Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 10:39 AM EDT

PDB ID	:	2JX9
BMRB ID	:	15553
Title	:	Solution structure of the Gal_lectin domain of mouse Latrophilin-1 GPCR
Authors	:	Vakonakis, I.; Campbell, I.D.
Deposited on	:	2007-11-09

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:

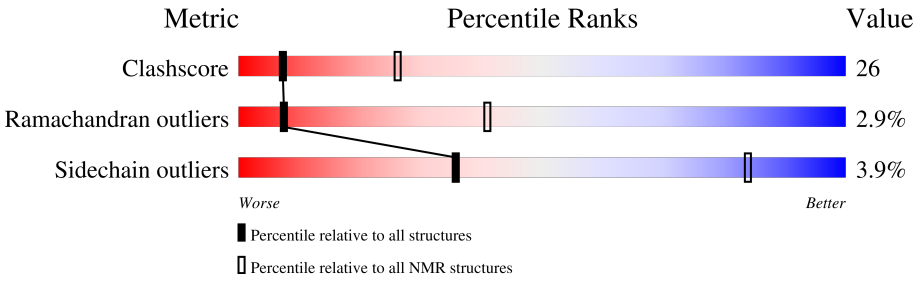
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 93%.

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	106	52% 35% • 10%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:36-A:130 (95)	0.25	1

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

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

The models can be grouped into 3 clusters and 4 single-model clusters were found.

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

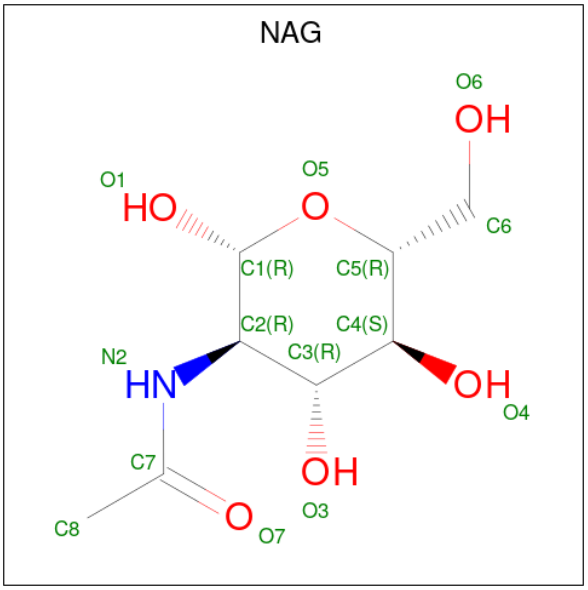
3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1649 atoms, of which 801 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Latrophilin 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	106	1621	522	787	138	162	12	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
2	A	1	28	8	14	1	5

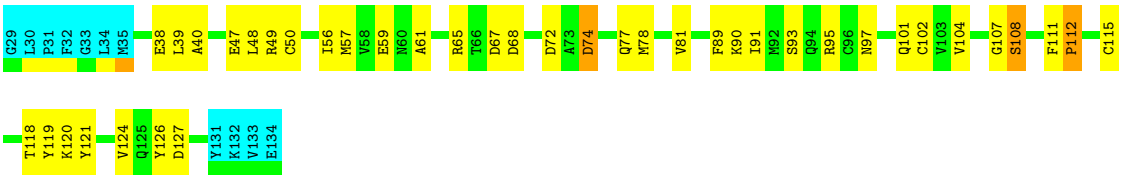
4 Residue-property plots (i)

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: Latrophilin 1

Chain A: 52% 35% • 10%



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

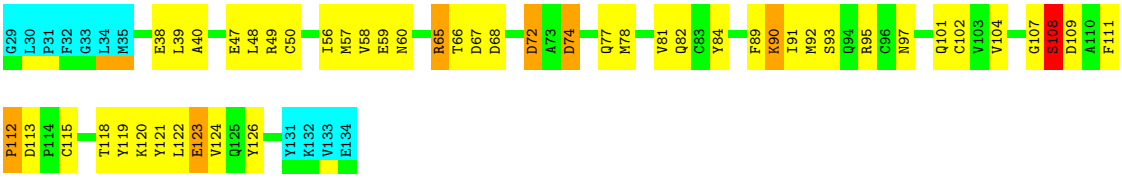
• Molecule 1: Latrophilin 1

Chain A: 54% 34% •• 10%

4.2.2 Score per residue for model 2

• Molecule 1: Latrophilin 1

Chain A: 44% 39% 6% • 10%



4.2.3 Score per residue for model 3

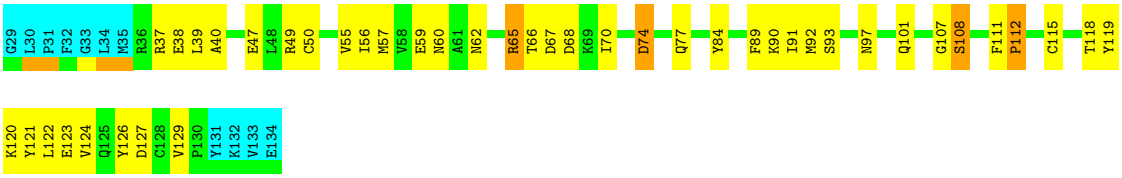
- Molecule 1: Latrophilin 1

Chain A:

4.2.4 Score per residue for model 4

- Molecule 1: Latrophilin 1

Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Latrophilin 1

Chain A:

4.2.6 Score per residue for model 6

- Molecule 1: Latrophilin 1

Chain A: 39% 45% 6% 10%

G29 L30 P31 F32 G33 L34 M35 R36 R37 E38 L39 A40 Y44 L48 R49 C50 P51 I56 M57 V58 E59 N60 A61 N62 R65 T66 D67 C71 D72 A73 D74 P75 F76 Q77 M78 E79 M80 V81 Q82 C83 Y84 F89 K90 I91 M92 S93 Q94 R95 C96 N97 Q101 C102 V103

V104 V105 A106 G107 S108 F111 P112 C115 T118 Y119 K120 Y121 L122 E123 Y126 D127 C128 Y131 K132 V133 E134

4.2.7 Score per residue for model 7

- Molecule 1: Latrophilin 1

Chain A: 48% 38% • 10%

G29 L30 P31 F32 G33 L34 M35 R36 R37 E38 L39 A40 Y44 L48 I56 M57 G64 R65 T66 D67 D68 D72 A73 D74 P75 F76 Q77 M78 V81 Q82 K90 I91 M92 S93 C96 N97 Q101 C102 A106 G107 S108 D109 A110 F111 P112 D113 P114 C115 T118

Y119 K120 Y121 L122 E123 Y126 D127 C128 Y131 K132 V133 E134

4.2.8 Score per residue for model 8

- Molecule 1: Latrophilin 1

Chain A: 54% 34% • 10%

G29 L30 P31 F32 G33 L34 M35 R36 R37 E38 L39 A40 E47 L48 R49 C50 I56 M57 V58 R65 T66 D67 D68 D72 A73 D74 Q77 M78 V81 Q82 F89 K90 I91 M92 S93 C96 N97 Q101 C102 G107 S108 F111 P112 C115 T118 Y119 K120

Y121 L122 E123 Y126 Y131 K132 V133 E134

4.2.9 Score per residue for model 9

- Molecule 1: Latrophilin 1

Chain A: 44% 43% • 10%

G29 L30 P31 F32 G33 L34 M35 R36 L39 A40 E47 L48 R49 C50 I56 M57 V58 A61 R65 T66 D67 D68 K69 D72 A73 D74 P75 F76 Q77 M78 E79 Y84 F89 K90 I91 M92 S93 Q94 R95 C96 N97 N98 R99 T100 Q101 C102 V103 V104 G107 S108

P112 D113 P114 C115 T118 Y119 K120 Y121 L122 E123 V124 Q125 Y126 D127 C128 Y131 K132 V133 E134

4.2.10 Score per residue for model 10

- Molecule 1: Latrophilin 1

Chain A: 48% 37% 5% 10%

G29 L30 P31 F32 G33 L34 M35 R36 R37 E38 L39 A40 E47 L48 P51 I56 M57 A61 R65 T66 D67 D68 K69 I70 C71 D72 A73 D74 P75 F76 Q77 M78 V81 Q82 D87 K90 I91 M92 S93 Q94 R95 C96 N97 N98 R99 T100 Q101 C102 V105 A106 G107

S108 F111 P112 T118 Y119 K120 Y121 V124 Q125 Y126 D127 C128 Y131 K132 V133 E134

4.2.11 Score per residue for model 11

- Molecule 1: Latrophilin 1

Chain A: 46% 40% • • 10%

G29 L30 P31 F32 G33 L34 M35 E38 L39 A40 E47 L48 R49 M57 V58 E59 G64 R65 D68 D72 A73 D74 P75 F76 Q77 M78 E79 N80 V81 Q82 L85 F89 K90 I91 M92 S93 Q94 R95 C96 N97 N98 R99 T100 Q101 C102 V103 V104 G107 S108 D109 A110

F111 P112 D113 P114 C115 T118 Y119 K120 Y121 L122 E123 V124 Q125 Y126 Y131 K132 V133 E134

4.2.12 Score per residue for model 12

- Molecule 1: Latrophilin 1

Chain A: 48% 39% • 10%

G29 L30 P31 F32 G33 L34 M35 R36 R37 E38 L39 A40 L48 R49 C50 I56 M57 V58 E59 N60 A61 N62 R65 T66 D67 I70 C71 D72 A73 D74 P75 F76 Q77 M78 E79 N80 V81 K90 I91 M92 S93 Q94 R95 C96 N97 Q101 C102 V103 V104 V105 A106 G107 S108 D109

A110 F111 P112 T118 Y121 L122 E123 V124 Q125 Y126 D127 Y131 K132 V133 E134

4.2.13 Score per residue for model 13

- Molecule 1: Latrophilin 1

Chain A: 50% 34% 5% • 10%

G29 L30 P31 F32 G33 L34 M35 R36 R37 E38 L39 A40 L48 R49 C50 I56 M57 A61 R65 T66 D67 D68 C71 D72 A73 D74 Q77 M78 V81 Q82 K90 I91 M92 S93 Q94 R95 C96 N97 Q101 C102 V103 V104 G107 S108 F111 P112 D113 Y119

K120 Y121 L122 E123 V124 Q125 Y126 D127 Y131 K132 V133 E134

4.2.14 Score per residue for model 14

- Molecule 1: Latrophilin 1

Chain A: 46% 41% • • 10%

G29 L30 P31 F32 G33 L34 M35 R36 R37 E38 L39 A40 E47 L48 R49 C50 I56 M57 V58 E59 N60 A61 N62 R65 T66 D67 D68 D74 P75 F76 Q77 M78 E79 N80 V81 Q82 C83 Y84 I91 M92 S93 Q94 R95 C96 N97 Q101 C102 V103 V104 G107 S108 F111

P112 D113 P116 G117 T118 Y119 K120 Y121 L122 E123 V124 Q125 Y126 V129 P130 Y131 K132 V133 E134

4.2.15 Score per residue for model 15

- Molecule 1: Latrophilin 1

Chain A: 54% 30% 6% 10%

G29 L30 P31 F32 G33 L34 M35 R36 L39 A40 E47 L48 R49 I56 M57 V58 G64 R65 T66 D67 D68 D72 A73 D74 P75 F76 Q77 M78 E79 C83 Y84 F89 K90 I91 M92 S93 N97 Q101 G107 S108 F111 P112 D113 P116 G117 T118 Y121

Y126 D127 C128 Y131 K132 V133 E134

4.2.16 Score per residue for model 16

- Molecule 1: Latrophilin 1

Chain A: 42% 43% • 10%

G29 L30 P31 F32 G33 L34 M35 R36 L39 A40 C41 E42 G43 Y44 E47 L48 R49 C50 P51 I56 M57 V58 E59 N60 A61 N62 Y63 G64 R65 D68 C71 D72 A73 D74 Q77 M78 F89 K90 I91 M92 S93 Q94 R95 C96 N97 Q101 C102 V103 V104 G107 S108

F111 P112 D113 P114 C115 P116 G117 T118 Y119 K120 V124 Q125 Y126 D127 C128 Y131 K132 V133 E134

4.2.17 Score per residue for model 17

- Molecule 1: Latrophilin 1

Chain A: 54% 29% 7% 10%

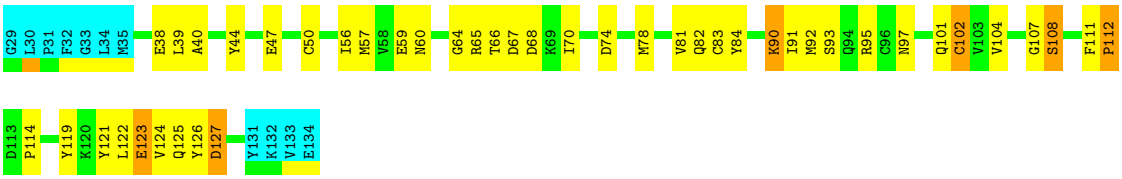
G29 L30 P31 F32 G33 L34 M35 R36 R37 E38 L39 A40 Y44 L48 V55 I56 M57 A61 R65 T66 D67 D68 K69 I70 G71 D72 A73 D74 P75 F76 Q77 M78 E79 K90 I91 R95 Q101 C102 V105 A106 G107 S108 F111 P112 C115 Y119 K120 Y121

V124 Q125 Y126 V129 P130 Y131 K132 V133 E134

4.2.18 Score per residue for model 18

- Molecule 1: Latrophilin 1

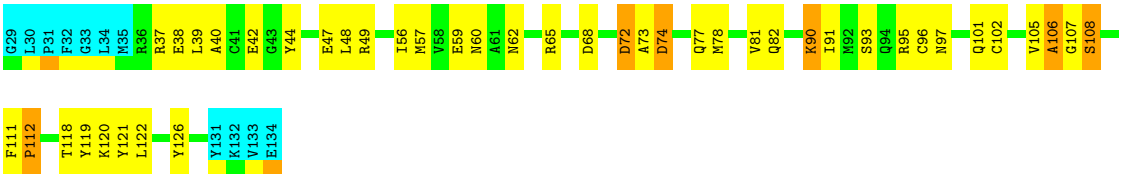
Chain A: 48% 36% 6% 10%



4.2.19 Score per residue for model 19

- Molecule 1: Latrophilin 1

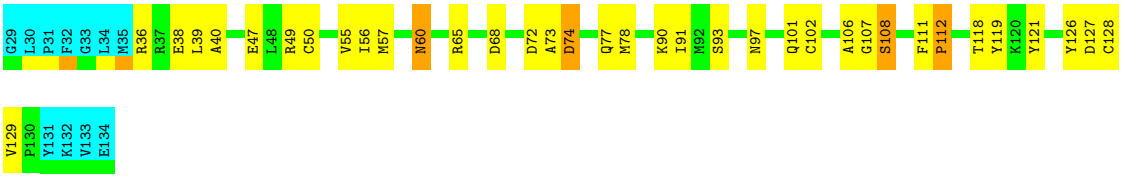
Chain A: 49% 35% 6% 10%



4.2.20 Score per residue for model 20

- Molecule 1: Latrophilin 1

Chain A: 56% 30% • 10%



4.2.21 Score per residue for model 21

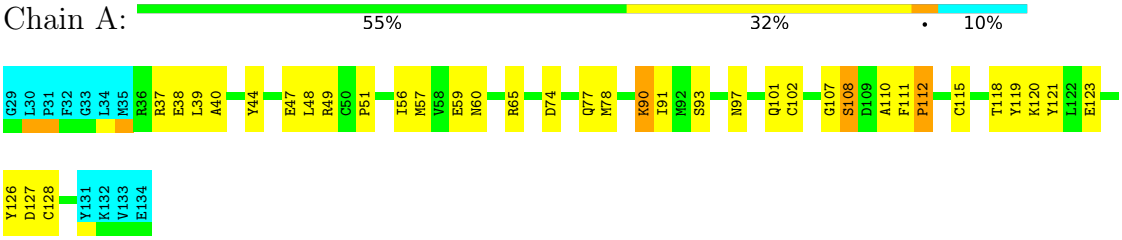
- Molecule 1: Latrophilin 1

Chain A: 47% 40% • 10%

4.2.22 Score per residue for model 22

- Molecule 1: Latrophilin 1

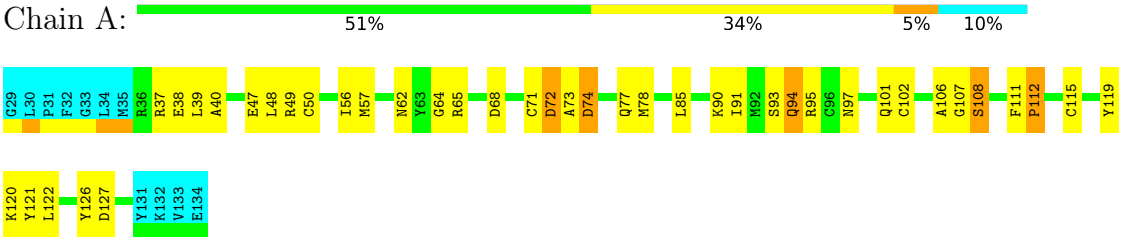
Chain A:



4.2.23 Score per residue for model 23

- Molecule 1: Latrophilin 1

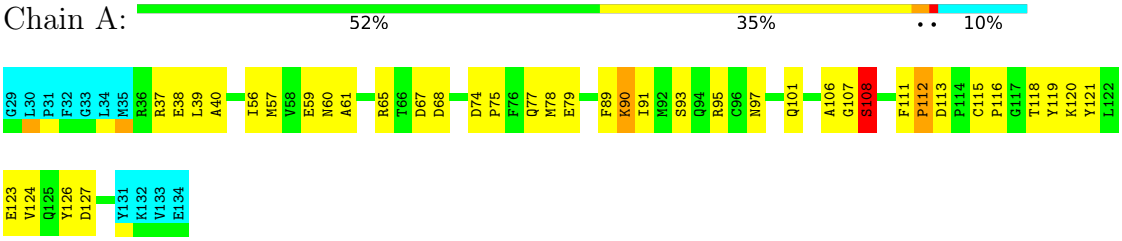
Chain A:



4.2.24 Score per residue for model 24

- Molecule 1: Latrophilin 1

Chain A:



4.2.25 Score per residue for model 25

- Molecule 1: Latrophilin 1

Chain A:

