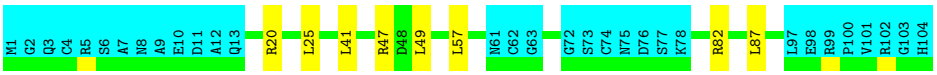
4 Residue-property plots (i)

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: Protein S100-A14

Chain A: 62% 8% 30%



• Molecule 1: Protein S100-A14

Chain B: 63% 6% 31%

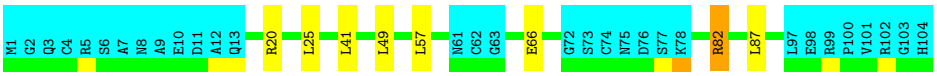
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

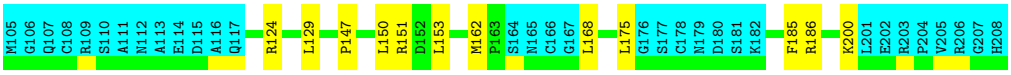
• Molecule 1: Protein S100-A14

Chain A: 62% 7% • 30%



• Molecule 1: Protein S100-A14

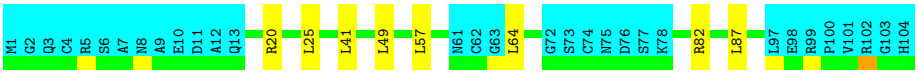
Chain B: 58% 12% 31%



4.2.2 Score per residue for model 2

- Molecule 1: Protein S100-A14

Chain A: 62% 8% 30%



- Molecule 1: Protein S100-A14

Chain B: 64% 5% 31%

4.2.3 Score per residue for model 3

- Molecule 1: Protein S100-A14

Chain A: 59% 12% 30%

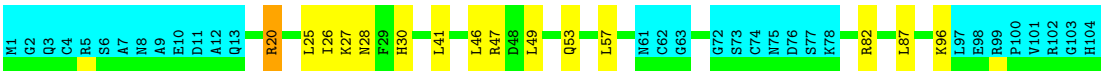
- Molecule 1: Protein S100-A14

Chain B: 61% 9% 31%

4.2.4 Score per residue for model 4

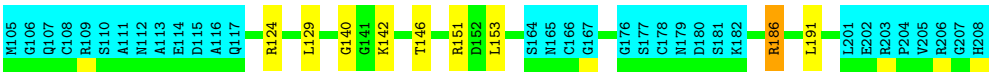
- Molecule 1: Protein S100-A14

Chain A: 56% 13% • 30%



- Molecule 1: Protein S100-A14

Chain B: 61% 8% • 31%



4.2.5 Score per residue for model 5

- Molecule 1: Protein S100-A14

Chain A: 60% 10% • 30%

M1 G2 Q3 C4 R5 S6 A7 N8 A9 E10 D11 A12 Q13 D17 R20 L25 S33 L41 T42 R47 D48 L49 L57 N61 C62 G63 G72 S73 C74 N75 D76 S77 K78 R82 L87 L97 E98 R99 P100 V101 R102 G103 H104

- Molecule 1: Protein S100-A14

Chain B: 58% 12% 31%

M105 G106 Q107 C108 R109 S110 A111 N112 A113 E114 D115 A116 Q117 R124 L129 I130 K142 L145 T146 R151 D152 L153 S164 N165 C166 G167 L175 G176 S177 C178 N179 D180 S181 K182 R186 S187 F188 I192 L201 E202 R203 P204 V205 R206 G207 H208

4.2.6 Score per residue for model 6

- Molecule 1: Protein S100-A14

Chain A: 57% 12% • 30%

M1 G2 Q3 C4 R5 S6 A7 N8 A9 E10 D11 A12 Q13 E14 F15 R20 L25 E39 R47 D48 L49 L57 M58 N61 C62 G63 G72 S73 C74 N75 D76 S77 K78 L79 E80 F81 R82 L87 I88 S94 L97 E98 R99 P100 V101 R102 G103 H104

- Molecule 1: Protein S100-A14

Chain B: 62% 8% 31%

M105 G106 Q107 C108 R109 S110 A111 N112 A113 E114 D115 A116 Q117 R124 L129 L145 R151 D152 L153 S164 N165 C166 G167 G176 S177 C178 N179 D180 S181 K182 F185 R186 K200 L201 E202 R203 P204 V205 R206 G207 H208

4.2.7 Score per residue for model 7

- Molecule 1: Protein S100-A14

Chain A: 59% 12% 30%

M1 G2 Q3 C4 R5 S6 A7 N8 A9 E10 D11 A12 Q13 R20 L25 N28 K38 L41 R47 D48 L49 Q53 L57 N61 C62 G63 L71 G72 S73 C74 N75 D76 S77 K78 R82 I88 L97 E98 R99 P100 V101 R102 G103 H104

- Molecule 1: Protein S100-A14

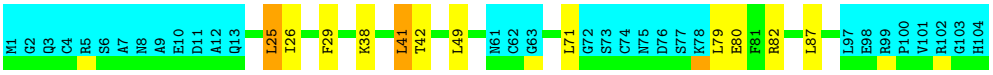
Chain B: 62% 7% • 31%

M105 G106 Q107 C108 R109 S110 A111 N112 A113 E114 D115 A116 Q117 D121 L129 L145 T146 R151 D152 L153 S164 N165 C166 G167 G176 S177 C178 N179 D180 S181 K182 R186 L191 L201 E202 R203 P204 V205 R206 G207 H208

