Full wwPDB NMR Structure Validation Report (i)

Nov 28, 2023 – 04:09 PM EST

PDB ID	:	2LB6
BMRB ID	:	17447
Title	:	Structure of 18694Da MUP, typical to the major urinary protein family: MUP9, MUP11, MUP15, MUP18 & MUP19
Authors	:	Phelan, M.M.; Mclean, L.; Beynon, R.J.; Hurst, J.L.; Lian, L.
Deposited on	:	2011-03-23

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

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

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

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

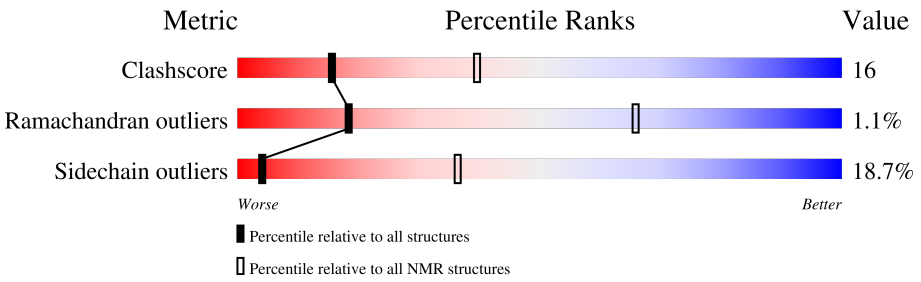
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 87%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	176	45% 33% • • 19%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 20 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:21-A:77, A:85-A:170 (143)	0.39	20

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 5 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2781 atoms, of which 1352 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major urinary protein 6.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	176	2781	885	1352	254	283	7	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MET	-	expression tag	UNP P02762
A	7	GLY	-	expression tag	UNP P02762
A	8	SER	-	expression tag	UNP P02762
A	9	SER	-	expression tag	UNP P02762
A	10	HIS	-	expression tag	UNP P02762
A	11	HIS	-	expression tag	UNP P02762
A	12	HIS	-	expression tag	UNP P02762
A	13	HIS	-	expression tag	UNP P02762
A	14	HIS	-	expression tag	UNP P02762
A	15	HIS	-	expression tag	UNP P02762
A	16	ILE	-	expression tag	UNP P02762
A	17	GLU	-	expression tag	UNP P02762
A	18	GLY	-	expression tag	UNP P02762
A	19	ARG	-	expression tag	UNP P02762

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: Major urinary protein 6

Chain A: 45% 33% • • 19%

M6 G7 S8 S9 H10 H11 H12 H13 H14 H15 I16 E17 G18 R19 E20 E21 A22 F29 N30 V31 I34 W38 H39 T40 I41 I42 L43 A44 S45 D46 K47 R48 E49 K50 I51 E52 R58 L59 F60 L61 E62 Q63 I64 E68 L71 V72 L73 K74 F75 H76 T77 V78 R79 D80

E81 E82 C83 S84 E85 L86 E98 Y103 N107 T108 F109 T110 I111 P112 K113 T114 D115 Y116 F119 L120 M121 A122 H123 L124 I125 F133 Q134 L135 M136 G137 L138 Y139 E142 L145 I149 F153 L163 R164 E165 N166 I167 I168 D169 L170 S171 N172 A173 N174 R175 C176

L177 Q178 A179 R180 E181

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: Major urinary protein 6

Chain A: 44% 34% • • 19%

M6 G7 S8 S9 H10 H11 H12 H13 H14 H15 I16 E17 G18 R19 E20 E21 A22 F29 N30 V31 I34 W38 H39 T40 I41 I42 L43 A44 S45 D46 K47 R48 E49 K50 I51 E52 L59 F60 L61 E62 Q63 I64 H65 N69 S70 L71 V72 L73 K74 F75 H76 T77 V78 R79 D80

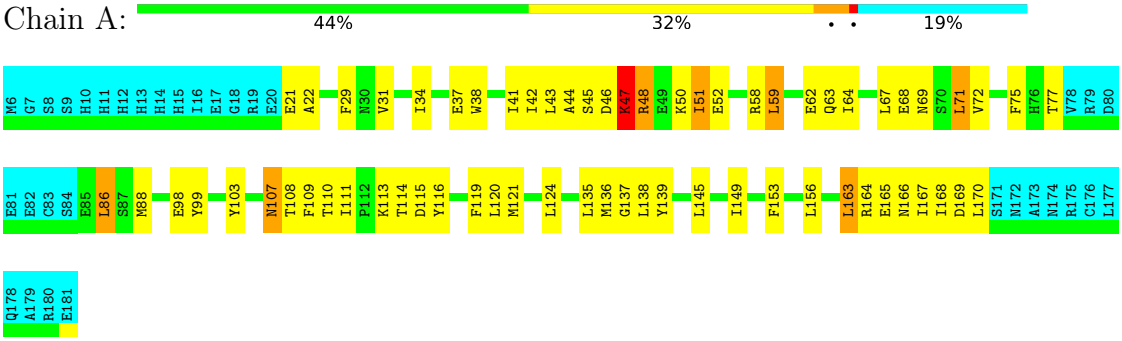
E81 E82 C83 S84 E85 L86 S87 M88 K95 E98 Y103 N107 T108 F109 T110 I111 P112 K113 T114 D115 Y116 F119 L120 M121 A122 H123 L124 I125 K128 F133 Q134 L135 M136 E142 L145 D148 I149 F153 A154 Q155 L156 L163 R164 E165 N166 I167 I168

S171 N172 A173 N174 R175 C176 L177 Q178 A179 R180 E181

4.2.2 Score per residue for model 2

- Molecule 1: Major urinary protein 6

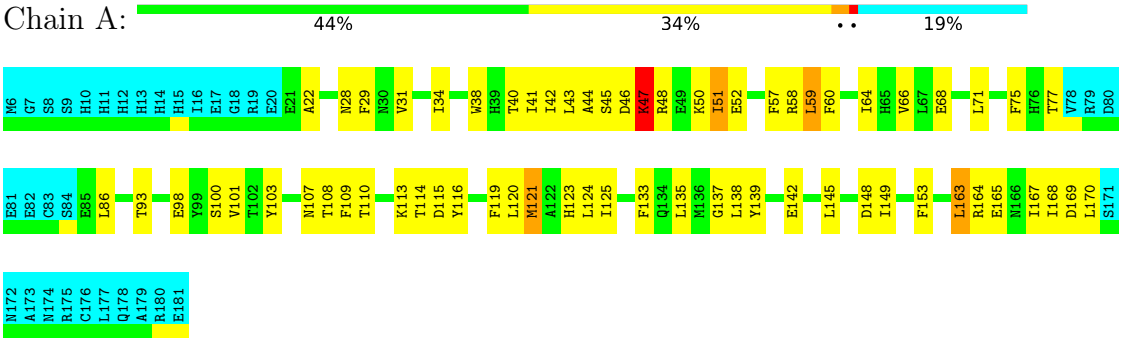
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Major urinary protein 6

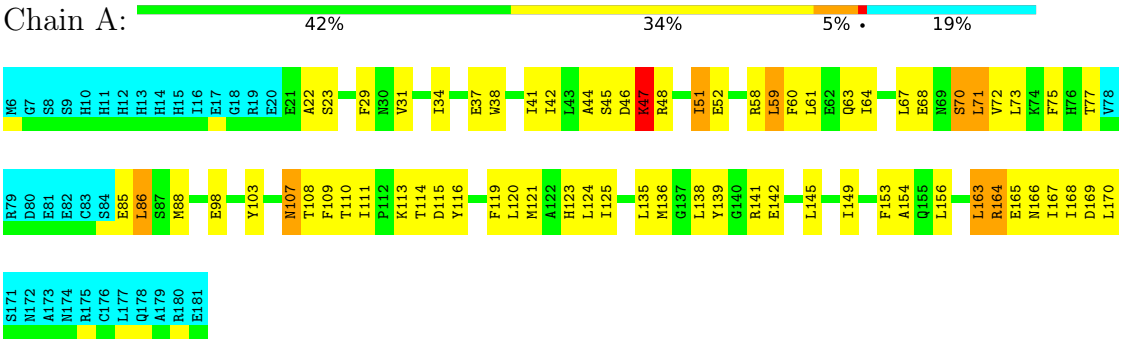
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Major urinary protein 6

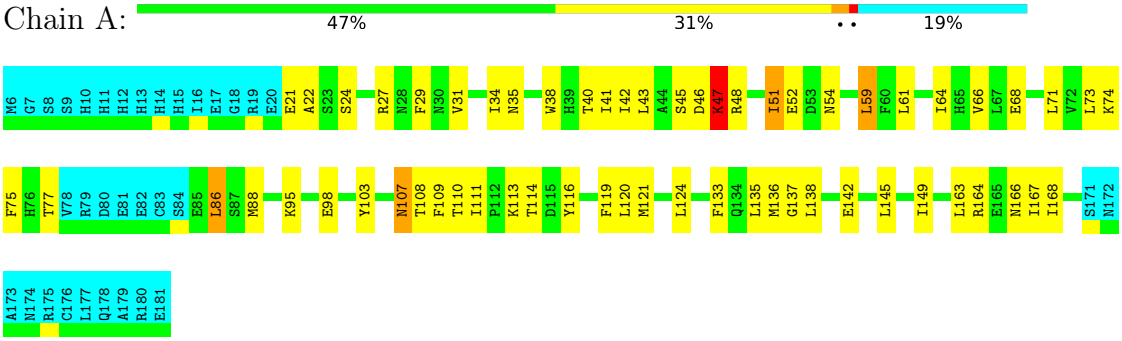
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Major urinary protein 6

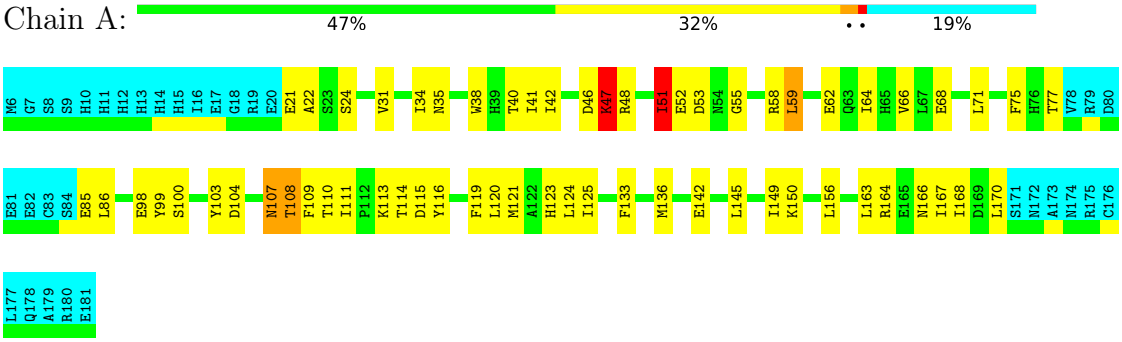
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Major urinary protein 6

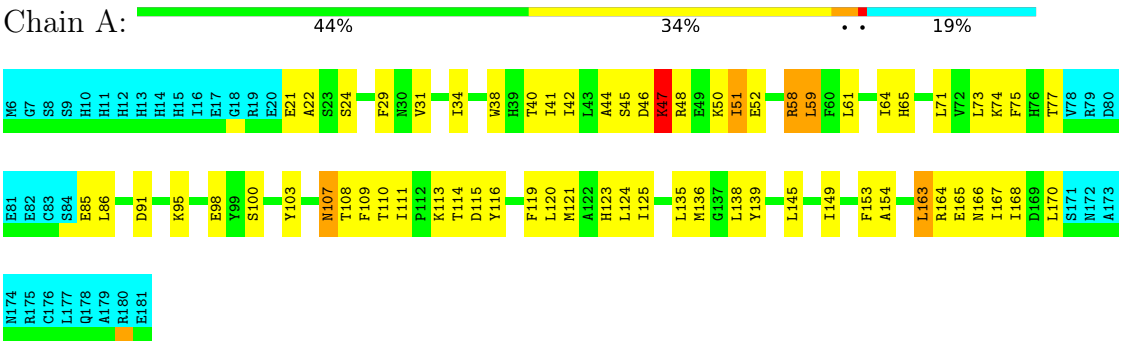
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: Major urinary protein 6

Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: Major urinary protein 6

Chain A: 45% 33% • • 19%

M6 G7 S8 S9 H10 H11 H12 H13 H14 H15 I16 E17 G18 R19 E20 E21 A22 V31 I34 E37 W38 H39 T40 I41 I42 L43 D46 K47 I51 E52 L59 F60 L61 E62 Q63 I64 L67 E68 N69 S70 L71 V72 L73 K74 F75 H76 T77 V78 R79 D80 E81 E82 C83

S84 E85 L86 S87 M88 D91 K95 E98 Y99 S100 Y103 N107 T108 F109 T110 I111 P112 K113 T114 D115 F119 L120 M121 A122 H123 L124 I125 F133 Q134 L135 M136 G137 L138 Y139 E142 L145 I149 F153 L156 L163 R164 E165 N166 I167 I168 S171

N172 A173 N174 R175 C176 L177 Q178 A179 R180 E181

4.2.9 Score per residue for model 9

- Molecule 1: Major urinary protein 6

Chain A: 51% 25% 5% • 19%

M6 G7 S8 S9 H10 H11 H12 H13 H14 H15 I16 E17 G18 R19 E20 E21 A22 V31 I34 W38 I41 I42 S45 D46 K47 K50 I51 E52 L59 I64 E68 L71 V72 L73 K74 F75 H76 T77 V78 R79 D80 E81 E82 C83 S84 E85 L86 E98 Y99

S100 Y103 N107 T108 F109 T110 T114 D115 Y116 F119 L120 L124 F133 Q134 L135 M136 G137 L138 Y139 G140 R141 E142 L145 D148 I149 K150 F153 L163 R164 E165 N166 I167 I168 D169 L170 S171 N172 A173 N174 R175 C176 L177 Q178 A179 R180 E181

4.2.10 Score per residue for model 10

- Molecule 1: Major urinary protein 6

Chain A: 44% 34% • • 19%

M6 G7 S8 S9 H10 H11 H12 H13 H14 H15 I16 E17 G18 R19 E20 E21 A22 F29 N30 V31 I34 E37 W38 I41 I42 L43 A44 S45 D46 K47 R48 E49 K50 I51 E52 R58 L59 F60 L61 E62 Q63 I64 L67 E68 N69 S70 L71 V72 L73 K74 F75 H76 T77 V78

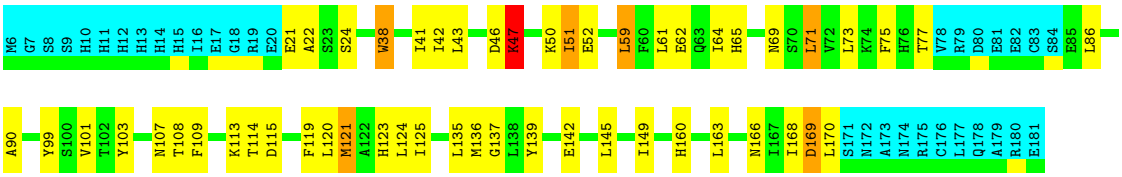
R79 D80 E81 E82 C83 S84 E85 L86 E98 Y99 Y103 N107 T108 F109 T110 K113 T114 D115 Y116 F119 L120 H123 L124 I125 F133 Q134 L135 M136 G137 L138 Y139 E142 P143 D144 L145 S146 S147 D148 I149 L163 R164 E165 N166 I167 I168 D169 L170 S171 N172 A173 N174

R175 C176 L177 Q178 A179 R180 E181

4.2.11 Score per residue for model 11

- Molecule 1: Major urinary protein 6

Chain A: 52% 26% • • 19%



4.2.12 Score per residue for model 12

- Molecule 1: Major urinary protein 6

Chain A: 47% 32% • • 19%

4.2.13 Score per residue for model 13

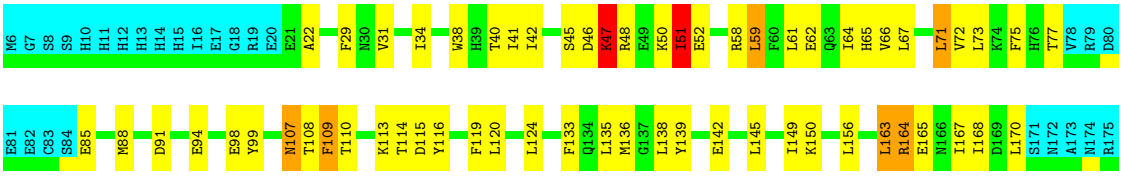
- Molecule 1: Major urinary protein 6

Chain A: 43% 34% • • 19%

4.2.14 Score per residue for model 14

- Molecule 1: Major urinary protein 6

Chain A: 47% 30% • • 19%



C176
L177
Q178
A179
R180
E181

4.2.15 Score per residue for model 15

- Molecule 1: Major urinary protein 6

Chain A: 47% 30% • • 19%

M6 G7 S8 S9 H10 H11 H12 H13 H14 H15 I16 E17 G18 R19 E20 E21 A22 R27 N28 F29 N30 V31 I34 W38 I41 I42 L43 A44 S45 D46 K47 I51 E52 L59 F60 L61 E62 Q63 I64 H65 V66 L71 F75 H76 T77 V78 R79 D80 E81 E82 C83 S84

E85 L86 S87 M88 V89 A90 Y99 Y103 N107 T108 F109 T110 I111 P112 K113 T114 D115 Y116 F119 L120 M121 A122 H123 L124 I125 K128 F133 Q134 L135 M136 G137 L138 Y139 L145 I149 K150 F153 A154 L163 R164 E165 N166 I167 I168 D169 L170 S171 N172 A173 N174

R175 C176 L177 Q178 A179 R180 E181

4.2.16 Score per residue for model 16

- Molecule 1: Major urinary protein 6

Chain A: 44% 33% • • 19%

M6 G7 S8 S9 H10 H11 H12 H13 H14 H15 I16 E17 G18 R19 E20 E21 A22 S23 S24 R27 N28 V31 I34 W38 H39 T40 I41 I42 L43 A44 S45 D46 K47 R48 E49 K50 I51 E52 L59 F60 L61 I64 L67 E68 L71 V72 L73 K74 F75 H76 T77 V78

R79 D80 E81 E82 C83 S84 E85 L86 E98 Y103 D104 N107 T108 F109 T110 I111 T114 D115 Y116 F119 L120 M121 A122 H123 L124 I125 L135 M136 G137 L138 Y139 G140 R141 L145 D148 I149 A154 L163 R164 E165 N166 I167 I168 S171 N172 A173 N174 R175 C176

L177 Q178 A179 R180 E181

4.2.17 Score per residue for model 17

- Molecule 1: Major urinary protein 6

Chain A: 41% 37% • • 19%

M6 G7 S8 S9 H10 H11 H12 H13 H14 H15 I16 E17 G18 R19 E20 E21 A22 S23 S24 R27 V31 E32 K33 I34 N35 W38 H39 T40 I41 I42 L43 A44 S45 D46 K47 R48 E49 K50 I51 E52 F57 R58 L59 F60 L61 I64 H65 V66 L67 E68 L71 V72 L73 K74

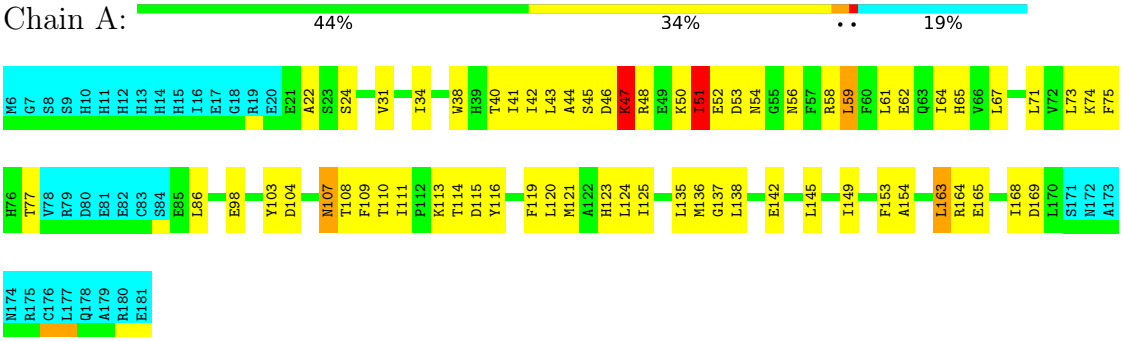
F75 H76 T77 V78 R79 D80 E81 E82 C83 S84 E85 L86 S87 M88 K92 E98 Y99 S100 V101 T102 Y103 N107 T108 F109 T110 I111 P112 K113 T114 D115 Y116 F119 L120 M121 A122 H123 L124 I125 N126 F133 Q134 L135 M136 G137 E142 L145 I149 K150 F153 A154