5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 25 were deposited, based on the following criterion: *Structures with lowest energy.*

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

Software name	Classification	Version
X-PLOR NIH	geometry optimization	2.17.0
X-PLOR NIH	refinement	2.17.0
X-PLOR NIH	structure solution	2.17.0

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	1301
Number of shifts mapped to atoms	1301
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

6 Model quality (i)

6.1 Standard geometry (i)

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

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	746	695	695	39±7
2	A	14	14	13	0±1
All	All	19000	17725	17700	968

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:MET:SD	1:A:122:LEU:HD21	0.99	1.97	4	8
1:A:48:LEU:HD12	1:A:102:CYS:SG	0.91	2.05	16	16
1:A:56:ILE:HG23	1:A:126:TYR:CD2	0.91	2.01	19	17
1:A:91:ILE:HG22	1:A:95:ARG:CZ	0.90	1.97	16	2
1:A:39:LEU:HD23	1:A:40:ALA:N	0.90	1.82	7	25
1:A:39:LEU:HD12	1:A:123:GLU:OE1	0.85	1.69	24	2
1:A:95:ARG:HE	1:A:104:VAL:HG22	0.82	1.35	3	3
1:A:61:ALA:HB2	1:A:124:VAL:HG13	0.81	1.51	9	5
1:A:56:ILE:HG23	1:A:126:TYR:CD1	0.79	2.12	21	6
1:A:97:ASN:N	1:A:99:ARG:NH2	0.77	2.32	11	1
1:A:92:MET:SD	1:A:95:ARG:NH2	0.77	2.58	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:ARG:NH1	1:A:119:TYR:O	0.76	2.19	17	9
1:A:92:MET:SD	1:A:124:VAL:HG21	0.75	2.21	13	8
1:A:61:ALA:HB1	1:A:124:VAL:HG22	0.74	1.57	24	9
1:A:65:ARG:NH1	1:A:78:MET:SD	0.74	2.61	22	4
1:A:36:ARG:NH1	1:A:128:CYS:SG	0.73	2.60	6	2
1:A:36:ARG:NE	1:A:128:CYS:SG	0.73	2.62	10	4
1:A:77:GLN:O	1:A:118:THR:HG23	0.71	1.85	11	20
1:A:95:ARG:O	1:A:99:ARG:NH1	0.71	2.23	9	2
1:A:108:SER:OG	1:A:109:ASP:N	0.71	2.20	11	5
1:A:65:ARG:CZ	1:A:78:MET:SD	0.71	2.78	23	3
1:A:74:ASP:N	1:A:74:ASP:OD1	0.70	2.23	12	25
1:A:65:ARG:NH1	1:A:77:GLN:O	0.70	2.23	11	3
1:A:65:ARG:NE	1:A:119:TYR:O	0.69	2.26	1	12
1:A:65:ARG:CZ	1:A:119:TYR:O	0.69	2.40	11	5
1:A:81:VAL:O	1:A:82:GLN:NE2	0.69	2.26	14	10
1:A:47:GLU:OE2	1:A:49:ARG:NE	0.69	2.26	9	12
1:A:74:ASP:OD2	1:A:77:GLN:NE2	0.69	2.25	21	5
1:A:38:GLU:N	1:A:38:GLU:OE1	0.69	2.26	23	11
1:A:90:LYS:O	1:A:94:GLN:NE2	0.69	2.26	13	2
1:A:47:GLU:OE2	1:A:49:ARG:NH2	0.69	2.26	23	9
1:A:36:ARG:HH12	1:A:51:PRO:CD	0.68	2.01	16	1
1:A:65:ARG:NE	1:A:67:ASP:O	0.68	2.26	6	6
1:A:95:ARG:O	1:A:99:ARG:NE	0.68	2.26	11	1
1:A:107:GLY:O	1:A:108:SER:O	0.68	2.12	8	25
1:A:61:ALA:CB	1:A:124:VAL:HG22	0.68	2.19	17	7
1:A:68:ASP:O	1:A:78:MET:CE	0.67	2.42	7	14
1:A:123:GLU:CD	1:A:124:VAL:N	0.67	2.48	2	1
1:A:113:ASP:OD1	1:A:120:LYS:NZ	0.67	2.26	5	8
1:A:48:LEU:HD12	1:A:96:CYS:SG	0.66	2.30	7	7
1:A:65:ARG:NH1	1:A:67:ASP:O	0.66	2.28	9	4
1:A:91:ILE:HG23	1:A:95:ARG:NH1	0.66	2.04	17	2
1:A:57:MET:O	1:A:57:MET:CG	0.65	2.45	16	15
1:A:113:ASP:CG	1:A:120:LYS:HZ3	0.65	1.94	5	1
1:A:123:GLU:OE1	1:A:124:VAL:N	0.65	2.29	2	1
1:A:97:ASN:N	1:A:99:ARG:HH21	0.65	1.90	11	1
1:A:62:ASN:O	1:A:122:LEU:HD12	0.64	1.93	23	6
1:A:95:ARG:NE	1:A:104:VAL:HG22	0.63	2.08	21	5
1:A:72:ASP:OD1	1:A:72:ASP:O	0.62	2.16	17	12
1:A:91:ILE:CG2	1:A:95:ARG:NH1	0.62	2.61	19	2
1:A:73:ALA:HB2	1:A:119:TYR:CD2	0.62	2.29	20	1
1:A:97:ASN:O	1:A:99:ARG:CZ	0.62	2.47	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:GLU:OE1	1:A:47:GLU:O	0.62	2.17	18	3
1:A:111:PHE:O	1:A:112:PRO:O	0.62	2.18	5	24
2:A:135:NAG:O3	2:A:135:NAG:O7	0.62	2.18	12	1
1:A:115:CYS:SG	1:A:120:LYS:CE	0.61	2.88	7	9
1:A:123:GLU:CD	1:A:125:GLN:NE2	0.61	2.54	18	1
1:A:50:CYS:SG	1:A:56:ILE:CG1	0.61	2.89	13	10
1:A:58:VAL:HG12	1:A:89:PHE:CE1	0.61	2.30	2	10
1:A:127:ASP:OD1	1:A:127:ASP:N	0.61	2.34	15	3
1:A:67:ASP:OD1	1:A:68:ASP:N	0.60	2.34	1	8
1:A:71:CYS:O	1:A:72:ASP:C	0.60	2.40	6	1
1:A:93:SER:O	1:A:97:ASN:CG	0.60	2.40	24	23
1:A:65:ARG:NH2	1:A:70:ILE:O	0.60	2.35	17	5
1:A:68:ASP:OD1	1:A:68:ASP:C	0.59	2.40	13	14
1:A:67:ASP:OD2	1:A:69:LYS:N	0.59	2.32	9	1
1:A:36:ARG:CD	1:A:128:CYS:SG	0.58	2.91	3	5
1:A:37:ARG:C	1:A:38:GLU:OE1	0.58	2.42	13	8
1:A:91:ILE:HG22	1:A:95:ARG:HE	0.58	1.57	14	1
1:A:74:ASP:OD2	1:A:77:GLN:CD	0.58	2.42	6	10
1:A:37:ARG:HE	1:A:123:GLU:CD	0.58	2.02	7	1
1:A:73:ALA:N	1:A:78:MET:SD	0.58	2.77	13	5
1:A:73:ALA:O	1:A:78:MET:SD	0.58	2.61	7	2
1:A:39:LEU:HD23	1:A:39:LEU:C	0.58	2.20	11	14
1:A:89:PHE:O	1:A:93:SER:OG	0.57	2.18	5	5
1:A:47:GLU:OE2	1:A:49:ARG:CZ	0.57	2.52	22	7
1:A:59:GLU:O	1:A:60:ASN:OD1	0.57	2.22	19	10
1:A:81:VAL:O	1:A:82:GLN:OE1	0.57	2.22	6	2
1:A:91:ILE:CG2	1:A:95:ARG:CZ	0.57	2.82	19	4
1:A:75:PRO:O	1:A:79:GLU:CG	0.56	2.52	12	5
1:A:74:ASP:CG	1:A:77:GLN:HE21	0.56	2.02	24	1
1:A:126:TYR:C	1:A:127:ASP:OD1	0.56	2.44	15	2
1:A:68:ASP:O	1:A:78:MET:HE3	0.55	2.01	21	2
2:A:135:NAG:O7	2:A:135:NAG:O3	0.55	2.21	6	2
1:A:44:TYR:CD1	1:A:44:TYR:N	0.54	2.75	7	6
1:A:125:GLN:NE2	1:A:125:GLN:N	0.54	2.55	13	1
1:A:95:ARG:HE	1:A:104:VAL:CG2	0.54	2.14	3	1
1:A:38:GLU:OE2	1:A:47:GLU:O	0.53	2.26	10	2
1:A:38:GLU:O	1:A:123:GLU:OE2	0.53	2.26	2	3
1:A:95:ARG:CZ	1:A:104:VAL:HG13	0.53	2.33	13	1
1:A:95:ARG:CZ	1:A:104:VAL:HG11	0.53	2.33	6	2
1:A:107:GLY:O	1:A:108:SER:C	0.53	2.47	15	25
1:A:95:ARG:CZ	1:A:104:VAL:HG22	0.53	2.34	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:VAL:N	1:A:129:VAL:O	0.53	2.40	20	4
1:A:84:TYR:CD1	1:A:84:TYR:N	0.53	2.77	18	3
1:A:47:GLU:CD	1:A:49:ARG:HE	0.53	2.07	4	5
1:A:66:THR:HG22	1:A:84:TYR:CZ	0.53	2.39	15	2
1:A:92:MET:SD	1:A:124:VAL:CG2	0.53	2.96	18	5
1:A:36:ARG:CZ	1:A:128:CYS:SG	0.53	2.97	7	1
1:A:47:GLU:OE2	1:A:49:ARG:NH1	0.53	2.42	15	1
1:A:76:PHE:CD1	1:A:76:PHE:N	0.52	2.74	10	1
1:A:42:GLU:OE2	1:A:63:TYR:OH	0.52	2.27	16	2
1:A:93:SER:O	1:A:97:ASN:CB	0.52	2.57	13	22
1:A:36:ARG:NH1	1:A:128:CYS:H	0.52	2.02	7	1
1:A:90:LYS:CG	1:A:91:ILE:N	0.52	2.72	16	19
1:A:64:GLY:O	1:A:121:TYR:N	0.52	2.42	18	5
1:A:67:ASP:CG	1:A:68:ASP:H	0.52	2.08	24	7
1:A:97:ASN:O	1:A:99:ARG:NH1	0.52	2.43	11	1
1:A:102:CYS:O	1:A:102:CYS:SG	0.52	2.68	18	4
1:A:59:GLU:OE2	1:A:127:ASP:OD2	0.51	2.28	16	5
1:A:59:GLU:OE2	1:A:127:ASP:CG	0.51	2.47	18	1
1:A:66:THR:N	1:A:121:TYR:OH	0.51	2.40	2	1
1:A:113:ASP:OD1	1:A:116:PRO:CD	0.51	2.58	15	3
1:A:56:ILE:HG23	1:A:126:TYR:CE2	0.51	2.41	19	1
1:A:85:LEU:HD23	1:A:88:ALA:HB2	0.51	1.82	21	1
1:A:123:GLU:CD	1:A:123:GLU:C	0.51	2.70	2	1
1:A:37:ARG:NH1	1:A:123:GLU:OE2	0.51	2.44	4	2
1:A:50:CYS:SG	1:A:56:ILE:HG13	0.50	2.47	13	2
1:A:68:ASP:O	1:A:78:MET:HE1	0.50	2.07	25	1
1:A:91:ILE:HG22	1:A:95:ARG:NE	0.50	2.19	14	1
1:A:37:ARG:C	1:A:38:GLU:CD	0.50	2.70	13	4
1:A:72:ASP:OD1	1:A:72:ASP:C	0.50	2.47	12	1
1:A:90:LYS:O	1:A:94:GLN:CD	0.50	2.50	13	2
1:A:65:ARG:NH2	1:A:78:MET:SD	0.50	2.84	23	1
1:A:65:ARG:NH1	1:A:68:ASP:HA	0.50	2.22	21	3
1:A:113:ASP:OD1	1:A:116:PRO:N	0.50	2.44	14	2
1:A:123:GLU:OE2	1:A:125:GLN:NE2	0.50	2.45	18	1
1:A:115:CYS:SG	1:A:120:LYS:HE2	0.49	2.47	24	10
1:A:37:ARG:HH21	1:A:123:GLU:CD	0.49	2.11	6	1
1:A:115:CYS:SG	1:A:120:LYS:HE3	0.49	2.48	16	2
1:A:50:CYS:SG	1:A:56:ILE:HG12	0.49	2.47	13	11
1:A:38:GLU:CD	1:A:47:GLU:O	0.49	2.51	10	3
1:A:91:ILE:HG22	1:A:95:ARG:NH2	0.49	2.23	6	3
1:A:95:ARG:HH11	1:A:104:VAL:HG21	0.49	1.67	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LYS:HG3	1:A:91:ILE:N	0.48	2.22	13	4
1:A:121:TYR:C	1:A:121:TYR:CD1	0.48	2.86	7	18
1:A:65:ARG:NH1	1:A:67:ASP:C	0.48	2.66	21	1
1:A:66:THR:HG21	1:A:84:TYR:CE2	0.48	2.44	4	2
1:A:58:VAL:HG12	1:A:89:PHE:HE1	0.48	1.66	2	1
1:A:44:TYR:O	1:A:106:ALA:HB3	0.48	2.09	6	2
1:A:77:GLN:HB3	1:A:119:TYR:N	0.48	2.24	13	4
1:A:67:ASP:C	1:A:81:VAL:HG12	0.47	2.28	18	3
1:A:95:ARG:HH11	1:A:104:VAL:CG1	0.47	2.22	1	1
1:A:126:TYR:CD1	1:A:126:TYR:C	0.47	2.88	13	2
1:A:57:MET:CG	1:A:127:ASP:O	0.47	2.63	7	9
1:A:91:ILE:CG2	1:A:95:ARG:HH21	0.47	2.21	14	1
1:A:97:ASN:O	1:A:99:ARG:NH2	0.47	2.46	11	1
1:A:95:ARG:NH2	1:A:111:PHE:CZ	0.47	2.83	14	1
1:A:102:CYS:SG	1:A:102:CYS:O	0.47	2.73	13	3
1:A:90:LYS:CD	1:A:90:LYS:C	0.47	2.82	15	1
1:A:97:ASN:HB3	2:A:135:NAG:H82	0.47	1.87	8	2
1:A:36:ARG:HD3	1:A:128:CYS:SG	0.47	2.50	9	2
1:A:91:ILE:HG23	1:A:95:ARG:NE	0.47	2.25	23	1
1:A:95:ARG:NH1	1:A:104:VAL:HG21	0.46	2.25	14	1
1:A:60:ASN:N	1:A:60:ASN:ND2	0.46	2.63	20	1
1:A:49:ARG:HH12	1:A:101:GLN:CD	0.46	2.14	5	1
1:A:94:GLN:O	1:A:99:ARG:NH2	0.46	2.48	11	1
1:A:95:ARG:NH1	1:A:104:VAL:HG13	0.46	2.26	9	1
1:A:90:LYS:HG2	1:A:91:ILE:N	0.46	2.25	24	6
1:A:66:THR:CG2	1:A:84:TYR:CE2	0.46	2.99	25	3
1:A:67:ASP:CG	1:A:68:ASP:N	0.46	2.69	24	1
1:A:77:GLN:O	1:A:118:THR:CG2	0.46	2.61	11	3
1:A:36:ARG:NH2	1:A:51:PRO:HG3	0.46	2.26	10	1
1:A:105:VAL:C	1:A:107:GLY:H	0.46	2.13	19	3
1:A:95:ARG:HH11	1:A:95:ARG:HG3	0.46	1.70	17	1
1:A:70:ILE:HG22	1:A:71:CYS:SG	0.46	2.50	3	1
1:A:65:ARG:HA	1:A:121:TYR:CE2	0.45	2.46	7	10
1:A:113:ASP:CG	1:A:120:LYS:HZ1	0.45	2.12	11	1
1:A:113:ASP:CG	1:A:120:LYS:NZ	0.45	2.70	5	1
1:A:110:ALA:O	1:A:111:PHE:CD1	0.45	2.70	22	2
1:A:56:ILE:HG23	1:A:126:TYR:CG	0.45	2.45	25	3
1:A:36:ARG:NH1	1:A:51:PRO:CD	0.45	2.75	16	1
1:A:92:MET:CG	1:A:95:ARG:HH21	0.45	2.25	16	1
1:A:75:PRO:O	1:A:79:GLU:HG3	0.45	2.10	9	7
1:A:91:ILE:CG2	1:A:95:ARG:NE	0.45	2.79	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:VAL:O	1:A:107:GLY:N	0.45	2.49	19	3
1:A:68:ASP:O	1:A:78:MET:HE2	0.45	2.12	8	3
1:A:91:ILE:HG22	1:A:95:ARG:NH1	0.44	2.27	19	1
1:A:75:PRO:O	1:A:79:GLU:HG2	0.44	2.12	14	1
1:A:91:ILE:HG22	1:A:95:ARG:HH21	0.44	1.71	14	1
1:A:66:THR:CG2	1:A:84:TYR:CZ	0.44	3.01	15	3
1:A:37:ARG:NE	1:A:123:GLU:OE2	0.44	2.51	6	2
1:A:66:THR:OG1	1:A:121:TYR:OH	0.44	2.29	2	2
1:A:36:ARG:HD2	1:A:128:CYS:SG	0.44	2.53	15	2
1:A:65:ARG:HH12	1:A:119:TYR:HB3	0.44	1.73	11	1
1:A:47:GLU:CG	1:A:49:ARG:HH11	0.44	2.25	16	1
1:A:57:MET:SD	1:A:129:VAL:CG1	0.44	3.06	14	1
1:A:89:PHE:CE1	1:A:93:SER:OG	0.43	2.71	4	1
1:A:57:MET:O	1:A:57:MET:HG3	0.43	2.12	2	13
1:A:97:ASN:CB	2:A:135:NAG:H82	0.43	2.44	15	2
1:A:42:GLU:OE1	1:A:120:LYS:N	0.43	2.38	19	2
1:A:91:ILE:CG2	1:A:95:ARG:HE	0.43	2.27	24	1
1:A:92:MET:HG2	1:A:95:ARG:HH22	0.43	1.72	14	1
1:A:37:ARG:CG	1:A:123:GLU:OE2	0.43	2.66	24	1
1:A:87:ASP:O	1:A:90:LYS:CG	0.43	2.67	10	1
1:A:65:ARG:NH1	1:A:78:MET:HA	0.43	2.29	25	4
1:A:72:ASP:O	1:A:72:ASP:CG	0.42	2.57	11	3
1:A:73:ALA:CB	1:A:119:TYR:CD2	0.42	3.00	20	1
1:A:93:SER:O	1:A:97:ASN:HB2	0.42	2.14	6	2
1:A:115:CYS:SG	1:A:120:LYS:HG2	0.42	2.53	7	1
1:A:71:CYS:O	1:A:73:ALA:N	0.42	2.52	16	3
1:A:85:LEU:HD21	1:A:112:PRO:HG2	0.42	1.91	11	2
1:A:39:LEU:HD21	1:A:121:TYR:HB2	0.42	1.90	22	1
1:A:64:GLY:HA3	1:A:83:CYS:SG	0.42	2.55	15	1
1:A:38:GLU:HG3	1:A:48:LEU:HD23	0.42	1.90	21	3
1:A:121:TYR:CD1	1:A:121:TYR:C	0.42	2.93	1	2
1:A:42:GLU:CD	1:A:63:TYR:OH	0.42	2.58	16	1
1:A:47:GLU:HG3	1:A:49:ARG:NH1	0.42	2.30	16	1
1:A:83:CYS:SG	1:A:114:PRO:HG2	0.42	2.55	18	1
1:A:61:ALA:HB3	1:A:89:PHE:HA	0.42	1.91	21	1
1:A:95:ARG:HH11	1:A:104:VAL:HG13	0.41	1.73	1	1
1:A:68:ASP:CB	1:A:78:MET:O	0.41	2.68	11	1
1:A:110:ALA:C	1:A:111:PHE:CD1	0.41	2.93	22	1
1:A:90:LYS:HD3	1:A:94:GLN:NE2	0.41	2.30	13	1
1:A:65:ARG:NH1	1:A:78:MET:HG2	0.41	2.31	14	1
1:A:72:ASP:O	1:A:72:ASP:OD1	0.41	2.39	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:MET:CE	1:A:122:LEU:HD21	0.41	2.45	14	1
1:A:44:TYR:N	1:A:44:TYR:CD1	0.41	2.89	18	1
1:A:93:SER:HA	1:A:97:ASN:ND2	0.41	2.31	24	1
1:A:51:PRO:HD2	1:A:128:CYS:SG	0.41	2.55	6	3
1:A:74:ASP:OD2	1:A:77:GLN:CG	0.41	2.69	12	1
1:A:49:ARG:NH1	1:A:49:ARG:CG	0.41	2.83	16	1
1:A:46:ILE:HG22	1:A:104:VAL:O	0.41	2.16	25	1
1:A:127:ASP:N	1:A:127:ASP:OD1	0.41	2.53	21	1
1:A:59:GLU:C	1:A:89:PHE:CE1	0.41	2.94	2	1
1:A:38:GLU:N	1:A:38:GLU:CD	0.41	2.74	6	2
1:A:36:ARG:HH12	1:A:51:PRO:CG	0.41	2.27	16	1
1:A:36:ARG:NH1	1:A:128:CYS:N	0.41	2.69	7	1
1:A:37:ARG:HH11	1:A:123:GLU:HG3	0.41	1.76	8	1
1:A:36:ARG:HG3	1:A:36:ARG:NH1	0.41	2.30	15	1
1:A:68:ASP:C	1:A:68:ASP:OD1	0.41	2.58	23	1
1:A:57:MET:HG3	1:A:127:ASP:O	0.41	2.16	7	1
1:A:57:MET:O	1:A:57:MET:HG2	0.41	2.16	16	1
1:A:93:SER:HB3	1:A:97:ASN:ND2	0.40	2.30	16	1
1:A:36:ARG:HG2	1:A:36:ARG:NH1	0.40	2.31	10	1
1:A:95:ARG:NE	1:A:104:VAL:CG2	0.40	2.83	11	1
1:A:93:SER:O	1:A:97:ASN:ND2	0.40	2.54	23	1
1:A:36:ARG:NH1	1:A:36:ARG:HG3	0.40	2.31	6	1
1:A:67:ASP:O	1:A:81:VAL:HG12	0.40	2.17	18	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	95/106 (90%)	84±1 (89±1%)	8±1 (9±1%)	3±1 (3±1%)	7	41
All	All	2375/2650 (90%)	2102 (89%)	203 (9%)	70 (3%)	7	41