4.2.8 Score per residue for model 8

- Molecule 1: Protein S100-A14

Chain A: 59% 10% • 30%



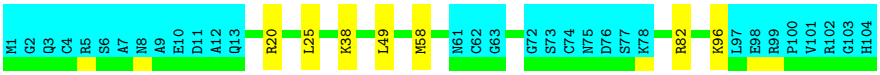
- Molecule 1: Protein S100-A14

Chain B: 60% 8% • 31%

4.2.9 Score per residue for model 9

- Molecule 1: Protein S100-A14

Chain A: 63% 7% 30%



- Molecule 1: Protein S100-A14

Chain B: 62% 7% • 31%

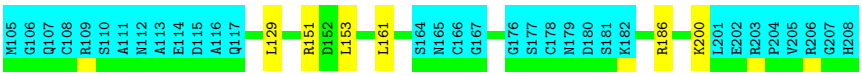
4.2.10 Score per residue for model 10

- Molecule 1: Protein S100-A14

Chain A: 63% 7% 30%

- Molecule 1: Protein S100-A14

Chain B: 63% 6% 31%



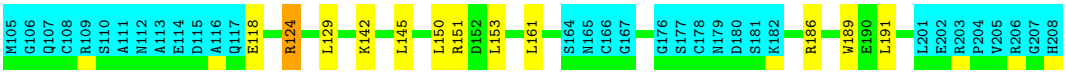
4.2.11 Score per residue for model 11

- Molecule 1: Protein S100-A14

Chain A: 61% 9% • 30%

- Molecule 1: Protein S100-A14

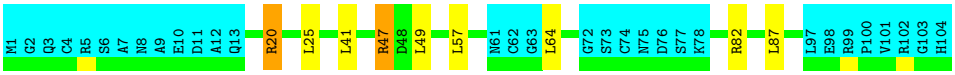
Chain B: 58% 11% • 31%



4.2.12 Score per residue for model 12

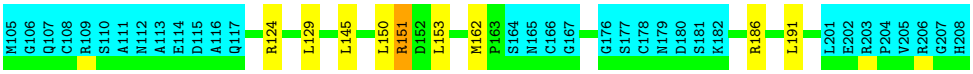
- Molecule 1: Protein S100-A14

Chain A: 62% 7% • 30%



- Molecule 1: Protein S100-A14

Chain B: 61% 8% • 31%



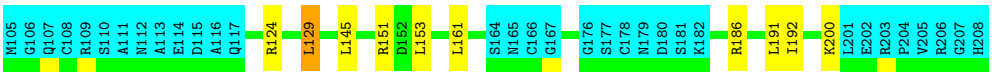
4.2.13 Score per residue for model 13

- Molecule 1: Protein S100-A14

Chain A: 60% 11% 30%

- Molecule 1: Protein S100-A14

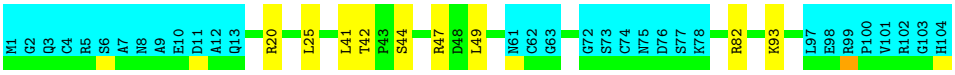
Chain B: 60% 9% • 31%



4.2.14 Score per residue for model 14

- Molecule 1: Protein S100-A14

Chain A: 62% 9% 30%



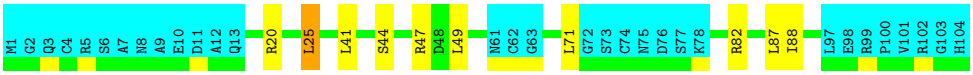
- Molecule 1: Protein S100-A14

Chain B: 63% 5% • 31%

4.2.15 Score per residue for model 15

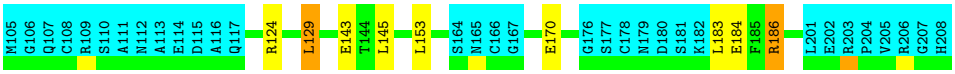
- Molecule 1: Protein S100-A14

Chain A: 61% 9% • 30%



- Molecule 1: Protein S100-A14

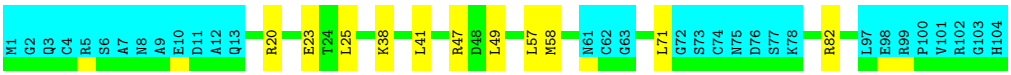
Chain B: 61% 7% • 31%



4.2.16 Score per residue for model 16 (medoid)

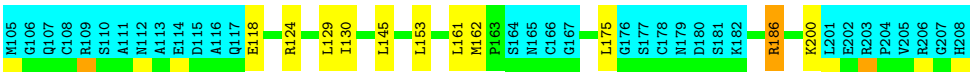
- Molecule 1: Protein S100-A14

Chain A: 60% 11% 30%



- Molecule 1: Protein S100-A14

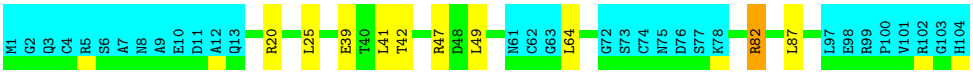
Chain B: 59% 10% • 31%



4.2.17 Score per residue for model 17

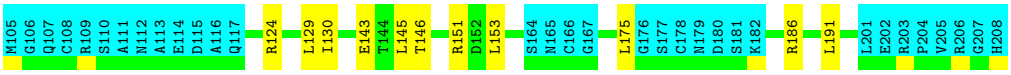
- Molecule 1: Protein S100-A14

Chain A: 61% 9% • 30%



- Molecule 1: Protein S100-A14

Chain B: 59% 11% 31%



4.2.18 Score per residue for model 18

- Molecule 1: Protein S100-A14

Chain A: 59% 11% • 30%

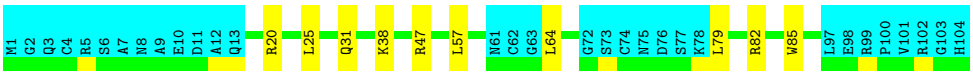
- Molecule 1: Protein S100-A14

Chain B: 62% 8% 31%

4.2.19 Score per residue for model 19

- Molecule 1: Protein S100-A14

Chain A: 61% 10% 30%



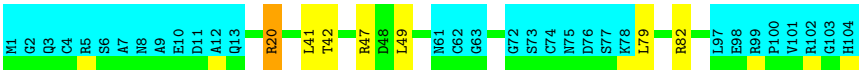
- Molecule 1: Protein S100-A14

Chain B: 61% 7% • 31%

4.2.20 Score per residue for model 20

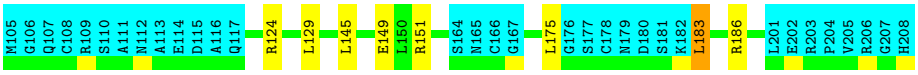
- Molecule 1: Protein S100-A14

Chain A: 63% 6% • 30%



- Molecule 1: Protein S100-A14

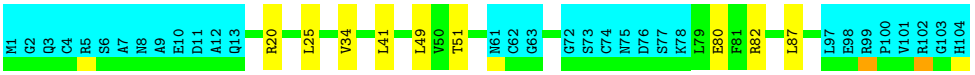
Chain B: 62% 7% • 31%



4.2.21 Score per residue for model 21

- Molecule 1: Protein S100-A14

Chain A: 62% 9% 30%



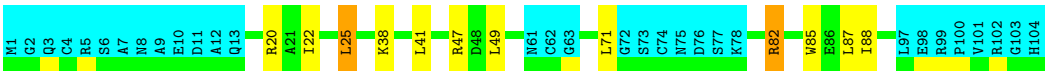
- Molecule 1: Protein S100-A14

Chain B: 61% 9% 31%

4.2.22 Score per residue for model 22

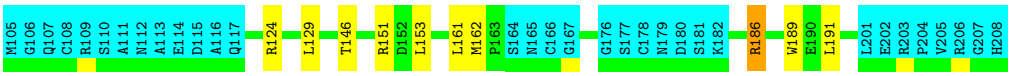
- Molecule 1: Protein S100-A14

Chain A: 59% 10% • 30%



- Molecule 1: Protein S100-A14

Chain B: 60% 9% • 31%



4.2.23 Score per residue for model 23

- Molecule 1: Protein S100-A14

Chain A: 61% 9% • 30%

M1 G2 Q3 C4 R5 S6 A7 N8 A9 E10 D11 A12 Q13 R20 L25 L41 L46 R47 D48 L49 L57 N61 C62 G63 L71 G72 S73 C74 N75 D76 S77 K78 R82 L87 L97 E98 R99 P100 V101 R102 G103 H104

- Molecule 1: Protein S100-A14

Chain B: 60% 10% 31%

M105 G106 Q107 C108 R109 S110 A111 N112 A113 E114 D115 A116 Q117 D121 R124 L129 L145 L150 R151 D152 L153 L161 S164 N165 C166 G167 L168 G176 S177 C178 N179 D180 S181 K182 L191 L201 E202 R203 P204 V205 R206 G207 H208

4.2.24 Score per residue for model 24

- Molecule 1: Protein S100-A14

Chain A: 61% 9% • 30%

M1 G2 Q3 C4 R5 S6 A7 N8 A9 E10 D11 A12 Q13 R20 L25 L41 T42 R47 D48 L49 L57 N61 C62 G63 G72 S73 C74 N75 D76 S77 K78 L79 E80 F81 R82 L87 L97 E98 R99 P100 V101 R102 G103 H104

- Molecule 1: Protein S100-A14

Chain B: 58% 12% 31%

M105 G106 Q107 C108 R109 S110 A111 N112 A113 E114 D115 A116 Q117 D121 R124 L129 I130 L145 R151 D152 L153 L161 S164 N165 C166 G167 L175 G176 S177 C178 N179 D180 S181 K182 R186 L191 K200 L201 E202 R203 P204 V205 R206 G207 H208

4.2.25 Score per residue for model 25

- Molecule 1: Protein S100-A14

Chain A: 64% 5% • 30%

M1 G2 Q3 C4 R5 S6 A7 N8 A9 E10 D11 A12 Q13 E23 T24 L25 E39 T40 L41 L49 N61 C62 G63 G72 S73 C74 N75 D76 S77 K78 R82 L97 E98 R99 P100 V101 R102 G103 H104

- Molecule 1: Protein S100-A14

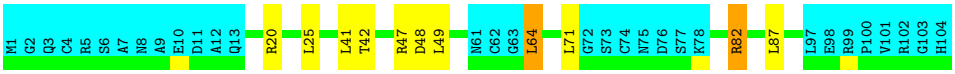
Chain B: 60% 9% • 31%

M105 G106 Q107 C108 R109 S110 A111 N112 A113 E114 D115 A116 Q117 R124 L129 I130 K131 T144 L145 R151 D152 L153 S164 N165 C166 G167 G176 S177 C178 N179 D180 S181 K182 R186 L191 K200 L201 E202 R203 P204 V205 R206 G207 H208