L163 R164 E165 N166 I167 I168 D169 L170 S171 N172 A173 N174 R175 C176 L177 Q178 A179 R180 E181

4.2.18 Score per residue for model 18

- Molecule 1: Major urinary protein 6

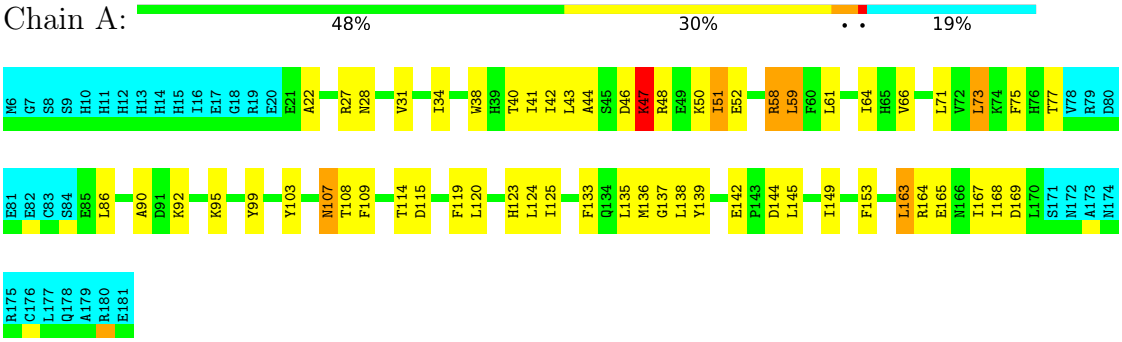
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Major urinary protein 6

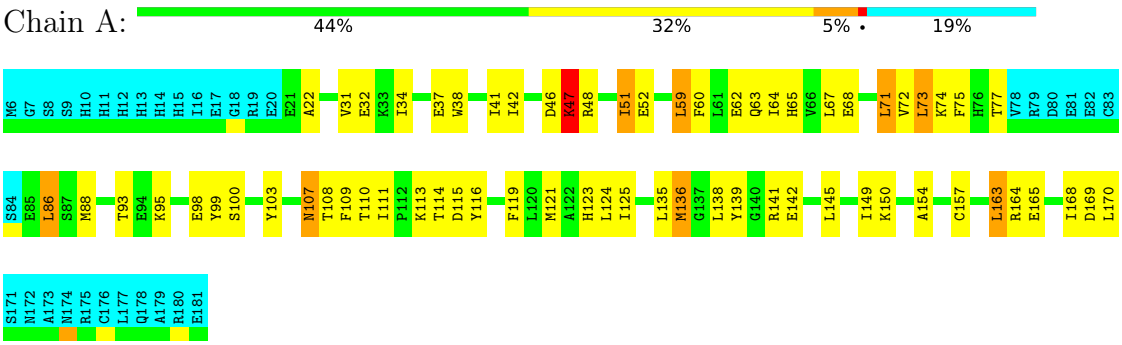
Chain A:



4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: Major urinary protein 6

Chain A:



5 Refinement protocol and experimental data overview (i)

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

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

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

Software name	**Classification**	**Version**
CYANA	structure solution	2.1 and 3
CYANA	refinement	2.1 and 3

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	1958
Number of shifts mapped to atoms	1958
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1162	1120	1120	37±4
All	All	23240	22400	22400	745

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:A:31:VAL:HG23	1:A:34:ILE:HD11	0.83	1.49	8	19
1:A:59:LEU:HD23	1:A:77:THR:HG23	0.80	1.52	16	2
1:A:38:TRP:CD1	1:A:64:ILE:HD12	0.73	2.19	3	20
1:A:41:ILE:HG21	1:A:145:LEU:HD12	0.72	1.62	4	20
1:A:170:LEU:HD22	1:A:170:LEU:O	0.68	1.87	9	1
1:A:51:ILE:HG13	1:A:168:ILE:HD13	0.66	1.67	14	14
1:A:73:LEU:HD12	1:A:75:PHE:CZ	0.66	2.26	20	15
1:A:59:LEU:HD23	1:A:77:THR:CG2	0.65	2.21	16	19
1:A:48:ARG:HD2	1:A:168:ILE:HD11	0.65	1.68	1	16
1:A:109:PHE:HB2	1:A:124:LEU:HD12	0.65	1.68	3	20
1:A:154:ALA:HB1	1:A:164:ARG:HD2	0.64	1.70	7	1
1:A:43:LEU:HD23	1:A:51:ILE:CG2	0.64	2.23	8	2
1:A:58:ARG:HG2	1:A:170:LEU:HD11	0.62	1.69	17	2
1:A:135:LEU:HD13	1:A:136:MET:N	0.62	2.09	9	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:LEU:HD13	1:A:121:MET:N	0.62	2.10	11	1
1:A:164:ARG:HA	1:A:167:ILE:HD13	0.62	1.72	14	11
1:A:58:ARG:CG	1:A:170:LEU:HD11	0.61	2.26	17	3
1:A:47:LYS:O	1:A:51:ILE:HD12	0.61	1.96	8	1
1:A:154:ALA:HB1	1:A:164:ARG:CD	0.61	2.25	4	4
1:A:59:LEU:HD22	1:A:75:PHE:HB3	0.61	1.73	16	11
1:A:107:ASN:OD1	1:A:124:LEU:HD11	0.60	1.97	19	15
1:A:67:LEU:HD11	1:A:72:VAL:CG2	0.60	2.26	12	2
1:A:22:ALA:O	1:A:114:THR:HG22	0.60	1.96	15	20
1:A:51:ILE:CG1	1:A:168:ILE:HD13	0.60	2.27	16	15
1:A:67:LEU:HD11	1:A:72:VAL:HG23	0.60	1.74	14	6
1:A:44:ALA:HB3	1:A:153:PHE:CZ	0.59	2.32	19	9
1:A:90:ALA:HB1	1:A:99:TYR:CB	0.59	2.28	19	1
1:A:123:HIS:CE1	1:A:125:ILE:HD11	0.58	2.32	6	15
1:A:154:ALA:HB1	1:A:164:ARG:HD3	0.58	1.75	18	7
1:A:86:LEU:HD12	1:A:88:MET:CE	0.58	2.29	17	5
1:A:45:SER:OG	1:A:135:LEU:HD22	0.57	1.99	5	1
1:A:38:TRP:HB3	1:A:61:LEU:HD23	0.57	1.77	4	11
1:A:59:LEU:HD22	1:A:75:PHE:CB	0.56	2.30	2	8
1:A:67:LEU:HD21	1:A:72:VAL:HG23	0.56	1.76	4	2
1:A:111:ILE:HG23	1:A:121:MET:O	0.56	2.01	18	13
1:A:109:PHE:CB	1:A:124:LEU:HD12	0.55	2.31	12	2
1:A:59:LEU:HD13	1:A:75:PHE:CD2	0.55	2.37	19	9
1:A:71:LEU:HD21	1:A:99:TYR:CE2	0.55	2.37	14	6
1:A:138:LEU:HD21	1:A:145:LEU:HD12	0.55	1.79	14	2
1:A:138:LEU:HD12	1:A:139:TYR:N	0.54	2.17	13	8
1:A:31:VAL:HG22	1:A:66:VAL:HG12	0.54	1.80	5	3
1:A:98:GLU:HA	1:A:110:THR:HG22	0.54	1.79	8	17
1:A:73:LEU:HD12	1:A:75:PHE:CE1	0.54	2.37	19	9
1:A:47:LYS:O	1:A:51:ILE:HD13	0.54	2.03	4	14
1:A:121:MET:CE	1:A:156:LEU:HD23	0.54	2.32	13	1
1:A:119:PHE:CD2	1:A:149:ILE:HG23	0.54	2.38	11	16
1:A:119:PHE:CD1	1:A:149:ILE:HG23	0.53	2.39	15	4
1:A:90:ALA:HB1	1:A:99:TYR:HB3	0.53	1.80	15	2
1:A:136:MET:SD	1:A:156:LEU:HD23	0.53	2.44	14	3
1:A:31:VAL:HG22	1:A:66:VAL:CG1	0.53	2.34	5	3
1:A:59:LEU:HD12	1:A:59:LEU:O	0.53	2.03	12	1
1:A:48:ARG:CD	1:A:168:ILE:HD11	0.53	2.34	13	6
1:A:156:LEU:O	1:A:156:LEU:HD23	0.53	2.04	1	1
1:A:41:ILE:HG21	1:A:145:LEU:CD1	0.53	2.32	4	10
1:A:138:LEU:HD23	1:A:139:TYR:N	0.53	2.18	2	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:PHE:CD2	1:A:135:LEU:HD13	0.53	2.39	3	2
1:A:166:ASN:O	1:A:168:ILE:HD12	0.53	2.04	16	14
1:A:58:ARG:HG3	1:A:170:LEU:HD11	0.52	1.81	6	2
1:A:71:LEU:HD12	1:A:71:LEU:O	0.52	2.04	15	1
1:A:43:LEU:HD12	1:A:137:GLY:HA2	0.52	1.82	18	12
1:A:170:LEU:HD22	1:A:170:LEU:C	0.52	2.25	9	1
1:A:145:LEU:HD22	1:A:149:ILE:HG21	0.52	1.81	11	2
1:A:145:LEU:HD13	1:A:149:ILE:CG2	0.51	2.35	12	1
1:A:41:ILE:O	1:A:42:ILE:HD13	0.51	2.05	1	20
1:A:29:PHE:CD2	1:A:114:THR:HG21	0.51	2.40	3	9
1:A:138:LEU:HD22	1:A:153:PHE:HB2	0.51	1.81	9	4
1:A:86:LEU:HD12	1:A:88:MET:HE2	0.51	1.81	17	1
1:A:67:LEU:N	1:A:67:LEU:HD22	0.50	2.22	16	4
1:A:121:MET:HE2	1:A:138:LEU:HD13	0.50	1.83	3	1
1:A:114:THR:HA	1:A:120:LEU:HD12	0.50	1.84	7	16
1:A:77:THR:CG2	1:A:86:LEU:HD22	0.50	2.36	13	1
1:A:86:LEU:HD12	1:A:88:MET:SD	0.49	2.46	2	1
1:A:86:LEU:HD23	1:A:86:LEU:H	0.49	1.67	13	1
1:A:120:LEU:HD13	1:A:120:LEU:C	0.49	2.27	11	1
1:A:75:PHE:HB2	1:A:86:LEU:HD21	0.49	1.85	13	1
1:A:163:LEU:HD12	1:A:165:GLU:HB2	0.49	1.82	14	17
1:A:29:PHE:CD1	1:A:114:THR:HG21	0.49	2.42	7	2
1:A:99:TYR:O	1:A:108:THR:HG22	0.49	2.08	6	1
1:A:38:TRP:HD1	1:A:64:ILE:HD12	0.48	1.68	2	9
1:A:38:TRP:CZ2	1:A:120:LEU:HD22	0.48	2.42	19	15
1:A:44:ALA:HB2	1:A:167:ILE:HG13	0.48	1.86	16	4
1:A:42:ILE:HD12	1:A:169:ASP:HA	0.48	1.85	4	7
1:A:86:LEU:HD12	1:A:88:MET:HE3	0.48	1.85	5	1
1:A:121:MET:CE	1:A:156:LEU:HD22	0.48	2.38	4	2
1:A:42:ILE:HG23	1:A:169:ASP:HA	0.48	1.85	20	3
1:A:22:ALA:C	1:A:114:THR:HG22	0.47	2.30	6	3
1:A:59:LEU:HD23	1:A:77:THR:HG22	0.47	1.84	13	2
1:A:61:LEU:HD22	1:A:139:TYR:CE1	0.47	2.44	19	1
1:A:45:SER:HB2	1:A:135:LEU:HD22	0.47	1.87	14	3
1:A:70:SER:C	1:A:71:LEU:HD23	0.47	2.29	4	3
1:A:22:ALA:HB1	1:A:27:ARG:O	0.47	2.09	16	2
1:A:46:ASP:O	1:A:47:LYS:HB2	0.46	2.10	8	20
1:A:50:LYS:NZ	1:A:135:LEU:HD23	0.46	2.24	13	1
1:A:41:ILE:HG22	1:A:42:ILE:HG12	0.46	1.86	4	3
1:A:41:ILE:HG21	1:A:145:LEU:CG	0.46	2.40	7	10
1:A:170:LEU:HD12	1:A:170:LEU:O	0.46	2.10	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:GLU:N	1:A:63:GLN:HE21	0.46	2.08	13	6
1:A:136:MET:CE	1:A:156:LEU:HD23	0.46	2.41	2	1
1:A:31:VAL:HG22	1:A:66:VAL:HG22	0.46	1.88	19	4
1:A:145:LEU:HD13	1:A:149:ILE:HG22	0.45	1.88	12	3
1:A:120:LEU:HD12	1:A:139:TYR:CD2	0.45	2.46	11	1
1:A:50:LYS:HZ1	1:A:135:LEU:HD23	0.45	1.72	13	1
1:A:44:ALA:HB3	1:A:153:PHE:CE2	0.45	2.47	1	1
1:A:41:ILE:HG21	1:A:145:LEU:HB2	0.45	1.88	5	10
1:A:73:LEU:H	1:A:73:LEU:HD23	0.44	1.71	14	4
1:A:43:LEU:HD23	1:A:51:ILE:HG23	0.44	1.90	8	1
1:A:120:LEU:HD12	1:A:139:TYR:HD2	0.44	1.73	11	1
1:A:121:MET:HE1	1:A:156:LEU:HD23	0.44	1.87	13	1
1:A:123:HIS:NE2	1:A:125:ILE:HD11	0.44	2.28	6	1
1:A:90:ALA:CA	1:A:101:VAL:HG12	0.44	2.43	11	1
1:A:138:LEU:HD21	1:A:145:LEU:CD1	0.43	2.42	14	2
1:A:35:ASN:ND2	1:A:66:VAL:HG22	0.43	2.28	17	2
1:A:93:THR:HG21	1:A:100:SER:HB3	0.43	1.90	20	2
1:A:121:MET:CE	1:A:138:LEU:HD13	0.43	2.42	3	1
1:A:46:ASP:O	1:A:47:LYS:CB	0.43	2.66	5	17
1:A:35:ASN:CG	1:A:66:VAL:HG22	0.43	2.34	5	1
1:A:51:ILE:HG12	1:A:168:ILE:HD13	0.42	1.91	5	1
1:A:45:SER:OG	1:A:51:ILE:HD12	0.42	2.14	7	6
1:A:59:LEU:HD13	1:A:75:PHE:CD1	0.42	2.49	15	1
1:A:135:LEU:HD13	1:A:135:LEU:C	0.42	2.35	16	4
1:A:43:LEU:HD23	1:A:51:ILE:HG22	0.42	1.90	19	2
1:A:77:THR:HG22	1:A:86:LEU:HD22	0.42	1.92	13	1
1:A:124:LEU:C	1:A:124:LEU:HD23	0.41	2.35	3	2
1:A:59:LEU:HD13	1:A:75:PHE:HB3	0.41	1.92	12	1
1:A:73:LEU:N	1:A:73:LEU:HD23	0.41	2.30	20	2
1:A:88:MET:HE3	1:A:103:TYR:CD1	0.41	2.51	13	1
1:A:31:VAL:CG2	1:A:34:ILE:HD11	0.41	2.39	5	1
1:A:58:ARG:NE	1:A:170:LEU:HD11	0.41	2.29	7	1
1:A:59:LEU:HD13	1:A:75:PHE:HD2	0.41	1.76	11	1
1:A:86:LEU:N	1:A:86:LEU:HD23	0.40	2.31	9	1
1:A:58:ARG:CD	1:A:170:LEU:HD11	0.40	2.45	7	1
1:A:170:LEU:N	1:A:170:LEU:CD1	0.40	2.85	9	1
1:A:22:ALA:HB3	1:A:114:THR:CG2	0.40	2.47	12	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	143/176 (81%)	125±2 (88±1%)	16±2 (11±1%)	2±1 (1±0%)	18 66
All	All	2860/3520 (81%)	2508 (88%)	320 (11%)	32 (1%)	18 66

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	A	47	LYS	20
1	A	51	ILE	6
1	A	95	LYS	5
1	A	55	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	A	128/157 (82%)	104±3 (81±2%)	24±3 (19±2%)	4 36
All	All	2560/3140 (82%)	2081 (81%)	479 (19%)	4 36

All 67 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	47	LYS	20
1	A	51	ILE	20
1	A	52	GLU	20
1	A	71	LEU	20
1	A	107	ASN	20
1	A	108	THR	20

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Mol	Chain	Res	Type	Models (Total)
1	A	163	LEU	20
1	A	59	LEU	19
1	A	103	TYR	19
1	A	86	LEU	18
1	A	115	ASP	18
1	A	116	TYR	17
1	A	113	LYS	16
1	A	142	GLU	16
1	A	68	GLU	13
1	A	40	THR	12
1	A	50	LYS	12
1	A	62	GLU	11
1	A	133	PHE	11
1	A	21	GLU	9
1	A	60	PHE	9
1	A	24	SER	8
1	A	65	HIS	7
1	A	58	ARG	7
1	A	150	LYS	7
1	A	85	GLU	6
1	A	164	ARG	6
1	A	170	LEU	6
1	A	148	ASP	5
1	A	28	ASN	5
1	A	100	SER	5
1	A	69	ASN	4
1	A	141	ARG	4
1	A	27	ARG	4
1	A	74	LYS	4
1	A	91	ASP	4
1	A	88	MET	3
1	A	128	LYS	3
1	A	104	ASP	3
1	A	95	LYS	3
1	A	109	PHE	3
1	A	169	ASP	3
1	A	92	LYS	3
1	A	136	MET	3
1	A	101	VAL	2
1	A	121	MET	2
1	A	23	SER	2
1	A	54	ASN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	53	ASP	2
1	A	77	THR	2
1	A	45	SER	2
1	A	144	ASP	2
1	A	33	LYS	2
1	A	73	LEU	2
1	A	48	ARG	1
1	A	70	SER	1
1	A	156	LEU	1
1	A	147	SER	1
1	A	38	TRP	1
1	A	160	HIS	1
1	A	146	SER	1
1	A	94	GLU	1
1	A	39	HIS	1
1	A	126	ASN	1
1	A	56	ASN	1
1	A	32	GLU	1
1	A	157	CYS	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 87% for the well-defined parts and 81% 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	1958
Number of shifts mapped to atoms	1958
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	165	-0.41 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	155	0.05 ± 0.14	None needed (< 0.5 ppm)
$^{13}C'$	165	0.31 ± 0.16	None needed (< 0.5 ppm)
^{15}N	162	0.16 ± 0.37	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 1724 atoms were assigned a chemical shift out of a possible 1975. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	718/720 (100%)	292/293 (100%)	285/286 (100%)	141/141 (100%)
Sidechain	897/1082 (83%)	603/696 (87%)	288/346 (83%)	6/40 (15%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	109/173 (63%)	55/87 (63%)	54/80 (68%)	0/6 (0%)
Overall	1724/1975 (87%)	950/1076 (88%)	627/712 (88%)	147/187 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1958 atoms were assigned a chemical shift out of a possible 2409. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	828/887 (93%)	336/361 (93%)	330/352 (94%)	162/174 (93%)
Sidechain	1021/1307 (78%)	683/838 (82%)	330/414 (80%)	8/55 (15%)
Aromatic	109/215 (51%)	55/111 (50%)	54/92 (59%)	0/12 (0%)
Overall	1958/2409 (81%)	1074/1310 (82%)	714/858 (83%)	170/241 (71%)

7.1.4 Statistically unusual chemical shifts (i)

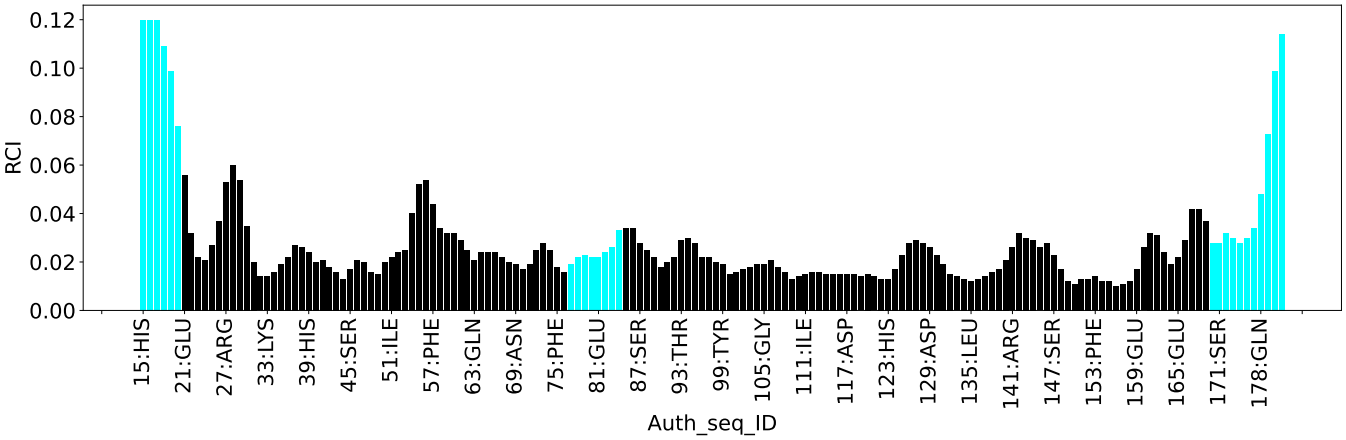
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	138	LEU	HB3	-0.72	-0.26 – 3.31	-6.3
1	A	24	SER	HB3	2.26	2.49 – 5.20	-5.9
1	A	104	ASP	HB3	1.13	1.32 – 4.00	-5.7
1	A	126	ASN	HB2	1.07	1.27 – 4.34	-5.7