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

Mol	Chain	Res	Type	Models (Total)
1	A	108	SER	25
1	A	112	PRO	25
1	A	106	ALA	10
1	A	72	ASP	9
1	A	71	CYS	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	84/93 (90%)	81±1 (96±2%)	3±1 (4±2%)	36 84
All	All	2100/2325 (90%)	2018 (96%)	82 (4%)	36 84

All 16 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	101	GLN	25
1	A	74	ASP	18
1	A	90	LYS	11
1	A	108	SER	6
1	A	65	ARG	6
1	A	127	ASP	3
1	A	123	GLU	2
1	A	94	GLN	2
1	A	102	CYS	2
1	A	78	MET	1
1	A	75	PRO	1
1	A	118	THR	1
1	A	125	GLN	1
1	A	47	GLU	1
1	A	116	PRO	1
1	A	60	ASN	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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	NAG	A	135	1	14,14,15	0.65±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	NAG	A	135	1	17,19,21	0.81±0.07	1±0 (4±2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	135	1	-	0±0,6,23,26	0±0,1,1,1

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	135	NAG	C2-N2-C7	3.04	118.58	122.90	14	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 93% for the well-defined parts and 91% 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	1301
Number of shifts mapped to atoms	1301
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	105	0.21 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	98	-0.46 ± 0.22	None needed (< 0.5 ppm)
$^{13}C'$	93	0.63 ± 0.18	Should be applied
^{15}N	95	-0.05 ± 0.20	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 93%, i.e. 1165 atoms were assigned a chemical shift out of a possible 1246. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	456/464 (98%)	187/187 (100%)	182/190 (96%)	87/87 (100%)
Sidechain	637/698 (91%)	424/449 (94%)	197/218 (90%)	16/31 (52%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	72/84 (86%)	37/39 (95%)	35/45 (78%)	0/0 (—%)
Overall	1165/1246 (93%)	648/675 (96%)	414/453 (91%)	103/118 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1281 atoms were assigned a chemical shift out of a possible 1401. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	500/519 (96%)	207/210 (99%)	198/212 (93%)	95/97 (98%)
Sidechain	701/779 (90%)	467/503 (93%)	218/244 (89%)	16/32 (50%)
Aromatic	80/103 (78%)	41/48 (85%)	39/55 (71%)	0/0 (—%)
Overall	1281/1401 (91%)	715/761 (94%)	455/511 (89%)	111/129 (86%)

7.1.4 Statistically unusual chemical shifts (i)

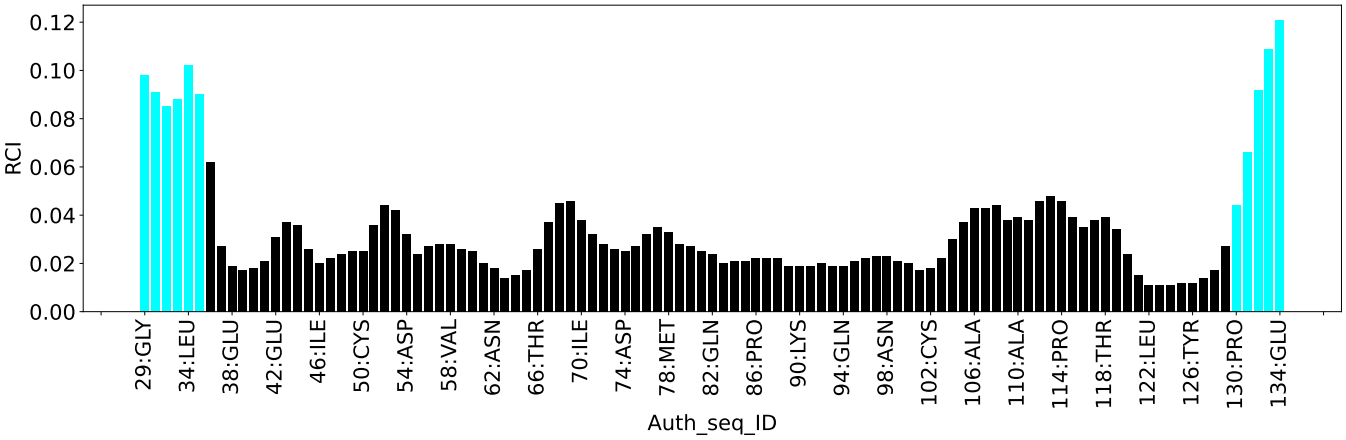
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	98	ASN	ND2	130.61	101.55 – 123.95	8.0
1	A	120	LYS	HD3	0.44	0.54 – 2.65	-5.5

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.00
0.02
0.04
0.06
0.08
0.10
0.12
29:GLY
34:LEU
38:GLU
42:GLU
46:ILE
50:CYS
54:ASP
58:VAL
62:ASN
66:THR
70:ILE
74:ASP
78:MET
82:GLN
86:PRO
90:LYS
94:GLN
98:ASN
102:CYS
106:ALA
110:ALA
114:PRO
118:THR
122:LEU
126:TYR
130:PRO
134:GLU
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	2889
Intra-residue (|i-j|=0)	499
Sequential (|i-j|=1)	703
Medium range (|i-j|>1 and |i-j|<5)	399
Long range (|i-j|≥5)	1288
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	225
Number of unmapped restraints	0
Number of restraints per residue	29.4
Number of long range restraints per residue[1]	12.2

[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)	20.6	0.2
0.2-0.5 (Medium)	1.1	0.29
>0.5 (Large)	None	None

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	6.2	4.3
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

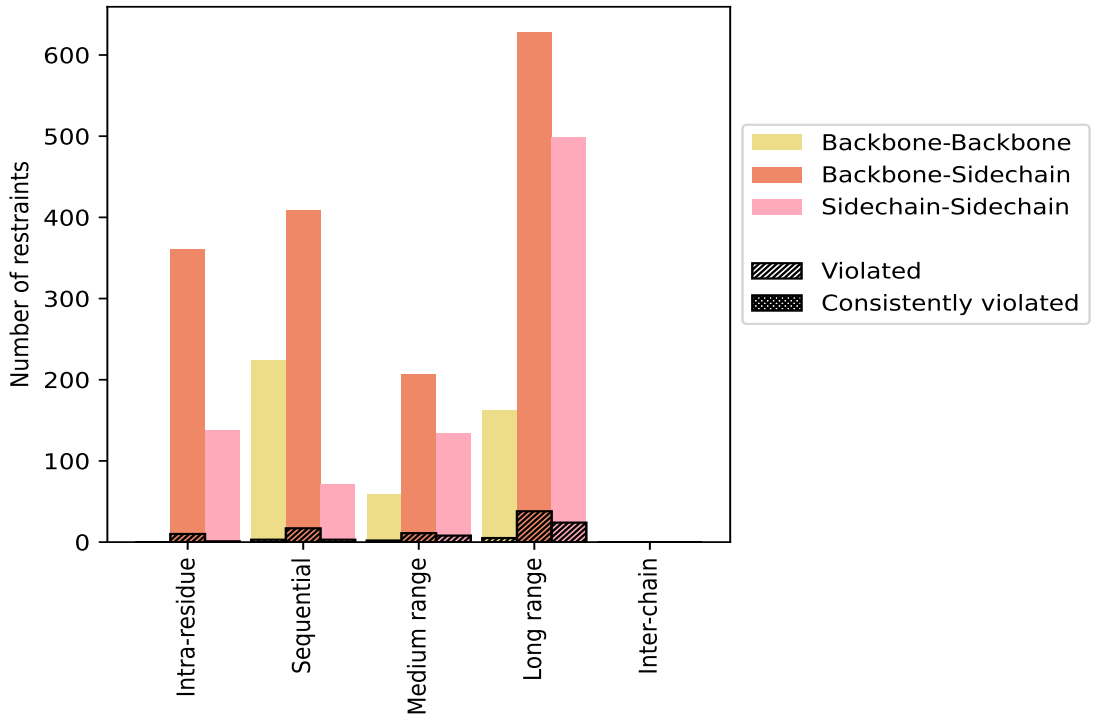
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	499	17.3	11	2.2	0.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	361	12.5	10	2.8	0.3	0	0.0	0.0
Sidechain-Sidechain	138	4.8	1	0.7	0.0	0	0.0	0.0
Sequential (|i-j|=1)	703	24.3	23	3.3	0.8	0	0.0	0.0
Backbone-Backbone	224	7.8	3	1.3	0.1	0	0.0	0.0
Backbone-Sidechain	408	14.1	17	4.2	0.6	0	0.0	0.0
Sidechain-Sidechain	71	2.5	3	4.2	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	399	13.8	21	5.3	0.7	0	0.0	0.0
Backbone-Backbone	59	2.0	2	3.4	0.1	0	0.0	0.0
Backbone-Sidechain	206	7.1	11	5.3	0.4	0	0.0	0.0
Sidechain-Sidechain	134	4.6	8	6.0	0.3	0	0.0	0.0
Long range (|i-j|≥5)	1288	44.6	67	5.2	2.3	0	0.0	0.0
Backbone-Backbone	162	5.6	5	3.1	0.2	0	0.0	0.0
Backbone-Sidechain	628	21.7	38	6.1	1.3	0	0.0	0.0
Sidechain-Sidechain	498	17.2	24	4.8	0.8	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	2889	100.0	122	4.2	4.2	0	0.0	0.0
Backbone-Backbone	445	15.4	10	2.2	0.3	0	0.0	0.0
Backbone-Sidechain	1603	55.5	76	4.7	2.6	0	0.0	0.0
Sidechain-Sidechain	841	29.1	36	4.3	1.2	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	3	7	2	11	0	23	0.15	0.24	0.03	0.16
2	3	6	0	9	0	18	0.14	0.2	0.03	0.14
3	2	2	1	6	0	11	0.15	0.2	0.03	0.15
4	2	7	0	12	0	21	0.14	0.19	0.02	0.14
5	4	9	5	11	0	29	0.14	0.18	0.02	0.15
6	3	8	0	9	0	20	0.13	0.17	0.02	0.13
7	0	11	3	8	0	22	0.15	0.26	0.04	0.15
8	2	6	1	16	0	25	0.14	0.21	0.03	0.13
9	2	6	2	7	0	17	0.13	0.18	0.02	0.12
10	3	5	2	11	0	21	0.15	0.26	0.04	0.13
11	1	6	1	11	0	19	0.14	0.21	0.03	0.14

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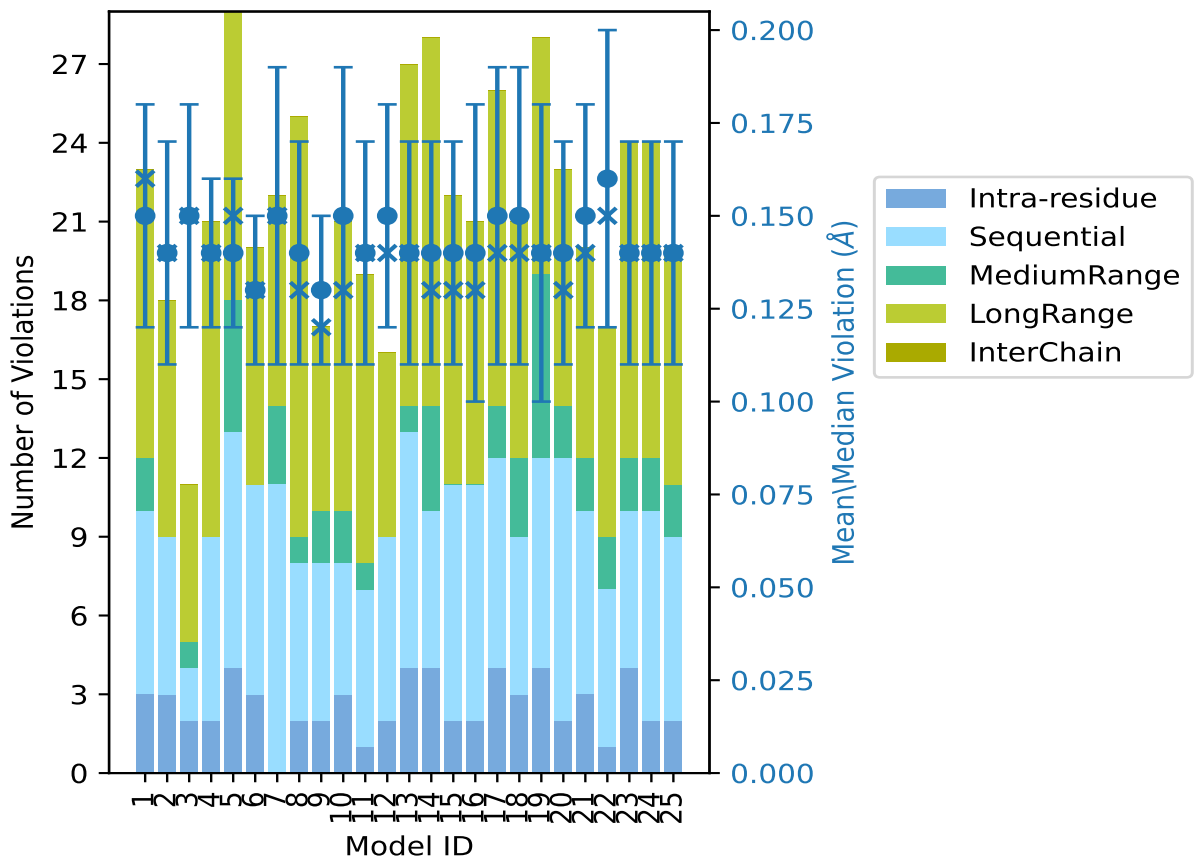
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	2	7	0	7	0	16	0.15	0.23	0.03	0.14
13	4	9	1	13	0	27	0.14	0.22	0.03	0.14
14	4	6	4	14	0	28	0.14	0.26	0.03	0.13
15	2	9	0	11	0	22	0.14	0.2	0.03	0.13
16	2	9	0	10	0	21	0.14	0.24	0.04	0.13
17	4	8	2	12	0	26	0.15	0.29	0.04	0.14
18	3	6	3	9	0	21	0.15	0.27	0.04	0.14
19	4	8	7	9	0	28	0.14	0.24	0.04	0.14
20	2	10	2	9	0	23	0.14	0.21	0.03	0.13
21	3	7	2	8	0	20	0.15	0.22	0.03	0.14
22	1	6	2	8	0	17	0.16	0.26	0.04	0.15
23	4	6	2	12	0	24	0.14	0.24	0.03	0.14
24	2	8	2	12	0	24	0.14	0.2	0.03	0.14
25	2	7	2	9	0	20	0.14	0.25	0.03	0.14