4.2.26 Score per residue for model 26

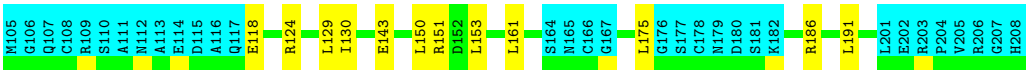
- Molecule 1: Protein S100-A14

Chain A: 60% 9% • 30%



- Molecule 1: Protein S100-A14

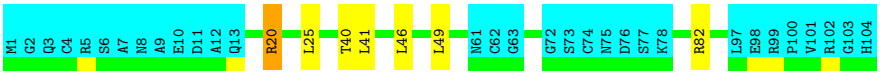
Chain B: 58% 12% 31%



4.2.27 Score per residue for model 27

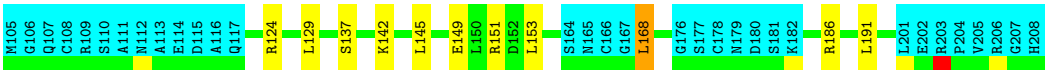
- Molecule 1: Protein S100-A14

Chain A: 63% 6% • 30%



- Molecule 1: Protein S100-A14

Chain B: 59% 10% • 31%



4.2.28 Score per residue for model 28

- Molecule 1: Protein S100-A14

Chain A: 59% 12% 30%

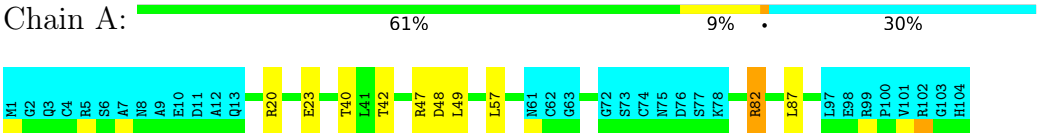
- Molecule 1: Protein S100-A14

Chain B: 62% 6% • 31%

4.2.29 Score per residue for model 29

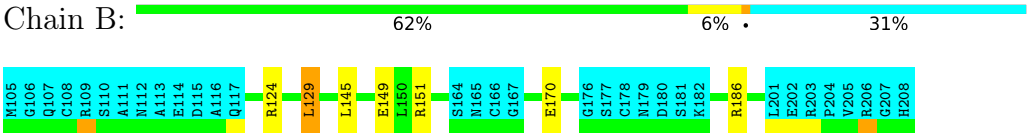
- Molecule 1: Protein S100-A14

Chain A:



- Molecule 1: Protein S100-A14

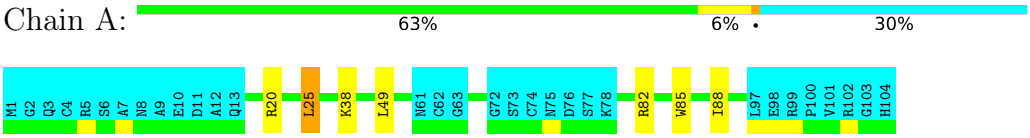
Chain B:



4.2.30 Score per residue for model 30

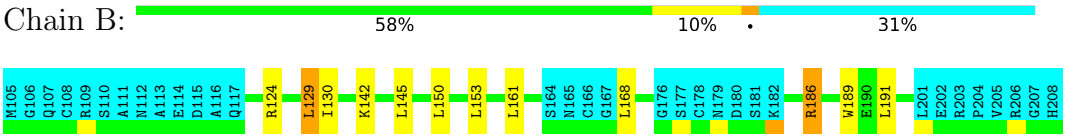
- Molecule 1: Protein S100-A14

Chain A:



- Molecule 1: Protein S100-A14

Chain B:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics, molecular dynamics.*

Of the 500 calculated structures, 30 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	2.1
Amber	refinement	11
CYANA	refinement	2.1

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	1077
Number of shifts mapped to atoms	1077
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	41%

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.69±0.01	0±0/603 (0.0± 0.0%)	1.11±0.03	3±1/815 (0.3± 0.1%)
1	B	0.69±0.01	0±0/597 (0.0± 0.0%)	1.12±0.03	3±1/807 (0.4± 0.1%)
All	All	0.69	0/36000 (0.0%)	1.12	172/48660 (0.4%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.2±0.4
1	B	0.0±0.0	0.2±0.5
All	All	0	13

There are no bond-length outliers.

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	B	124	ARG	NE-CZ-NH1	9.23	124.92	120.30	29	26
1	A	82	ARG	NE-CZ-NH1	9.17	124.89	120.30	21	28
1	A	20	ARG	NE-CZ-NH1	8.75	124.67	120.30	26	27
1	B	186	ARG	NE-CZ-NH1	8.72	124.66	120.30	8	25
1	B	151	ARG	NE-CZ-NH1	8.33	124.46	120.30	5	25
1	A	47	ARG	NE-CZ-NH1	7.69	124.15	120.30	19	20
1	B	186	ARG	NE-CZ-NH2	-7.68	116.46	120.30	11	5
1	A	82	ARG	NE-CZ-NH2	-6.36	117.12	120.30	1	3
1	A	20	ARG	NE-CZ-NH2	-5.93	117.33	120.30	1	2
1	B	151	ARG	NE-CZ-NH2	-5.49	117.55	120.30	24	1
1	B	129	LEU	CB-CG-CD2	5.29	119.99	111.00	8	5
1	A	23	GLU	N-CA-CB	-5.27	101.11	110.60	16	1
1	A	25	LEU	CB-CG-CD2	5.17	119.79	111.00	5	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	15	PHE	CB-CG-CD2	-5.08	117.24	120.80	6	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	A	20	ARG	Sidechain	2
1	A	47	ARG	Sidechain	2
1	B	200	LYS	Peptide	2
1	A	82	ARG	Sidechain	2
1	B	186	ARG	Sidechain	1
1	B	151	ARG	Sidechain	1
1	B	183	LEU	Peptide	1
1	B	145	LEU	Peptide	1
1	A	40	THR	Peptide	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	591	590	590	1±1
1	B	585	585	585	0±1
All	All	35280	35250	35250	23

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:168:LEU:H	1:B:168:LEU:HD12	0.52	1.63	27	2
1:B:183:LEU:H	1:B:183:LEU:HD13	0.47	1.70	20	1
1:A:25:LEU:CD1	1:A:88:ILE:HD13	0.45	2.41	7	7
1:B:129:LEU:CD1	1:B:192:ILE:HD13	0.45	2.42	13	2
1:A:85:TRP:CZ2	1:B:189:TRP:CZ2	0.44	3.05	22	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:PHE:CZ	1:B:200:LYS:HE2	0.44	2.48	6	1
1:B:188:PHE:CE2	1:B:192:ILE:HD11	0.43	2.48	5	1
1:A:29:PHE:CE2	1:A:41:LEU:HB2	0.43	2.49	8	1
1:A:96:LYS:HE2	1:B:185:PHE:CE1	0.43	2.48	3	1
1:A:27:LYS:HE2	1:A:30:HIS:CE1	0.42	2.49	4	1
1:A:25:LEU:HD12	1:A:88:ILE:HD13	0.41	1.91	22	1
1:A:64:LEU:H	1:A:64:LEU:HD12	0.41	1.76	26	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	73/104 (70%)	69±2 (95±2%)	4±2 (5±2%)	0±0 (0±1%)	38	78
1	B	72/104 (69%)	69±1 (95±2%)	3±1 (4±2%)	0±1 (0±1%)	38	78
All	All	4350/6240 (70%)	4132 (95%)	200 (5%)	18 (0%)	38	78

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	38	LYS	8
1	B	142	LYS	6
1	B	140	GLY	1
1	A	33	SER	1
1	B	118	GLU	1
1	B	137	SER	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	66/90 (73%)	59±2 (90±2%)	7±2 (10±2%)	11 56
1	B	65/90 (72%)	59±2 (90±3%)	6±2 (10±3%)	11 57
All	All	3930/5400 (73%)	3541 (90%)	389 (10%)	11 57