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.12
0.10
0.08
0.06
0.04
0.02
0.00
15:HIS
21:GLU
27:ARG
33:LYS
39:HIS
45:SER
51:ILE
57:PHE
63:GLN
69:ASN
75:PHE
81:GLU
87:SER
93:THR
99:TYR
105:GLY
111:ILE
117:ASP
123:HIS
129:ASP
135:LEU
141:ARG
147:SER
153:PHE
159:GLU
165:GLU
171:SER
178:GLN
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	3626
Intra-residue (|i-j|=0)	749
Sequential (|i-j|=1)	1009
Medium range (|i-j|>1 and |i-j|<5)	568
Long range (|i-j|≥5)	1300
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	252
Number of unmapped restraints	0
Number of restraints per residue	22.0
Number of long range restraints per residue[1]	7.4

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations (i)

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model (i)

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	12.6	0.2
0.2-0.5 (Medium)	4.0	0.49
>0.5 (Large)	0.1	0.55

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	15.2	9.75
10.0-20.0 (Medium)	1.1	19.88
>20.0 (Large)	0.1	20.69

9 Distance violation analysis (i)

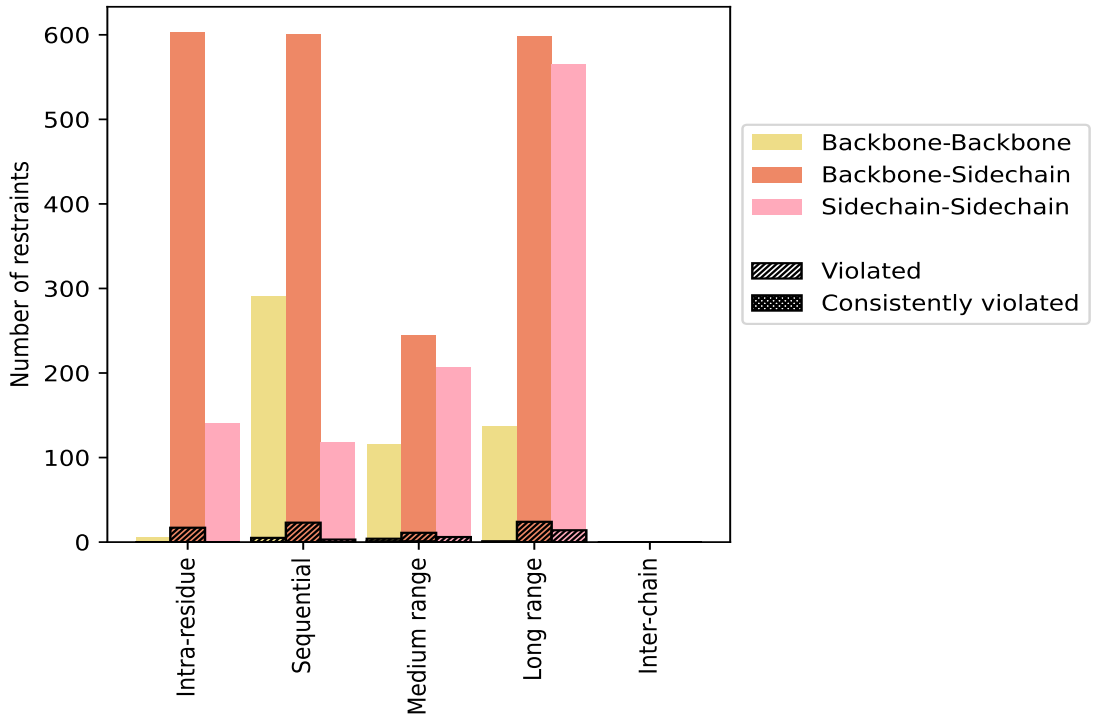
9.1 Summary of distance violations (i)

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)	749	20.7	17	2.3	0.5	0	0.0	0.0
Backbone-Backbone	6	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	603	16.6	17	2.8	0.5	0	0.0	0.0
Sidechain-Sidechain	140	3.9	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	1009	27.8	31	3.1	0.9	0	0.0	0.0
Backbone-Backbone	291	8.0	5	1.7	0.1	0	0.0	0.0
Backbone-Sidechain	600	16.5	23	3.8	0.6	0	0.0	0.0
Sidechain-Sidechain	118	3.3	3	2.5	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	568	15.7	21	3.7	0.6	2	0.4	0.1
Backbone-Backbone	116	3.2	4	3.4	0.1	1	0.9	0.0
Backbone-Sidechain	245	6.8	11	4.5	0.3	1	0.4	0.0
Sidechain-Sidechain	207	5.7	6	2.9	0.2	0	0.0	0.0
Long range (|i-j|≥5)	1300	35.9	39	3.0	1.1	0	0.0	0.0
Backbone-Backbone	137	3.8	1	0.7	0.0	0	0.0	0.0
Backbone-Sidechain	598	16.5	24	4.0	0.7	0	0.0	0.0
Sidechain-Sidechain	565	15.6	14	2.5	0.4	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3626	100.0	108	3.0	3.0	2	0.1	0.1
Backbone-Backbone	550	15.2	10	1.8	0.3	1	0.2	0.0
Backbone-Sidechain	2046	56.4	75	3.7	2.1	1	0.0	0.0
Sidechain-Sidechain	1030	28.4	23	2.2	0.6	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	4	8	3	9	0	24	0.17	0.37	0.08	0.13
2	1	3	4	3	0	11	0.16	0.33	0.07	0.14
3	1	4	5	4	0	14	0.19	0.43	0.09	0.15
4	2	4	5	3	0	14	0.17	0.33	0.07	0.14
5	4	7	3	1	0	15	0.19	0.41	0.08	0.15
6	2	7	2	4	0	15	0.18	0.33	0.08	0.16
7	4	5	4	5	0	18	0.15	0.28	0.05	0.14
8	4	7	3	6	0	20	0.16	0.29	0.05	0.15
9	2	1	5	5	0	13	0.18	0.36	0.08	0.15
10	1	8	6	3	0	18	0.2	0.41	0.09	0.15
11	3	7	5	5	0	20	0.18	0.49	0.1	0.14

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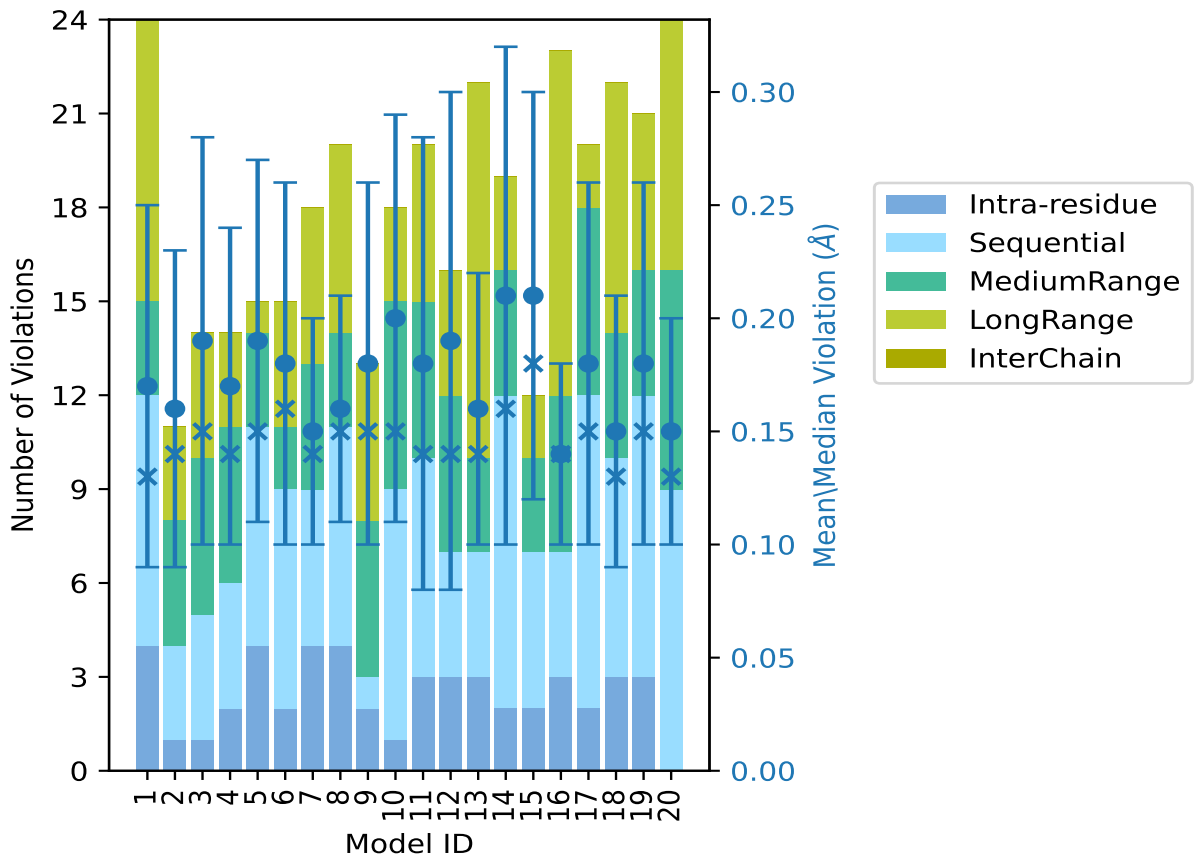
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	3	4	5	4	0	16	0.19	0.55	0.11	0.14
13	3	4	3	12	0	22	0.16	0.32	0.06	0.14
14	2	10	4	3	0	19	0.21	0.48	0.11	0.16
15	2	5	3	2	0	12	0.21	0.43	0.09	0.18
16	3	4	5	11	0	23	0.14	0.27	0.04	0.14
17	2	10	6	2	0	20	0.18	0.38	0.08	0.15
18	3	7	4	8	0	22	0.15	0.33	0.06	0.13
19	3	9	4	5	0	21	0.18	0.37	0.08	0.15
20	0	9	7	8	0	24	0.15	0.33	0.05	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

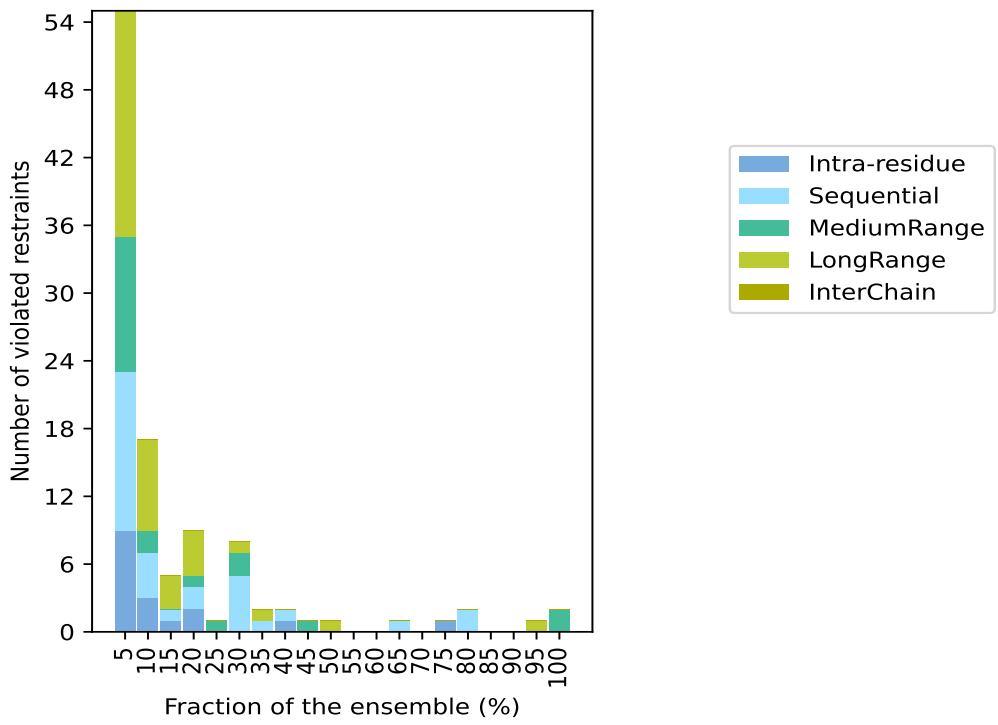
9.3 Distance violation statistics for the ensemble (i)

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, 3518(IR:732, SQ:978, MR:547, LR:1261, 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]	%
9	14	12	20	0	55	1	5.0
3	4	2	8	0	17	2	10.0
1	1	0	3	0	5	3	15.0
2	2	1	4	0	9	4	20.0
0	0	1	0	0	1	5	25.0
0	5	2	1	0	8	6	30.0
0	1	0	1	0	2	7	35.0
1	1	0	0	0	2	8	40.0
0	0	1	0	0	1	9	45.0
0	0	0	1	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	1	0	0	0	1	13	65.0
0	0	0	0	0	0	14	70.0
1	0	0	0	0	1	15	75.0
0	2	0	0	0	2	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	1	0	1	19	95.0
0	0	2	0	0	2	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

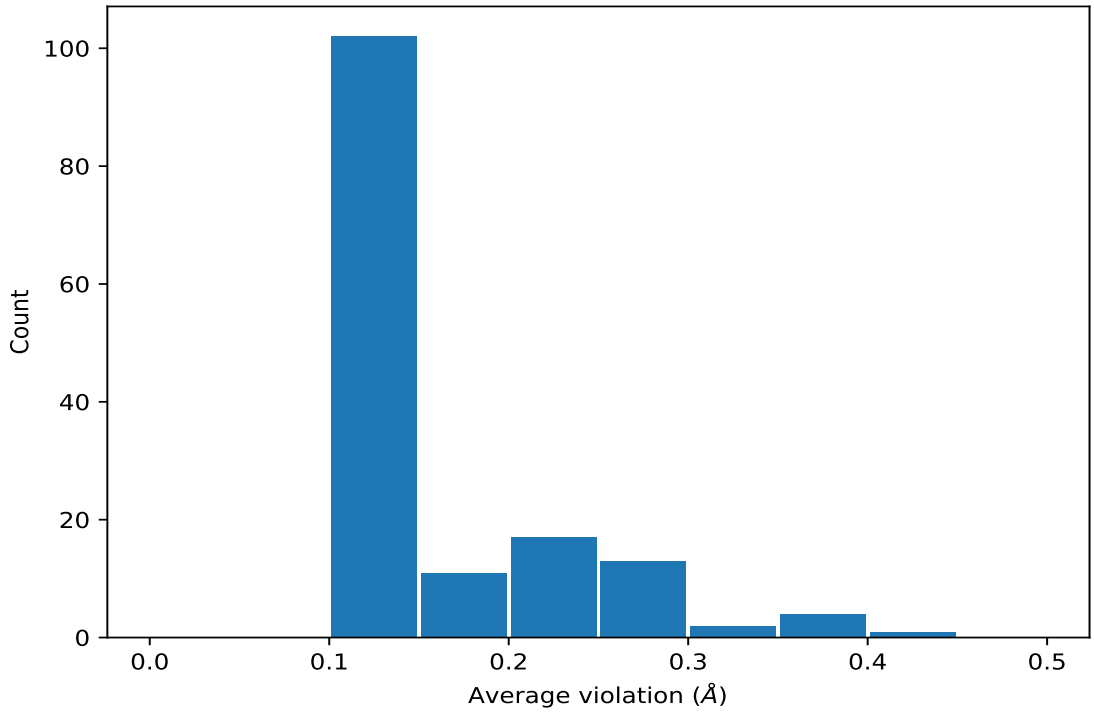
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	20	0.27	0.04	0.29
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	20	0.17	0.03	0.18
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	20	0.17	0.03	0.18
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	20	0.17	0.03	0.18
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	19	0.13	0.01	0.13
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	19	0.13	0.01	0.13
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	19	0.13	0.01	0.13
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	16	0.13	0.01	0.13
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	16	0.13	0.01	0.13
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	16	0.13	0.01	0.13
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	16	0.13	0.01	0.13
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	16	0.13	0.01	0.13
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	16	0.13	0.01	0.13
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	16	0.13	0.01	0.13
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	15	0.15	0.05	0.14
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	15	0.15	0.05	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	15	0.15	0.05	0.14
(1,2158)	1:120:A:LEU:HD21	1:121:A:MET:HA	13	0.13	0.02	0.13
(1,2158)	1:120:A:LEU:HD22	1:121:A:MET:HA	13	0.13	0.02	0.13
(1,2158)	1:120:A:LEU:HD23	1:121:A:MET:HA	13	0.13	0.02	0.13
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD1	10	0.14	0.02	0.14
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD2	10	0.14	0.02	0.14
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD1	10	0.14	0.02	0.14
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD2	10	0.14	0.02	0.14
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD1	10	0.14	0.02	0.14
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD2	10	0.14	0.02	0.14
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD1	10	0.14	0.02	0.14
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD2	10	0.14	0.02	0.14
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD1	10	0.14	0.02	0.14
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD2	10	0.14	0.02	0.14
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD1	10	0.14	0.02	0.14
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD2	10	0.14	0.02	0.14
(1,2123)	1:73:A:LEU:HD21	1:75:A:PHE:HZ	9	0.14	0.01	0.15
(1,2123)	1:73:A:LEU:HD22	1:75:A:PHE:HZ	9	0.14	0.01	0.15
(1,2123)	1:73:A:LEU:HD23	1:75:A:PHE:HZ	9	0.14	0.01	0.15
(1,15)	1:17:A:GLU:HA	1:18:A:GLY:H	8	0.41	0.03	0.41
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD11	8	0.2	0.0	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD12	8	0.2	0.0	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD13	8	0.2	0.0	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD21	8	0.2	0.0	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD22	8	0.2	0.0	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD23	8	0.2	0.0	0.2
(1,3187)	1:101:A:VAL:HG11	1:102:A:THR:HB	7	0.21	0.03	0.21
(1,3187)	1:101:A:VAL:HG12	1:102:A:THR:HB	7	0.21	0.03	0.21
(1,3187)	1:101:A:VAL:HG13	1:102:A:THR:HB	7	0.21	0.03	0.21
(1,3187)	1:101:A:VAL:HG21	1:102:A:THR:HB	7	0.21	0.03	0.21
(1,3187)	1:101:A:VAL:HG22	1:102:A:THR:HB	7	0.21	0.03	0.21
(1,3187)	1:101:A:VAL:HG23	1:102:A:THR:HB	7	0.21	0.03	0.21
(1,2036)	1:118:A:ASN:HA	1:141:A:ARG:HB2	7	0.16	0.02	0.16
(1,195)	1:53:A:ASP:H	1:54:A:ASN:H	6	0.33	0.01	0.33
(1,1963)	1:138:A:LEU:HG	1:139:A:TYR:HA	6	0.32	0.02	0.32
(1,2805)	1:53:A:ASP:HB2	1:54:A:ASN:HA	6	0.27	0.03	0.26
(1,2805)	1:53:A:ASP:HB3	1:54:A:ASN:HA	6	0.27	0.03	0.26
(1,2224)	1:138:A:LEU:HD11	1:140:A:GLY:HA3	6	0.19	0.03	0.18
(1,2224)	1:138:A:LEU:HD12	1:140:A:GLY:HA3	6	0.19	0.03	0.18
(1,2224)	1:138:A:LEU:HD13	1:140:A:GLY:HA3	6	0.19	0.03	0.18
(1,2501)	1:17:A:GLU:HG2	1:18:A:GLY:HA2	6	0.13	0.01	0.14
(1,2501)	1:17:A:GLU:HG2	1:18:A:GLY:HA3	6	0.13	0.01	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2501)	1:17:A:GLU:HG3	1:18:A:GLY:HA2	6	0.13	0.01	0.14
(1,2501)	1:17:A:GLU:HG3	1:18:A:GLY:HA3	6	0.13	0.01	0.14
(1,2834)	1:59:A:LEU:HB2	1:75:A:PHE:HE1	6	0.13	0.03	0.12
(1,2834)	1:59:A:LEU:HB2	1:75:A:PHE:HE2	6	0.13	0.03	0.12
(1,2834)	1:59:A:LEU:HB3	1:75:A:PHE:HE1	6	0.13	0.03	0.12
(1,2834)	1:59:A:LEU:HB3	1:75:A:PHE:HE2	6	0.13	0.03	0.12
(1,2716)	1:45:A:SER:HB2	1:47:A:LYS:H	6	0.13	0.02	0.12
(1,2716)	1:45:A:SER:HB3	1:47:A:LYS:H	6	0.13	0.02	0.12
(1,1947)	1:135:A:LEU:HG	1:136:A:MET:H	6	0.12	0.03	0.11
(1,2050)	1:101:A:VAL:HB	1:103:A:TYR:HD1	5	0.14	0.01	0.14
(1,2050)	1:101:A:VAL:HB	1:103:A:TYR:HD2	5	0.14	0.01	0.14
(1,2508)	1:19:A:ARG:HA	1:19:A:ARG:HG2	4	0.29	0.01	0.3
(1,2508)	1:19:A:ARG:HA	1:19:A:ARG:HG3	4	0.29	0.01	0.3
(1,1269)	1:66:A:VAL:HA	1:67:A:LEU:HG	4	0.24	0.01	0.25
(1,1628)	1:78:A:VAL:HB	1:82:A:GLU:HA	4	0.24	0.04	0.24
(1,264)	1:67:A:LEU:H	1:67:A:LEU:HG	4	0.14	0.03	0.15
(1,2359)	1:86:A:LEU:HG	1:103:A:TYR:HE1	4	0.14	0.02	0.14
(1,2359)	1:86:A:LEU:HG	1:103:A:TYR:HE2	4	0.14	0.02	0.14
(1,771)	1:162:A:ILE:H	1:167:A:ILE:HD11	4	0.13	0.01	0.12
(1,771)	1:162:A:ILE:H	1:167:A:ILE:HD12	4	0.13	0.01	0.12
(1,771)	1:162:A:ILE:H	1:167:A:ILE:HD13	4	0.13	0.01	0.12
(1,3179)	1:100:A:SER:HB2	1:101:A:VAL:H	4	0.12	0.02	0.12
(1,3179)	1:100:A:SER:HB3	1:101:A:VAL:H	4	0.12	0.02	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD11	4	0.12	0.0	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD12	4	0.12	0.0	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD13	4	0.12	0.0	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD21	4	0.12	0.0	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD22	4	0.12	0.0	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD23	4	0.12	0.0	0.12
(1,1213)	1:39:A:HIS:H	1:61:A:LEU:HD11	4	0.11	0.0	0.11
(1,1213)	1:39:A:HIS:H	1:61:A:LEU:HD12	4	0.11	0.0	0.11
(1,1213)	1:39:A:HIS:H	1:61:A:LEU:HD13	4	0.11	0.0	0.11
(1,2399)	1:65:A:HIS:HA	1:65:A:HIS:HD2	3	0.15	0.04	0.13
(1,166)	1:47:A:LYS:H	1:133:A:PHE:HB2	3	0.14	0.02	0.15
(1,1834)	1:154:A:ALA:HA	1:167:A:ILE:HD11	3	0.14	0.04	0.13
(1,1834)	1:154:A:ALA:HA	1:167:A:ILE:HD12	3	0.14	0.04	0.13
(1,1834)	1:154:A:ALA:HA	1:167:A:ILE:HD13	3	0.14	0.04	0.13
(1,103)	1:39:A:HIS:H	1:64:A:ILE:HD11	3	0.13	0.03	0.11
(1,103)	1:39:A:HIS:H	1:64:A:ILE:HD12	3	0.13	0.03	0.11
(1,103)	1:39:A:HIS:H	1:64:A:ILE:HD13	3	0.13	0.03	0.11
(1,16)	1:17:A:GLU:HB3	1:18:A:GLY:H	3	0.12	0.01	0.13
(1,2505)	1:18:A:GLY:HA2	1:19:A:ARG:HG2	2	0.36	0.04	0.36