[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, 2767(IR:488, SQ:680, MR:378, LR:1221, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
5	4	7	26	0	42	1	4.0
1	2	10	12	0	25	2	8.0
1	2	1	6	0	10	3	12.0
0	0	1	3	0	4	4	16.0
1	1	1	5	0	8	5	20.0
0	3	0	3	0	6	6	24.0

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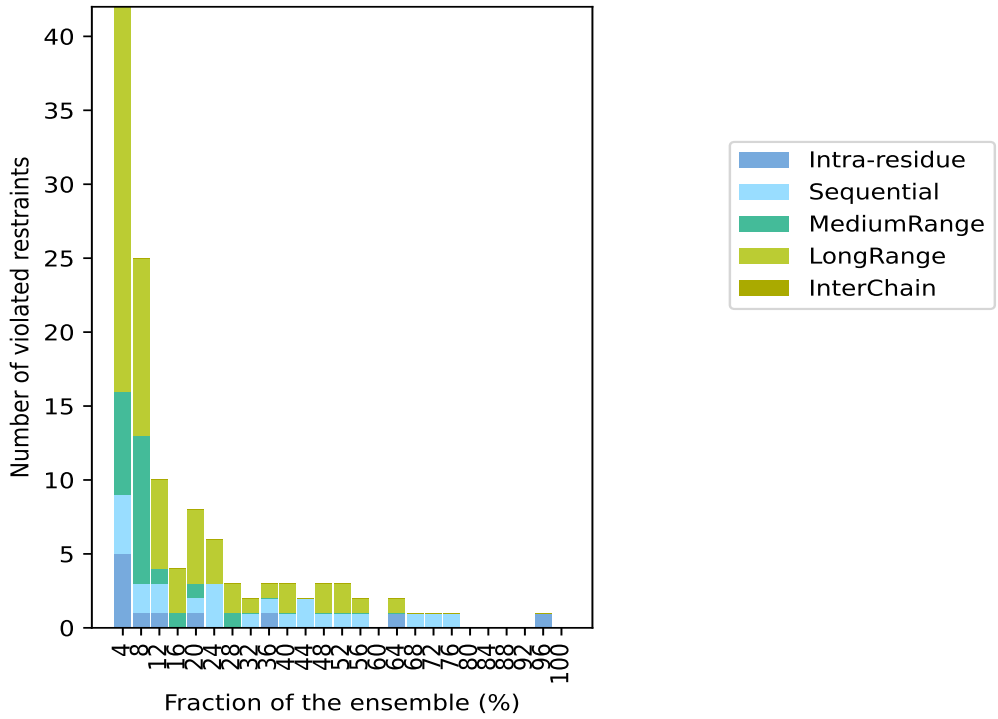
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	1	2	0	3	7	28.0
0	1	0	1	0	2	8	32.0
1	1	0	1	0	3	9	36.0
0	1	0	2	0	3	10	40.0
0	2	0	0	0	2	11	44.0
0	1	0	2	0	3	12	48.0
0	1	0	2	0	3	13	52.0
0	1	0	1	0	2	14	56.0
0	0	0	0	0	0	15	60.0
1	0	0	1	0	2	16	64.0
0	1	0	0	0	1	17	68.0
0	1	0	0	0	1	18	72.0
0	1	0	0	0	1	19	76.0
0	0	0	0	0	0	20	80.0
0	0	0	0	0	0	21	84.0
0	0	0	0	0	0	22	88.0
0	0	0	0	0	0	23	92.0
1	0	0	0	0	1	24	96.0
0	0	0	0	0	0	25	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

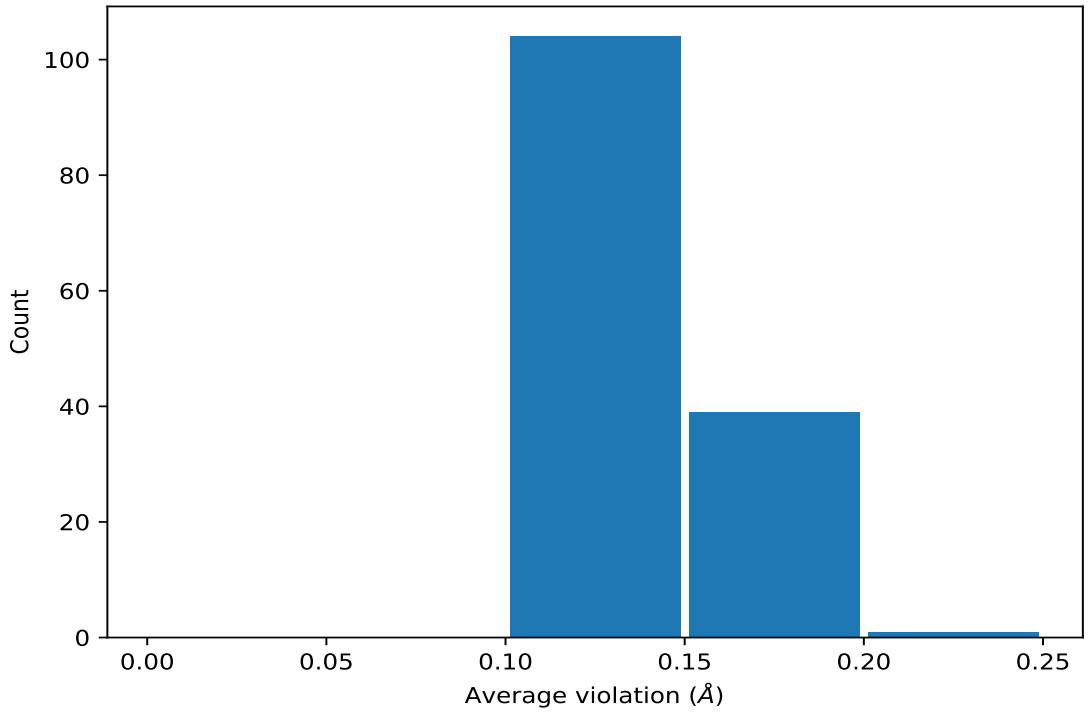
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	24	0.16	0.02	0.16
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	24	0.16	0.02	0.16
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	19	0.16	0.04	0.15
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	18	0.12	0.01	0.11
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	17	0.14	0.02	0.13
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	16	0.15	0.03	0.15
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	16	0.15	0.03	0.15
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	16	0.13	0.02	0.13
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	16	0.13	0.02	0.13
(1,1229)	1:A:111:PHE:HB3	1:A:112:PRO:HG2	14	0.16	0.02	0.16
(1,533)	1:A:57:MET:HE1	2:A:135:NAG:H1	14	0.15	0.04	0.15
(1,533)	1:A:57:MET:HE2	2:A:135:NAG:H1	14	0.15	0.04	0.15
(1,533)	1:A:57:MET:HE3	2:A:135:NAG:H1	14	0.15	0.04	0.15
(1,1490)	1:A:39:LEU:HA	1:A:124:VAL:H	13	0.15	0.03	0.14
(1,1980)	1:A:64:GLY:H	1:A:122:LEU:HB3	13	0.15	0.03	0.14
(1,2102)	1:A:70:ILE:HG12	1:A:71:CYS:H	13	0.14	0.03	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2088)	1:A:69:LYS:HG2	1:A:70:ILE:H	12	0.14	0.03	0.13
(1,2307)	1:A:85:LEU:HB2	1:A:115:CYS:H	12	0.14	0.02	0.14
(1,730)	1:A:66:THR:HA	1:A:81:VAL:HB	12	0.14	0.01	0.14
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD2	11	0.18	0.06	0.16
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD3	11	0.18	0.06	0.16
(1,2725)	1:A:37:ARG:HB2	1:A:38:GLU:H	11	0.16	0.04	0.15
(1,2725)	1:A:37:ARG:HB3	1:A:38:GLU:H	11	0.16	0.04	0.15
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG21	10	0.14	0.02	0.15
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG22	10	0.14	0.02	0.15
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG23	10	0.14	0.02	0.15
(1,1627)	1:A:48:LEU:HG	1:A:49:ARG:H	10	0.14	0.02	0.14
(1,1608)	1:A:46:ILE:H	1:A:105:VAL:HA	10	0.13	0.02	0.13
(1,1454)	1:A:38:GLU:HG2	1:A:47:GLU:H	9	0.18	0.04	0.18
(1,2200)	1:A:78:MET:HG2	1:A:79:GLU:H	9	0.15	0.02	0.14
(1,905)	1:A:82:GLN:HG2	1:A:82:GLN:HA	9	0.14	0.02	0.13
(1,905)	1:A:82:GLN:HG3	1:A:82:GLN:HA	9	0.14	0.02	0.13
(1,134)	1:A:39:LEU:HD21	1:A:123:GLU:HB3	8	0.16	0.03	0.16
(1,134)	1:A:39:LEU:HD22	1:A:123:GLU:HB3	8	0.16	0.03	0.16
(1,134)	1:A:39:LEU:HD23	1:A:123:GLU:HB3	8	0.16	0.03	0.16
(1,2389)	1:A:92:MET:H	1:A:93:SER:HB3	8	0.12	0.01	0.11
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB2	7	0.16	0.02	0.16
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB3	7	0.16	0.02	0.16
(1,1398)	1:A:35:MET:HG3	1:A:126:TYR:H	7	0.14	0.03	0.14
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG2	7	0.13	0.02	0.12
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG3	7	0.13	0.02	0.12
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG2	7	0.13	0.02	0.12
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG3	7	0.13	0.02	0.12
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE1	6	0.19	0.04	0.18
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE2	6	0.19	0.04	0.18
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE3	6	0.19	0.04	0.18
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG21	6	0.17	0.04	0.15
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG22	6	0.17	0.04	0.15
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG23	6	0.17	0.04	0.15
(1,1455)	1:A:38:GLU:HG3	1:A:47:GLU:H	6	0.15	0.02	0.15
(1,1994)	1:A:65:ARG:HE	1:A:66:THR:H	6	0.14	0.02	0.15
(1,2014)	1:A:65:ARG:HG3	1:A:81:VAL:H	6	0.14	0.04	0.12
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD11	6	0.14	0.02	0.14
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD12	6	0.14	0.02	0.14
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD13	6	0.14	0.02	0.14
(1,1630)	1:A:48:LEU:H	1:A:101:GLN:HG2	5	0.16	0.06	0.13
(1,1630)	1:A:48:LEU:H	1:A:101:GLN:HG3	5	0.16	0.06	0.13
(1,2733)	1:A:45:PRO:HG2	1:A:44:TYR:H	5	0.15	0.03	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2733)	1:A:122:LEU:HB3	1:A:44:TYR:H	5	0.15	0.03	0.14
(1,2112)	1:A:70:ILE:H	1:A:121:TYR:HE1	5	0.15	0.05	0.14
(1,2112)	1:A:70:ILE:H	1:A:121:TYR:HE2	5	0.15	0.05	0.14
(1,1391)	1:A:131:TYR:HE1	2:A:135:NAG:H1	5	0.14	0.02	0.14
(1,1391)	1:A:131:TYR:HE2	2:A:135:NAG:H1	5	0.14	0.02	0.14
(1,414)	1:A:51:PRO:HD3	1:A:56:ILE:HG12	5	0.13	0.01	0.13
(1,185)	1:A:42:GLU:HG3	1:A:119:TYR:HD1	5	0.13	0.03	0.13
(1,185)	1:A:42:GLU:HG3	1:A:119:TYR:HD2	5	0.13	0.03	0.13
(1,2383)	1:A:92:MET:HG3	1:A:92:MET:H	5	0.13	0.01	0.13
(1,2021)	1:A:65:ARG:H	1:A:83:CYS:HB3	5	0.13	0.01	0.13
(1,2784)	1:A:62:ASN:HD21	1:A:86:PRO:HG3	4	0.16	0.02	0.16
(1,2784)	1:A:62:ASN:HD21	1:A:114:PRO:HG3	4	0.16	0.02	0.16
(1,1122)	1:A:95:ARG:HG2	1:A:104:VAL:HG21	4	0.16	0.06	0.13
(1,1122)	1:A:95:ARG:HG2	1:A:104:VAL:HG22	4	0.16	0.06	0.13
(1,1122)	1:A:95:ARG:HG2	1:A:104:VAL:HG23	4	0.16	0.06	0.13
(1,2073)	1:A:68:ASP:H	1:A:70:ILE:HG13	4	0.15	0.03	0.14
(1,1916)	1:A:62:ASN:HD22	1:A:84:TYR:HA	4	0.13	0.02	0.12
(1,1161)	1:A:104:VAL:HG11	1:A:105:VAL:HA	3	0.15	0.03	0.13
(1,1161)	1:A:104:VAL:HG12	1:A:105:VAL:HA	3	0.15	0.03	0.13
(1,1161)	1:A:104:VAL:HG13	1:A:105:VAL:HA	3	0.15	0.03	0.13
(1,2660)	1:A:123:GLU:HB2	1:A:125:GLN:HE22	3	0.15	0.02	0.16
(1,29)	1:A:37:ARG:HB2	1:A:37:ARG:HD2	3	0.15	0.02	0.15
(1,29)	1:A:37:ARG:HB2	1:A:37:ARG:HD3	3	0.15	0.02	0.15
(1,188)	1:A:42:GLU:HG2	1:A:119:TYR:HE1	3	0.14	0.01	0.13
(1,188)	1:A:42:GLU:HG2	1:A:119:TYR:HE2	3	0.14	0.01	0.13
(1,2004)	1:A:65:ARG:HE	1:A:78:MET:HG3	3	0.14	0.02	0.12
(1,419)	1:A:53:SER:HA	1:A:100:THR:HB	3	0.13	0.0	0.13
(1,2008)	1:A:65:ARG:HD2	1:A:79:GLU:H	3	0.13	0.01	0.12
(1,2710)	1:A:130:PRO:HB2	1:A:131:TYR:H	3	0.13	0.01	0.14
(1,689)	1:A:64:GLY:HA2	1:A:84:TYR:HA	3	0.13	0.02	0.12
(1,492)	1:A:56:ILE:HG21	1:A:97:ASN:HA	3	0.12	0.01	0.11
(1,492)	1:A:56:ILE:HG22	1:A:97:ASN:HA	3	0.12	0.01	0.11
(1,492)	1:A:56:ILE:HG23	1:A:97:ASN:HA	3	0.12	0.01	0.11
(1,625)	1:A:62:ASN:HB2	1:A:123:GLU:HB3	2	0.2	0.04	0.2
(1,1001)	1:A:87:ASP:HA	1:A:90:LYS:HB3	2	0.18	0.08	0.18
(1,287)	1:A:46:ILE:HD11	1:A:124:VAL:HG11	2	0.17	0.03	0.17
(1,287)	1:A:46:ILE:HD11	1:A:124:VAL:HG12	2	0.17	0.03	0.17
(1,287)	1:A:46:ILE:HD11	1:A:124:VAL:HG13	2	0.17	0.03	0.17
(1,287)	1:A:46:ILE:HD12	1:A:124:VAL:HG11	2	0.17	0.03	0.17
(1,287)	1:A:46:ILE:HD12	1:A:124:VAL:HG12	2	0.17	0.03	0.17
(1,287)	1:A:46:ILE:HD12	1:A:124:VAL:HG13	2	0.17	0.03	0.17
(1,287)	1:A:46:ILE:HD13	1:A:124:VAL:HG11	2	0.17	0.03	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,287)	1:A:46:ILE:HD13	1:A:124:VAL:HG12	2	0.17	0.03	0.17
(1,287)	1:A:46:ILE:HD13	1:A:124:VAL:HG13	2	0.17	0.03	0.17
(1,2574)	1:A:111:PHE:HD1	1:A:111:PHE:H	2	0.16	0.06	0.16
(1,2574)	1:A:111:PHE:HD2	1:A:111:PHE:H	2	0.16	0.06	0.16
(1,1059)	1:A:91:ILE:HA	1:A:94:GLN:HA	2	0.15	0.01	0.15
(1,1307)	1:A:121:TYR:HD1	1:A:123:GLU:HG2	2	0.15	0.01	0.15
(1,1307)	1:A:121:TYR:HD1	1:A:123:GLU:HG3	2	0.15	0.01	0.15
(1,1307)	1:A:121:TYR:HD2	1:A:123:GLU:HG2	2	0.15	0.01	0.15
(1,1307)	1:A:121:TYR:HD2	1:A:123:GLU:HG3	2	0.15	0.01	0.15
(1,1182)	1:A:105:VAL:HB	1:A:108:SER:HA	2	0.14	0.03	0.14
(1,2108)	1:A:70:ILE:H	1:A:72:ASP:HB2	2	0.14	0.0	0.14
(1,2108)	1:A:70:ILE:H	1:A:72:ASP:HB3	2	0.14	0.0	0.14
(1,1586)	1:A:45:PRO:HB3	1:A:105:VAL:H	2	0.14	0.02	0.14
(1,1661)	1:A:49:ARG:H	1:A:126:TYR:HD1	2	0.14	0.01	0.14
(1,1661)	1:A:49:ARG:H	1:A:126:TYR:HD2	2	0.14	0.01	0.14
(1,2515)	1:A:102:CYS:HB2	1:A:103:VAL:H	2	0.14	0.02	0.14
(1,2515)	1:A:102:CYS:HB3	1:A:103:VAL:H	2	0.14	0.02	0.14
(1,11)	1:A:35:MET:HE1	1:A:127:ASP:HA	2	0.13	0.02	0.13
(1,11)	1:A:35:MET:HE2	1:A:127:ASP:HA	2	0.13	0.02	0.13
(1,11)	1:A:35:MET:HE3	1:A:127:ASP:HA	2	0.13	0.02	0.13
(1,296)	1:A:47:GLU:HG2	1:A:48:LEU:HG	2	0.13	0.01	0.13
(1,850)	1:A:75:PRO:HA	1:A:78:MET:HG2	2	0.13	0.02	0.13
(1,1538)	1:A:42:GLU:HA	1:A:44:TYR:H	2	0.13	0.0	0.13
(1,1892)	1:A:61:ALA:HB1	1:A:126:TYR:H	2	0.13	0.0	0.13
(1,1892)	1:A:61:ALA:HB2	1:A:126:TYR:H	2	0.13	0.0	0.13
(1,1892)	1:A:61:ALA:HB3	1:A:126:TYR:H	2	0.13	0.0	0.13
(1,2055)	1:A:67:ASP:H	1:A:70:ILE:HD11	2	0.13	0.01	0.13
(1,2055)	1:A:67:ASP:H	1:A:70:ILE:HD12	2	0.13	0.01	0.13
(1,2055)	1:A:67:ASP:H	1:A:70:ILE:HD13	2	0.13	0.01	0.13
(1,1436)	1:A:37:ARG:HB3	1:A:126:TYR:H	2	0.12	0.02	0.12
(1,2445)	1:A:96:CYS:HB2	1:A:101:GLN:H	2	0.12	0.02	0.12
(1,2445)	1:A:96:CYS:HB3	1:A:101:GLN:H	2	0.12	0.02	0.12
(1,238)	1:A:45:PRO:HG2	1:A:105:VAL:HG21	2	0.12	0.01	0.12
(1,238)	1:A:45:PRO:HG2	1:A:105:VAL:HG22	2	0.12	0.01	0.12
(1,238)	1:A:45:PRO:HG2	1:A:105:VAL:HG23	2	0.12	0.01	0.12
(1,818)	1:A:73:ALA:HB1	1:A:77:GLN:HG2	2	0.12	0.01	0.12
(1,818)	1:A:73:ALA:HB2	1:A:77:GLN:HG2	2	0.12	0.01	0.12
(1,818)	1:A:73:ALA:HB3	1:A:77:GLN:HG2	2	0.12	0.01	0.12
(1,585)	1:A:60:ASN:HA	1:A:89:PHE:HA	2	0.12	0.0	0.12
(1,974)	1:A:85:LEU:HD11	1:A:113:ASP:HA	2	0.12	0.0	0.12
(1,974)	1:A:85:LEU:HD12	1:A:113:ASP:HA	2	0.12	0.0	0.12
(1,974)	1:A:85:LEU:HD13	1:A:113:ASP:HA	2	0.12	0.0	0.12