All 65 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	49	LEU	29
1	B	129	LEU	29
1	B	153	LEU	28
1	A	25	LEU	24
1	A	41	LEU	23
1	B	145	LEU	22
1	A	87	LEU	18
1	A	57	LEU	17
1	B	191	LEU	15
1	B	161	LEU	13
1	B	175	LEU	9
1	A	42	THR	8
1	A	71	LEU	8
1	B	168	LEU	7
1	B	150	LEU	6
1	A	64	LEU	6
1	B	130	ILE	6
1	B	186	ARG	6
1	A	82	ARG	5
1	B	162	MET	5
1	A	46	LEU	5
1	A	96	LYS	5
1	B	146	THR	5
1	A	80	GLU	5
1	A	79	LEU	5
1	B	124	ARG	5
1	B	200	LYS	4
1	A	39	GLU	4
1	B	143	GLU	4
1	B	183	LEU	4
1	B	149	GLU	4
1	A	20	ARG	4
1	A	23	GLU	3
1	A	53	GLN	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	58	MET	3
1	B	121	ASP	3
1	B	170	GLU	3
1	B	185	PHE	2
1	A	26	ILE	2
1	A	28	ASN	2
1	A	40	THR	2
1	A	44	SER	2
1	B	118	GLU	2
1	A	31	GLN	2
1	A	48	ASP	2
1	A	66	GLU	1
1	B	147	PRO	1
1	B	169	GLU	1
1	A	17	ASP	1
1	A	47	ARG	1
1	A	94	SER	1
1	B	127	GLU	1
1	A	43	PRO	1
1	A	27	LYS	1
1	A	93	LYS	1
1	B	184	GLU	1
1	B	157	GLN	1
1	A	34	VAL	1
1	A	51	THR	1
1	B	148	SER	1
1	A	22	ILE	1
1	B	131	LYS	1
1	B	144	THR	1
1	B	137	SER	1
1	A	15	PHE	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 41% for the well-defined parts and 39% 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	1077
Number of shifts mapped to atoms	1077
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
$^{13}C_{\alpha}$	100	-0.28 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	94	0.56 ± 0.09	Should be checked
$^{13}C'$	99	-0.17 ± 0.14	None needed (< 0.5 ppm)
^{15}N	96	0.41 ± 0.25	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 41%, i.e. 840 atoms were assigned a chemical shift out of a possible 2044. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	357/719 (50%)	142/290 (49%)	145/290 (50%)	70/139 (50%)
Sidechain	469/1175 (40%)	295/762 (39%)	170/375 (45%)	4/38 (11%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Aromatic	14/150 (9%)	14/76 (18%)	0/68 (0%)	0/6 (0%)
Overall	840/2044 (41%)	451/1128 (40%)	315/733 (43%)	74/183 (40%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 39%, i.e. 1077 atoms were assigned a chemical shift out of a possible 2790. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	487/1038 (47%)	192/422 (45%)	199/416 (48%)	96/200 (48%)
Sidechain	574/1588 (36%)	350/1022 (34%)	218/498 (44%)	6/68 (9%)
Aromatic	16/164 (10%)	16/84 (19%)	0/72 (0%)	0/8 (0%)
Overall	1077/2790 (39%)	558/1528 (37%)	417/986 (42%)	102/276 (37%)

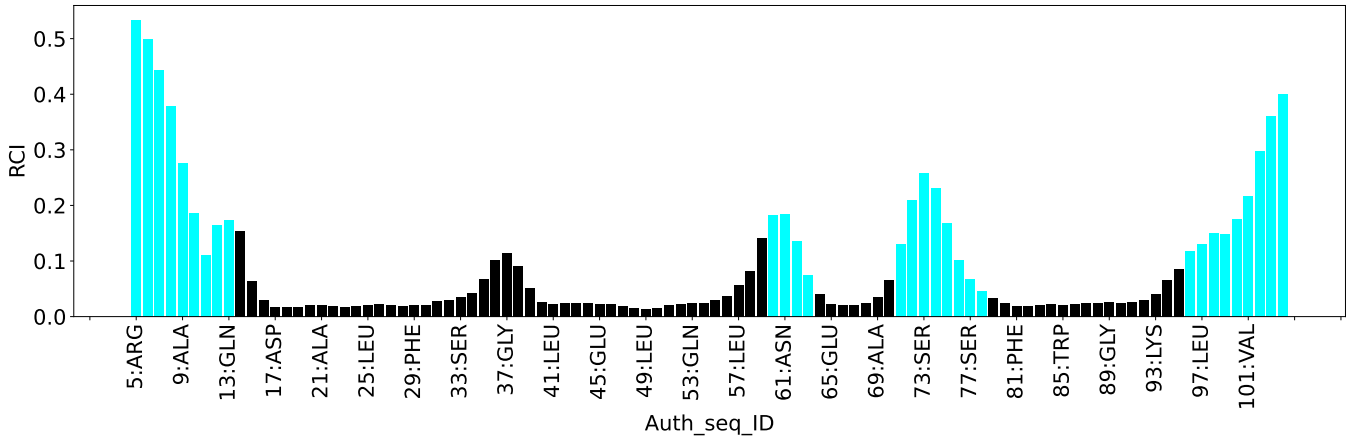
7.1.4 Statistically unusual chemical shifts (i)

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 A:



8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1590
Intra-residue (|i-j|=0)	575
Sequential (|i-j|=1)	394
Medium range (|i-j|>1 and |i-j|<5)	276
Long range (|i-j|≥5)	227
Inter-chain	118
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	7.6
Number of long range restraints per residue[1]	1.1

[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)	2.7	0.2
0.2-0.5 (Medium)	0.2	0.49
>0.5 (Large)	0.9	2.78

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

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

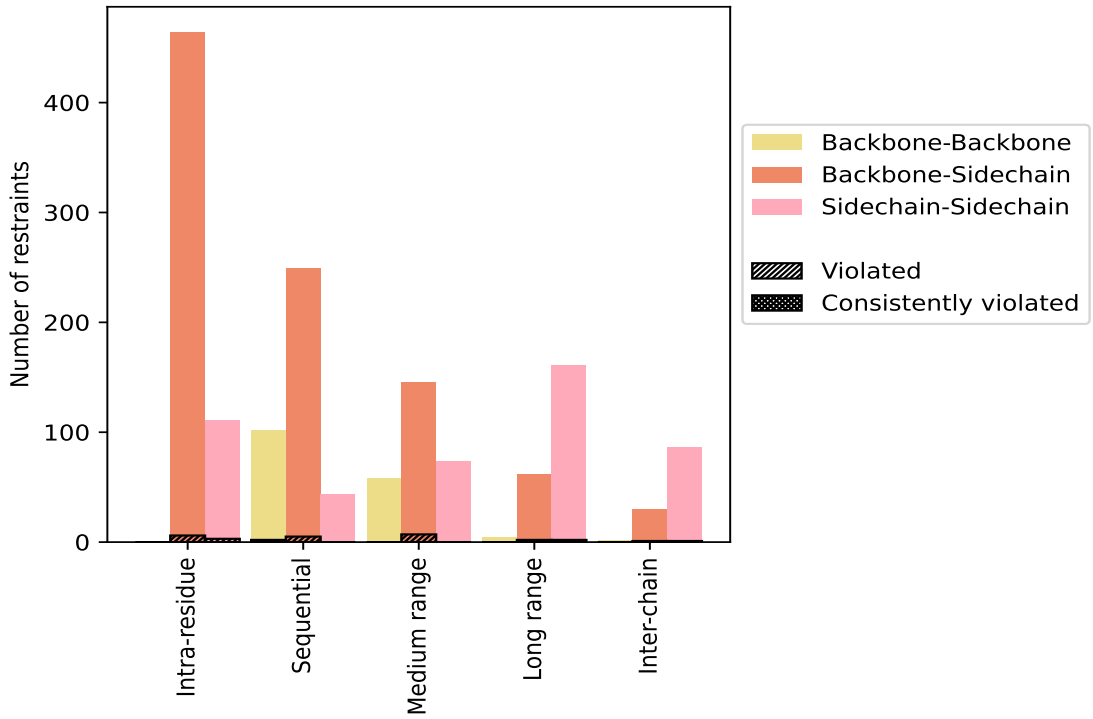
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	575	36.2	9	1.6	0.6	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	464	29.2	6	1.3	0.4	0	0.0	0.0
Sidechain-Sidechain	111	7.0	3	2.7	0.2	0	0.0	0.0
Sequential (|i-j|=1)	394	24.8	7	1.8	0.4	0	0.0	0.0
Backbone-Backbone	102	6.4	2	2.0	0.1	0	0.0	0.0
Backbone-Sidechain	249	15.7	5	2.0	0.3	0	0.0	0.0
Sidechain-Sidechain	43	2.7	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	276	17.4	7	2.5	0.4	0	0.0	0.0
Backbone-Backbone	58	3.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	145	9.1	7	4.8	0.4	0	0.0	0.0
Sidechain-Sidechain	73	4.6	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	227	14.3	4	1.8	0.3	0	0.0	0.0
Backbone-Backbone	4	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	62	3.9	2	3.2	0.1	0	0.0	0.0
Sidechain-Sidechain	161	10.1	2	1.2	0.1	0	0.0	0.0
Inter-chain	118	7.4	2	1.7	0.1	0	0.0	0.0
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	30	1.9	1	3.3	0.1	0	0.0	0.0
Sidechain-Sidechain	86	5.4	1	1.2	0.1	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1590	100.0	29	1.8	1.8	0	0.0	0.0
Backbone-Backbone	166	10.4	2	1.2	0.1	0	0.0	0.0
Backbone-Sidechain	950	59.7	21	2.2	1.3	0	0.0	0.0
Sidechain-Sidechain	474	29.8	6	1.3	0.4	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	1	1	3	0	0	5	0.64	1.51	0.65	0.11
2	1	0	3	0	1	5	0.37	1.1	0.38	0.17
3	1	2	0	0	0	3	0.11	0.11	0.0	0.11
4	0	0	3	0	0	3	0.31	0.63	0.23	0.16
5	0	0	2	1	0	3	0.5	0.79	0.27	0.58
6	0	0	2	0	0	2	0.28	0.45	0.17	0.28
7	1	1	1	0	0	3	0.11	0.12	0.0	0.11
8	1	0	3	0	0	4	0.44	0.87	0.33	0.4
9	0	2	0	0	0	2	0.11	0.11	0.0	0.11
10	1	0	1	0	0	2	0.12	0.14	0.02	0.12
11	0	0	0	0	0	0	0.0	0.0	0.0	0.0