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2505)	1:18:A:GLY:HA2	1:19:A:ARG:HG3	2	0.36	0.04	0.36
(1,2505)	1:18:A:GLY:HA3	1:19:A:ARG:HG2	2	0.36	0.04	0.36
(1,2505)	1:18:A:GLY:HA3	1:19:A:ARG:HG3	2	0.36	0.04	0.36
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD11	2	0.29	0.07	0.29
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD12	2	0.29	0.07	0.29
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD13	2	0.29	0.07	0.29
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD21	2	0.29	0.07	0.29
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD22	2	0.29	0.07	0.29
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD23	2	0.29	0.07	0.29
(1,2541)	1:27:A:ARG:HA	1:27:A:ARG:HG2	2	0.26	0.03	0.26
(1,2541)	1:27:A:ARG:HA	1:27:A:ARG:HG3	2	0.26	0.03	0.26
(1,2179)	1:101:A:VAL:HG21	1:102:A:THR:HB	2	0.22	0.02	0.22
(1,2179)	1:101:A:VAL:HG22	1:102:A:THR:HB	2	0.22	0.02	0.22
(1,2179)	1:101:A:VAL:HG23	1:102:A:THR:HB	2	0.22	0.02	0.22
(1,2507)	1:19:A:ARG:H	1:19:A:ARG:HG2	2	0.18	0.04	0.18
(1,2507)	1:19:A:ARG:H	1:19:A:ARG:HG3	2	0.18	0.04	0.18
(1,3408)	1:141:A:ARG:HB2	1:142:A:GLU:HA	2	0.16	0.01	0.16
(1,3408)	1:141:A:ARG:HB3	1:142:A:GLU:HA	2	0.16	0.01	0.16
(1,1984)	1:94:A:GLU:HA	1:94:A:GLU:HG2	2	0.15	0.0	0.15
(1,1922)	1:133:A:PHE:HE1	1:135:A:LEU:HB3	2	0.15	0.0	0.15
(1,1922)	1:133:A:PHE:HE2	1:135:A:LEU:HB3	2	0.15	0.0	0.15
(1,1899)	1:154:A:ALA:HA	1:167:A:ILE:HG21	2	0.14	0.01	0.14
(1,1899)	1:154:A:ALA:HA	1:167:A:ILE:HG22	2	0.14	0.01	0.14
(1,1899)	1:154:A:ALA:HA	1:167:A:ILE:HG23	2	0.14	0.01	0.14
(1,3500)	1:158:A:GLU:H	1:164:A:ARG:HD2	2	0.14	0.04	0.14
(1,3500)	1:158:A:GLU:H	1:164:A:ARG:HD3	2	0.14	0.04	0.14
(1,3061)	1:79:A:ARG:H	1:82:A:GLU:HB2	2	0.12	0.02	0.12
(1,3061)	1:79:A:ARG:H	1:82:A:GLU:HB3	2	0.12	0.02	0.12
(1,1327)	1:109:A:PHE:H	1:124:A:LEU:HD21	2	0.12	0.0	0.12
(1,1327)	1:109:A:PHE:H	1:124:A:LEU:HD22	2	0.12	0.0	0.12
(1,1327)	1:109:A:PHE:H	1:124:A:LEU:HD23	2	0.12	0.0	0.12
(1,3193)	1:101:A:VAL:HG11	1:107:A:ASN:HA	2	0.12	0.0	0.12
(1,3193)	1:101:A:VAL:HG12	1:107:A:ASN:HA	2	0.12	0.0	0.12
(1,3193)	1:101:A:VAL:HG13	1:107:A:ASN:HA	2	0.12	0.0	0.12
(1,3193)	1:101:A:VAL:HG21	1:107:A:ASN:HA	2	0.12	0.0	0.12
(1,3193)	1:101:A:VAL:HG22	1:107:A:ASN:HA	2	0.12	0.0	0.12
(1,3193)	1:101:A:VAL:HG23	1:107:A:ASN:HA	2	0.12	0.0	0.12
(1,3283)	1:120:A:LEU:HD11	1:138:A:LEU:HA	2	0.12	0.0	0.12
(1,3283)	1:120:A:LEU:HD12	1:138:A:LEU:HA	2	0.12	0.0	0.12
(1,3283)	1:120:A:LEU:HD13	1:138:A:LEU:HA	2	0.12	0.0	0.12
(1,3283)	1:120:A:LEU:HD21	1:138:A:LEU:HA	2	0.12	0.0	0.12
(1,3283)	1:120:A:LEU:HD22	1:138:A:LEU:HA	2	0.12	0.0	0.12