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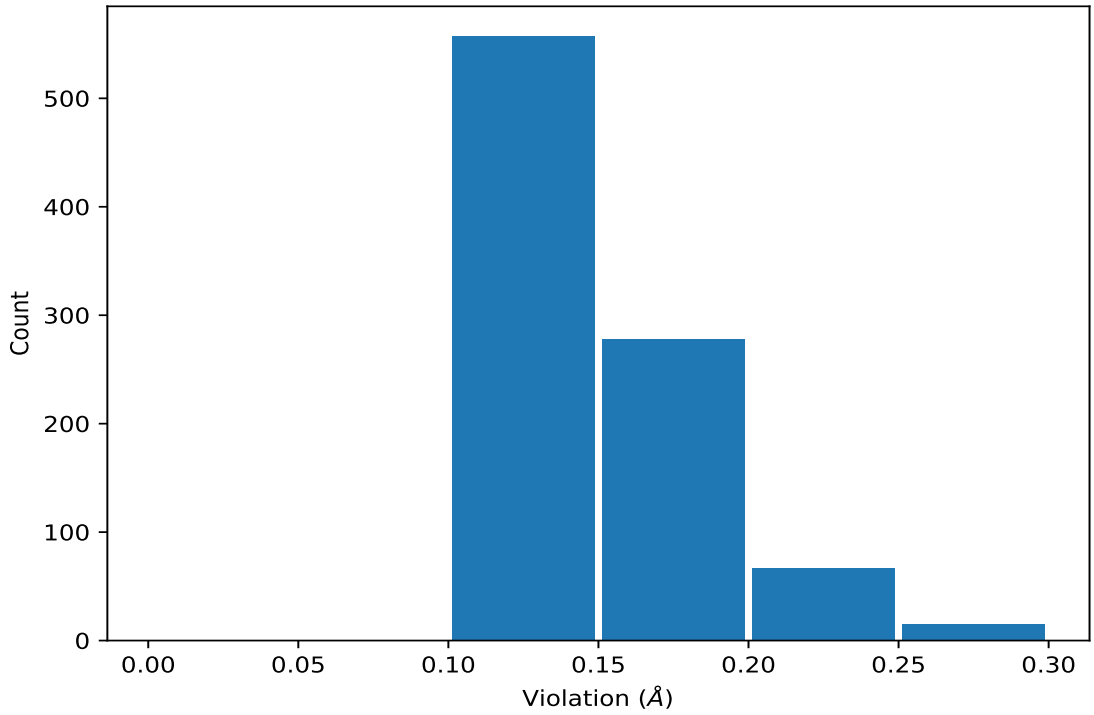
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,749)	1:A:67:ASP:HB2	1:A:70:ILE:HB	2	0.11	0.0	0.11
(1,1603)	1:A:46:ILE:HG13	1:A:104:VAL:H	2	0.11	0.0	0.11