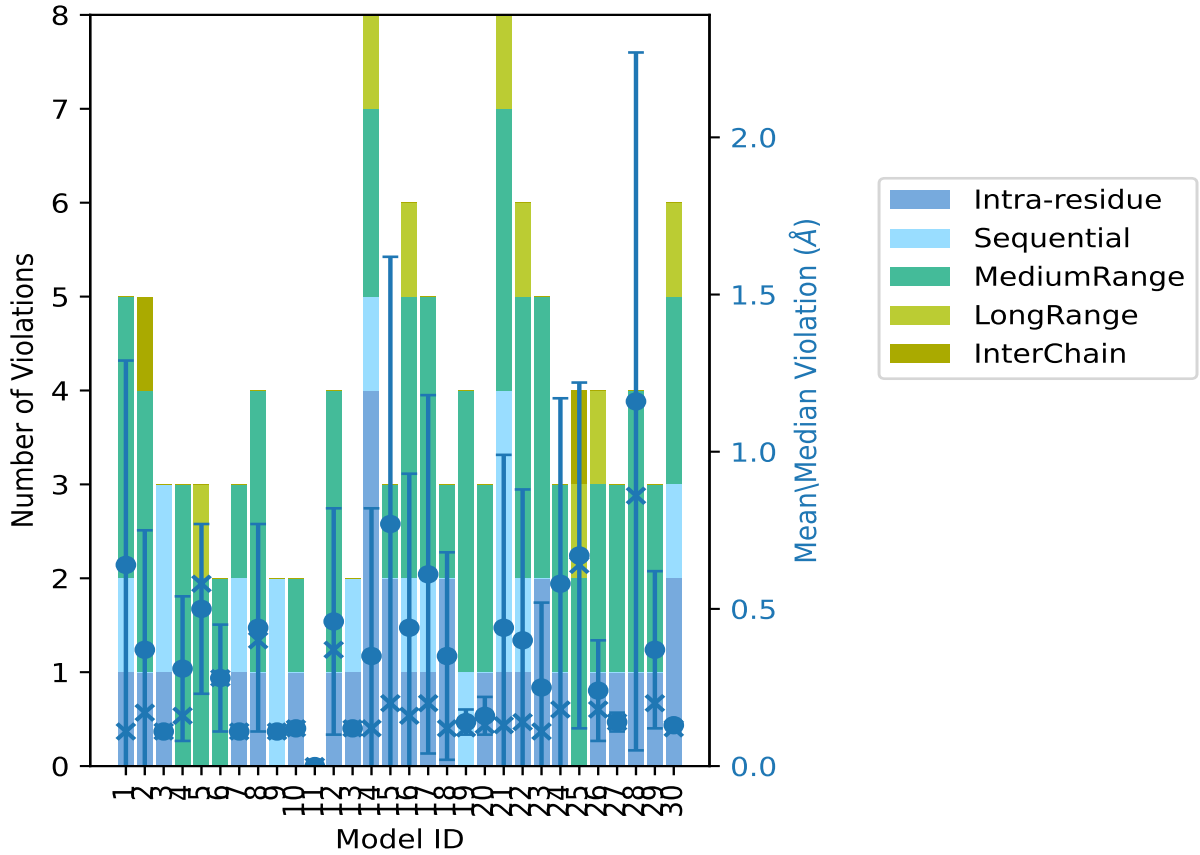
Continued on next page...

Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	0	3	0	0	4	0.46	0.99	0.36	0.37
13	1	1	0	0	0	2	0.12	0.13	0.01	0.12
14	4	1	2	1	0	8	0.35	1.54	0.47	0.12
15	2	0	1	0	0	3	0.77	1.97	0.85	0.2
16	1	1	3	1	0	6	0.44	1.45	0.49	0.16
17	1	1	3	0	0	5	0.61	1.32	0.57	0.2
18	2	0	1	0	0	3	0.35	0.81	0.33	0.12
19	0	1	3	0	0	4	0.14	0.22	0.04	0.12
20	1	0	2	0	0	3	0.16	0.25	0.06	0.13
21	1	3	3	1	0	8	0.44	1.45	0.55	0.13
22	1	1	3	1	0	6	0.4	1.43	0.48	0.14
23	2	0	3	0	0	5	0.25	0.8	0.27	0.11
24	1	0	2	0	0	3	0.58	1.42	0.59	0.18
25	0	0	2	1	1	4	0.67	1.3	0.55	0.64
26	1	0	2	1	0	4	0.24	0.49	0.16	0.18
27	1	0	2	0	0	3	0.14	0.18	0.03	0.14
28	1	0	3	0	0	4	1.16	2.78	1.11	0.86
29	1	0	2	0	0	3	0.37	0.73	0.25	0.2
30	2	1	2	1	0	6	0.13	0.15	0.01	0.12

[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, 1561(IR:566, SQ:387, MR:269, LR:223, IC:116) 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]	%
4	2	2	2	2	12	1	3.3
0	2	0	0	0	2	2	6.7
2	2	0	2	0	6	3	10.0
0	1	1	0	0	2	4	13.3
1	0	0	0	0	1	5	16.7
1	0	0	0	0	1	6	20.0

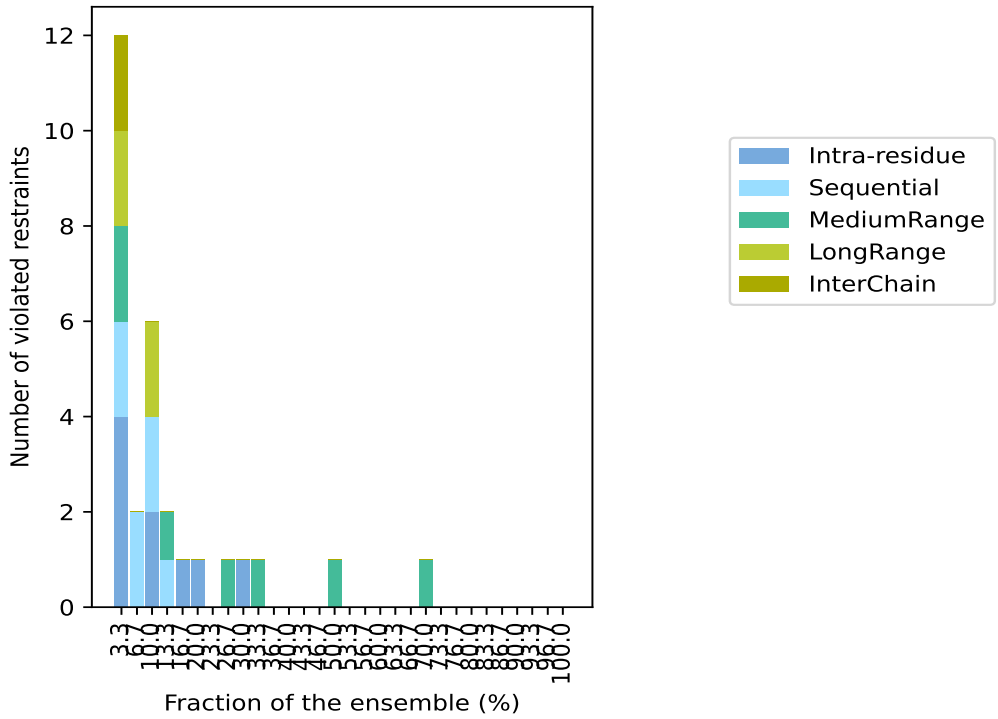
Continued on next page...

Continued from previous page...