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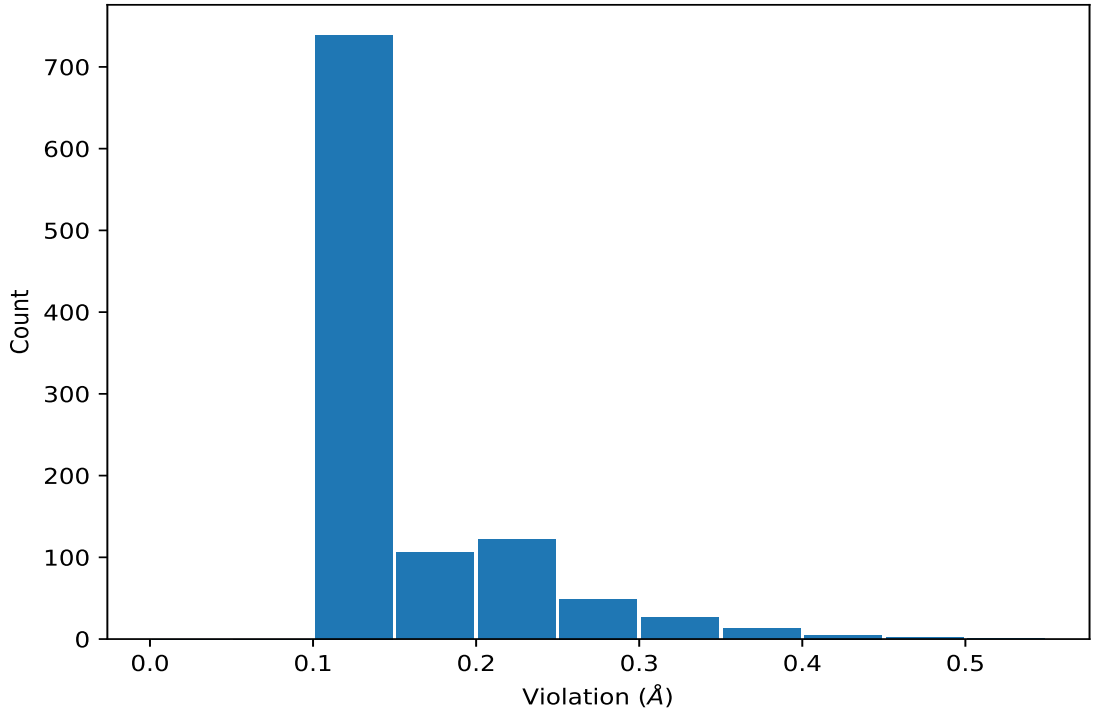
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3283)	1:120:A:LEU:HD23	1:138:A:LEU:HA	2	0.12	0.0	0.12
(1,2282)	1:154:A:ALA:HB1	1:164:A:ARG:H	2	0.11	0.01	0.11
(1,2282)	1:154:A:ALA:HB2	1:164:A:ARG:H	2	0.11	0.01	0.11
(1,2282)	1:154:A:ALA:HB3	1:164:A:ARG:H	2	0.11	0.01	0.11
(1,2293)	1:57:A:PHE:HB3	1:135:A:LEU:HD11	2	0.11	0.01	0.11
(1,2293)	1:57:A:PHE:HB3	1:135:A:LEU:HD12	2	0.11	0.01	0.11
(1,2293)	1:57:A:PHE:HB3	1:135:A:LEU:HD13	2	0.11	0.01	0.11
(1,819)	1:173:A:ALA:H	1:174:A:ASN:H	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)
(1,2393)	1:65:A:HIS:H	1:65:A:HIS:HD2	12	0.55
(1,1637)	1:120:A:LEU:HG	1:121:A:MET:HA	11	0.49
(1,15)	1:17:A:GLU:HA	1:18:A:GLY:H	14	0.48
(1,15)	1:17:A:GLU:HA	1:18:A:GLY:H	3	0.43
(1,15)	1:17:A:GLU:HA	1:18:A:GLY:H	15	0.43
(1,848)	1:15:A:HIS:HA	1:16:A:ILE:H	14	0.42
(1,15)	1:17:A:GLU:HA	1:18:A:GLY:H	5	0.41
(1,15)	1:17:A:GLU:HA	1:18:A:GLY:H	10	0.41
(1,2505)	1:18:A:GLY:HA2	1:19:A:ARG:HG2	11	0.39
(1,2505)	1:18:A:GLY:HA2	1:19:A:ARG:HG3	11	0.39
(1,2505)	1:18:A:GLY:HA3	1:19:A:ARG:HG2	11	0.39
(1,2505)	1:18:A:GLY:HA3	1:19:A:ARG:HG3	11	0.39
(1,15)	1:17:A:GLU:HA	1:18:A:GLY:H	17	0.38
(1,15)	1:17:A:GLU:HA	1:18:A:GLY:H	1	0.37
(1,15)	1:17:A:GLU:HA	1:18:A:GLY:H	19	0.37
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD11	9	0.36
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD12	9	0.36
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD13	9	0.36
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD21	9	0.36
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD22	9	0.36
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD23	9	0.36
(1,1963)	1:138:A:LEU:HG	1:139:A:TYR:HA	19	0.35
(1,195)	1:53:A:ASP:H	1:54:A:ASN:H	10	0.34
(1,195)	1:53:A:ASP:H	1:54:A:ASN:H	17	0.34
(1,2805)	1:53:A:ASP:HB2	1:54:A:ASN:HA	6	0.33
(1,2805)	1:53:A:ASP:HB3	1:54:A:ASN:HA	6	0.33
(1,1963)	1:138:A:LEU:HG	1:139:A:TYR:HA	2	0.33
(1,1963)	1:138:A:LEU:HG	1:139:A:TYR:HA	4	0.33
(1,762)	1:159:A:GLU:HB2	1:160:A:HIS:H	20	0.33
(1,195)	1:53:A:ASP:H	1:54:A:ASN:H	14	0.33
(1,195)	1:53:A:ASP:H	1:54:A:ASN:H	18	0.33
(1,2505)	1:18:A:GLY:HA2	1:19:A:ARG:HG2	19	0.32
(1,2505)	1:18:A:GLY:HA2	1:19:A:ARG:HG3	19	0.32
(1,2505)	1:18:A:GLY:HA3	1:19:A:ARG:HG2	19	0.32
(1,2505)	1:18:A:GLY:HA3	1:19:A:ARG:HG3	19	0.32
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	13	0.32
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	13	0.32
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	13	0.32
(1,1963)	1:138:A:LEU:HG	1:139:A:TYR:HA	12	0.32
(1,195)	1:53:A:ASP:H	1:54:A:ASN:H	1	0.32
(1,2169)	1:15:A:HIS:HA	1:16:A:ILE:HG21	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2169)	1:15:A:HIS:HA	1:16:A:ILE:HG22	14	0.31
(1,2169)	1:15:A:HIS:HA	1:16:A:ILE:HG23	14	0.31
(1,1963)	1:138:A:LEU:HG	1:139:A:TYR:HA	15	0.31
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	6	0.31
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	11	0.31
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	15	0.31
(1,2508)	1:19:A:ARG:HA	1:19:A:ARG:HG2	1	0.3
(1,2508)	1:19:A:ARG:HA	1:19:A:ARG:HG3	1	0.3
(1,2508)	1:19:A:ARG:HA	1:19:A:ARG:HG2	10	0.3
(1,2508)	1:19:A:ARG:HA	1:19:A:ARG:HG3	10	0.3
(1,1628)	1:78:A:VAL:HB	1:82:A:GLU:HA	9	0.3
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	1	0.3
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	9	0.3
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	10	0.3
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	18	0.3
(1,195)	1:53:A:ASP:H	1:54:A:ASN:H	6	0.3
(1,2805)	1:53:A:ASP:HB2	1:54:A:ASN:HA	1	0.29
(1,2805)	1:53:A:ASP:HB3	1:54:A:ASN:HA	1	0.29
(1,2508)	1:19:A:ARG:HA	1:19:A:ARG:HG2	13	0.29
(1,2508)	1:19:A:ARG:HA	1:19:A:ARG:HG3	13	0.29
(1,1963)	1:138:A:LEU:HG	1:139:A:TYR:HA	10	0.29
(1,1150)	1:51:A:ILE:H	1:51:A:ILE:HG21	8	0.29
(1,1150)	1:51:A:ILE:H	1:51:A:ILE:HG22	8	0.29
(1,1150)	1:51:A:ILE:H	1:51:A:ILE:HG23	8	0.29
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	4	0.29
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	5	0.29
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	20	0.29
(1,2541)	1:27:A:ARG:HA	1:27:A:ARG:HG2	3	0.28
(1,2541)	1:27:A:ARG:HA	1:27:A:ARG:HG3	3	0.28
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	7	0.28
(1,2805)	1:53:A:ASP:HB2	1:54:A:ASN:HA	14	0.27
(1,2805)	1:53:A:ASP:HB3	1:54:A:ASN:HA	14	0.27
(1,2508)	1:19:A:ARG:HA	1:19:A:ARG:HG2	5	0.27
(1,2508)	1:19:A:ARG:HA	1:19:A:ARG:HG3	5	0.27
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	3	0.27
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	12	0.27
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	16	0.27
(1,3187)	1:101:A:VAL:HG11	1:102:A:THR:HB	15	0.26
(1,3187)	1:101:A:VAL:HG12	1:102:A:THR:HB	15	0.26
(1,3187)	1:101:A:VAL:HG13	1:102:A:THR:HB	15	0.26
(1,3187)	1:101:A:VAL:HG21	1:102:A:THR:HB	15	0.26
(1,3187)	1:101:A:VAL:HG22	1:102:A:THR:HB	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3187)	1:101:A:VAL:HG23	1:102:A:THR:HB	15	0.26
(1,1628)	1:78:A:VAL:HB	1:82:A:GLU:HA	10	0.26
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	2	0.26
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	17	0.26
(1,2805)	1:53:A:ASP:HB2	1:54:A:ASN:HA	17	0.25
(1,2805)	1:53:A:ASP:HB3	1:54:A:ASN:HA	17	0.25
(1,1269)	1:66:A:VAL:HA	1:67:A:LEU:HG	4	0.25
(1,1269)	1:66:A:VAL:HA	1:67:A:LEU:HG	8	0.25
(1,1269)	1:66:A:VAL:HA	1:67:A:LEU:HG	18	0.25
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	19	0.25
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	19	0.25
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	19	0.25
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	14	0.25
(1,3187)	1:101:A:VAL:HG11	1:102:A:THR:HB	5	0.24
(1,3187)	1:101:A:VAL:HG12	1:102:A:THR:HB	5	0.24
(1,3187)	1:101:A:VAL:HG13	1:102:A:THR:HB	5	0.24
(1,3187)	1:101:A:VAL:HG21	1:102:A:THR:HB	5	0.24
(1,3187)	1:101:A:VAL:HG22	1:102:A:THR:HB	5	0.24
(1,3187)	1:101:A:VAL:HG23	1:102:A:THR:HB	5	0.24
(1,2805)	1:53:A:ASP:HB2	1:54:A:ASN:HA	10	0.24
(1,2805)	1:53:A:ASP:HB3	1:54:A:ASN:HA	10	0.24
(1,2224)	1:138:A:LEU:HD11	1:140:A:GLY:HA3	15	0.24
(1,2224)	1:138:A:LEU:HD12	1:140:A:GLY:HA3	15	0.24
(1,2224)	1:138:A:LEU:HD13	1:140:A:GLY:HA3	15	0.24
(1,2805)	1:53:A:ASP:HB2	1:54:A:ASN:HA	18	0.23
(1,2805)	1:53:A:ASP:HB3	1:54:A:ASN:HA	18	0.23
(1,2541)	1:27:A:ARG:HA	1:27:A:ARG:HG2	5	0.23
(1,2541)	1:27:A:ARG:HA	1:27:A:ARG:HG3	5	0.23
(1,2179)	1:101:A:VAL:HG21	1:102:A:THR:HB	19	0.23
(1,2179)	1:101:A:VAL:HG22	1:102:A:THR:HB	19	0.23
(1,2179)	1:101:A:VAL:HG23	1:102:A:THR:HB	19	0.23
(1,1269)	1:66:A:VAL:HA	1:67:A:LEU:HG	16	0.23
(1,3356)	1:133:A:PHE:HZ	1:135:A:LEU:HD11	13	0.22
(1,3356)	1:133:A:PHE:HZ	1:135:A:LEU:HD12	13	0.22
(1,3356)	1:133:A:PHE:HZ	1:135:A:LEU:HD13	13	0.22
(1,3356)	1:133:A:PHE:HZ	1:135:A:LEU:HD21	13	0.22
(1,3356)	1:133:A:PHE:HZ	1:135:A:LEU:HD22	13	0.22
(1,3356)	1:133:A:PHE:HZ	1:135:A:LEU:HD23	13	0.22
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD11	13	0.22
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD12	13	0.22
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD13	13	0.22
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD21	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD22	13	0.22
(1,3036)	1:77:A:THR:HA	1:86:A:LEU:HD23	13	0.22
(1,2507)	1:19:A:ARG:H	1:19:A:ARG:HG2	11	0.22
(1,2507)	1:19:A:ARG:H	1:19:A:ARG:HG3	11	0.22
(1,2224)	1:138:A:LEU:HD11	1:140:A:GLY:HA3	4	0.22
(1,2224)	1:138:A:LEU:HD12	1:140:A:GLY:HA3	4	0.22
(1,2224)	1:138:A:LEU:HD13	1:140:A:GLY:HA3	4	0.22
(1,850)	1:15:A:HIS:HA	1:16:A:ILE:HB	14	0.22
(1,3187)	1:101:A:VAL:HG11	1:102:A:THR:HB	7	0.21
(1,3187)	1:101:A:VAL:HG12	1:102:A:THR:HB	7	0.21
(1,3187)	1:101:A:VAL:HG13	1:102:A:THR:HB	7	0.21
(1,3187)	1:101:A:VAL:HG21	1:102:A:THR:HB	7	0.21
(1,3187)	1:101:A:VAL:HG22	1:102:A:THR:HB	7	0.21
(1,3187)	1:101:A:VAL:HG23	1:102:A:THR:HB	7	0.21
(1,3187)	1:101:A:VAL:HG11	1:102:A:THR:HB	8	0.21
(1,3187)	1:101:A:VAL:HG12	1:102:A:THR:HB	8	0.21
(1,3187)	1:101:A:VAL:HG13	1:102:A:THR:HB	8	0.21
(1,3187)	1:101:A:VAL:HG21	1:102:A:THR:HB	8	0.21
(1,3187)	1:101:A:VAL:HG22	1:102:A:THR:HB	8	0.21
(1,3187)	1:101:A:VAL:HG23	1:102:A:THR:HB	8	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD11	1	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD12	1	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD13	1	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD21	1	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD22	1	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD23	1	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD11	7	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD12	7	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD13	7	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD21	7	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD22	7	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD23	7	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD11	17	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD12	17	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD13	17	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD21	17	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD22	17	0.21
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD23	17	0.21
(1,1628)	1:78:A:VAL:HB	1:82:A:GLU:HA	17	0.21
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	19	0.21
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD1	1	0.2
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD2	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD1	1	0.2
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD2	1	0.2
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD1	1	0.2
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD2	1	0.2
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD1	1	0.2
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD2	1	0.2
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD1	1	0.2
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD2	1	0.2
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD1	1	0.2
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD2	1	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD11	5	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD12	5	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD13	5	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD21	5	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD22	5	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD23	5	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD11	6	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD12	6	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD13	6	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD21	6	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD22	6	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD23	6	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD11	9	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD12	9	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD13	9	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD21	9	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD22	9	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD23	9	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD11	15	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD12	15	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD13	15	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD21	15	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD22	15	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD23	15	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD11	19	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD12	19	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD13	19	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD21	19	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD22	19	0.2
(1,2961)	1:71:A:LEU:HA	1:71:A:LEU:HD23	19	0.2
(1,2399)	1:65:A:HIS:HA	1:65:A:HIS:HD2	12	0.2
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	14	0.2
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	14	0.2
(1,2179)	1:101:A:VAL:HG21	1:102:A:THR:HB	6	0.2
(1,2179)	1:101:A:VAL:HG22	1:102:A:THR:HB	6	0.2
(1,2179)	1:101:A:VAL:HG23	1:102:A:THR:HB	6	0.2
(1,1628)	1:78:A:VAL:HB	1:82:A:GLU:HA	3	0.2
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	3	0.2
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	3	0.2
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	3	0.2
(1,3187)	1:101:A:VAL:HG11	1:102:A:THR:HB	3	0.19
(1,3187)	1:101:A:VAL:HG12	1:102:A:THR:HB	3	0.19
(1,3187)	1:101:A:VAL:HG13	1:102:A:THR:HB	3	0.19
(1,3187)	1:101:A:VAL:HG21	1:102:A:THR:HB	3	0.19
(1,3187)	1:101:A:VAL:HG22	1:102:A:THR:HB	3	0.19
(1,3187)	1:101:A:VAL:HG23	1:102:A:THR:HB	3	0.19
(1,3187)	1:101:A:VAL:HG11	1:102:A:THR:HB	17	0.19
(1,3187)	1:101:A:VAL:HG12	1:102:A:THR:HB	17	0.19
(1,3187)	1:101:A:VAL:HG13	1:102:A:THR:HB	17	0.19
(1,3187)	1:101:A:VAL:HG21	1:102:A:THR:HB	17	0.19
(1,3187)	1:101:A:VAL:HG22	1:102:A:THR:HB	17	0.19
(1,3187)	1:101:A:VAL:HG23	1:102:A:THR:HB	17	0.19
(1,3086)	1:82:A:GLU:HB2	1:83:A:CYS:H	17	0.19
(1,3086)	1:82:A:GLU:HB3	1:83:A:CYS:H	17	0.19
(1,2224)	1:138:A:LEU:HD11	1:140:A:GLY:HA3	12	0.19
(1,2224)	1:138:A:LEU:HD12	1:140:A:GLY:HA3	12	0.19
(1,2224)	1:138:A:LEU:HD13	1:140:A:GLY:HA3	12	0.19
(1,1834)	1:154:A:ALA:HA	1:167:A:ILE:HD11	16	0.19
(1,1834)	1:154:A:ALA:HA	1:167:A:ILE:HD12	16	0.19
(1,1834)	1:154:A:ALA:HA	1:167:A:ILE:HD13	16	0.19
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	7	0.19
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	7	0.19
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	7	0.19
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	9	0.19
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	9	0.19
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	9	0.19
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	8	0.19
(1,1114)	1:45:A:SER:H	1:48:A:ARG:HA	13	0.19
(1,823)	1:180:A:ARG:HA	1:181:A:GLU:H	20	0.19
(1,10)	1:17:A:GLU:H	1:17:A:GLU:HB2	11	0.19
(1,3187)	1:101:A:VAL:HG11	1:102:A:THR:HB	11	0.18
(1,3187)	1:101:A:VAL:HG12	1:102:A:THR:HB	11	0.18
(1,3187)	1:101:A:VAL:HG13	1:102:A:THR:HB	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3187)	1:101:A:VAL:HG21	1:102:A:THR:HB	11	0.18
(1,3187)	1:101:A:VAL:HG22	1:102:A:THR:HB	11	0.18
(1,3187)	1:101:A:VAL:HG23	1:102:A:THR:HB	11	0.18
(1,2834)	1:59:A:LEU:HB2	1:75:A:PHE:HE1	12	0.18
(1,2834)	1:59:A:LEU:HB2	1:75:A:PHE:HE2	12	0.18
(1,2834)	1:59:A:LEU:HB3	1:75:A:PHE:HE1	12	0.18
(1,2834)	1:59:A:LEU:HB3	1:75:A:PHE:HE2	12	0.18
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	1	0.18
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	1	0.18
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	1	0.18
(1,2036)	1:118:A:ASN:HA	1:141:A:ARG:HB2	20	0.18
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	1	0.18
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	1	0.18
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	1	0.18
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	6	0.18
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	6	0.18
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	6	0.18
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	10	0.18
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	10	0.18
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	10	0.18
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	12	0.18
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	12	0.18
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	12	0.18
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	13	0.18
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	13	0.18
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	13	0.18
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	14	0.18
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	14	0.18
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	14	0.18
(1,1079)	1:45:A:SER:HB2	1:51:A:ILE:HG21	8	0.18
(1,1079)	1:45:A:SER:HB2	1:51:A:ILE:HG22	8	0.18
(1,1079)	1:45:A:SER:HB2	1:51:A:ILE:HG23	8	0.18
(1,3500)	1:158:A:GLU:H	1:164:A:ARG:HD2	16	0.17
(1,3500)	1:158:A:GLU:H	1:164:A:ARG:HD3	16	0.17
(1,3408)	1:141:A:ARG:HB2	1:142:A:GLU:HA	20	0.17
(1,3408)	1:141:A:ARG:HB3	1:142:A:GLU:HA	20	0.17
(1,2224)	1:138:A:LEU:HD11	1:140:A:GLY:HA3	19	0.17
(1,2224)	1:138:A:LEU:HD12	1:140:A:GLY:HA3	19	0.17
(1,2224)	1:138:A:LEU:HD13	1:140:A:GLY:HA3	19	0.17
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	8	0.17
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	8	0.17
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	9	0.17
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	9	0.17
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	9	0.17
(1,2036)	1:118:A:ASN:HA	1:141:A:ARG:HB2	6	0.17
(1,2036)	1:118:A:ASN:HA	1:141:A:ARG:HB2	18	0.17
(1,1947)	1:135:A:LEU:HG	1:136:A:MET:H	13	0.17
(1,1362)	1:120:A:LEU:HG	1:122:A:ALA:H	11	0.17
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	2	0.17
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	2	0.17
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	2	0.17
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	5	0.17
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	5	0.17
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	5	0.17
(1,264)	1:67:A:LEU:H	1:67:A:LEU:HG	4	0.17
(1,103)	1:39:A:HIS:H	1:64:A:ILE:HD11	11	0.17
(1,103)	1:39:A:HIS:H	1:64:A:ILE:HD12	11	0.17
(1,103)	1:39:A:HIS:H	1:64:A:ILE:HD13	11	0.17
(1,2224)	1:138:A:LEU:HD11	1:140:A:GLY:HA3	2	0.16
(1,2224)	1:138:A:LEU:HD12	1:140:A:GLY:HA3	2	0.16
(1,2224)	1:138:A:LEU:HD13	1:140:A:GLY:HA3	2	0.16
(1,2158)	1:120:A:LEU:HD21	1:121:A:MET:HA	6	0.16
(1,2158)	1:120:A:LEU:HD22	1:121:A:MET:HA	6	0.16
(1,2158)	1:120:A:LEU:HD23	1:121:A:MET:HA	6	0.16
(1,2036)	1:118:A:ASN:HA	1:141:A:ARG:HB2	13	0.16
(1,2036)	1:118:A:ASN:HA	1:141:A:ARG:HB2	16	0.16
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	17	0.16
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	17	0.16
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	17	0.16
(1,264)	1:67:A:LEU:H	1:67:A:LEU:HG	8	0.16
(1,166)	1:47:A:LYS:H	1:133:A:PHE:HB2	19	0.16
(1,11)	1:16:A:ILE:HB	1:17:A:GLU:H	14	0.16
(1,3408)	1:141:A:ARG:HB2	1:142:A:GLU:HA	8	0.15
(1,3408)	1:141:A:ARG:HB3	1:142:A:GLU:HA	8	0.15
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD1	14	0.15
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD2	14	0.15
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD1	14	0.15
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD2	14	0.15
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD1	14	0.15
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD2	14	0.15
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD1	14	0.15
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD2	14	0.15
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD1	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD2	14	0.15
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD1	14	0.15
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD2	14	0.15
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD1	16	0.15
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD2	16	0.15
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD1	16	0.15
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD2	16	0.15
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD1	16	0.15
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD2	16	0.15
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD1	16	0.15
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD2	16	0.15
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD1	16	0.15
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD2	16	0.15
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD1	16	0.15
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD2	16	0.15
(1,2834)	1:59:A:LEU:HB2	1:75:A:PHE:HE1	2	0.15
(1,2834)	1:59:A:LEU:HB2	1:75:A:PHE:HE2	2	0.15
(1,2834)	1:59:A:LEU:HB3	1:75:A:PHE:HE1	2	0.15
(1,2834)	1:59:A:LEU:HB3	1:75:A:PHE:HE2	2	0.15
(1,2716)	1:45:A:SER:HB2	1:47:A:LYS:H	3	0.15
(1,2716)	1:45:A:SER:HB3	1:47:A:LYS:H	3	0.15
(1,2716)	1:45:A:SER:HB2	1:47:A:LYS:H	17	0.15
(1,2716)	1:45:A:SER:HB3	1:47:A:LYS:H	17	0.15
(1,2514)	1:20:A:GLU:H	1:20:A:GLU:HG2	1	0.15
(1,2514)	1:20:A:GLU:H	1:20:A:GLU:HG3	1	0.15
(1,2507)	1:19:A:ARG:H	1:19:A:ARG:HG2	19	0.15
(1,2507)	1:19:A:ARG:H	1:19:A:ARG:HG3	19	0.15
(1,2501)	1:17:A:GLU:HG2	1:18:A:GLY:HA2	5	0.15
(1,2501)	1:17:A:GLU:HG2	1:18:A:GLY:HA3	5	0.15
(1,2501)	1:17:A:GLU:HG3	1:18:A:GLY:HA2	5	0.15
(1,2501)	1:17:A:GLU:HG3	1:18:A:GLY:HA3	5	0.15
(1,2501)	1:17:A:GLU:HG2	1:18:A:GLY:HA2	17	0.15
(1,2501)	1:17:A:GLU:HG2	1:18:A:GLY:HA3	17	0.15
(1,2501)	1:17:A:GLU:HG3	1:18:A:GLY:HA2	17	0.15
(1,2501)	1:17:A:GLU:HG3	1:18:A:GLY:HA3	17	0.15
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	19	0.15
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	19	0.15
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	19	0.15
(1,2359)	1:86:A:LEU:HG	1:103:A:TYR:HE1	7	0.15
(1,2359)	1:86:A:LEU:HG	1:103:A:TYR:HE2	7	0.15
(1,2359)	1:86:A:LEU:HG	1:103:A:TYR:HE1	9	0.15
(1,2359)	1:86:A:LEU:HG	1:103:A:TYR:HE2	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2300)	1:65:A:HIS:HD2	1:72:A:VAL:HG11	12	0.15
(1,2300)	1:65:A:HIS:HD2	1:72:A:VAL:HG12	12	0.15
(1,2300)	1:65:A:HIS:HD2	1:72:A:VAL:HG13	12	0.15
(1,2224)	1:138:A:LEU:HD11	1:140:A:GLY:HA3	10	0.15
(1,2224)	1:138:A:LEU:HD12	1:140:A:GLY:HA3	10	0.15
(1,2224)	1:138:A:LEU:HD13	1:140:A:GLY:HA3	10	0.15
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	7	0.15
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	7	0.15
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	7	0.15
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	15	0.15
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	15	0.15
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	15	0.15
(1,2158)	1:120:A:LEU:HD21	1:121:A:MET:HA	18	0.15
(1,2158)	1:120:A:LEU:HD22	1:121:A:MET:HA	18	0.15
(1,2158)	1:120:A:LEU:HD23	1:121:A:MET:HA	18	0.15
(1,2123)	1:73:A:LEU:HD21	1:75:A:PHE:HZ	4	0.15
(1,2123)	1:73:A:LEU:HD22	1:75:A:PHE:HZ	4	0.15
(1,2123)	1:73:A:LEU:HD23	1:75:A:PHE:HZ	4	0.15
(1,2123)	1:73:A:LEU:HD21	1:75:A:PHE:HZ	10	0.15
(1,2123)	1:73:A:LEU:HD22	1:75:A:PHE:HZ	10	0.15
(1,2123)	1:73:A:LEU:HD23	1:75:A:PHE:HZ	10	0.15
(1,2123)	1:73:A:LEU:HD21	1:75:A:PHE:HZ	16	0.15
(1,2123)	1:73:A:LEU:HD22	1:75:A:PHE:HZ	16	0.15
(1,2123)	1:73:A:LEU:HD23	1:75:A:PHE:HZ	16	0.15
(1,2123)	1:73:A:LEU:HD21	1:75:A:PHE:HZ	18	0.15
(1,2123)	1:73:A:LEU:HD22	1:75:A:PHE:HZ	18	0.15
(1,2123)	1:73:A:LEU:HD23	1:75:A:PHE:HZ	18	0.15
(1,2123)	1:73:A:LEU:HD21	1:75:A:PHE:HZ	20	0.15
(1,2123)	1:73:A:LEU:HD22	1:75:A:PHE:HZ	20	0.15
(1,2123)	1:73:A:LEU:HD23	1:75:A:PHE:HZ	20	0.15
(1,2050)	1:101:A:VAL:HB	1:103:A:TYR:HD1	1	0.15
(1,2050)	1:101:A:VAL:HB	1:103:A:TYR:HD2	1	0.15
(1,2050)	1:101:A:VAL:HB	1:103:A:TYR:HD1	14	0.15
(1,2050)	1:101:A:VAL:HB	1:103:A:TYR:HD2	14	0.15
(1,2036)	1:118:A:ASN:HA	1:141:A:ARG:HB2	8	0.15
(1,1984)	1:94:A:GLU:HA	1:94:A:GLU:HG2	7	0.15
(1,1984)	1:94:A:GLU:HA	1:94:A:GLU:HG2	8	0.15
(1,1922)	1:133:A:PHE:HE1	1:135:A:LEU:HB3	5	0.15
(1,1922)	1:133:A:PHE:HE2	1:135:A:LEU:HB3	5	0.15
(1,1899)	1:154:A:ALA:HA	1:167:A:ILE:HG21	16	0.15
(1,1899)	1:154:A:ALA:HA	1:167:A:ILE:HG22	16	0.15
(1,1899)	1:154:A:ALA:HA	1:167:A:ILE:HG23	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1802)	1:101:A:VAL:HG11	1:103:A:TYR:HD1	7	0.15
(1,1802)	1:101:A:VAL:HG11	1:103:A:TYR:HD2	7	0.15
(1,1802)	1:101:A:VAL:HG12	1:103:A:TYR:HD1	7	0.15
(1,1802)	1:101:A:VAL:HG12	1:103:A:TYR:HD2	7	0.15
(1,1802)	1:101:A:VAL:HG13	1:103:A:TYR:HD1	7	0.15
(1,1802)	1:101:A:VAL:HG13	1:103:A:TYR:HD2	7	0.15
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	8	0.15
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	8	0.15
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	8	0.15
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	11	0.15
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	11	0.15
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	11	0.15
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	20	0.15
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	20	0.15
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	20	0.15
(1,166)	1:47:A:LYS:H	1:133:A:PHE:HB2	13	0.15
(1,3513)	1:159:A:GLU:HB2	1:160:A:HIS:H	20	0.14
(1,3513)	1:159:A:GLU:HB3	1:160:A:HIS:H	20	0.14
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD1	13	0.14
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD2	13	0.14
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD1	13	0.14
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD2	13	0.14
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD1	13	0.14
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD2	13	0.14
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD1	13	0.14
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD2	13	0.14
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD1	13	0.14
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD2	13	0.14
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD1	13	0.14
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD2	13	0.14
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD1	18	0.14
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD2	18	0.14
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD1	18	0.14
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD2	18	0.14
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD1	18	0.14
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD2	18	0.14
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD1	18	0.14
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD2	18	0.14
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD1	18	0.14
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD2	18	0.14
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD1	18	0.14
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD2	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3179)	1:100:A:SER:HB2	1:101:A:VAL:H	16	0.14
(1,3179)	1:100:A:SER:HB3	1:101:A:VAL:H	16	0.14
(1,3077)	1:80:A:ASP:HB2	1:82:A:GLU:HG2	17	0.14
(1,3077)	1:80:A:ASP:HB2	1:82:A:GLU:HG3	17	0.14
(1,3077)	1:80:A:ASP:HB3	1:82:A:GLU:HG2	17	0.14
(1,3077)	1:80:A:ASP:HB3	1:82:A:GLU:HG3	17	0.14
(1,3061)	1:79:A:ARG:H	1:82:A:GLU:HB2	17	0.14
(1,3061)	1:79:A:ARG:H	1:82:A:GLU:HB3	17	0.14
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	2	0.14
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	2	0.14
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	2	0.14
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	2	0.14
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	2	0.14
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	2	0.14
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	11	0.14
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	11	0.14
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	11	0.14
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	11	0.14
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	11	0.14
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	11	0.14
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	13	0.14
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	13	0.14
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	13	0.14
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	13	0.14
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	13	0.14
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	13	0.14
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	15	0.14
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	15	0.14
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	15	0.14
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	15	0.14
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	15	0.14
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	15	0.14
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	16	0.14
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	16	0.14
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	16	0.14
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	16	0.14
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	16	0.14
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	16	0.14
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	18	0.14
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	18	0.14
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	18	0.14
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	18	0.14
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	18	0.14
(1,2834)	1:59:A:LEU:HB2	1:75:A:PHE:HE1	3	0.14
(1,2834)	1:59:A:LEU:HB2	1:75:A:PHE:HE2	3	0.14
(1,2834)	1:59:A:LEU:HB3	1:75:A:PHE:HE1	3	0.14
(1,2834)	1:59:A:LEU:HB3	1:75:A:PHE:HE2	3	0.14
(1,2818)	1:57:A:PHE:H	1:135:A:LEU:HD11	13	0.14
(1,2818)	1:57:A:PHE:H	1:135:A:LEU:HD12	13	0.14
(1,2818)	1:57:A:PHE:H	1:135:A:LEU:HD13	13	0.14
(1,2818)	1:57:A:PHE:H	1:135:A:LEU:HD21	13	0.14
(1,2818)	1:57:A:PHE:H	1:135:A:LEU:HD22	13	0.14
(1,2818)	1:57:A:PHE:H	1:135:A:LEU:HD23	13	0.14
(1,2501)	1:17:A:GLU:HG2	1:18:A:GLY:HA2	19	0.14
(1,2501)	1:17:A:GLU:HG2	1:18:A:GLY:HA3	19	0.14
(1,2501)	1:17:A:GLU:HG3	1:18:A:GLY:HA2	19	0.14