[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)
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD2	17	0.29
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD3	17	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	18	0.27
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD2	22	0.26
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD3	22	0.26
(1,1630)	1:A:48:LEU:H	1:A:101:GLN:HG2	7	0.26
(1,1630)	1:A:48:LEU:H	1:A:101:GLN:HG3	7	0.26
(1,1122)	1:A:95:ARG:HG2	1:A:104:VAL:HG21	14	0.26
(1,1122)	1:A:95:ARG:HG2	1:A:104:VAL:HG22	14	0.26
(1,1122)	1:A:95:ARG:HG2	1:A:104:VAL:HG23	14	0.26
(1,1001)	1:A:87:ASP:HA	1:A:90:LYS:HB3	10	0.26
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD2	25	0.25
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD3	25	0.25
(1,2112)	1:A:70:ILE:H	1:A:121:TYR:HE1	18	0.25
(1,2112)	1:A:70:ILE:H	1:A:121:TYR:HE2	18	0.25
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE1	22	0.24
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE2	22	0.24
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE3	22	0.24
(1,625)	1:A:62:ASN:HB2	1:A:123:GLU:HB3	23	0.24
(1,2054)	1:A:67:ASP:H	1:A:70:ILE:HG12	19	0.24
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG21	17	0.24
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG22	17	0.24
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG23	17	0.24
(1,1454)	1:A:38:GLU:HG2	1:A:47:GLU:H	1	0.24
(1,1454)	1:A:38:GLU:HG2	1:A:47:GLU:H	16	0.24
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE1	12	0.23
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE2	12	0.23
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE3	12	0.23
(1,533)	1:A:57:MET:HE1	2:A:135:NAG:H1	19	0.23
(1,533)	1:A:57:MET:HE2	2:A:135:NAG:H1	19	0.23
(1,533)	1:A:57:MET:HE3	2:A:135:NAG:H1	19	0.23
(1,1401)	1:A:51:PRO:HG2	1:A:128:CYS:H	10	0.23
(1,2725)	1:A:37:ARG:HB2	1:A:38:GLU:H	7	0.22
(1,2725)	1:A:37:ARG:HB3	1:A:38:GLU:H	7	0.22
(1,2725)	1:A:37:ARG:HB2	1:A:38:GLU:H	21	0.22
(1,2725)	1:A:37:ARG:HB3	1:A:38:GLU:H	21	0.22
(1,2574)	1:A:111:PHE:HD1	1:A:111:PHE:H	13	0.22
(1,2574)	1:A:111:PHE:HD2	1:A:111:PHE:H	13	0.22
(1,1980)	1:A:64:GLY:H	1:A:122:LEU:HB3	16	0.22
(1,134)	1:A:39:LEU:HD21	1:A:123:GLU:HB3	21	0.22
(1,134)	1:A:39:LEU:HD22	1:A:123:GLU:HB3	21	0.22
(1,134)	1:A:39:LEU:HD23	1:A:123:GLU:HB3	21	0.22
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	12	0.22
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD2	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD3	11	0.21
(1,533)	1:A:57:MET:HE1	2:A:135:NAG:H1	20	0.21
(1,533)	1:A:57:MET:HE2	2:A:135:NAG:H1	20	0.21
(1,533)	1:A:57:MET:HE3	2:A:135:NAG:H1	20	0.21
(1,2014)	1:A:65:ARG:HG3	1:A:81:VAL:H	8	0.21
(1,1229)	1:A:111:PHE:HB3	1:A:112:PRO:HG2	8	0.21
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE1	18	0.2
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE2	18	0.2
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE3	18	0.2
(1,287)	1:A:46:ILE:HD11	1:A:124:VAL:HG11	22	0.2
(1,287)	1:A:46:ILE:HD11	1:A:124:VAL:HG12	22	0.2
(1,287)	1:A:46:ILE:HD11	1:A:124:VAL:HG13	22	0.2
(1,287)	1:A:46:ILE:HD12	1:A:124:VAL:HG11	22	0.2
(1,287)	1:A:46:ILE:HD12	1:A:124:VAL:HG12	22	0.2
(1,287)	1:A:46:ILE:HD12	1:A:124:VAL:HG13	22	0.2
(1,287)	1:A:46:ILE:HD13	1:A:124:VAL:HG11	22	0.2
(1,287)	1:A:46:ILE:HD13	1:A:124:VAL:HG12	22	0.2
(1,287)	1:A:46:ILE:HD13	1:A:124:VAL:HG13	22	0.2
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	3	0.2
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	3	0.2
(1,2733)	1:A:45:PRO:HG2	1:A:44:TYR:H	1	0.2
(1,2733)	1:A:122:LEU:HB3	1:A:44:TYR:H	1	0.2
(1,2307)	1:A:85:LEU:HB2	1:A:115:CYS:H	24	0.2
(1,2102)	1:A:70:ILE:HG12	1:A:71:CYS:H	16	0.2
(1,2073)	1:A:68:ASP:H	1:A:70:ILE:HG13	7	0.2
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG21	20	0.2
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG22	20	0.2
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG23	20	0.2
(1,1490)	1:A:39:LEU:HA	1:A:124:VAL:H	15	0.2
(1,1490)	1:A:39:LEU:HA	1:A:124:VAL:H	21	0.2
(1,1454)	1:A:38:GLU:HG2	1:A:47:GLU:H	8	0.2
(1,134)	1:A:39:LEU:HD21	1:A:123:GLU:HB3	2	0.2
(1,134)	1:A:39:LEU:HD22	1:A:123:GLU:HB3	2	0.2
(1,134)	1:A:39:LEU:HD23	1:A:123:GLU:HB3	2	0.2
(1,1161)	1:A:104:VAL:HG11	1:A:105:VAL:HA	19	0.2
(1,1161)	1:A:104:VAL:HG12	1:A:105:VAL:HA	19	0.2
(1,1161)	1:A:104:VAL:HG13	1:A:105:VAL:HA	19	0.2
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	19	0.2
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB2	3	0.19
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB3	3	0.19
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	24	0.19
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	24	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2784)	1:A:62:ASN:HD21	1:A:86:PRO:HG3	22	0.19
(1,2784)	1:A:62:ASN:HD21	1:A:114:PRO:HG3	22	0.19
(1,2725)	1:A:37:ARG:HB2	1:A:38:GLU:H	2	0.19
(1,2725)	1:A:37:ARG:HB3	1:A:38:GLU:H	2	0.19
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	10	0.19
(1,2622)	1:A:120:LYS:HE3	1:A:120:LYS:H	1	0.19
(1,2200)	1:A:78:MET:HG2	1:A:79:GLU:H	14	0.19
(1,2088)	1:A:69:LYS:HG2	1:A:70:ILE:H	15	0.19
(1,185)	1:A:42:GLU:HG3	1:A:119:TYR:HD1	25	0.19
(1,185)	1:A:42:GLU:HG3	1:A:119:TYR:HD2	25	0.19
(1,1630)	1:A:48:LEU:H	1:A:101:GLN:HG2	1	0.19
(1,1630)	1:A:48:LEU:H	1:A:101:GLN:HG3	1	0.19
(1,1608)	1:A:46:ILE:H	1:A:105:VAL:HA	2	0.19
(1,1490)	1:A:39:LEU:HA	1:A:124:VAL:H	12	0.19
(1,1455)	1:A:38:GLU:HG3	1:A:47:GLU:H	24	0.19
(1,1454)	1:A:38:GLU:HG2	1:A:47:GLU:H	2	0.19
(1,1398)	1:A:35:MET:HG3	1:A:126:TYR:H	20	0.19
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	1	0.19
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	4	0.19
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	17	0.19
(1,905)	1:A:82:GLN:HG2	1:A:82:GLN:HA	9	0.18
(1,905)	1:A:82:GLN:HG3	1:A:82:GLN:HA	9	0.18
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB2	20	0.18
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB3	20	0.18
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	3	0.18
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	3	0.18
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	5	0.18
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	5	0.18
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	9	0.18
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	9	0.18
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	23	0.18
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	23	0.18
(1,779)	1:A:69:LYS:HE2	1:A:78:MET:HE1	25	0.18
(1,779)	1:A:69:LYS:HE2	1:A:78:MET:HE2	25	0.18
(1,779)	1:A:69:LYS:HE2	1:A:78:MET:HE3	25	0.18
(1,779)	1:A:69:LYS:HE3	1:A:78:MET:HE1	25	0.18
(1,779)	1:A:69:LYS:HE3	1:A:78:MET:HE2	25	0.18
(1,779)	1:A:69:LYS:HE3	1:A:78:MET:HE3	25	0.18
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD2	13	0.18
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD3	13	0.18
(1,533)	1:A:57:MET:HE1	2:A:135:NAG:H1	13	0.18
(1,533)	1:A:57:MET:HE2	2:A:135:NAG:H1	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,533)	1:A:57:MET:HE3	2:A:135:NAG:H1	13	0.18
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG2	4	0.18
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG3	4	0.18
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG2	4	0.18
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG3	4	0.18
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	11	0.18
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	11	0.18
(1,2725)	1:A:37:ARG:HB2	1:A:38:GLU:H	12	0.18
(1,2725)	1:A:37:ARG:HB3	1:A:38:GLU:H	12	0.18
(1,2200)	1:A:78:MET:HG2	1:A:79:GLU:H	13	0.18
(1,2102)	1:A:70:ILE:HG12	1:A:71:CYS:H	3	0.18
(1,2088)	1:A:69:LYS:HG2	1:A:70:ILE:H	18	0.18
(1,1980)	1:A:64:GLY:H	1:A:122:LEU:HB3	5	0.18
(1,1627)	1:A:48:LEU:HG	1:A:49:ARG:H	5	0.18
(1,1490)	1:A:39:LEU:HA	1:A:124:VAL:H	18	0.18
(1,1454)	1:A:38:GLU:HG2	1:A:47:GLU:H	21	0.18
(1,134)	1:A:39:LEU:HD21	1:A:123:GLU:HB3	4	0.18
(1,134)	1:A:39:LEU:HD22	1:A:123:GLU:HB3	4	0.18
(1,134)	1:A:39:LEU:HD23	1:A:123:GLU:HB3	4	0.18
(1,1229)	1:A:111:PHE:HB3	1:A:112:PRO:HG2	4	0.18
(1,1229)	1:A:111:PHE:HB3	1:A:112:PRO:HG2	14	0.18
(1,1229)	1:A:111:PHE:HB3	1:A:112:PRO:HG2	24	0.18
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	13	0.18
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	2	0.17
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	2	0.17
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	6	0.17
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	6	0.17
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	11	0.17
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	11	0.17
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	12	0.17
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	12	0.17
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	22	0.17
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	22	0.17
(1,533)	1:A:57:MET:HE1	2:A:135:NAG:H1	10	0.17
(1,533)	1:A:57:MET:HE2	2:A:135:NAG:H1	10	0.17
(1,533)	1:A:57:MET:HE3	2:A:135:NAG:H1	10	0.17
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG21	14	0.17
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG22	14	0.17
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG23	14	0.17
(1,298)	1:A:47:GLU:HG2	1:A:56:ILE:HD11	13	0.17
(1,298)	1:A:47:GLU:HG2	1:A:56:ILE:HD12	13	0.17
(1,298)	1:A:47:GLU:HG2	1:A:56:ILE:HD13	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:A:37:ARG:HB2	1:A:37:ARG:HD2	4	0.17
(1,29)	1:A:37:ARG:HB2	1:A:37:ARG:HD3	4	0.17
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	1	0.17
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	1	0.17
(1,2784)	1:A:62:ASN:HD21	1:A:86:PRO:HG3	5	0.17
(1,2784)	1:A:62:ASN:HD21	1:A:114:PRO:HG3	5	0.17
(1,2733)	1:A:45:PRO:HG2	1:A:44:TYR:H	19	0.17
(1,2733)	1:A:122:LEU:HB3	1:A:44:TYR:H	19	0.17
(1,2660)	1:A:123:GLU:HB2	1:A:125:GLN:HE22	7	0.17
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	20	0.17
(1,2088)	1:A:69:LYS:HG2	1:A:70:ILE:H	4	0.17
(1,2004)	1:A:65:ARG:HE	1:A:78:MET:HG3	21	0.17
(1,1994)	1:A:65:ARG:HE	1:A:66:THR:H	6	0.17
(1,1980)	1:A:64:GLY:H	1:A:122:LEU:HB3	21	0.17
(1,1980)	1:A:64:GLY:H	1:A:122:LEU:HB3	22	0.17
(1,1980)	1:A:64:GLY:H	1:A:122:LEU:HB3	25	0.17
(1,1627)	1:A:48:LEU:HG	1:A:49:ARG:H	15	0.17
(1,1454)	1:A:38:GLU:HG2	1:A:47:GLU:H	5	0.17
(1,1229)	1:A:111:PHE:HB3	1:A:112:PRO:HG2	1	0.17
(1,1182)	1:A:105:VAL:HB	1:A:108:SER:HA	1	0.17
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	15	0.17
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB2	10	0.16
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB3	10	0.16
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB2	19	0.16
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB3	19	0.16
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB2	25	0.16
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB3	25	0.16
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	1	0.16
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	1	0.16
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	13	0.16
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	13	0.16
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	15	0.16
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	15	0.16
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	18	0.16
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	18	0.16
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	21	0.16
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	21	0.16
(1,808)	1:A:71:CYS:HB2	1:A:121:TYR:HE1	19	0.16
(1,808)	1:A:71:CYS:HB2	1:A:121:TYR:HE2	19	0.16
(1,808)	1:A:71:CYS:HB3	1:A:121:TYR:HE1	19	0.16
(1,808)	1:A:71:CYS:HB3	1:A:121:TYR:HE2	19	0.16
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE1	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE2	15	0.16
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE3	15	0.16
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE1	17	0.16
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE2	17	0.16
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE3	17	0.16
(1,730)	1:A:66:THR:HA	1:A:81:VAL:HB	7	0.16
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD2	21	0.16
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD3	21	0.16
(1,533)	1:A:57:MET:HE1	2:A:135:NAG:H1	15	0.16
(1,533)	1:A:57:MET:HE2	2:A:135:NAG:H1	15	0.16
(1,533)	1:A:57:MET:HE3	2:A:135:NAG:H1	15	0.16
(1,533)	1:A:57:MET:HE1	2:A:135:NAG:H1	24	0.16
(1,533)	1:A:57:MET:HE2	2:A:135:NAG:H1	24	0.16
(1,533)	1:A:57:MET:HE3	2:A:135:NAG:H1	24	0.16
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG21	13	0.16
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG22	13	0.16
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG23	13	0.16
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG21	18	0.16
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG22	18	0.16
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG23	18	0.16
(1,414)	1:A:51:PRO:HD3	1:A:56:ILE:HG12	1	0.16
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG2	5	0.16
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG3	5	0.16
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG2	5	0.16
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG3	5	0.16
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	7	0.16
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	7	0.16
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	13	0.16
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	13	0.16
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	22	0.16
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	22	0.16
(1,2725)	1:A:37:ARG:HB2	1:A:38:GLU:H	5	0.16
(1,2725)	1:A:37:ARG:HB3	1:A:38:GLU:H	5	0.16
(1,2660)	1:A:123:GLU:HB2	1:A:125:GLN:HE22	18	0.16
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	1	0.16
(1,2515)	1:A:102:CYS:HB2	1:A:103:VAL:H	5	0.16
(1,2515)	1:A:102:CYS:HB3	1:A:103:VAL:H	5	0.16
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	1	0.16
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	1	0.16
(1,2307)	1:A:85:LEU:HB2	1:A:115:CYS:H	10	0.16
(1,2264)	1:A:82:GLN:H	1:A:83:CYS:H	5	0.16
(1,1916)	1:A:62:ASN:HD22	1:A:84:TYR:HA	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1627)	1:A:48:LEU:HG	1:A:49:ARG:H	21	0.16
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG21	24	0.16
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG22	24	0.16
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG23	24	0.16
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD11	6	0.16
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD12	6	0.16
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD13	6	0.16
(1,1608)	1:A:46:ILE:H	1:A:105:VAL:HA	11	0.16
(1,1455)	1:A:38:GLU:HG3	1:A:47:GLU:H	4	0.16
(1,1454)	1:A:38:GLU:HG2	1:A:47:GLU:H	12	0.16
(1,1398)	1:A:35:MET:HG3	1:A:126:TYR:H	17	0.16
(1,1391)	1:A:131:TYR:HE1	2:A:135:NAG:H1	24	0.16
(1,1391)	1:A:131:TYR:HE2	2:A:135:NAG:H1	24	0.16
(1,134)	1:A:39:LEU:HD21	1:A:123:GLU:HB3	5	0.16
(1,134)	1:A:39:LEU:HD22	1:A:123:GLU:HB3	5	0.16
(1,134)	1:A:39:LEU:HD23	1:A:123:GLU:HB3	5	0.16
(1,134)	1:A:39:LEU:HD21	1:A:123:GLU:HB3	8	0.16
(1,134)	1:A:39:LEU:HD22	1:A:123:GLU:HB3	8	0.16
(1,134)	1:A:39:LEU:HD23	1:A:123:GLU:HB3	8	0.16
(1,134)	1:A:39:LEU:HD21	1:A:123:GLU:HB3	11	0.16
(1,134)	1:A:39:LEU:HD22	1:A:123:GLU:HB3	11	0.16
(1,134)	1:A:39:LEU:HD23	1:A:123:GLU:HB3	11	0.16
(1,1307)	1:A:121:TYR:HD1	1:A:123:GLU:HG2	7	0.16
(1,1307)	1:A:121:TYR:HD1	1:A:123:GLU:HG3	7	0.16
(1,1307)	1:A:121:TYR:HD2	1:A:123:GLU:HG2	7	0.16
(1,1307)	1:A:121:TYR:HD2	1:A:123:GLU:HG3	7	0.16
(1,1229)	1:A:111:PHE:HB3	1:A:112:PRO:HG2	10	0.16
(1,1229)	1:A:111:PHE:HB3	1:A:112:PRO:HG2	16	0.16
(1,1210)	1:A:108:SER:HA	1:A:111:PHE:HB2	14	0.16
(1,1059)	1:A:91:ILE:HA	1:A:94:GLN:HA	23	0.16
(1,905)	1:A:82:GLN:HG2	1:A:82:GLN:HA	2	0.15
(1,905)	1:A:82:GLN:HG3	1:A:82:GLN:HA	2	0.15
(1,850)	1:A:75:PRO:HA	1:A:78:MET:HG2	5	0.15
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	8	0.15
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	8	0.15
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	24	0.15
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	24	0.15
(1,730)	1:A:66:THR:HA	1:A:81:VAL:HB	16	0.15
(1,730)	1:A:66:THR:HA	1:A:81:VAL:HB	19	0.15
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD2	23	0.15
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD3	23	0.15
(1,689)	1:A:64:GLY:HA2	1:A:84:TYR:HA	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,625)	1:A:62:ASN:HB2	1:A:123:GLU:HB3	14	0.15
(1,598)	1:A:61:ALA:HB1	1:A:88:ALA:HA	23	0.15
(1,598)	1:A:61:ALA:HB2	1:A:88:ALA:HA	23	0.15
(1,598)	1:A:61:ALA:HB3	1:A:88:ALA:HA	23	0.15
(1,533)	1:A:57:MET:HE1	2:A:135:NAG:H1	16	0.15
(1,533)	1:A:57:MET:HE2	2:A:135:NAG:H1	16	0.15
(1,533)	1:A:57:MET:HE3	2:A:135:NAG:H1	16	0.15
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG21	1	0.15
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG22	1	0.15
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG23	1	0.15
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG21	25	0.15
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG22	25	0.15
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG23	25	0.15
(1,29)	1:A:37:ARG:HB2	1:A:37:ARG:HD2	19	0.15
(1,29)	1:A:37:ARG:HB2	1:A:37:ARG:HD3	19	0.15
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	20	0.15
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	20	0.15
(1,2784)	1:A:62:ASN:HD21	1:A:86:PRO:HG3	15	0.15
(1,2784)	1:A:62:ASN:HD21	1:A:114:PRO:HG3	15	0.15
(1,2784)	1:A:62:ASN:HD21	1:A:86:PRO:HG3	24	0.15
(1,2784)	1:A:62:ASN:HD21	1:A:114:PRO:HG3	24	0.15
(1,2725)	1:A:37:ARG:HB2	1:A:38:GLU:H	16	0.15
(1,2725)	1:A:37:ARG:HB3	1:A:38:GLU:H	16	0.15
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	2	0.15
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	6	0.15
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	14	0.15
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	24	0.15
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	25	0.15
(1,2405)	1:A:93:SER:HB3	1:A:97:ASN:HD22	5	0.15
(1,2383)	1:A:92:MET:HG3	1:A:92:MET:H	17	0.15
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	3	0.15
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	3	0.15
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	8	0.15
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	8	0.15
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	23	0.15
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	23	0.15
(1,2307)	1:A:85:LEU:HB2	1:A:115:CYS:H	5	0.15
(1,2200)	1:A:78:MET:HG2	1:A:79:GLU:H	7	0.15
(1,2200)	1:A:78:MET:HG2	1:A:79:GLU:H	20	0.15
(1,2102)	1:A:70:ILE:HG12	1:A:71:CYS:H	18	0.15
(1,2021)	1:A:65:ARG:H	1:A:83:CYS:HB3	3	0.15
(1,2008)	1:A:65:ARG:HD2	1:A:79:GLU:H	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1994)	1:A:65:ARG:HE	1:A:66:THR:H	4	0.15
(1,1994)	1:A:65:ARG:HE	1:A:66:THR:H	7	0.15
(1,1980)	1:A:64:GLY:H	1:A:122:LEU:HB3	8	0.15
(1,188)	1:A:42:GLU:HG2	1:A:119:TYR:HE1	8	0.15
(1,188)	1:A:42:GLU:HG2	1:A:119:TYR:HE2	8	0.15
(1,1627)	1:A:48:LEU:HG	1:A:49:ARG:H	22	0.15
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD11	4	0.15
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD12	4	0.15
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD13	4	0.15
(1,1586)	1:A:45:PRO:HB3	1:A:105:VAL:H	7	0.15
(1,1490)	1:A:39:LEU:HA	1:A:124:VAL:H	5	0.15
(1,1490)	1:A:39:LEU:HA	1:A:124:VAL:H	17	0.15
(1,1455)	1:A:38:GLU:HG3	1:A:47:GLU:H	22	0.15
(1,1391)	1:A:131:TYR:HE1	2:A:135:NAG:H1	11	0.15
(1,1391)	1:A:131:TYR:HE2	2:A:135:NAG:H1	11	0.15
(1,1229)	1:A:111:PHE:HB3	1:A:112:PRO:HG2	5	0.15
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	7	0.15
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	8	0.15
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	9	0.15
(1,11)	1:A:35:MET:HE1	1:A:127:ASP:HA	7	0.15
(1,11)	1:A:35:MET:HE2	1:A:127:ASP:HA	7	0.15
(1,11)	1:A:35:MET:HE3	1:A:127:ASP:HA	7	0.15
(1,905)	1:A:82:GLN:HG2	1:A:82:GLN:HA	13	0.14
(1,905)	1:A:82:GLN:HG3	1:A:82:GLN:HA	13	0.14
(1,905)	1:A:82:GLN:HG2	1:A:82:GLN:HA	14	0.14
(1,905)	1:A:82:GLN:HG3	1:A:82:GLN:HA	14	0.14
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB2	18	0.14
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB3	18	0.14
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	4	0.14
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	4	0.14
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	10	0.14
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	10	0.14
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	14	0.14
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	14	0.14
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	17	0.14
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	17	0.14
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	20	0.14
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	20	0.14
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE1	20	0.14
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE2	20	0.14
(1,778)	1:A:69:LYS:HA	1:A:78:MET:HE3	20	0.14
(1,736)	1:A:66:THR:HG21	1:A:82:GLN:HA	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:A:66:THR:HG22	1:A:82:GLN:HA	12	0.14
(1,736)	1:A:66:THR:HG23	1:A:82:GLN:HA	12	0.14
(1,730)	1:A:66:THR:HA	1:A:81:VAL:HB	4	0.14
(1,730)	1:A:66:THR:HA	1:A:81:VAL:HB	15	0.14
(1,730)	1:A:66:THR:HA	1:A:81:VAL:HB	18	0.14
(1,730)	1:A:66:THR:HA	1:A:81:VAL:HB	23	0.14
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD2	5	0.14
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD3	5	0.14
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD2	12	0.14
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD3	12	0.14
(1,533)	1:A:57:MET:HE1	2:A:135:NAG:H1	17	0.14
(1,533)	1:A:57:MET:HE2	2:A:135:NAG:H1	17	0.14
(1,533)	1:A:57:MET:HE3	2:A:135:NAG:H1	17	0.14
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG21	23	0.14
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG22	23	0.14
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG23	23	0.14
(1,414)	1:A:51:PRO:HD3	1:A:56:ILE:HG12	7	0.14
(1,296)	1:A:47:GLU:HG2	1:A:48:LEU:HG	18	0.14
(1,287)	1:A:46:ILE:HD11	1:A:124:VAL:HG11	13	0.14
(1,287)	1:A:46:ILE:HD11	1:A:124:VAL:HG12	13	0.14
(1,287)	1:A:46:ILE:HD11	1:A:124:VAL:HG13	13	0.14
(1,287)	1:A:46:ILE:HD12	1:A:124:VAL:HG11	13	0.14
(1,287)	1:A:46:ILE:HD12	1:A:124:VAL:HG12	13	0.14
(1,287)	1:A:46:ILE:HD12	1:A:124:VAL:HG13	13	0.14
(1,287)	1:A:46:ILE:HD13	1:A:124:VAL:HG11	13	0.14
(1,287)	1:A:46:ILE:HD13	1:A:124:VAL:HG12	13	0.14
(1,287)	1:A:46:ILE:HD13	1:A:124:VAL:HG13	13	0.14
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	12	0.14
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	12	0.14
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	16	0.14
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	16	0.14
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	19	0.14
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	19	0.14
(1,2733)	1:A:45:PRO:HG2	1:A:44:TYR:H	17	0.14
(1,2733)	1:A:122:LEU:HB3	1:A:44:TYR:H	17	0.14
(1,2733)	1:A:45:PRO:HG2	1:A:44:TYR:H	24	0.14
(1,2733)	1:A:122:LEU:HB3	1:A:44:TYR:H	24	0.14
(1,2725)	1:A:37:ARG:HB2	1:A:38:GLU:H	15	0.14
(1,2725)	1:A:37:ARG:HB3	1:A:38:GLU:H	15	0.14
(1,2725)	1:A:37:ARG:HB2	1:A:38:GLU:H	23	0.14
(1,2725)	1:A:37:ARG:HB3	1:A:38:GLU:H	23	0.14
(1,2710)	1:A:130:PRO:HB2	1:A:131:TYR:H	22	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2710)	1:A:130:PRO:HB2	1:A:131:TYR:H	25	0.14
(1,2597)	1:A:115:CYS:H	1:A:120:LYS:HE2	3	0.14
(1,2445)	1:A:96:CYS:HB2	1:A:101:GLN:H	14	0.14
(1,2445)	1:A:96:CYS:HB3	1:A:101:GLN:H	14	0.14
(1,2389)	1:A:92:MET:H	1:A:93:SER:HB3	24	0.14
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	2	0.14
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	2	0.14
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	6	0.14
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	6	0.14
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	20	0.14
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	20	0.14
(1,2307)	1:A:85:LEU:HB2	1:A:115:CYS:H	13	0.14
(1,2307)	1:A:85:LEU:HB2	1:A:115:CYS:H	18	0.14
(1,2307)	1:A:85:LEU:HB2	1:A:115:CYS:H	21	0.14
(1,2307)	1:A:85:LEU:HB2	1:A:115:CYS:H	25	0.14
(1,2200)	1:A:78:MET:HG2	1:A:79:GLU:H	8	0.14
(1,2119)	1:A:71:CYS:HA	1:A:72:ASP:H	6	0.14
(1,2112)	1:A:70:ILE:H	1:A:121:TYR:HE1	5	0.14
(1,2112)	1:A:70:ILE:H	1:A:121:TYR:HE2	5	0.14
(1,2112)	1:A:70:ILE:H	1:A:121:TYR:HE1	8	0.14
(1,2112)	1:A:70:ILE:H	1:A:121:TYR:HE2	8	0.14
(1,2108)	1:A:70:ILE:H	1:A:72:ASP:HB2	5	0.14