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	7	23.3
0	0	1	0	0	1	8	26.7
1	0	0	0	0	1	9	30.0
0	0	1	0	0	1	10	33.3
0	0	0	0	0	0	11	36.7
0	0	0	0	0	0	12	40.0
0	0	0	0	0	0	13	43.3
0	0	0	0	0	0	14	46.7
0	0	1	0	0	1	15	50.0
0	0	0	0	0	0	16	53.3
0	0	0	0	0	0	17	56.7
0	0	0	0	0	0	18	60.0
0	0	0	0	0	0	19	63.3
0	0	0	0	0	0	20	66.7
0	0	1	0	0	1	21	70.0
0	0	0	0	0	0	22	73.3
0	0	0	0	0	0	23	76.7
0	0	0	0	0	0	24	80.0
0	0	0	0	0	0	25	83.3
0	0	0	0	0	0	26	86.7
0	0	0	0	0	0	27	90.0
0	0	0	0	0	0	28	93.3
0	0	0	0	0	0	29	96.7
0	0	0	0	0	0	30	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

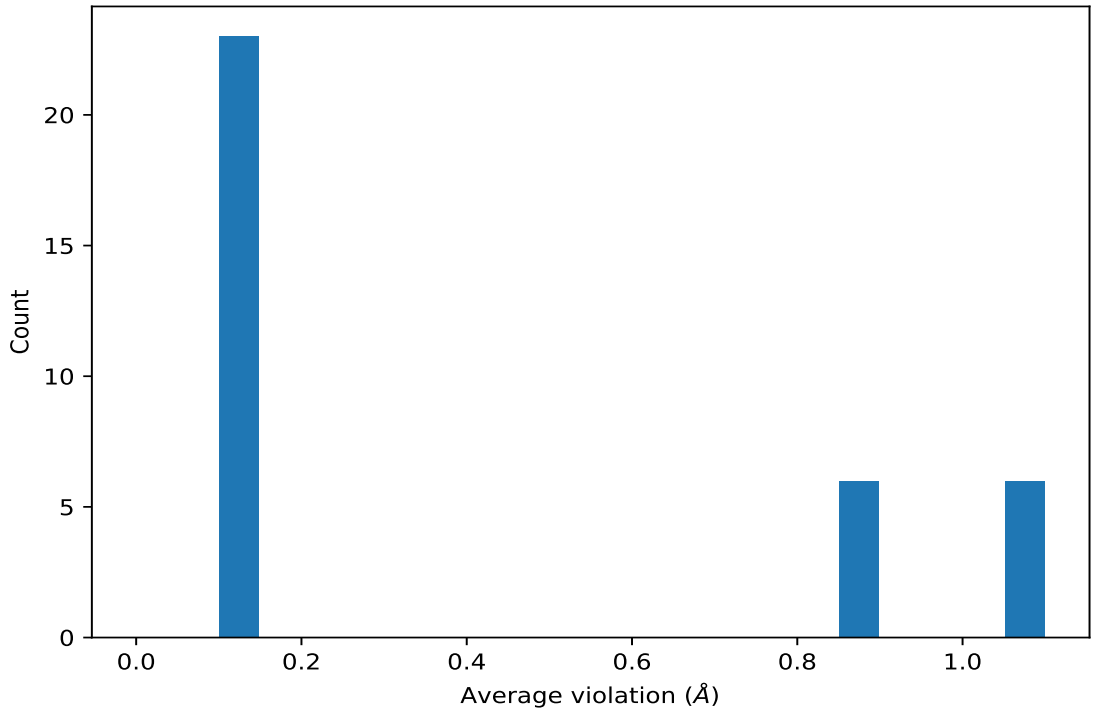
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	21	1.05	0.63	0.99
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	21	1.05	0.63	0.99
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	21	1.05	0.63	0.99
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	21	1.05	0.63	0.99
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	21	1.05	0.63	0.99
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	21	1.05	0.63	0.99
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	15	0.88	0.43	0.8
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	15	0.88	0.43	0.8
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	15	0.88	0.43	0.8
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	15	0.88	0.43	0.8
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	15	0.88	0.43	0.8
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	15	0.88	0.43	0.8
(1,1503)	1:B:132:ASN:HA	1:B:134:HIS:HD2	10	0.15	0.03	0.14
(1,877)	1:B:127:GLU:H	1:B:127:GLU:HG3	9	0.15	0.03	0.14
(1,160)	1:A:28:ASN:HA	1:A:30:HIS:HD2	8	0.15	0.03	0.14
(1,1117)	1:B:171:LYS:HB3	1:B:171:LYS:HE2	6	0.12	0.02	0.12

Continued on next page...

Continued from previous page...

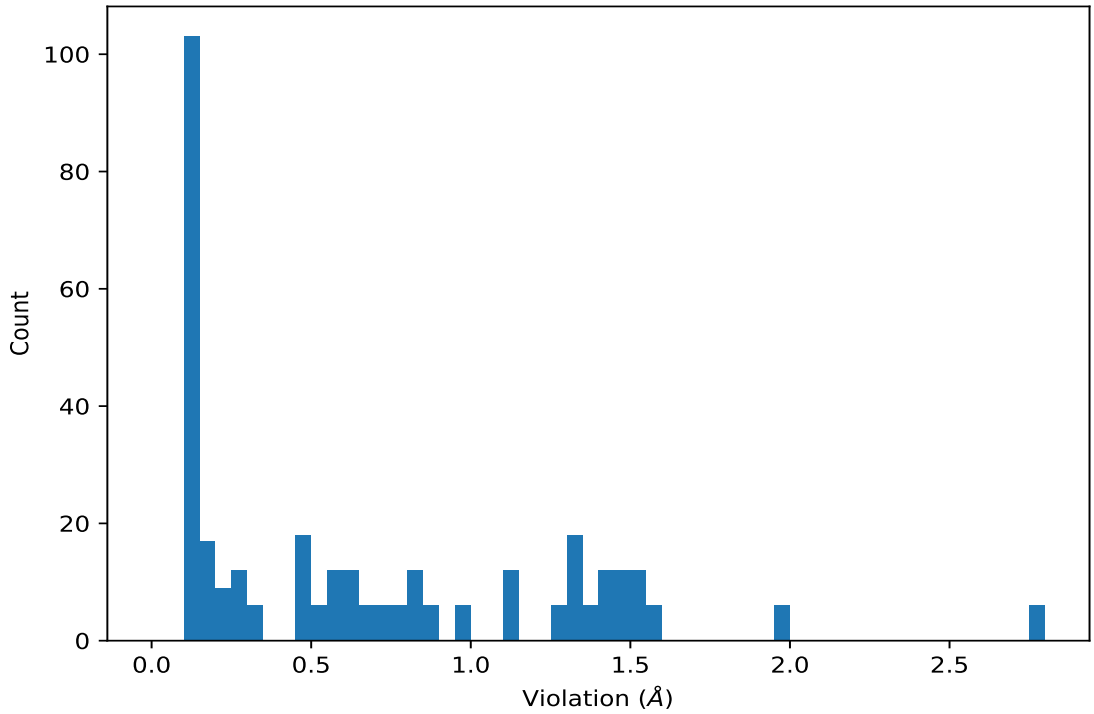
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1117)	1:B:171:LYS:HB3	1:B:171:LYS:HE3	6	0.12	0.02	0.12
(1,430)	1:A:67:LYS:HB3	1:A:67:LYS:HE2	5	0.12	0.01	0.11
(1,430)	1:A:67:LYS:HB3	1:A:67:LYS:HE3	5	0.12	0.01	0.11
(1,896)	1:B:127:GLU:HG3	1:B:128:THR:H	4	0.12	0.01	0.12
(1,1221)	1:B:126:ILE:H	1:B:129:LEU:HD21	4	0.11	0.0	0.11
(1,1221)	1:B:126:ILE:H	1:B:129:LEU:HD22	4	0.11	0.0	0.11
(1,1221)	1:B:126:ILE:H	1:B:129:LEU:HD23	4	0.11	0.0	0.11
(1,1558)	1:B:145:LEU:HG	1:B:188:PHE:HA	3	0.13	0.02	0.14
(1,539)	1:A:41:LEU:HG	1:A:84:PHE:HA	3	0.12	0.01	0.12
(1,1407)	1:B:201:LEU:HA	1:B:201:LEU:HD11	3	0.12	0.0	0.12
(1,1407)	1:B:201:LEU:HA	1:B:201:LEU:HD12	3	0.12	0.0	0.12
(1,1407)	1:B:201:LEU:HA	1:B:201:LEU:HD13	3	0.12	0.0	0.12
(1,98)	1:A:23:GLU:HG3	1:A:24:THR:H	3	0.12	0.01	0.12
(1,997)	1:B:114:GLU:HA	1:B:115:ASP:H	3	0.11	0.0	0.11
(1,1465)	1:B:129:LEU:HA	1:B:129:LEU:HD21	3	0.11	0.0	0.11
(1,1465)	1:B:129:LEU:HA	1:B:129:LEU:HD22	3	0.11	0.0	0.11
(1,1465)	1:B:129:LEU:HA	1:B:129:LEU:HD23	3	0.11	0.0	0.11
(1,11)	1:A:10:GLU:HA	1:A:11:ASP:H	2	0.11	0.0	0.11
(1,1184)	1:B:153:LEU:HB2	1:B:154:VAL:HA	2	0.11	0.0	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	28	2.78
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	28	2.78
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	28	2.78
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	28	2.78
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	28	2.78
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	28	2.78
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	15	1.97
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	15	1.97
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	15	1.97
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	15	1.97
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	15	1.97
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	15	1.97
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	28	1.59
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	28	1.59
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	28	1.59
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	28	1.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	28	1.59
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	28	1.59
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	14	1.54
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	14	1.54
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	14	1.54
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	14	1.54
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	14	1.54
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	14	1.54
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	1	1.51
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	1	1.51
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	1	1.51
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	1	1.51
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	1	1.51
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	1	1.51
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	21	1.45
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	21	1.45
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	21	1.45
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	21	1.45
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	21	1.45
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	21	1.45
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	16	1.45
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	16	1.45
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	16	1.45
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	16	1.45
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	16	1.45
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	16	1.45
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	22	1.43
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	22	1.43
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	22	1.43
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	22	1.43
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	22	1.43
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	22	1.43
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	24	1.42
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	24	1.42
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	24	1.42
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	24	1.42
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	24	1.42
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	24	1.42
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	21	1.36
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	21	1.36
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	21	1.36
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	21	1.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	21	1.36
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	21	1.36
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	1	1.34
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	1	1.34
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	1	1.34
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	1	1.34
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	1	1.34
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	1	1.34
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	17	1.32
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	17	1.32
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	17	1.32
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	17	1.32
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	17	1.32
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	17	1.32
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	25	1.3
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	25	1.3
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	25	1.3
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	25	1.3
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	25	1.3
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	25	1.3
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	17	1.28
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	17	1.28
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	17	1.28
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	17	1.28
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	17	1.28
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	17	1.28
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	25	1.13
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	25	1.13
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	25	1.13
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	25	1.13
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	25	1.13
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	25	1.13
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	2	1.1
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	2	1.1
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	2	1.1
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	2	1.1
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	2	1.1
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	2	1.1
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	12	0.99
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	12	0.99
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	12	0.99
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	12	0.99