(1,2501)	1:17:A:GLU:HG3	1:18:A:GLY:HA3	19	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	4	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	4	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	4	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	5	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	5	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	5	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	7	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	7	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	7	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	8	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	8	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	8	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	15	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	15	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	15	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	16	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	16	0.14
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	16	0.14
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	19	0.14
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	19	0.14
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	19	0.14
(1,2158)	1:120:A:LEU:HD21	1:121:A:MET:HA	16	0.14
(1,2158)	1:120:A:LEU:HD22	1:121:A:MET:HA	16	0.14
(1,2158)	1:120:A:LEU:HD23	1:121:A:MET:HA	16	0.14
(1,2158)	1:120:A:LEU:HD21	1:121:A:MET:HA	20	0.14
(1,2158)	1:120:A:LEU:HD22	1:121:A:MET:HA	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2158)	1:120:A:LEU:HD23	1:121:A:MET:HA	20	0.14
(1,2123)	1:73:A:LEU:HD21	1:75:A:PHE:HZ	8	0.14
(1,2123)	1:73:A:LEU:HD22	1:75:A:PHE:HZ	8	0.14
(1,2123)	1:73:A:LEU:HD23	1:75:A:PHE:HZ	8	0.14
(1,2123)	1:73:A:LEU:HD21	1:75:A:PHE:HZ	11	0.14
(1,2123)	1:73:A:LEU:HD22	1:75:A:PHE:HZ	11	0.14
(1,2123)	1:73:A:LEU:HD23	1:75:A:PHE:HZ	11	0.14
(1,2123)	1:73:A:LEU:HD21	1:75:A:PHE:HZ	19	0.14
(1,2123)	1:73:A:LEU:HD22	1:75:A:PHE:HZ	19	0.14
(1,2123)	1:73:A:LEU:HD23	1:75:A:PHE:HZ	19	0.14
(1,2050)	1:101:A:VAL:HB	1:103:A:TYR:HD1	9	0.14
(1,2050)	1:101:A:VAL:HB	1:103:A:TYR:HD2	9	0.14
(1,1947)	1:135:A:LEU:HG	1:136:A:MET:H	5	0.14
(1,1922)	1:133:A:PHE:HE1	1:135:A:LEU:HB3	10	0.14
(1,1922)	1:133:A:PHE:HE2	1:135:A:LEU:HB3	10	0.14
(1,1740)	1:94:A:GLU:HA	1:94:A:GLU:HG3	14	0.14
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	14	0.14
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	15	0.14
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	20	0.14
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	16	0.14
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	16	0.14
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	16	0.14
(1,771)	1:162:A:ILE:H	1:167:A:ILE:HD11	18	0.14
(1,771)	1:162:A:ILE:H	1:167:A:ILE:HD12	18	0.14
(1,771)	1:162:A:ILE:H	1:167:A:ILE:HD13	18	0.14
(1,264)	1:67:A:LEU:H	1:67:A:LEU:HG	16	0.14
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD1	2	0.13
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD2	2	0.13
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD1	2	0.13
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD2	2	0.13
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD1	2	0.13
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD2	2	0.13
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD1	2	0.13
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD2	2	0.13
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD1	2	0.13
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD2	2	0.13
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD1	2	0.13
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD2	2	0.13
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD1	4	0.13
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD2	4	0.13
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD1	4	0.13
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD2	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD1	4	0.13
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD2	4	0.13
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD1	4	0.13
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD2	4	0.13
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD1	4	0.13
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD2	4	0.13
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD1	4	0.13
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD2	4	0.13
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD1	20	0.13
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD2	20	0.13
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD1	20	0.13
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD2	20	0.13
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD1	20	0.13
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD2	20	0.13
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD1	20	0.13
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD2	20	0.13
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD1	20	0.13
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD2	20	0.13
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD1	20	0.13
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD2	20	0.13
(1,3179)	1:100:A:SER:HB2	1:101:A:VAL:H	18	0.13
(1,3179)	1:100:A:SER:HB3	1:101:A:VAL:H	18	0.13
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	4	0.13
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	4	0.13
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	4	0.13
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	4	0.13
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	4	0.13
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	4	0.13
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	5	0.13
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	5	0.13
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	5	0.13
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	5	0.13
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	5	0.13
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	5	0.13
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	6	0.13
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	6	0.13
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	6	0.13
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	6	0.13
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	6	0.13
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	6	0.13
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	12	0.13
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	12	0.13
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	12	0.13
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	12	0.13
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	12	0.13
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	14	0.13
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	14	0.13
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	14	0.13
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	14	0.13
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	14	0.13
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	14	0.13
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	19	0.13
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	19	0.13
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	19	0.13
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	19	0.13
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	19	0.13
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	19	0.13
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	20	0.13
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	20	0.13
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	20	0.13
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	20	0.13
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	20	0.13
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	20	0.13
(1,2885)	1:63:A:GLN:HG2	1:64:A:ILE:H	19	0.13
(1,2885)	1:63:A:GLN:HG3	1:64:A:ILE:H	19	0.13
(1,2869)	1:61:A:LEU:HD11	1:76:A:HIS:H	13	0.13
(1,2869)	1:61:A:LEU:HD12	1:76:A:HIS:H	13	0.13
(1,2869)	1:61:A:LEU:HD13	1:76:A:HIS:H	13	0.13
(1,2869)	1:61:A:LEU:HD21	1:76:A:HIS:H	13	0.13
(1,2869)	1:61:A:LEU:HD22	1:76:A:HIS:H	13	0.13
(1,2869)	1:61:A:LEU:HD23	1:76:A:HIS:H	13	0.13
(1,2716)	1:45:A:SER:HB2	1:47:A:LYS:H	20	0.13
(1,2716)	1:45:A:SER:HB3	1:47:A:LYS:H	20	0.13
(1,2511)	1:19:A:ARG:HB2	1:20:A:GLU:H	11	0.13
(1,2511)	1:19:A:ARG:HB3	1:20:A:GLU:H	11	0.13
(1,2501)	1:17:A:GLU:HG2	1:18:A:GLY:HA2	1	0.13
(1,2501)	1:17:A:GLU:HG2	1:18:A:GLY:HA3	1	0.13
(1,2501)	1:17:A:GLU:HG3	1:18:A:GLY:HA2	1	0.13
(1,2501)	1:17:A:GLU:HG3	1:18:A:GLY:HA3	1	0.13
(1,2399)	1:65:A:HIS:HA	1:65:A:HIS:HD2	18	0.13
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	6	0.13
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	6	0.13
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	13	0.13
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	13	0.13
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	13	0.13
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	18	0.13
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	18	0.13
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	18	0.13
(1,2359)	1:86:A:LEU:HG	1:103:A:TYR:HE1	14	0.13
(1,2359)	1:86:A:LEU:HG	1:103:A:TYR:HE2	14	0.13
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	5	0.13
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	5	0.13
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	5	0.13
(1,2203)	1:147:A:SER:HA	1:150:A:LYS:HA	3	0.13
(1,2158)	1:120:A:LEU:HD21	1:121:A:MET:HA	7	0.13
(1,2158)	1:120:A:LEU:HD22	1:121:A:MET:HA	7	0.13
(1,2158)	1:120:A:LEU:HD23	1:121:A:MET:HA	7	0.13
(1,2158)	1:120:A:LEU:HD21	1:121:A:MET:HA	8	0.13
(1,2158)	1:120:A:LEU:HD22	1:121:A:MET:HA	8	0.13
(1,2158)	1:120:A:LEU:HD23	1:121:A:MET:HA	8	0.13
(1,2158)	1:120:A:LEU:HD21	1:121:A:MET:HA	10	0.13
(1,2158)	1:120:A:LEU:HD22	1:121:A:MET:HA	10	0.13
(1,2158)	1:120:A:LEU:HD23	1:121:A:MET:HA	10	0.13
(1,2036)	1:118:A:ASN:HA	1:141:A:ARG:HB2	9	0.13
(1,1899)	1:154:A:ALA:HA	1:167:A:ILE:HG21	20	0.13
(1,1899)	1:154:A:ALA:HA	1:167:A:ILE:HG22	20	0.13
(1,1899)	1:154:A:ALA:HA	1:167:A:ILE:HG23	20	0.13
(1,1865)	1:156:A:LEU:HA	1:159:A:GLU:HG3	20	0.13
(1,1834)	1:154:A:ALA:HA	1:167:A:ILE:HD11	17	0.13
(1,1834)	1:154:A:ALA:HA	1:167:A:ILE:HD12	17	0.13
(1,1834)	1:154:A:ALA:HA	1:167:A:ILE:HD13	17	0.13
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	1	0.13
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	2	0.13
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	3	0.13
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	7	0.13
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	10	0.13
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	11	0.13
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	12	0.13
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	19	0.13
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	15	0.13
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	15	0.13
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	15	0.13
(1,1156)	1:51:A:ILE:HG21	1:135:A:LEU:HG	13	0.13
(1,1156)	1:51:A:ILE:HG22	1:135:A:LEU:HG	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1156)	1:51:A:ILE:HG23	1:135:A:LEU:HG	13	0.13
(1,1067)	1:44:A:ALA:HA	1:167:A:ILE:HB	16	0.13
(1,771)	1:162:A:ILE:H	1:167:A:ILE:HD11	1	0.13
(1,771)	1:162:A:ILE:H	1:167:A:ILE:HD12	1	0.13
(1,771)	1:162:A:ILE:H	1:167:A:ILE:HD13	1	0.13
(1,16)	1:17:A:GLU:HB3	1:18:A:GLY:H	1	0.13
(1,16)	1:17:A:GLU:HB3	1:18:A:GLY:H	19	0.13
(1,3283)	1:120:A:LEU:HD11	1:138:A:LEU:HA	19	0.12
(1,3283)	1:120:A:LEU:HD12	1:138:A:LEU:HA	19	0.12
(1,3283)	1:120:A:LEU:HD13	1:138:A:LEU:HA	19	0.12
(1,3283)	1:120:A:LEU:HD21	1:138:A:LEU:HA	19	0.12
(1,3283)	1:120:A:LEU:HD22	1:138:A:LEU:HA	19	0.12
(1,3283)	1:120:A:LEU:HD23	1:138:A:LEU:HA	19	0.12
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD1	10	0.12
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD2	10	0.12
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD1	10	0.12
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD2	10	0.12
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD1	10	0.12
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD2	10	0.12
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD1	10	0.12
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD2	10	0.12
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD1	10	0.12
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD2	10	0.12
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD1	10	0.12
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD2	10	0.12
(1,3193)	1:101:A:VAL:HG11	1:107:A:ASN:HA	6	0.12
(1,3193)	1:101:A:VAL:HG12	1:107:A:ASN:HA	6	0.12
(1,3193)	1:101:A:VAL:HG13	1:107:A:ASN:HA	6	0.12
(1,3193)	1:101:A:VAL:HG21	1:107:A:ASN:HA	6	0.12
(1,3193)	1:101:A:VAL:HG22	1:107:A:ASN:HA	6	0.12
(1,3193)	1:101:A:VAL:HG23	1:107:A:ASN:HA	6	0.12
(1,3087)	1:82:A:GLU:HB2	1:83:A:CYS:HA	17	0.12
(1,3087)	1:82:A:GLU:HB3	1:83:A:CYS:HA	17	0.12
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	1	0.12
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	1	0.12
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	1	0.12
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	1	0.12
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	1	0.12
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	1	0.12
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	7	0.12
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	7	0.12
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	7	0.12
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	7	0.12
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	7	0.12
(1,3043)	1:78:A:VAL:HG11	1:79:A:ARG:H	8	0.12
(1,3043)	1:78:A:VAL:HG12	1:79:A:ARG:H	8	0.12
(1,3043)	1:78:A:VAL:HG13	1:79:A:ARG:H	8	0.12
(1,3043)	1:78:A:VAL:HG21	1:79:A:ARG:H	8	0.12
(1,3043)	1:78:A:VAL:HG22	1:79:A:ARG:H	8	0.12
(1,3043)	1:78:A:VAL:HG23	1:79:A:ARG:H	8	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD11	8	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD12	8	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD13	8	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD21	8	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD22	8	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD23	8	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD11	16	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD12	16	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD13	16	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD21	16	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD22	16	0.12
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD23	16	0.12
(1,2716)	1:45:A:SER:HB2	1:47:A:LYS:H	4	0.12
(1,2716)	1:45:A:SER:HB3	1:47:A:LYS:H	4	0.12
(1,2501)	1:17:A:GLU:HG2	1:18:A:GLY:HA2	10	0.12
(1,2501)	1:17:A:GLU:HG2	1:18:A:GLY:HA3	10	0.12
(1,2501)	1:17:A:GLU:HG3	1:18:A:GLY:HA2	10	0.12
(1,2501)	1:17:A:GLU:HG3	1:18:A:GLY:HA3	10	0.12
(1,2497)	1:17:A:GLU:H	1:17:A:GLU:HG2	18	0.12
(1,2497)	1:17:A:GLU:H	1:17:A:GLU:HG3	18	0.12
(1,2496)	1:16:A:ILE:HG21	1:18:A:GLY:HA2	18	0.12
(1,2496)	1:16:A:ILE:HG21	1:18:A:GLY:HA3	18	0.12
(1,2496)	1:16:A:ILE:HG22	1:18:A:GLY:HA2	18	0.12
(1,2496)	1:16:A:ILE:HG22	1:18:A:GLY:HA3	18	0.12
(1,2496)	1:16:A:ILE:HG23	1:18:A:GLY:HA2	18	0.12
(1,2496)	1:16:A:ILE:HG23	1:18:A:GLY:HA3	18	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	1	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	1	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	1	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	2	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	2	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	2	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	3	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	3	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	9	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	9	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	9	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	10	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	10	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	10	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	12	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	12	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	12	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	20	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	20	0.12
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	20	0.12
(1,2293)	1:57:A:PHE:HB3	1:135:A:LEU:HD11	13	0.12
(1,2293)	1:57:A:PHE:HB3	1:135:A:LEU:HD12	13	0.12
(1,2293)	1:57:A:PHE:HB3	1:135:A:LEU:HD13	13	0.12
(1,2282)	1:154:A:ALA:HB1	1:164:A:ARG:H	18	0.12
(1,2282)	1:154:A:ALA:HB2	1:164:A:ARG:H	18	0.12
(1,2282)	1:154:A:ALA:HB3	1:164:A:ARG:H	18	0.12
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	12	0.12
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	12	0.12
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	12	0.12
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	16	0.12
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	16	0.12
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	16	0.12
(1,2158)	1:120:A:LEU:HD21	1:121:A:MET:HA	1	0.12
(1,2158)	1:120:A:LEU:HD22	1:121:A:MET:HA	1	0.12
(1,2158)	1:120:A:LEU:HD23	1:121:A:MET:HA	1	0.12
(1,2158)	1:120:A:LEU:HD21	1:121:A:MET:HA	3	0.12
(1,2158)	1:120:A:LEU:HD22	1:121:A:MET:HA	3	0.12
(1,2158)	1:120:A:LEU:HD23	1:121:A:MET:HA	3	0.12
(1,2158)	1:120:A:LEU:HD21	1:121:A:MET:HA	17	0.12
(1,2158)	1:120:A:LEU:HD22	1:121:A:MET:HA	17	0.12
(1,2158)	1:120:A:LEU:HD23	1:121:A:MET:HA	17	0.12
(1,2050)	1:101:A:VAL:HB	1:103:A:TYR:HD1	2	0.12
(1,2050)	1:101:A:VAL:HB	1:103:A:TYR:HD2	2	0.12
(1,2050)	1:101:A:VAL:HB	1:103:A:TYR:HD1	12	0.12
(1,2050)	1:101:A:VAL:HB	1:103:A:TYR:HD2	12	0.12
(1,1463)	1:109:A:PHE:HB3	1:124:A:LEU:HA	8	0.12
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	6	0.12
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	13	0.12
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	17	0.12
(1,1327)	1:109:A:PHE:H	1:124:A:LEU:HD21	3	0.12
(1,1327)	1:109:A:PHE:H	1:124:A:LEU:HD22	3	0.12
(1,1327)	1:109:A:PHE:H	1:124:A:LEU:HD23	3	0.12
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	4	0.12
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	4	0.12
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	4	0.12
(1,1217)	1:61:A:LEU:HD21	1:64:A:ILE:HA	18	0.12
(1,1217)	1:61:A:LEU:HD22	1:64:A:ILE:HA	18	0.12
(1,1217)	1:61:A:LEU:HD23	1:64:A:ILE:HA	18	0.12
(1,1142)	1:44:A:ALA:HA	1:51:A:ILE:HD11	8	0.12
(1,1142)	1:44:A:ALA:HA	1:51:A:ILE:HD12	8	0.12
(1,1142)	1:44:A:ALA:HA	1:51:A:ILE:HD13	8	0.12
(1,771)	1:162:A:ILE:H	1:167:A:ILE:HD11	7	0.12
(1,771)	1:162:A:ILE:H	1:167:A:ILE:HD12	7	0.12
(1,771)	1:162:A:ILE:H	1:167:A:ILE:HD13	7	0.12
(1,771)	1:162:A:ILE:H	1:167:A:ILE:HD11	16	0.12
(1,771)	1:162:A:ILE:H	1:167:A:ILE:HD12	16	0.12
(1,771)	1:162:A:ILE:H	1:167:A:ILE:HD13	16	0.12
(1,3592)	1:172:A:ASN:HB2	1:173:A:ALA:HB1	20	0.11
(1,3592)	1:172:A:ASN:HB2	1:173:A:ALA:HB2	20	0.11
(1,3592)	1:172:A:ASN:HB2	1:173:A:ALA:HB3	20	0.11
(1,3592)	1:172:A:ASN:HB3	1:173:A:ALA:HB1	20	0.11
(1,3592)	1:172:A:ASN:HB3	1:173:A:ALA:HB2	20	0.11
(1,3592)	1:172:A:ASN:HB3	1:173:A:ALA:HB3	20	0.11
(1,3577)	1:170:A:LEU:HA	1:170:A:LEU:HD11	13	0.11
(1,3577)	1:170:A:LEU:HA	1:170:A:LEU:HD12	13	0.11
(1,3577)	1:170:A:LEU:HA	1:170:A:LEU:HD13	13	0.11
(1,3577)	1:170:A:LEU:HA	1:170:A:LEU:HD21	13	0.11
(1,3577)	1:170:A:LEU:HA	1:170:A:LEU:HD22	13	0.11
(1,3577)	1:170:A:LEU:HA	1:170:A:LEU:HD23	13	0.11
(1,3492)	1:157:A:CYS:HB2	1:162:A:ILE:H	20	0.11
(1,3492)	1:157:A:CYS:HB3	1:162:A:ILE:H	20	0.11
(1,3417)	1:142:A:GLU:HG2	1:144:A:ASP:H	12	0.11
(1,3417)	1:142:A:GLU:HG3	1:144:A:ASP:H	12	0.11
(1,3365)	1:134:A:GLN:HG2	1:162:A:ILE:HD11	11	0.11
(1,3365)	1:134:A:GLN:HG2	1:162:A:ILE:HD12	11	0.11
(1,3365)	1:134:A:GLN:HG2	1:162:A:ILE:HD13	11	0.11
(1,3365)	1:134:A:GLN:HG3	1:162:A:ILE:HD11	11	0.11
(1,3365)	1:134:A:GLN:HG3	1:162:A:ILE:HD12	11	0.11
(1,3365)	1:134:A:GLN:HG3	1:162:A:ILE:HD13	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3283)	1:120:A:LEU:HD11	1:138:A:LEU:HA	12	0.11
(1,3283)	1:120:A:LEU:HD12	1:138:A:LEU:HA	12	0.11
(1,3283)	1:120:A:LEU:HD13	1:138:A:LEU:HA	12	0.11
(1,3283)	1:120:A:LEU:HD21	1:138:A:LEU:HA	12	0.11
(1,3283)	1:120:A:LEU:HD22	1:138:A:LEU:HA	12	0.11
(1,3283)	1:120:A:LEU:HD23	1:138:A:LEU:HA	12	0.11
(1,3224)	1:109:A:PHE:HB3	1:124:A:LEU:HB2	11	0.11
(1,3224)	1:109:A:PHE:HB3	1:124:A:LEU:HB3	11	0.11
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD1	9	0.11
(1,3199)	1:101:A:VAL:HG11	1:109:A:PHE:HD2	9	0.11
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD1	9	0.11
(1,3199)	1:101:A:VAL:HG12	1:109:A:PHE:HD2	9	0.11
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD1	9	0.11
(1,3199)	1:101:A:VAL:HG13	1:109:A:PHE:HD2	9	0.11
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD1	9	0.11
(1,3199)	1:101:A:VAL:HG21	1:109:A:PHE:HD2	9	0.11
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD1	9	0.11
(1,3199)	1:101:A:VAL:HG22	1:109:A:PHE:HD2	9	0.11
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD1	9	0.11
(1,3199)	1:101:A:VAL:HG23	1:109:A:PHE:HD2	9	0.11
(1,3193)	1:101:A:VAL:HG11	1:107:A:ASN:HA	19	0.11
(1,3193)	1:101:A:VAL:HG12	1:107:A:ASN:HA	19	0.11
(1,3193)	1:101:A:VAL:HG13	1:107:A:ASN:HA	19	0.11
(1,3193)	1:101:A:VAL:HG21	1:107:A:ASN:HA	19	0.11
(1,3193)	1:101:A:VAL:HG22	1:107:A:ASN:HA	19	0.11
(1,3193)	1:101:A:VAL:HG23	1:107:A:ASN:HA	19	0.11
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD11	4	0.11
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD12	4	0.11
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD13	4	0.11
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD21	4	0.11
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD22	4	0.11
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD23	4	0.11
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD11	18	0.11
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD12	18	0.11
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD13	18	0.11
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD21	18	0.11
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD22	18	0.11
(1,2912)	1:66:A:VAL:HA	1:71:A:LEU:HD23	18	0.11
(1,2834)	1:59:A:LEU:HB2	1:75:A:PHE:HE1	18	0.11
(1,2834)	1:59:A:LEU:HB2	1:75:A:PHE:HE2	18	0.11
(1,2834)	1:59:A:LEU:HB3	1:75:A:PHE:HE1	18	0.11
(1,2834)	1:59:A:LEU:HB3	1:75:A:PHE:HE2	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2716)	1:45:A:SER:HB2	1:47:A:LYS:H	7	0.11
(1,2716)	1:45:A:SER:HB3	1:47:A:LYS:H	7	0.11
(1,2501)	1:17:A:GLU:HG2	1:18:A:GLY:HA2	18	0.11
(1,2501)	1:17:A:GLU:HG2	1:18:A:GLY:HA3	18	0.11
(1,2501)	1:17:A:GLU:HG3	1:18:A:GLY:HA2	18	0.11
(1,2501)	1:17:A:GLU:HG3	1:18:A:GLY:HA3	18	0.11
(1,2399)	1:65:A:HIS:HA	1:65:A:HIS:HD2	16	0.11
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	14	0.11
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	14	0.11
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	14	0.11
(1,2359)	1:86:A:LEU:HG	1:103:A:TYR:HE1	1	0.11
(1,2359)	1:86:A:LEU:HG	1:103:A:TYR:HE2	1	0.11
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	6	0.11
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	6	0.11
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	6	0.11
(1,2158)	1:120:A:LEU:HD21	1:121:A:MET:HA	5	0.11
(1,2158)	1:120:A:LEU:HD22	1:121:A:MET:HA	5	0.11
(1,2158)	1:120:A:LEU:HD23	1:121:A:MET:HA	5	0.11
(1,2158)	1:120:A:LEU:HD21	1:121:A:MET:HA	13	0.11
(1,2158)	1:120:A:LEU:HD22	1:121:A:MET:HA	13	0.11
(1,2158)	1:120:A:LEU:HD23	1:121:A:MET:HA	13	0.11
(1,2129)	1:113:A:LYS:HB3	1:119:A:PHE:HE1	19	0.11
(1,2129)	1:113:A:LYS:HB3	1:119:A:PHE:HE2	19	0.11
(1,2123)	1:73:A:LEU:HD21	1:75:A:PHE:HZ	14	0.11
(1,2123)	1:73:A:LEU:HD22	1:75:A:PHE:HZ	14	0.11
(1,2123)	1:73:A:LEU:HD23	1:75:A:PHE:HZ	14	0.11
(1,1947)	1:135:A:LEU:HG	1:136:A:MET:H	10	0.11
(1,1947)	1:135:A:LEU:HG	1:136:A:MET:H	11	0.11
(1,1730)	1:158:A:GLU:HA	1:163:A:LEU:HB3	20	0.11
(1,1523)	1:34:A:ILE:HG13	1:120:A:LEU:HD11	11	0.11
(1,1523)	1:34:A:ILE:HG13	1:120:A:LEU:HD12	11	0.11
(1,1523)	1:34:A:ILE:HG13	1:120:A:LEU:HD13	11	0.11
(1,1458)	1:67:A:LEU:HG	1:68:A:GLU:H	5	0.11
(1,1349)	1:65:A:HIS:HD2	1:72:A:VAL:HG21	18	0.11
(1,1349)	1:65:A:HIS:HD2	1:72:A:VAL:HG22	18	0.11
(1,1349)	1:65:A:HIS:HD2	1:72:A:VAL:HG23	18	0.11
(1,1327)	1:109:A:PHE:H	1:124:A:LEU:HD21	11	0.11
(1,1327)	1:109:A:PHE:H	1:124:A:LEU:HD22	11	0.11
(1,1327)	1:109:A:PHE:H	1:124:A:LEU:HD23	11	0.11
(1,1213)	1:39:A:HIS:H	1:61:A:LEU:HD11	7	0.11
(1,1213)	1:39:A:HIS:H	1:61:A:LEU:HD12	7	0.11
(1,1213)	1:39:A:HIS:H	1:61:A:LEU:HD13	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1213)	1:39:A:HIS:H	1:61:A:LEU:HD11	13	0.11
(1,1213)	1:39:A:HIS:H	1:61:A:LEU:HD12	13	0.11
(1,1213)	1:39:A:HIS:H	1:61:A:LEU:HD13	13	0.11
(1,929)	1:142:A:GLU:HA	1:142:A:GLU:HG3	7	0.11
(1,819)	1:173:A:ALA:H	1:174:A:ASN:H	20	0.11
(1,538)	1:41:A:ILE:HG12	1:120:A:LEU:H	10	0.11
(1,511)	1:116:A:TYR:H	1:119:A:PHE:H	20	0.11
(1,450)	1:101:A:VAL:H	1:107:A:ASN:H	1	0.11
(1,188)	1:50:A:LYS:H	1:51:A:ILE:HD11	8	0.11
(1,188)	1:50:A:LYS:H	1:51:A:ILE:HD12	8	0.11
(1,188)	1:50:A:LYS:H	1:51:A:ILE:HD13	8	0.11
(1,166)	1:47:A:LYS:H	1:133:A:PHE:HB2	15	0.11
(1,165)	1:47:A:LYS:H	1:133:A:PHE:HD1	13	0.11
(1,165)	1:47:A:LYS:H	1:133:A:PHE:HD2	13	0.11
(1,103)	1:39:A:HIS:H	1:64:A:ILE:HD11	3	0.11
(1,103)	1:39:A:HIS:H	1:64:A:ILE:HD12	3	0.11
(1,103)	1:39:A:HIS:H	1:64:A:ILE:HD13	3	0.11
(1,103)	1:39:A:HIS:H	1:64:A:ILE:HD11	20	0.11
(1,103)	1:39:A:HIS:H	1:64:A:ILE:HD12	20	0.11
(1,103)	1:39:A:HIS:H	1:64:A:ILE:HD13	20	0.11
(1,16)	1:17:A:GLU:HB3	1:18:A:GLY:H	17	0.11
(1,3541)	1:163:A:LEU:HD11	1:165:A:GLU:HA	11	0.1
(1,3541)	1:163:A:LEU:HD12	1:165:A:GLU:HA	11	0.1
(1,3541)	1:163:A:LEU:HD13	1:165:A:GLU:HA	11	0.1
(1,3541)	1:163:A:LEU:HD21	1:165:A:GLU:HA	11	0.1
(1,3541)	1:163:A:LEU:HD22	1:165:A:GLU:HA	11	0.1
(1,3541)	1:163:A:LEU:HD23	1:165:A:GLU:HA	11	0.1
(1,3500)	1:158:A:GLU:H	1:164:A:ARG:HD2	1	0.1
(1,3500)	1:158:A:GLU:H	1:164:A:ARG:HD3	1	0.1
(1,3179)	1:100:A:SER:HB2	1:101:A:VAL:H	4	0.1
(1,3179)	1:100:A:SER:HB3	1:101:A:VAL:H	4	0.1
(1,3179)	1:100:A:SER:HB2	1:101:A:VAL:H	6	0.1
(1,3179)	1:100:A:SER:HB3	1:101:A:VAL:H	6	0.1
(1,3061)	1:79:A:ARG:H	1:82:A:GLU:HB2	9	0.1
(1,3061)	1:79:A:ARG:H	1:82:A:GLU:HB3	9	0.1
(1,2834)	1:59:A:LEU:HB2	1:75:A:PHE:HE1	6	0.1
(1,2834)	1:59:A:LEU:HB2	1:75:A:PHE:HE2	6	0.1
(1,2834)	1:59:A:LEU:HB3	1:75:A:PHE:HE1	6	0.1
(1,2834)	1:59:A:LEU:HB3	1:75:A:PHE:HE2	6	0.1
(1,2834)	1:59:A:LEU:HB2	1:75:A:PHE:HE1	16	0.1
(1,2834)	1:59:A:LEU:HB2	1:75:A:PHE:HE2	16	0.1
(1,2834)	1:59:A:LEU:HB3	1:75:A:PHE:HE1	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2834)	1:59:A:LEU:HB3	1:75:A:PHE:HE2	16	0.1
(1,2791)	1:51:A:ILE:HA	1:135:A:LEU:HD11	13	0.1
(1,2791)	1:51:A:ILE:HA	1:135:A:LEU:HD12	13	0.1
(1,2791)	1:51:A:ILE:HA	1:135:A:LEU:HD13	13	0.1
(1,2791)	1:51:A:ILE:HA	1:135:A:LEU:HD21	13	0.1
(1,2791)	1:51:A:ILE:HA	1:135:A:LEU:HD22	13	0.1
(1,2791)	1:51:A:ILE:HA	1:135:A:LEU:HD23	13	0.1
(1,2716)	1:45:A:SER:HB2	1:47:A:LYS:H	16	0.1
(1,2716)	1:45:A:SER:HB3	1:47:A:LYS:H	16	0.1
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD21	17	0.1
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD22	17	0.1
(1,2361)	1:111:A:ILE:HB	1:120:A:LEU:HD23	17	0.1
(1,2293)	1:57:A:PHE:HB3	1:135:A:LEU:HD11	7	0.1
(1,2293)	1:57:A:PHE:HB3	1:135:A:LEU:HD12	7	0.1
(1,2293)	1:57:A:PHE:HB3	1:135:A:LEU:HD13	7	0.1
(1,2282)	1:154:A:ALA:HB1	1:164:A:ARG:H	16	0.1
(1,2282)	1:154:A:ALA:HB2	1:164:A:ARG:H	16	0.1
(1,2282)	1:154:A:ALA:HB3	1:164:A:ARG:H	16	0.1
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	2	0.1
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	2	0.1
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	2	0.1
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	4	0.1
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	4	0.1
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	4	0.1
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD11	17	0.1
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD12	17	0.1
(1,2214)	1:86:A:LEU:H	1:86:A:LEU:HD13	17	0.1
(1,2158)	1:120:A:LEU:HD21	1:121:A:MET:HA	14	0.1
(1,2158)	1:120:A:LEU:HD22	1:121:A:MET:HA	14	0.1
(1,2158)	1:120:A:LEU:HD23	1:121:A:MET:HA	14	0.1
(1,1947)	1:135:A:LEU:HG	1:136:A:MET:H	7	0.1
(1,1947)	1:135:A:LEU:HG	1:136:A:MET:H	8	0.1
(1,1913)	1:158:A:GLU:HA	1:160:A:HIS:H	20	0.1
(1,1834)	1:154:A:ALA:HA	1:167:A:ILE:HD11	1	0.1
(1,1834)	1:154:A:ALA:HA	1:167:A:ILE:HD12	1	0.1
(1,1834)	1:154:A:ALA:HA	1:167:A:ILE:HD13	1	0.1
(1,1769)	1:111:A:ILE:HG21	1:116:A:TYR:HE1	1	0.1
(1,1769)	1:111:A:ILE:HG21	1:116:A:TYR:HE2	1	0.1
(1,1769)	1:111:A:ILE:HG22	1:116:A:TYR:HE1	1	0.1
(1,1769)	1:111:A:ILE:HG22	1:116:A:TYR:HE2	1	0.1
(1,1769)	1:111:A:ILE:HG23	1:116:A:TYR:HE1	1	0.1
(1,1769)	1:111:A:ILE:HG23	1:116:A:TYR:HE2	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1281)	1:138:A:LEU:HD21	1:140:A:GLY:HA3	16	0.1
(1,1281)	1:138:A:LEU:HD22	1:140:A:GLY:HA3	16	0.1
(1,1281)	1:138:A:LEU:HD23	1:140:A:GLY:HA3	16	0.1
(1,1213)	1:39:A:HIS:H	1:61:A:LEU:HD11	1	0.1
(1,1213)	1:39:A:HIS:H	1:61:A:LEU:HD12	1	0.1
(1,1213)	1:39:A:HIS:H	1:61:A:LEU:HD13	1	0.1
(1,1213)	1:39:A:HIS:H	1:61:A:LEU:HD11	20	0.1
(1,1213)	1:39:A:HIS:H	1:61:A:LEU:HD12	20	0.1
(1,1213)	1:39:A:HIS:H	1:61:A:LEU:HD13	20	0.1
(1,819)	1:173:A:ALA:H	1:174:A:ASN:H	12	0.1
(1,568)	1:124:A:LEU:H	1:124:A:LEU:HD11	11	0.1
(1,568)	1:124:A:LEU:H	1:124:A:LEU:HD12	11	0.1
(1,568)	1:124:A:LEU:H	1:124:A:LEU:HD13	11	0.1
(1,264)	1:67:A:LEU:H	1:67:A:LEU:HG	18	0.1