(1,2108)	1:A:70:ILE:H	1:A:72:ASP:HB3	5	0.14
(1,2108)	1:A:70:ILE:H	1:A:72:ASP:HB2	19	0.14
(1,2108)	1:A:70:ILE:H	1:A:72:ASP:HB3	19	0.14
(1,2102)	1:A:70:ILE:HG12	1:A:71:CYS:H	4	0.14
(1,2102)	1:A:70:ILE:HG12	1:A:71:CYS:H	12	0.14
(1,2102)	1:A:70:ILE:HG12	1:A:71:CYS:H	14	0.14
(1,2088)	1:A:69:LYS:HG2	1:A:70:ILE:H	1	0.14
(1,2088)	1:A:69:LYS:HG2	1:A:70:ILE:H	22	0.14
(1,2077)	1:A:68:ASP:HB2	1:A:78:MET:H	20	0.14
(1,2073)	1:A:68:ASP:H	1:A:70:ILE:HG13	22	0.14
(1,2055)	1:A:67:ASP:H	1:A:70:ILE:HD11	17	0.14
(1,2055)	1:A:67:ASP:H	1:A:70:ILE:HD12	17	0.14
(1,2055)	1:A:67:ASP:H	1:A:70:ILE:HD13	17	0.14
(1,2014)	1:A:65:ARG:HG3	1:A:81:VAL:H	1	0.14
(1,2014)	1:A:65:ARG:HG3	1:A:81:VAL:H	25	0.14
(1,1994)	1:A:65:ARG:HE	1:A:66:THR:H	17	0.14
(1,1980)	1:A:64:GLY:H	1:A:122:LEU:HB3	9	0.14
(1,1916)	1:A:62:ASN:HD22	1:A:84:TYR:HA	25	0.14
(1,1661)	1:A:49:ARG:H	1:A:126:TYR:HD1	11	0.14
(1,1661)	1:A:49:ARG:H	1:A:126:TYR:HD2	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1627)	1:A:48:LEU:HG	1:A:49:ARG:H	7	0.14
(1,1627)	1:A:48:LEU:HG	1:A:49:ARG:H	11	0.14
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG21	7	0.14
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG22	7	0.14
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG23	7	0.14
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD11	11	0.14
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD12	11	0.14
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD13	11	0.14
(1,1608)	1:A:46:ILE:H	1:A:105:VAL:HA	23	0.14
(1,1490)	1:A:39:LEU:HA	1:A:124:VAL:H	24	0.14
(1,1455)	1:A:38:GLU:HG3	1:A:47:GLU:H	23	0.14
(1,1436)	1:A:37:ARG:HB3	1:A:126:TYR:H	14	0.14
(1,1398)	1:A:35:MET:HG3	1:A:126:TYR:H	6	0.14
(1,1398)	1:A:35:MET:HG3	1:A:126:TYR:H	13	0.14
(1,1391)	1:A:131:TYR:HE1	2:A:135:NAG:H1	19	0.14
(1,1391)	1:A:131:TYR:HE2	2:A:135:NAG:H1	19	0.14
(1,1307)	1:A:121:TYR:HD1	1:A:123:GLU:HG2	19	0.14
(1,1307)	1:A:121:TYR:HD1	1:A:123:GLU:HG3	19	0.14
(1,1307)	1:A:121:TYR:HD2	1:A:123:GLU:HG2	19	0.14
(1,1307)	1:A:121:TYR:HD2	1:A:123:GLU:HG3	19	0.14
(1,1229)	1:A:111:PHE:HB3	1:A:112:PRO:HG2	6	0.14
(1,1229)	1:A:111:PHE:HB3	1:A:112:PRO:HG2	13	0.14
(1,1229)	1:A:111:PHE:HB3	1:A:112:PRO:HG2	19	0.14
(1,1229)	1:A:111:PHE:HB3	1:A:112:PRO:HG2	23	0.14
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	2	0.14
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	6	0.14
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	22	0.14
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	23	0.14
(1,1122)	1:A:95:ARG:HG2	1:A:104:VAL:HG21	16	0.14
(1,1122)	1:A:95:ARG:HG2	1:A:104:VAL:HG22	16	0.14
(1,1122)	1:A:95:ARG:HG2	1:A:104:VAL:HG23	16	0.14
(1,1059)	1:A:91:ILE:HA	1:A:94:GLN:HA	13	0.14
(1,911)	1:A:82:GLN:HB2	1:A:84:TYR:HE1	9	0.13
(1,911)	1:A:82:GLN:HB2	1:A:84:TYR:HE2	9	0.13
(1,905)	1:A:82:GLN:HG2	1:A:82:GLN:HA	6	0.13
(1,905)	1:A:82:GLN:HG3	1:A:82:GLN:HA	6	0.13
(1,905)	1:A:82:GLN:HG2	1:A:82:GLN:HA	17	0.13
(1,905)	1:A:82:GLN:HG3	1:A:82:GLN:HA	17	0.13
(1,905)	1:A:82:GLN:HG2	1:A:82:GLN:HA	24	0.13
(1,905)	1:A:82:GLN:HG3	1:A:82:GLN:HA	24	0.13
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	25	0.13
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	25	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,818)	1:A:73:ALA:HB1	1:A:77:GLN:HG2	5	0.13
(1,818)	1:A:73:ALA:HB2	1:A:77:GLN:HG2	5	0.13
(1,818)	1:A:73:ALA:HB3	1:A:77:GLN:HG2	5	0.13
(1,797)	1:A:70:ILE:HD11	1:A:121:TYR:HE1	22	0.13
(1,797)	1:A:70:ILE:HD11	1:A:121:TYR:HE2	22	0.13
(1,797)	1:A:70:ILE:HD12	1:A:121:TYR:HE1	22	0.13
(1,797)	1:A:70:ILE:HD12	1:A:121:TYR:HE2	22	0.13
(1,797)	1:A:70:ILE:HD13	1:A:121:TYR:HE1	22	0.13
(1,797)	1:A:70:ILE:HD13	1:A:121:TYR:HE2	22	0.13
(1,730)	1:A:66:THR:HA	1:A:81:VAL:HB	12	0.13
(1,730)	1:A:66:THR:HA	1:A:81:VAL:HB	13	0.13
(1,730)	1:A:66:THR:HA	1:A:81:VAL:HB	14	0.13
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD2	15	0.13
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD3	15	0.13
(1,694)	1:A:64:GLY:HA3	1:A:120:LYS:HG3	8	0.13
(1,533)	1:A:57:MET:HE1	2:A:135:NAG:H1	2	0.13
(1,533)	1:A:57:MET:HE2	2:A:135:NAG:H1	2	0.13
(1,533)	1:A:57:MET:HE3	2:A:135:NAG:H1	2	0.13
(1,533)	1:A:57:MET:HE1	2:A:135:NAG:H1	8	0.13
(1,533)	1:A:57:MET:HE2	2:A:135:NAG:H1	8	0.13
(1,533)	1:A:57:MET:HE3	2:A:135:NAG:H1	8	0.13
(1,533)	1:A:57:MET:HE1	2:A:135:NAG:H1	23	0.13
(1,533)	1:A:57:MET:HE2	2:A:135:NAG:H1	23	0.13
(1,533)	1:A:57:MET:HE3	2:A:135:NAG:H1	23	0.13
(1,492)	1:A:56:ILE:HG21	1:A:97:ASN:HA	23	0.13
(1,492)	1:A:56:ILE:HG22	1:A:97:ASN:HA	23	0.13
(1,492)	1:A:56:ILE:HG23	1:A:97:ASN:HA	23	0.13
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG21	10	0.13
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG22	10	0.13
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG23	10	0.13
(1,419)	1:A:53:SER:HA	1:A:100:THR:HB	11	0.13
(1,419)	1:A:53:SER:HA	1:A:100:THR:HB	17	0.13
(1,419)	1:A:53:SER:HA	1:A:100:THR:HB	19	0.13
(1,414)	1:A:51:PRO:HD3	1:A:56:ILE:HG12	8	0.13
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG2	16	0.13
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG3	16	0.13
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG2	16	0.13
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG3	16	0.13
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	17	0.13
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	17	0.13
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	7	0.13
(1,2389)	1:A:92:MET:H	1:A:93:SER:HB3	23	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2383)	1:A:92:MET:HG3	1:A:92:MET:H	5	0.13
(1,2383)	1:A:92:MET:HG3	1:A:92:MET:H	15	0.13
(1,238)	1:A:45:PRO:HG2	1:A:105:VAL:HG21	8	0.13
(1,238)	1:A:45:PRO:HG2	1:A:105:VAL:HG22	8	0.13
(1,238)	1:A:45:PRO:HG2	1:A:105:VAL:HG23	8	0.13
(1,2348)	1:A:90:LYS:HB2	1:A:90:LYS:H	10	0.13
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	12	0.13
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	12	0.13
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	18	0.13
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	18	0.13
(1,2243)	1:A:80:ASN:HD22	1:A:118:THR:HB	4	0.13
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	6	0.13
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	7	0.13
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	20	0.13
(1,2200)	1:A:78:MET:HG2	1:A:79:GLU:H	5	0.13
(1,2200)	1:A:78:MET:HG2	1:A:79:GLU:H	24	0.13
(1,2186)	1:A:77:GLN:HB3	1:A:119:TYR:H	4	0.13
(1,2149)	1:A:74:ASP:H	1:A:77:GLN:HE21	25	0.13
(1,2102)	1:A:70:ILE:HG12	1:A:71:CYS:H	2	0.13
(1,2102)	1:A:70:ILE:HG12	1:A:71:CYS:H	7	0.13
(1,2088)	1:A:69:LYS:HG2	1:A:70:ILE:H	9	0.13
(1,2088)	1:A:69:LYS:HG2	1:A:70:ILE:H	16	0.13
(1,2088)	1:A:69:LYS:HG2	1:A:70:ILE:H	25	0.13
(1,2073)	1:A:68:ASP:H	1:A:70:ILE:HG13	20	0.13
(1,2021)	1:A:65:ARG:H	1:A:83:CYS:HB3	10	0.13
(1,2021)	1:A:65:ARG:H	1:A:83:CYS:HB3	17	0.13
(1,1994)	1:A:65:ARG:HE	1:A:66:THR:H	21	0.13
(1,1980)	1:A:64:GLY:H	1:A:122:LEU:HB3	14	0.13
(1,1980)	1:A:64:GLY:H	1:A:122:LEU:HB3	24	0.13
(1,1892)	1:A:61:ALA:HB1	1:A:126:TYR:H	4	0.13
(1,1892)	1:A:61:ALA:HB2	1:A:126:TYR:H	4	0.13
(1,1892)	1:A:61:ALA:HB3	1:A:126:TYR:H	4	0.13
(1,1892)	1:A:61:ALA:HB1	1:A:126:TYR:H	13	0.13
(1,1892)	1:A:61:ALA:HB2	1:A:126:TYR:H	13	0.13
(1,1892)	1:A:61:ALA:HB3	1:A:126:TYR:H	13	0.13
(1,188)	1:A:42:GLU:HG2	1:A:119:TYR:HE1	1	0.13
(1,188)	1:A:42:GLU:HG2	1:A:119:TYR:HE2	1	0.13
(1,188)	1:A:42:GLU:HG2	1:A:119:TYR:HE1	9	0.13
(1,188)	1:A:42:GLU:HG2	1:A:119:TYR:HE2	9	0.13
(1,185)	1:A:42:GLU:HG3	1:A:119:TYR:HD1	6	0.13
(1,185)	1:A:42:GLU:HG3	1:A:119:TYR:HD2	6	0.13
(1,185)	1:A:42:GLU:HG3	1:A:119:TYR:HD1	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,185)	1:A:42:GLU:HG3	1:A:119:TYR:HD2	12	0.13
(1,1661)	1:A:49:ARG:H	1:A:126:TYR:HD1	17	0.13
(1,1661)	1:A:49:ARG:H	1:A:126:TYR:HD2	17	0.13
(1,1630)	1:A:48:LEU:H	1:A:101:GLN:HG2	3	0.13
(1,1630)	1:A:48:LEU:H	1:A:101:GLN:HG3	3	0.13
(1,1627)	1:A:48:LEU:HG	1:A:49:ARG:H	1	0.13
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG21	14	0.13
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG22	14	0.13
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG23	14	0.13
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG21	19	0.13
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG22	19	0.13
(1,1623)	1:A:47:GLU:H	1:A:46:ILE:HG23	19	0.13
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD11	20	0.13
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD12	20	0.13
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD13	20	0.13
(1,1608)	1:A:46:ILE:H	1:A:105:VAL:HA	9	0.13
(1,1608)	1:A:46:ILE:H	1:A:105:VAL:HA	13	0.13
(1,1608)	1:A:46:ILE:H	1:A:105:VAL:HA	14	0.13
(1,1538)	1:A:42:GLU:HA	1:A:44:TYR:H	18	0.13
(1,1538)	1:A:42:GLU:HA	1:A:44:TYR:H	21	0.13
(1,1490)	1:A:39:LEU:HA	1:A:124:VAL:H	4	0.13
(1,1490)	1:A:39:LEU:HA	1:A:124:VAL:H	8	0.13
(1,1490)	1:A:39:LEU:HA	1:A:124:VAL:H	10	0.13
(1,1455)	1:A:38:GLU:HG3	1:A:47:GLU:H	10	0.13
(1,1455)	1:A:38:GLU:HG3	1:A:47:GLU:H	25	0.13
(1,1454)	1:A:38:GLU:HG2	1:A:47:GLU:H	3	0.13
(1,1229)	1:A:111:PHE:HB3	1:A:112:PRO:HG2	15	0.13
(1,1161)	1:A:104:VAL:HG11	1:A:105:VAL:HA	16	0.13
(1,1161)	1:A:104:VAL:HG12	1:A:105:VAL:HA	16	0.13
(1,1161)	1:A:104:VAL:HG13	1:A:105:VAL:HA	16	0.13
(1,1161)	1:A:104:VAL:HG11	1:A:105:VAL:HA	17	0.13
(1,1161)	1:A:104:VAL:HG12	1:A:105:VAL:HA	17	0.13
(1,1161)	1:A:104:VAL:HG13	1:A:105:VAL:HA	17	0.13
(1,974)	1:A:85:LEU:HD11	1:A:113:ASP:HA	6	0.12
(1,974)	1:A:85:LEU:HD12	1:A:113:ASP:HA	6	0.12
(1,974)	1:A:85:LEU:HD13	1:A:113:ASP:HA	6	0.12
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	16	0.12
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	16	0.12
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG2	19	0.12
(1,845)	1:A:75:PRO:HA	1:A:75:PRO:HG3	19	0.12
(1,689)	1:A:64:GLY:HA2	1:A:84:TYR:HA	19	0.12
(1,585)	1:A:60:ASN:HA	1:A:89:PHE:HA	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	1:A:58:VAL:HG21	1:A:92:MET:HG3	14	0.12
(1,552)	1:A:58:VAL:HG22	1:A:92:MET:HG3	14	0.12
(1,552)	1:A:58:VAL:HG23	1:A:92:MET:HG3	14	0.12
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG21	5	0.12
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG22	5	0.12
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG23	5	0.12
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG21	6	0.12
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG22	6	0.12
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG23	6	0.12
(1,414)	1:A:51:PRO:HD3	1:A:56:ILE:HG12	17	0.12
(1,414)	1:A:51:PRO:HD3	1:A:56:ILE:HG12	20	0.12
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG2	11	0.12
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG3	11	0.12
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG2	11	0.12
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG3	11	0.12
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG2	18	0.12
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG3	18	0.12
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG2	18	0.12
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG3	18	0.12
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG2	25	0.12
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG3	25	0.12
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG2	25	0.12
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG3	25	0.12
(1,382)	1:A:49:ARG:HD3	1:A:101:GLN:HA	10	0.12
(1,341)	1:A:48:LEU:HG	1:A:102:CYS:HB2	24	0.12
(1,341)	1:A:48:LEU:HG	1:A:102:CYS:HB3	24	0.12
(1,296)	1:A:47:GLU:HG2	1:A:48:LEU:HG	13	0.12
(1,29)	1:A:37:ARG:HB2	1:A:37:ARG:HD2	21	0.12
(1,29)	1:A:37:ARG:HB2	1:A:37:ARG:HD3	21	0.12
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	15	0.12
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	15	0.12
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	23	0.12
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	23	0.12
(1,2817)	1:A:70:ILE:HG12	1:A:66:THR:H	19	0.12
(1,2817)	1:A:120:LYS:HB3	1:A:66:THR:H	19	0.12
(1,2802)	1:A:65:ARG:HD3	1:A:70:ILE:H	2	0.12
(1,2802)	1:A:121:TYR:HB3	1:A:70:ILE:H	2	0.12
(1,2733)	1:A:45:PRO:HG2	1:A:44:TYR:H	9	0.12
(1,2733)	1:A:122:LEU:HB3	1:A:44:TYR:H	9	0.12
(1,2660)	1:A:123:GLU:HB2	1:A:125:GLN:HE22	5	0.12
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	3	0.12
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	9	0.12
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	13	0.12
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	21	0.12
(1,2389)	1:A:92:MET:H	1:A:93:SER:HB3	8	0.12
(1,2383)	1:A:92:MET:HG3	1:A:92:MET:H	23	0.12
(1,2376)	1:A:91:ILE:HG21	1:A:110:ALA:H	16	0.12
(1,2376)	1:A:91:ILE:HG22	1:A:110:ALA:H	16	0.12
(1,2376)	1:A:91:ILE:HG23	1:A:110:ALA:H	16	0.12
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	13	0.12
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	13	0.12
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	14	0.12
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	14	0.12
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	16	0.12
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	16	0.12
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	17	0.12
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	17	0.12
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	19	0.12
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	19	0.12
(1,2307)	1:A:85:LEU:HB2	1:A:115:CYS:H	8	0.12
(1,2307)	1:A:85:LEU:HB2	1:A:115:CYS:H	14	0.12
(1,2307)	1:A:85:LEU:HB2	1:A:115:CYS:H	17	0.12
(1,2307)	1:A:85:LEU:HB2	1:A:115:CYS:H	22	0.12
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	9	0.12
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	10	0.12
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	11	0.12
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	21	0.12
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	23	0.12
(1,2200)	1:A:78:MET:HG2	1:A:79:GLU:H	2	0.12
(1,2200)	1:A:78:MET:HG2	1:A:79:GLU:H	25	0.12
(1,2112)	1:A:70:ILE:H	1:A:121:TYR:HE1	21	0.12
(1,2112)	1:A:70:ILE:H	1:A:121:TYR:HE2	21	0.12
(1,2102)	1:A:70:ILE:HG12	1:A:71:CYS:H	11	0.12
(1,2088)	1:A:69:LYS:HG2	1:A:70:ILE:H	12	0.12
(1,2088)	1:A:69:LYS:HG2	1:A:70:ILE:H	20	0.12
(1,2073)	1:A:68:ASP:H	1:A:70:ILE:HG13	23	0.12
(1,2055)	1:A:67:ASP:H	1:A:70:ILE:HD11	21	0.12
(1,2055)	1:A:67:ASP:H	1:A:70:ILE:HD12	21	0.12
(1,2055)	1:A:67:ASP:H	1:A:70:ILE:HD13	21	0.12
(1,2008)	1:A:65:ARG:HD2	1:A:79:GLU:H	2	0.12
(1,2008)	1:A:65:ARG:HD2	1:A:79:GLU:H	4	0.12
(1,2004)	1:A:65:ARG:HE	1:A:78:MET:HG3	16	0.12
(1,2004)	1:A:65:ARG:HE	1:A:78:MET:HG3	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1980)	1:A:64:GLY:H	1:A:122:LEU:HB3	1	0.12
(1,1980)	1:A:64:GLY:H	1:A:122:LEU:HB3	11	0.12
(1,1869)	1:A:60:ASN:HD21	1:A:125:GLN:HG3	2	0.12
(1,1630)	1:A:48:LEU:H	1:A:101:GLN:HG2	15	0.12
(1,1630)	1:A:48:LEU:H	1:A:101:GLN:HG3	15	0.12
(1,1627)	1:A:48:LEU:HG	1:A:49:ARG:H	12	0.12
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD11	15	0.12
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD12	15	0.12
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD13	15	0.12
(1,1608)	1:A:46:ILE:H	1:A:105:VAL:HA	5	0.12
(1,1608)	1:A:46:ILE:H	1:A:105:VAL:HA	19	0.12
(1,1586)	1:A:45:PRO:HB3	1:A:105:VAL:H	21	0.12
(1,1490)	1:A:39:LEU:HA	1:A:124:VAL:H	14	0.12
(1,1490)	1:A:39:LEU:HA	1:A:124:VAL:H	20	0.12
(1,1398)	1:A:35:MET:HG3	1:A:126:TYR:H	15	0.12
(1,1398)	1:A:35:MET:HG3	1:A:126:TYR:H	24	0.12
(1,1391)	1:A:131:TYR:HE1	2:A:135:NAG:H1	1	0.12
(1,1391)	1:A:131:TYR:HE2	2:A:135:NAG:H1	1	0.12
(1,134)	1:A:39:LEU:HD21	1:A:123:GLU:HB3	15	0.12
(1,134)	1:A:39:LEU:HD22	1:A:123:GLU:HB3	15	0.12
(1,134)	1:A:39:LEU:HD23	1:A:123:GLU:HB3	15	0.12
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	16	0.12
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	20	0.12
(1,1122)	1:A:95:ARG:HG2	1:A:104:VAL:HG21	15	0.12
(1,1122)	1:A:95:ARG:HG2	1:A:104:VAL:HG22	15	0.12
(1,1122)	1:A:95:ARG:HG2	1:A:104:VAL:HG23	15	0.12
(1,104)	1:A:39:LEU:HD21	1:A:70:ILE:HG12	4	0.12
(1,104)	1:A:39:LEU:HD22	1:A:70:ILE:HG12	4	0.12
(1,104)	1:A:39:LEU:HD23	1:A:70:ILE:HG12	4	0.12
(1,974)	1:A:85:LEU:HD11	1:A:113:ASP:HA	11	0.11
(1,974)	1:A:85:LEU:HD12	1:A:113:ASP:HA	11	0.11
(1,974)	1:A:85:LEU:HD13	1:A:113:ASP:HA	11	0.11
(1,905)	1:A:82:GLN:HG2	1:A:82:GLN:HA	5	0.11
(1,905)	1:A:82:GLN:HG3	1:A:82:GLN:HA	5	0.11
(1,905)	1:A:82:GLN:HG2	1:A:82:GLN:HA	21	0.11
(1,905)	1:A:82:GLN:HG3	1:A:82:GLN:HA	21	0.11
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB2	22	0.11
(1,857)	1:A:76:PHE:HA	1:A:79:GLU:HB3	22	0.11
(1,850)	1:A:75:PRO:HA	1:A:78:MET:HG2	24	0.11
(1,840)	1:A:74:ASP:HB2	1:A:77:GLN:HG2	8	0.11
(1,840)	1:A:74:ASP:HB3	1:A:77:GLN:HG2	8	0.11
(1,818)	1:A:73:ALA:HB1	1:A:77:GLN:HG2	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,818)	1:A:73:ALA:HB2	1:A:77:GLN:HG2	17	0.11
(1,818)	1:A:73:ALA:HB3	1:A:77:GLN:HG2	17	0.11
(1,811)	1:A:72:ASP:HB2	1:A:78:MET:HE1	1	0.11
(1,811)	1:A:72:ASP:HB2	1:A:78:MET:HE2	1	0.11
(1,811)	1:A:72:ASP:HB2	1:A:78:MET:HE3	1	0.11
(1,811)	1:A:72:ASP:HB3	1:A:78:MET:HE1	1	0.11
(1,811)	1:A:72:ASP:HB3	1:A:78:MET:HE2	1	0.11
(1,811)	1:A:72:ASP:HB3	1:A:78:MET:HE3	1	0.11
(1,749)	1:A:67:ASP:HB2	1:A:70:ILE:HB	14	0.11
(1,749)	1:A:67:ASP:HB2	1:A:70:ILE:HB	19	0.11
(1,730)	1:A:66:THR:HA	1:A:81:VAL:HB	2	0.11
(1,730)	1:A:66:THR:HA	1:A:81:VAL:HB	6	0.11
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD2	16	0.11
(1,7)	1:A:35:MET:HA	1:A:36:ARG:HD3	16	0.11
(1,689)	1:A:64:GLY:HA2	1:A:84:TYR:HA	15	0.11
(1,585)	1:A:60:ASN:HA	1:A:89:PHE:HA	23	0.11
(1,533)	1:A:57:MET:HE1	2:A:135:NAG:H1	1	0.11
(1,533)	1:A:57:MET:HE2	2:A:135:NAG:H1	1	0.11
(1,533)	1:A:57:MET:HE3	2:A:135:NAG:H1	1	0.11
(1,533)	1:A:57:MET:HE1	2:A:135:NAG:H1	6	0.11
(1,533)	1:A:57:MET:HE2	2:A:135:NAG:H1	6	0.11
(1,533)	1:A:57:MET:HE3	2:A:135:NAG:H1	6	0.11
(1,533)	1:A:57:MET:HE1	2:A:135:NAG:H1	18	0.11
(1,533)	1:A:57:MET:HE2	2:A:135:NAG:H1	18	0.11
(1,533)	1:A:57:MET:HE3	2:A:135:NAG:H1	18	0.11
(1,492)	1:A:56:ILE:HG21	1:A:97:ASN:HA	4	0.11
(1,492)	1:A:56:ILE:HG22	1:A:97:ASN:HA	4	0.11
(1,492)	1:A:56:ILE:HG23	1:A:97:ASN:HA	4	0.11
(1,492)	1:A:56:ILE:HG21	1:A:97:ASN:HA	24	0.11
(1,492)	1:A:56:ILE:HG22	1:A:97:ASN:HA	24	0.11
(1,492)	1:A:56:ILE:HG23	1:A:97:ASN:HA	24	0.11
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG21	7	0.11
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG22	7	0.11
(1,420)	1:A:53:SER:HB3	1:A:100:THR:HG23	7	0.11
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG2	8	0.11
(1,384)	1:A:49:ARG:HB2	1:A:101:GLN:HG3	8	0.11
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG2	8	0.11
(1,384)	1:A:49:ARG:HB3	1:A:101:GLN:HG3	8	0.11
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	8	0.11
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	8	0.11
(1,2869)	1:A:56:ILE:HG13	1:A:101:GLN:H	9	0.11
(1,2869)	1:A:99:ARG:HB2	1:A:101:GLN:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2781)	1:A:61:ALA:H	1:A:89:PHE:H	23	0.11
(1,2781)	1:A:62:ASN:H	1:A:89:PHE:H	23	0.11
(1,2778)	1:A:61:ALA:H	1:A:60:ASN:HD21	10	0.11
(1,2778)	1:A:125:GLN:H	1:A:60:ASN:HD21	10	0.11
(1,2725)	1:A:37:ARG:HB2	1:A:38:GLU:H	4	0.11
(1,2725)	1:A:37:ARG:HB3	1:A:38:GLU:H	4	0.11
(1,2725)	1:A:37:ARG:HB2	1:A:38:GLU:H	13	0.11
(1,2725)	1:A:37:ARG:HB3	1:A:38:GLU:H	13	0.11
(1,2725)	1:A:37:ARG:HB2	1:A:38:GLU:H	14	0.11
(1,2725)	1:A:37:ARG:HB3	1:A:38:GLU:H	14	0.11
(1,2710)	1:A:130:PRO:HB2	1:A:131:TYR:H	16	0.11
(1,2631)	1:A:120:LYS:HE3	1:A:121:TYR:H	15	0.11
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	5	0.11
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	11	0.11
(1,2625)	1:A:120:LYS:HB3	1:A:121:TYR:H	18	0.11
(1,2574)	1:A:111:PHE:HD1	1:A:111:PHE:H	25	0.11
(1,2574)	1:A:111:PHE:HD2	1:A:111:PHE:H	25	0.11
(1,2515)	1:A:102:CYS:HB2	1:A:103:VAL:H	25	0.11
(1,2515)	1:A:102:CYS:HB3	1:A:103:VAL:H	25	0.11
(1,2453)	1:A:97:ASN:HB3	1:A:97:ASN:H	18	0.11
(1,2445)	1:A:96:CYS:HB2	1:A:101:GLN:H	8	0.11
(1,2445)	1:A:96:CYS:HB3	1:A:101:GLN:H	8	0.11
(1,2389)	1:A:92:MET:H	1:A:93:SER:HB3	7	0.11
(1,2389)	1:A:92:MET:H	1:A:93:SER:HB3	13	0.11
(1,2389)	1:A:92:MET:H	1:A:93:SER:HB3	19	0.11
(1,2389)	1:A:92:MET:H	1:A:93:SER:HB3	20	0.11
(1,2389)	1:A:92:MET:H	1:A:93:SER:HB3	22	0.11
(1,2383)	1:A:92:MET:HG3	1:A:92:MET:H	19	0.11
(1,2380)	1:A:92:MET:HB3	1:A:92:MET:H	14	0.11
(1,238)	1:A:45:PRO:HG2	1:A:105:VAL:HG21	9	0.11
(1,238)	1:A:45:PRO:HG2	1:A:105:VAL:HG22	9	0.11
(1,238)	1:A:45:PRO:HG2	1:A:105:VAL:HG23	9	0.11
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	5	0.11
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	5	0.11
(1,2334)	1:A:89:PHE:HE1	1:A:89:PHE:H	10	0.11
(1,2334)	1:A:89:PHE:HE2	1:A:89:PHE:H	10	0.11
(1,2307)	1:A:85:LEU:HB2	1:A:115:CYS:H	6	0.11
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	1	0.11
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	2	0.11
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	8	0.11
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	13	0.11
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	17	0.11
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	18	0.11
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	19	0.11
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	24	0.11
(1,2210)	1:A:79:GLU:HA	1:A:80:ASN:H	25	0.11
(1,2173)	1:A:77:GLN:HG2	1:A:77:GLN:H	23	0.11
(1,2112)	1:A:70:ILE:H	1:A:121:TYR:HE1	13	0.11
(1,2112)	1:A:70:ILE:H	1:A:121:TYR:HE2	13	0.11
(1,2102)	1:A:70:ILE:HG12	1:A:71:CYS:H	5	0.11
(1,2102)	1:A:70:ILE:HG12	1:A:71:CYS:H	15	0.11
(1,2102)	1:A:70:ILE:HG12	1:A:71:CYS:H	17	0.11
(1,2102)	1:A:70:ILE:HG12	1:A:71:CYS:H	20	0.11
(1,2088)	1:A:69:LYS:HG2	1:A:70:ILE:H	19	0.11
(1,2088)	1:A:69:LYS:HG2	1:A:70:ILE:H	24	0.11
(1,2021)	1:A:65:ARG:H	1:A:83:CYS:HB3	8	0.11
(1,2021)	1:A:65:ARG:H	1:A:83:CYS:HB3	14	0.11
(1,2014)	1:A:65:ARG:HG3	1:A:81:VAL:H	5	0.11
(1,2014)	1:A:65:ARG:HG3	1:A:81:VAL:H	19	0.11
(1,2014)	1:A:65:ARG:HG3	1:A:81:VAL:H	20	0.11
(1,2007)	1:A:65:ARG:HD2	1:A:78:MET:H	10	0.11
(1,1994)	1:A:65:ARG:HE	1:A:66:THR:H	12	0.11
(1,1980)	1:A:64:GLY:H	1:A:122:LEU:HB3	4	0.11
(1,1980)	1:A:64:GLY:H	1:A:122:LEU:HB3	20	0.11
(1,1934)	1:A:62:ASN:H	1:A:123:GLU:HG2	2	0.11
(1,1934)	1:A:62:ASN:H	1:A:123:GLU:HG3	2	0.11
(1,1916)	1:A:62:ASN:HD22	1:A:84:TYR:HA	10	0.11
(1,1916)	1:A:62:ASN:HD22	1:A:84:TYR:HA	24	0.11
(1,1890)	1:A:61:ALA:H	1:A:125:GLN:HE22	23	0.11
(1,185)	1:A:42:GLU:HG3	1:A:119:TYR:HD1	7	0.11
(1,185)	1:A:42:GLU:HG3	1:A:119:TYR:HD2	7	0.11
(1,185)	1:A:42:GLU:HG3	1:A:119:TYR:HD1	13	0.11
(1,185)	1:A:42:GLU:HG3	1:A:119:TYR:HD2	13	0.11
(1,1630)	1:A:48:LEU:H	1:A:101:GLN:HG2	9	0.11
(1,1630)	1:A:48:LEU:H	1:A:101:GLN:HG3	9	0.11
(1,1627)	1:A:48:LEU:HG	1:A:49:ARG:H	6	0.11
(1,1627)	1:A:48:LEU:HG	1:A:49:ARG:H	20	0.11
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD11	7	0.11
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD12	7	0.11
(1,1619)	1:A:47:GLU:H	1:A:48:LEU:HD13	7	0.11
(1,1608)	1:A:46:ILE:H	1:A:105:VAL:HA	16	0.11
(1,1608)	1:A:46:ILE:H	1:A:105:VAL:HA	24	0.11
(1,1603)	1:A:46:ILE:HG13	1:A:104:VAL:H	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1603)	1:A:46:ILE:HG13	1:A:104:VAL:H	18	0.11
(1,1576)	1:A:44:TYR:H	1:A:105:VAL:HG21	13	0.11
(1,1576)	1:A:44:TYR:H	1:A:105:VAL:HG22	13	0.11
(1,1576)	1:A:44:TYR:H	1:A:105:VAL:HG23	13	0.11
(1,1490)	1:A:39:LEU:HA	1:A:124:VAL:H	3	0.11
(1,1454)	1:A:38:GLU:HG2	1:A:47:GLU:H	9	0.11
(1,1436)	1:A:37:ARG:HB3	1:A:126:TYR:H	11	0.11
(1,1398)	1:A:35:MET:HG3	1:A:126:TYR:H	1	0.11
(1,1391)	1:A:131:TYR:HE1	2:A:135:NAG:H1	14	0.11
(1,1391)	1:A:131:TYR:HE2	2:A:135:NAG:H1	14	0.11
(1,134)	1:A:39:LEU:HD21	1:A:123:GLU:HB3	17	0.11
(1,134)	1:A:39:LEU:HD22	1:A:123:GLU:HB3	17	0.11
(1,134)	1:A:39:LEU:HD23	1:A:123:GLU:HB3	17	0.11
(1,1229)	1:A:111:PHE:HB3	1:A:112:PRO:HG2	9	0.11
(1,1182)	1:A:105:VAL:HB	1:A:108:SER:HA	9	0.11
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	10	0.11
(1,1139)	1:A:99:ARG:HG2	1:A:100:THR:HB	21	0.11
(1,1122)	1:A:95:ARG:HG2	1:A:104:VAL:HG21	11	0.11
(1,1122)	1:A:95:ARG:HG2	1:A:104:VAL:HG22	11	0.11
(1,1122)	1:A:95:ARG:HG2	1:A:104:VAL:HG23	11	0.11
(1,11)	1:A:35:MET:HE1	1:A:127:ASP:HA	6	0.11
(1,11)	1:A:35:MET:HE2	1:A:127:ASP:HA	6	0.11
(1,11)	1:A:35:MET:HE3	1:A:127:ASP:HA	6	0.11
(1,105)	1:A:39:LEU:HD21	1:A:70:ILE:HD11	6	0.11
(1,105)	1:A:39:LEU:HD21	1:A:70:ILE:HD12	6	0.11
(1,105)	1:A:39:LEU:HD21	1:A:70:ILE:HD13	6	0.11
(1,105)	1:A:39:LEU:HD22	1:A:70:ILE:HD11	6	0.11
(1,105)	1:A:39:LEU:HD22	1:A:70:ILE:HD12	6	0.11
(1,105)	1:A:39:LEU:HD22	1:A:70:ILE:HD13	6	0.11
(1,105)	1:A:39:LEU:HD23	1:A:70:ILE:HD11	6	0.11
(1,105)	1:A:39:LEU:HD23	1:A:70:ILE:HD12	6	0.11
(1,105)	1:A:39:LEU:HD23	1:A:70:ILE:HD13	6	0.11
(1,1001)	1:A:87:ASP:HA	1:A:90:LYS:HB3	14	0.11