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	12	0.99
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	12	0.99
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	8	0.87
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	8	0.87
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	8	0.87
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	8	0.87
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	8	0.87
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	8	0.87
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	18	0.81
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	18	0.81
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	18	0.81
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	18	0.81
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	18	0.81
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	18	0.81
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	23	0.8
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	23	0.8
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	23	0.8
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	23	0.8
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	23	0.8
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	23	0.8
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	5	0.79
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	5	0.79
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	5	0.79
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	5	0.79
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	5	0.79
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	5	0.79
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	29	0.73
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	29	0.73
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	29	0.73
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	29	0.73
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	29	0.73
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	29	0.73
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	8	0.65
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	8	0.65
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	8	0.65
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	8	0.65
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	8	0.65
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	8	0.65
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	16	0.63
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	16	0.63
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	16	0.63
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	16	0.63

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	16	0.63
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	16	0.63
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	4	0.63
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	4	0.63
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	4	0.63
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	4	0.63
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	4	0.63
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	4	0.63
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	5	0.58
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	5	0.58
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	5	0.58
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	5	0.58
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	5	0.58
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	5	0.58
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	12	0.58
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	12	0.58
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	12	0.58
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	12	0.58
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	12	0.58
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	12	0.58
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	14	0.51
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	14	0.51
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	14	0.51
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	14	0.51
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	14	0.51
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	14	0.51
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	26	0.49
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	26	0.49
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	26	0.49
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	26	0.49
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	26	0.49
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	26	0.49
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	22	0.47
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	22	0.47
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	22	0.47
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	22	0.47
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	22	0.47
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	22	0.47
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	6	0.45
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	6	0.45
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	6	0.45
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	6	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	6	0.45
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	6	0.45
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	2	0.33
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	2	0.33
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	2	0.33
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	2	0.33
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	2	0.33
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	2	0.33
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	26	0.26
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	26	0.26
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	26	0.26
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	26	0.26
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	26	0.26
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	26	0.26
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	20	0.25
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	20	0.25
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	20	0.25
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	20	0.25
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	20	0.25