10 Dihedral-angle violation analysis (i)

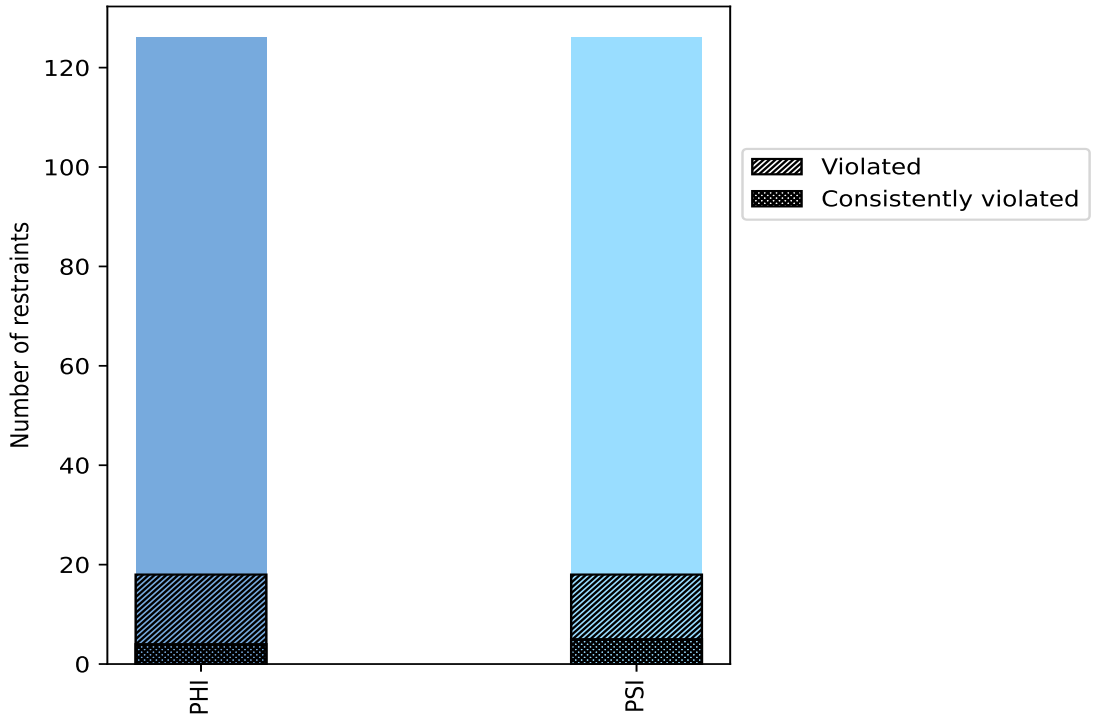
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	126	50.0	18	14.3	7.1	4	3.2	1.6
PSI	126	50.0	18	14.3	7.1	5	4.0	2.0
Total	252	100.0	36	14.3	14.3	9	3.6	3.6

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations (i)



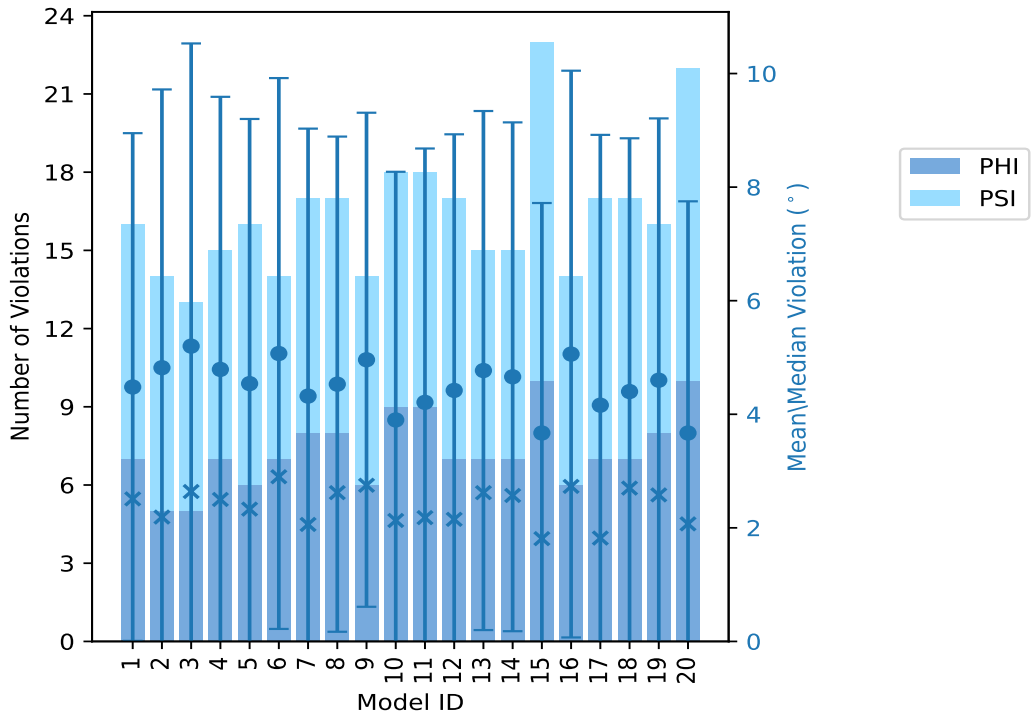
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	7	9	16	4.48	18.59	4.47	2.51
2	5	9	14	4.82	19.09	4.9	2.19
3	5	8	13	5.2	20.69	5.33	2.64
4	7	8	15	4.79	19.39	4.8	2.5
5	6	10	16	4.54	18.95	4.66	2.33
6	7	7	14	5.07	18.69	4.85	2.9
7	8	9	17	4.32	19.69	4.71	2.06
8	8	9	17	4.53	18.03	4.36	2.62
9	6	8	14	4.96	18.31	4.35	2.75
10	9	9	18	3.9	18.74	4.37	2.13
11	9	9	18	4.21	18.54	4.47	2.18
12	7	10	17	4.42	18.6	4.51	2.15
13	7	8	15	4.77	18.73	4.57	2.62
14	7	8	15	4.66	18.5	4.48	2.57
15	10	13	23	3.67	18.75	4.05	1.81
16	6	8	14	5.06	19.67	4.99	2.73
17	7	10	17	4.16	19.88	4.76	1.82
18	7	10	17	4.4	18.7	4.46	2.7
19	8	8	16	4.6	18.48	4.61	2.58
20	10	12	22	3.67	19.18	4.08	2.07

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



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

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

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

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

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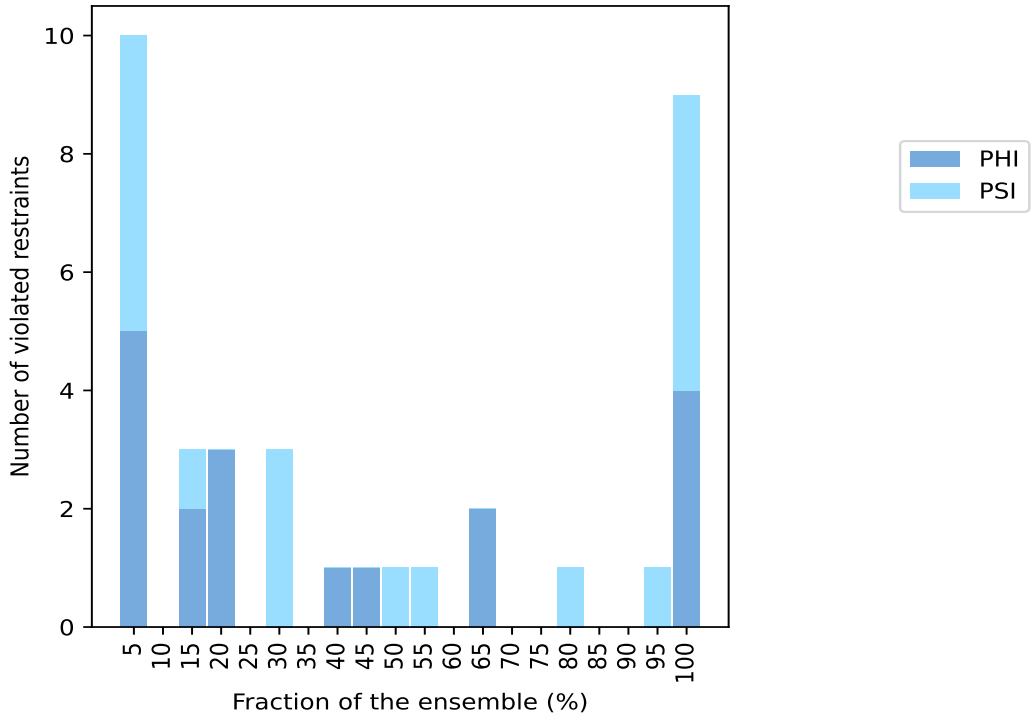
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
2	0	2	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	1	1	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	1	1	19	95.0
4	5	9	20	100.0