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	20	0.25
(1,1122)	1:B:205:VAL:HG11	1:B:208:HIS:HA	19	0.22
(1,1122)	1:B:205:VAL:HG12	1:B:208:HIS:HA	19	0.22
(1,1122)	1:B:205:VAL:HG13	1:B:208:HIS:HA	19	0.22
(1,1122)	1:B:205:VAL:HG21	1:B:208:HIS:HA	19	0.22
(1,1122)	1:B:205:VAL:HG22	1:B:208:HIS:HA	19	0.22
(1,1122)	1:B:205:VAL:HG23	1:B:208:HIS:HA	19	0.22
(1,877)	1:B:127:GLU:H	1:B:127:GLU:HG3	15	0.2
(1,160)	1:A:28:ASN:HA	1:A:30:HIS:HD2	17	0.2
(1,1503)	1:B:132:ASN:HA	1:B:134:HIS:HD2	29	0.2
(1,877)	1:B:127:GLU:H	1:B:127:GLU:HG3	29	0.18
(1,160)	1:A:28:ASN:HA	1:A:30:HIS:HD2	27	0.18
(1,1503)	1:B:132:ASN:HA	1:B:134:HIS:HD2	24	0.18
(1,160)	1:A:28:ASN:HA	1:A:30:HIS:HD2	2	0.17
(1,1503)	1:B:132:ASN:HA	1:B:134:HIS:HD2	16	0.17
(1,877)	1:B:127:GLU:H	1:B:127:GLU:HG3	14	0.16
(1,685)	1:A:101:VAL:HG11	1:A:104:HIS:HA	4	0.16
(1,685)	1:A:101:VAL:HG12	1:A:104:HIS:HA	4	0.16
(1,685)	1:A:101:VAL:HG13	1:A:104:HIS:HA	4	0.16
(1,685)	1:A:101:VAL:HG21	1:A:104:HIS:HA	4	0.16
(1,685)	1:A:101:VAL:HG22	1:A:104:HIS:HA	4	0.16
(1,685)	1:A:101:VAL:HG23	1:A:104:HIS:HA	4	0.16
(1,1503)	1:B:132:ASN:HA	1:B:134:HIS:HD2	12	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,877)	1:B:127:GLU:H	1:B:127:GLU:HG3	24	0.15
(1,1558)	1:B:145:LEU:HG	1:B:188:PHE:HA	30	0.15
(1,1117)	1:B:171:LYS:HB3	1:B:171:LYS:HE2	15	0.15
(1,1117)	1:B:171:LYS:HB3	1:B:171:LYS:HE3	15	0.15
(1,877)	1:B:127:GLU:H	1:B:127:GLU:HG3	10	0.14
(1,877)	1:B:127:GLU:H	1:B:127:GLU:HG3	30	0.14
(1,583)	1:A:25:LEU:HD11	1:A:88:ILE:HG12	25	0.14
(1,583)	1:A:25:LEU:HD12	1:A:88:ILE:HG12	25	0.14
(1,583)	1:A:25:LEU:HD13	1:A:88:ILE:HG12	25	0.14
(1,539)	1:A:41:LEU:HG	1:A:84:PHE:HA	21	0.14
(1,430)	1:A:67:LYS:HB3	1:A:67:LYS:HE2	16	0.14
(1,430)	1:A:67:LYS:HB3	1:A:67:LYS:HE3	16	0.14
(1,160)	1:A:28:ASN:HA	1:A:30:HIS:HD2	8	0.14
(1,1558)	1:B:145:LEU:HG	1:B:188:PHE:HA	5	0.14
(1,1503)	1:B:132:ASN:HA	1:B:134:HIS:HD2	22	0.14
(1,1503)	1:B:132:ASN:HA	1:B:134:HIS:HD2	27	0.14
(1,1117)	1:B:171:LYS:HB3	1:B:171:LYS:HE2	28	0.14
(1,1117)	1:B:171:LYS:HB3	1:B:171:LYS:HE3	28	0.14
(1,98)	1:A:23:GLU:HG3	1:A:24:THR:H	21	0.13
(1,896)	1:B:127:GLU:HG3	1:B:128:THR:H	19	0.13
(1,896)	1:B:127:GLU:HG3	1:B:128:THR:H	21	0.13
(1,160)	1:A:28:ASN:HA	1:A:30:HIS:HD2	20	0.13
(1,160)	1:A:28:ASN:HA	1:A:30:HIS:HD2	23	0.13
(1,1503)	1:B:132:ASN:HA	1:B:134:HIS:HD2	4	0.13
(1,1407)	1:B:201:LEU:HA	1:B:201:LEU:HD11	13	0.13
(1,1407)	1:B:201:LEU:HA	1:B:201:LEU:HD12	13	0.13
(1,1407)	1:B:201:LEU:HA	1:B:201:LEU:HD13	13	0.13
(1,1249)	1:B:144:THR:HB	1:B:183:LEU:HG	22	0.13
(1,1068)	1:B:124:ARG:H	1:B:124:ARG:HG2	30	0.13
(1,997)	1:B:114:GLU:HA	1:B:115:ASP:H	16	0.12
(1,98)	1:A:23:GLU:HG3	1:A:24:THR:H	17	0.12
(1,896)	1:B:127:GLU:HG3	1:B:128:THR:H	30	0.12
(1,877)	1:B:127:GLU:H	1:B:127:GLU:HG3	22	0.12
(1,676)	1:A:99:ARG:HB3	1:A:99:ARG:HD2	7	0.12
(1,539)	1:A:41:LEU:HG	1:A:84:PHE:HA	14	0.12
(1,430)	1:A:67:LYS:HB3	1:A:67:LYS:HE2	21	0.12
(1,430)	1:A:67:LYS:HB3	1:A:67:LYS:HE3	21	0.12
(1,160)	1:A:28:ASN:HA	1:A:30:HIS:HD2	19	0.12
(1,160)	1:A:28:ASN:HA	1:A:30:HIS:HD2	21	0.12
(1,1503)	1:B:132:ASN:HA	1:B:134:HIS:HD2	30	0.12
(1,1407)	1:B:201:LEU:HA	1:B:201:LEU:HD11	2	0.12
(1,1407)	1:B:201:LEU:HA	1:B:201:LEU:HD12	2	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1407)	1:B:201:LEU:HA	1:B:201:LEU:HD13	2	0.12
(1,1407)	1:B:201:LEU:HA	1:B:201:LEU:HD11	18	0.12
(1,1407)	1:B:201:LEU:HA	1:B:201:LEU:HD12	18	0.12
(1,1407)	1:B:201:LEU:HA	1:B:201:LEU:HD13	18	0.12
(1,1221)	1:B:126:ILE:H	1:B:129:LEU:HD21	30	0.12
(1,1221)	1:B:126:ILE:H	1:B:129:LEU:HD22	30	0.12
(1,1221)	1:B:126:ILE:H	1:B:129:LEU:HD23	30	0.12
(1,1117)	1:B:171:LYS:HB3	1:B:171:LYS:HE2	14	0.12
(1,1117)	1:B:171:LYS:HB3	1:B:171:LYS:HE3	14	0.12
(1,997)	1:B:114:GLU:HA	1:B:115:ASP:H	13	0.11
(1,997)	1:B:114:GLU:HA	1:B:115:ASP:H	22	0.11
(1,98)	1:A:23:GLU:HG3	1:A:24:THR:H	3	0.11
(1,896)	1:B:127:GLU:HG3	1:B:128:THR:H	9	0.11
(1,877)	1:B:127:GLU:H	1:B:127:GLU:HG3	17	0.11
(1,877)	1:B:127:GLU:H	1:B:127:GLU:HG3	20	0.11
(1,782)	1:B:200:LYS:HA	1:A:30:HIS:HD2	2	0.11
(1,707)	1:A:88:ILE:HD11	1:B:126:ILE:HB	25	0.11
(1,707)	1:A:88:ILE:HD12	1:B:126:ILE:HB	25	0.11
(1,707)	1:A:88:ILE:HD13	1:B:126:ILE:HB	25	0.11
(1,539)	1:A:41:LEU:HG	1:A:84:PHE:HA	16	0.11
(1,530)	1:A:82:ARG:HA	1:A:82:ARG:HD3	14	0.11
(1,430)	1:A:67:LYS:HB3	1:A:67:LYS:HE2	1	0.11
(1,430)	1:A:67:LYS:HB3	1:A:67:LYS:HE3	1	0.11
(1,430)	1:A:67:LYS:HB3	1:A:67:LYS:HE2	12	0.11
(1,430)	1:A:67:LYS:HB3	1:A:67:LYS:HE3	12	0.11
(1,430)	1:A:67:LYS:HB3	1:A:67:LYS:HE2	23	0.11
(1,430)	1:A:67:LYS:HB3	1:A:67:LYS:HE3	23	0.11
(1,1558)	1:B:145:LEU:HG	1:B:188:PHE:HA	26	0.11
(1,1529)	1:B:119:PHE:HB2	1:B:123:GLU:HA	10	0.11
(1,1503)	1:B:132:ASN:HA	1:B:134:HIS:HD2	1	0.11
(1,1503)	1:B:132:ASN:HA	1:B:134:HIS:HD2	19	0.11
(1,1465)	1:B:129:LEU:HA	1:B:129:LEU:HD21	3	0.11
(1,1465)	1:B:129:LEU:HA	1:B:129:LEU:HD22	3	0.11
(1,1465)	1:B:129:LEU:HA	1:B:129:LEU:HD23	3	0.11
(1,1465)	1:B:129:LEU:HA	1:B:129:LEU:HD21	14	0.11
(1,1465)	1:B:129:LEU:HA	1:B:129:LEU:HD22	14	0.11
(1,1465)	1:B:129:LEU:HA	1:B:129:LEU:HD23	14	0.11
(1,1465)	1:B:129:LEU:HA	1:B:129:LEU:HD21	18	0.11
(1,1465)	1:B:129:LEU:HA	1:B:129:LEU:HD22	18	0.11
(1,1465)	1:B:129:LEU:HA	1:B:129:LEU:HD23	18	0.11
(1,1254)	1:B:186:ARG:HA	1:B:186:ARG:HD3	27	0.11
(1,1221)	1:B:126:ILE:H	1:B:129:LEU:HD21	6	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1221)	1:B:126:ILE:H	1:B:129:LEU:HD22	6	0.11
(1,1221)	1:B:126:ILE:H	1:B:129:LEU:HD23	6	0.11
(1,1221)	1:B:126:ILE:H	1:B:129:LEU:HD21	7	0.11
(1,1221)	1:B:126:ILE:H	1:B:129:LEU:HD22	7	0.11
(1,1221)	1:B:126:ILE:H	1:B:129:LEU:HD23	7	0.11
(1,1221)	1:B:126:ILE:H	1:B:129:LEU:HD21	28	0.11
(1,1221)	1:B:126:ILE:H	1:B:129:LEU:HD22	28	0.11
(1,1221)	1:B:126:ILE:H	1:B:129:LEU:HD23	28	0.11
(1,1184)	1:B:153:LEU:HB2	1:B:154:VAL:HA	9	0.11
(1,1184)	1:B:153:LEU:HB2	1:B:154:VAL:HA	21	0.11
(1,1117)	1:B:171:LYS:HB3	1:B:171:LYS:HE2	8	0.11
(1,1117)	1:B:171:LYS:HB3	1:B:171:LYS:HE3	8	0.11
(1,1117)	1:B:171:LYS:HB3	1:B:171:LYS:HE2	23	0.11
(1,1117)	1:B:171:LYS:HB3	1:B:171:LYS:HE3	23	0.11
(1,1117)	1:B:171:LYS:HB3	1:B:171:LYS:HE2	26	0.11
(1,1117)	1:B:171:LYS:HB3	1:B:171:LYS:HE3	26	0.11
(1,1101)	1:B:128:THR:H	1:B:129:LEU:HG	14	0.11
(1,11)	1:A:10:GLU:HA	1:A:11:ASP:H	3	0.11
(1,11)	1:A:10:GLU:HA	1:A:11:ASP:H	7	0.11
(1,107)	1:A:24:THR:H	1:A:25:LEU:HG	1	0.11
(1,102)	1:A:22:ILE:H	1:A:25:LEU:HD21	23	0.11
(1,102)	1:A:22:ILE:H	1:A:25:LEU:HD22	23	0.11
(1,102)	1:A:22:ILE:H	1:A:25:LEU:HD23	23	0.11

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value