[1] Number of models with violations

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

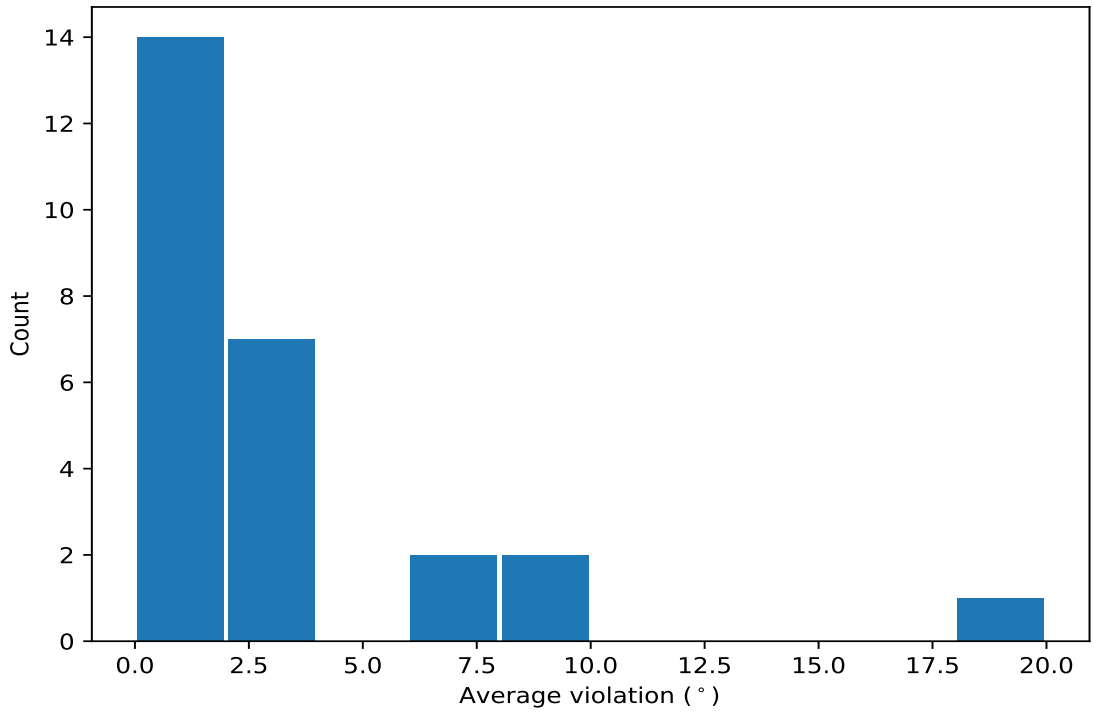


10.4 Most violated dihedral-angle restraints in the ensemble (i)

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

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints (i)

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	20	18.96	0.62	18.74
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	20	9.16	0.8	9.07
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	20	8.01	0.75	7.96
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	20	7.86	0.59	7.71
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	20	7.07	0.48	7.08
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	20	2.65	0.33	2.7
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	20	2.56	0.41	2.62
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	20	2.47	0.71	2.48
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	20	2.28	0.61	2.33
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	19	2.06	0.36	2.04
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	16	1.56	0.38	1.5
(1,155)	1:117:A:ASP:C	1:118:A:ASN:N	1:118:A:ASN:CA	1:118:A:ASN:C	13	1.75	0.65	1.87
(1,201)	1:144:A:ASP:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	13	1.18	0.15	1.14
(1,92)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:ARG:N	11	1.28	0.13	1.29
(1,186)	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	1:135:A:LEU:N	10	2.53	0.62	2.56
(1,61)	1:61:A:LEU:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	9	1.29	0.12	1.3
(1,75)	1:69:A:ASN:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	8	1.66	0.26	1.67
(1,220)	1:154:A:ALA:N	1:154:A:ALA:CA	1:154:A:ALA:C	1:155:A:GLN:N	6	2.55	0.92	2.19
(1,150)	1:114:A:THR:N	1:114:A:THR:CA	1:114:A:THR:C	1:115:A:ASP:N	6	1.52	0.22	1.47
(1,10)	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	1:23:A:SER:N	6	1.27	0.17	1.25

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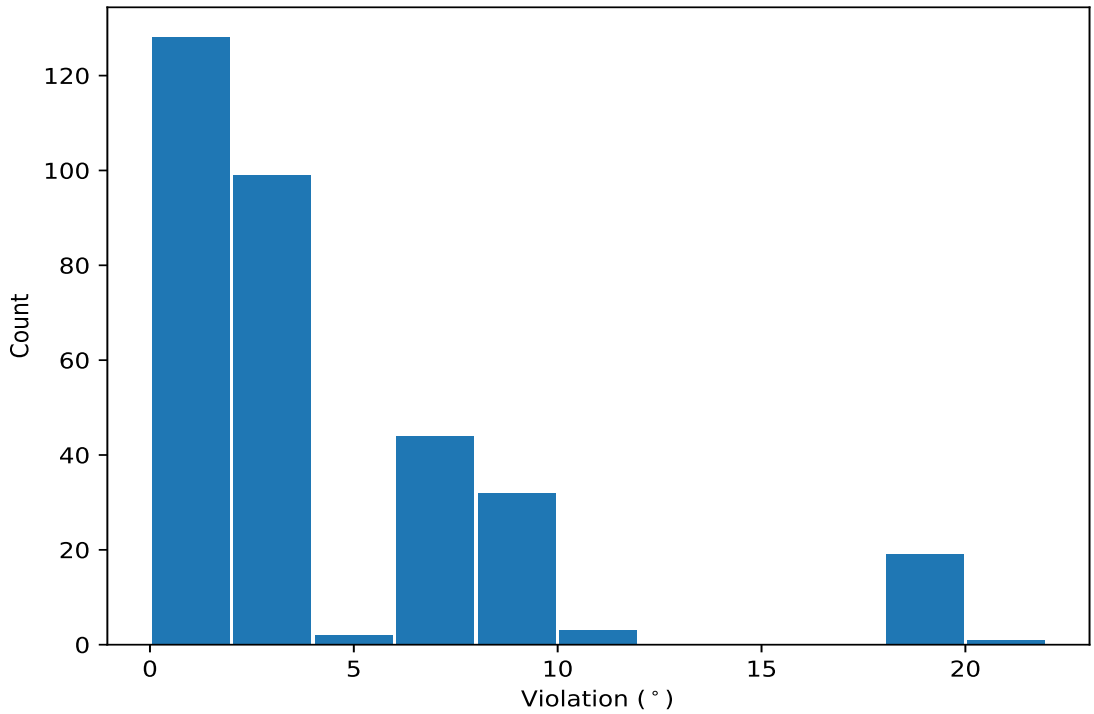
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,223)	1:155:A:GLN:C	1:156:A:LEU:N	1:156:A:LEU:CA	1:156:A:LEU:C	4	1.5	0.33	1.46
(1,141)	1:108:A:THR:C	1:109:A:PHE:N	1:109:A:PHE:CA	1:109:A:PHE:C	4	1.3	0.2	1.23
(1,209)	1:148:A:ASP:C	1:149:A:ILE:N	1:149:A:ILE:CA	1:149:A:ILE:C	4	1.1	0.07	1.08
(1,51)	1:49:A:GLU:C	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	3	1.4	0.43	1.13
(1,43)	1:44:A:ALA:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	3	1.29	0.13	1.34
(1,190)	1:136:A:MET:N	1:136:A:MET:CA	1:136:A:MET:C	1:137:A:GLY:N	3	1.07	0.06	1.03

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints (i)

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	3	20.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	17	19.88
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	7	19.69
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	16	19.67
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	4	19.39
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	20	19.18
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	2	19.09
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	5	18.95
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	15	18.75
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	10	18.74
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	13	18.73
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	18	18.7
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	6	18.69
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	12	18.6
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	1	18.59
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	11	18.54
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	14	18.5
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	19	18.48
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	9	18.31
(1,46)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	8	18.03
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	19	11.29
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	6	10.3
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	8	10.07
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	12	9.75
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	6	9.72
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	16	9.68
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	4	9.48
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	3	9.46
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	5	9.4
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	18	9.18
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1	9.15
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	12	9.08
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	7	8.98
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	11	8.92
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	13	8.87
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	11	8.86
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	16	8.85
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	5	8.81
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	9	8.8
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	17	8.8
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	19	8.8
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	7	8.73
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	2	8.6
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	15	8.55
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	11	8.47
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	2	8.46
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	3	8.45
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	13	8.45
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	15	8.43
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	14	8.38
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	17	8.35
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	4	8.23

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	2	8.22
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	18	8.2
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	8	8.11
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	15	7.97
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	14	7.94
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	20	7.92
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	10	7.87
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	1	7.87
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	16	7.81
(1,63)	1:62:A:GLU:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	10	7.79
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	8	7.79
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	8	7.75
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	18	7.67
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	12	7.56
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	5	7.54
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	3	7.5
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	14	7.49
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	20	7.49
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	13	7.48
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	11	7.45
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	4	7.45
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	20	7.44
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	4	7.41
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	15	7.41
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	18	7.41
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	1	7.4
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	10	7.34
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	6	7.32
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	7	7.32
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	2	7.31
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	7	7.29
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	5	7.28
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	17	7.22
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	17	7.08
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	20	7.08
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	13	7.06
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	9	7.01
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	10	6.98
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	9	6.97
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1	6.84
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	14	6.83
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	16	6.83
(1,132)	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	1:103:A:TYR:N	19	6.81
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLN:N	3	6.71
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	12	6.61
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	9	6.47
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	6	6.32
(1,133)	1:102:A:THR:C	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	19	5.93
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	12	4.11
(1,220)	1:154:A:ALA:N	1:154:A:ALA:CA	1:154:A:ALA:C	1:155:A:GLN:N	15	3.83
(1,220)	1:154:A:ALA:N	1:154:A:ALA:CA	1:154:A:ALA:C	1:155:A:GLN:N	4	3.76

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,186)	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	1:135:A:LEU:N	14	3.52
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	9	3.3
(1,186)	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	1:135:A:LEU:N	19	3.28
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	20	3.27
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	3	3.25
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	6	3.25
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	11	3.24
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	8	3.2
(1,155)	1:117:A:ASP:C	1:118:A:ASN:N	1:118:A:ASN:CA	1:118:A:ASN:C	20	3.14
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	15	3.12
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	7	3.12
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	19	3.05
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	1	3.05
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	20	3.04
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	20	3.03
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	6	3.02
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	14	3.02
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	13	3.0
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	19	2.97
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	16	2.97
(1,186)	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	1:135:A:LEU:N	15	2.92
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	11	2.9
(1,186)	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	1:135:A:LEU:N	8	2.88
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	16	2.88
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	18	2.87
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	18	2.85
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	10	2.84
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	15	2.83
(1,186)	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	1:135:A:LEU:N	9	2.8
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	18	2.79
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	6	2.78
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	8	2.73
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	18	2.7
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	1	2.7
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	9	2.7
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	12	2.7
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	13	2.69
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	1	2.69
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	9	2.69
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	20	2.67
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	4	2.64
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	12	2.64
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	3	2.64
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	8	2.62
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	13	2.62
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	11	2.61
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	8	2.61
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	5	2.59
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	16	2.58
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	14	2.57
(1,42)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:SER:N	5	2.56

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	9	2.53
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	10	2.53
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	13	2.53
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	4	2.5
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	9	2.5
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	2	2.5
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	6	2.47
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	5	2.45
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	10	2.45
(1,155)	1:117:A:ASP:C	1:118:A:ASN:N	1:118:A:ASN:CA	1:118:A:ASN:C	6	2.43
(1,220)	1:154:A:ALA:N	1:154:A:ALA:CA	1:154:A:ALA:C	1:155:A:GLN:N	7	2.39
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	17	2.39
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	17	2.38
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	4	2.35
(1,186)	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	1:135:A:LEU:N	1	2.33
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	9	2.33
(1,155)	1:117:A:ASP:C	1:118:A:ASN:N	1:118:A:ASN:CA	1:118:A:ASN:C	13	2.32
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	8	2.26
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	4	2.25
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	17	2.24
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	11	2.23
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	5	2.2
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	2	2.2
(1,186)	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	1:135:A:LEU:N	10	2.19
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	19	2.19
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	2	2.18
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	2	2.18
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	15	2.17
(1,250)	1:173:A:ALA:N	1:173:A:ALA:CA	1:173:A:ALA:C	1:174:A:ASN:N	20	2.16
(1,186)	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	1:135:A:LEU:N	5	2.16
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	12	2.15
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	7	2.15
(1,75)	1:69:A:ASN:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	11	2.14
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	3	2.14
(1,155)	1:117:A:ASP:C	1:118:A:ASN:N	1:118:A:ASN:CA	1:118:A:ASN:C	16	2.11
(1,155)	1:117:A:ASP:C	1:118:A:ASN:N	1:118:A:ASN:CA	1:118:A:ASN:C	8	2.09
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	16	2.08
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	10	2.07
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	7	2.06
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	8	2.04
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	2	2.03
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	13	2.03
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	14	2.01
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	5	2.01
(1,51)	1:49:A:GLU:C	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	14	2.01
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	1	2.0
(1,220)	1:154:A:ALA:N	1:154:A:ALA:CA	1:154:A:ALA:C	1:155:A:GLN:N	18	1.99
(1,155)	1:117:A:ASP:C	1:118:A:ASN:N	1:118:A:ASN:CA	1:118:A:ASN:C	9	1.99
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	15	1.99
(1,223)	1:155:A:GLN:C	1:156:A:LEU:N	1:156:A:LEU:CA	1:156:A:LEU:C	20	1.98
(1,150)	1:114:A:THR:N	1:114:A:THR:CA	1:114:A:THR:C	1:115:A:ASP:N	12	1.92

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	7	1.91
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	12	1.91
(1,155)	1:117:A:ASP:C	1:118:A:ASN:N	1:118:A:ASN:CA	1:118:A:ASN:C	18	1.87
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	19	1.87
(1,75)	1:69:A:ASN:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	1	1.85
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	5	1.82
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	7	1.82
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	17	1.82
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	14	1.82
(1,33)	1:38:A:TRP:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	15	1.81
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	18	1.79
(1,75)	1:69:A:ASN:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	19	1.77
(1,186)	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	1:135:A:LEU:N	18	1.75
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	17	1.74
(1,220)	1:154:A:ALA:N	1:154:A:ALA:CA	1:154:A:ALA:C	1:155:A:GLN:N	1	1.73
(1,134)	1:103:A:TYR:N	1:103:A:TYR:CA	1:103:A:TYR:C	1:104:A:ASP:N	3	1.7
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	14	1.69
(1,75)	1:69:A:ASN:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	7	1.69
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	14	1.66
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	1	1.65
(1,150)	1:114:A:THR:N	1:114:A:THR:CA	1:114:A:THR:C	1:115:A:ASP:N	15	1.65
(1,75)	1:69:A:ASN:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	13	1.65
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	20	1.65
(1,223)	1:155:A:GLN:C	1:156:A:LEU:N	1:156:A:LEU:CA	1:156:A:LEU:C	4	1.64
(1,141)	1:108:A:THR:C	1:109:A:PHE:N	1:109:A:PHE:CA	1:109:A:PHE:C	19	1.63
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	1	1.62
(1,220)	1:154:A:ALA:N	1:154:A:ALA:CA	1:154:A:ALA:C	1:155:A:GLN:N	17	1.59
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	13	1.58
(1,10)	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	1:23:A:SER:N	15	1.58
(1,150)	1:114:A:THR:N	1:114:A:THR:CA	1:114:A:THR:C	1:115:A:ASP:N	17	1.57
(1,75)	1:69:A:ASN:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	15	1.57
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	6	1.56
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	12	1.56
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	19	1.52
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	10	1.51
(1,201)	1:144:A:ASP:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	15	1.49
(1,186)	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	1:135:A:LEU:N	12	1.49
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	2	1.49
(1,61)	1:61:A:LEU:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	19	1.46
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	16	1.45
(1,92)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:ARG:N	12	1.44
(1,92)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:ARG:N	15	1.43
(1,64)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	4	1.43
(1,92)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:ARG:N	13	1.42
(1,201)	1:144:A:ASP:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	7	1.41
(1,155)	1:117:A:ASP:C	1:118:A:ASN:N	1:118:A:ASN:CA	1:118:A:ASN:C	11	1.41
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	3	1.41
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	7	1.41
(1,43)	1:44:A:ALA:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	19	1.41
(1,6)	1:20:A:GLU:N	1:20:A:GLU:CA	1:20:A:GLU:C	1:21:A:GLU:N	11	1.4
(1,61)	1:61:A:LEU:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	14	1.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,150)	1:114:A:THR:N	1:114:A:THR:CA	1:114:A:THR:C	1:115:A:ASP:N	20	1.37
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	11	1.37
(1,201)	1:144:A:ASP:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	8	1.36
(1,92)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:ARG:N	11	1.36
(1,61)	1:61:A:LEU:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	18	1.36
(1,10)	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	1:23:A:SER:N	5	1.36
(1,92)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:ARG:N	18	1.35
(1,75)	1:69:A:ASN:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	5	1.35
(1,61)	1:61:A:LEU:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	11	1.34
(1,43)	1:44:A:ALA:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	12	1.34
(1,150)	1:114:A:THR:N	1:114:A:THR:CA	1:114:A:THR:C	1:115:A:ASP:N	3	1.33
(1,10)	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	1:23:A:SER:N	16	1.32
(1,157)	1:119:A:PHE:C	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	11	1.31
(1,61)	1:61:A:LEU:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	20	1.3
(1,150)	1:114:A:THR:N	1:114:A:THR:CA	1:114:A:THR:C	1:115:A:ASP:N	16	1.29
(1,141)	1:108:A:THR:C	1:109:A:PHE:N	1:109:A:PHE:CA	1:109:A:PHE:C	20	1.29
(1,92)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:ARG:N	20	1.29
(1,92)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:ARG:N	7	1.28
(1,61)	1:61:A:LEU:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	17	1.28
(1,223)	1:155:A:GLN:C	1:156:A:LEU:N	1:156:A:LEU:CA	1:156:A:LEU:C	15	1.27
(1,61)	1:61:A:LEU:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	10	1.27
(1,201)	1:144:A:ASP:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	16	1.26
(1,75)	1:69:A:ASN:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	17	1.25
(1,13)	1:25:A:THR:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	15	1.24
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	3	1.23
(1,209)	1:148:A:ASP:C	1:149:A:ILE:N	1:149:A:ILE:CA	1:149:A:ILE:C	4	1.22
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	20	1.2
(1,201)	1:144:A:ASP:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	1	1.19
(1,141)	1:108:A:THR:C	1:109:A:PHE:N	1:109:A:PHE:CA	1:109:A:PHE:C	8	1.18
(1,10)	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	1:23:A:SER:N	18	1.18
(1,190)	1:136:A:MET:N	1:136:A:MET:CA	1:136:A:MET:C	1:137:A:GLY:N	19	1.16
(1,201)	1:144:A:ASP:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	11	1.15
(1,92)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:ARG:N	2	1.15
(1,92)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:ARG:N	8	1.15
(1,201)	1:144:A:ASP:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	10	1.14
(1,155)	1:117:A:ASP:C	1:118:A:ASN:N	1:118:A:ASN:CA	1:118:A:ASN:C	12	1.14
(1,92)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:ARG:N	5	1.14
(1,61)	1:61:A:LEU:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	4	1.14
(1,7)	1:20:A:GLU:C	1:21:A:GLU:N	1:21:A:GLU:CA	1:21:A:GLU:C	15	1.14
(1,201)	1:144:A:ASP:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	3	1.13
(1,201)	1:144:A:ASP:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	12	1.13
(1,51)	1:49:A:GLU:C	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	10	1.13
(1,10)	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	1:23:A:SER:N	20	1.13
(1,223)	1:155:A:GLN:C	1:156:A:LEU:N	1:156:A:LEU:CA	1:156:A:LEU:C	18	1.12
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	10	1.11
(1,43)	1:44:A:ALA:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	8	1.11
(1,141)	1:108:A:THR:C	1:109:A:PHE:N	1:109:A:PHE:CA	1:109:A:PHE:C	10	1.1
(1,209)	1:148:A:ASP:C	1:149:A:ILE:N	1:149:A:ILE:CA	1:149:A:ILE:C	20	1.09
(1,155)	1:117:A:ASP:C	1:118:A:ASN:N	1:118:A:ASN:CA	1:118:A:ASN:C	5	1.09
(1,209)	1:148:A:ASP:C	1:149:A:ILE:N	1:149:A:ILE:CA	1:149:A:ILE:C	7	1.08
(1,193)	1:137:A:GLY:C	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	11	1.08

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	15	1.08
(1,155)	1:117:A:ASP:C	1:118:A:ASN:N	1:118:A:ASN:CA	1:118:A:ASN:C	7	1.07
(1,155)	1:117:A:ASP:C	1:118:A:ASN:N	1:118:A:ASN:CA	1:118:A:ASN:C	15	1.06
(1,76)	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	1:71:A:LEU:N	20	1.06
(1,201)	1:144:A:ASP:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	17	1.05
(1,137)	1:106:A:PHE:C	1:107:A:ASN:N	1:107:A:ASN:CA	1:107:A:ASN:C	6	1.05
(1,124)	1:96:A:ALA:N	1:96:A:ALA:CA	1:96:A:ALA:C	1:97:A:GLY:N	2	1.05
(1,51)	1:49:A:GLU:C	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	13	1.05
(1,10)	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	1:23:A:SER:N	10	1.05
(1,148)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:THR:N	17	1.04
(1,201)	1:144:A:ASP:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	9	1.03
(1,190)	1:136:A:MET:N	1:136:A:MET:CA	1:136:A:MET:C	1:137:A:GLY:N	15	1.03
(1,115)	1:89:A:VAL:C	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	14	1.03
(1,61)	1:61:A:LEU:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1	1.03
(1,209)	1:148:A:ASP:C	1:149:A:ILE:N	1:149:A:ILE:CA	1:149:A:ILE:C	6	1.02
(1,201)	1:144:A:ASP:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	2	1.02
(1,201)	1:144:A:ASP:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	20	1.02
(1,190)	1:136:A:MET:N	1:136:A:MET:CA	1:136:A:MET:C	1:137:A:GLY:N	17	1.02
(1,155)	1:117:A:ASP:C	1:118:A:ASN:N	1:118:A:ASN:CA	1:118:A:ASN:C	10	1.02
(1,92)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:ARG:N	4	1.02
(1,84)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:PHE:N	6	1.0