10 Dihedral-angle violation analysis (i)

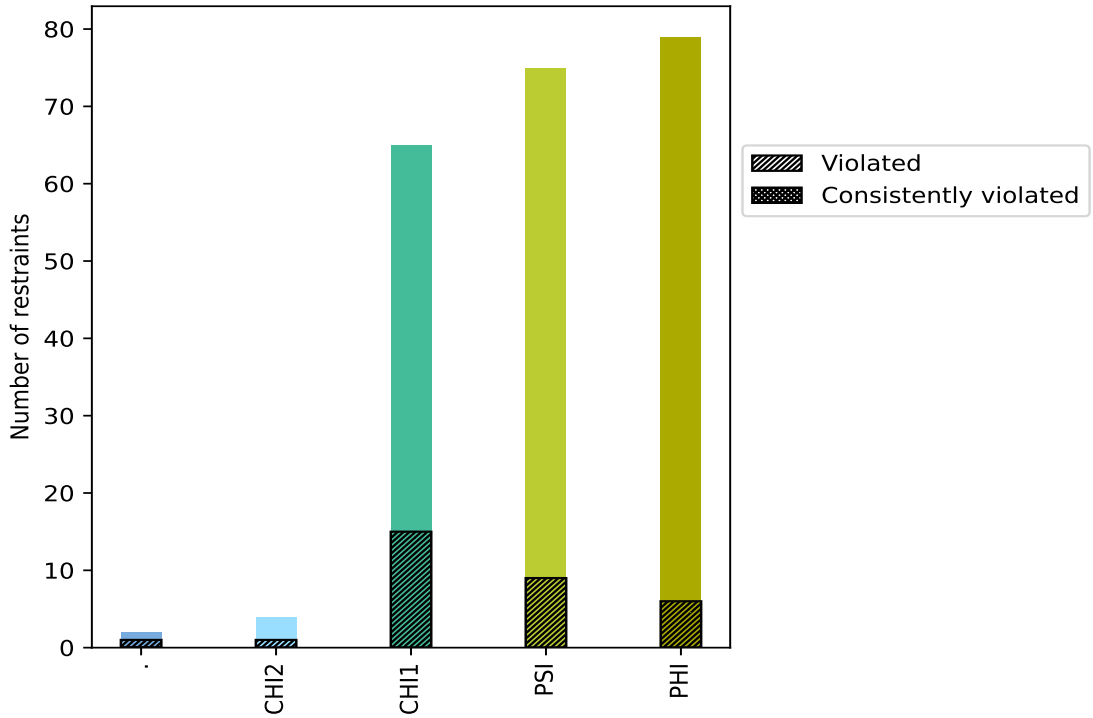
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
.	2	0.9	1	50.0	0.4	0	0.0	0.0
CHI2	4	1.8	1	25.0	0.4	0	0.0	0.0
CHI1	65	28.9	15	23.1	6.7	0	0.0	0.0
PSI	75	33.3	9	12.0	4.0	0	0.0	0.0
PHI	79	35.1	6	7.6	2.7	0	0.0	0.0
Total	225	100.0	32	14.2	14.2	0	0.0	0.0

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

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



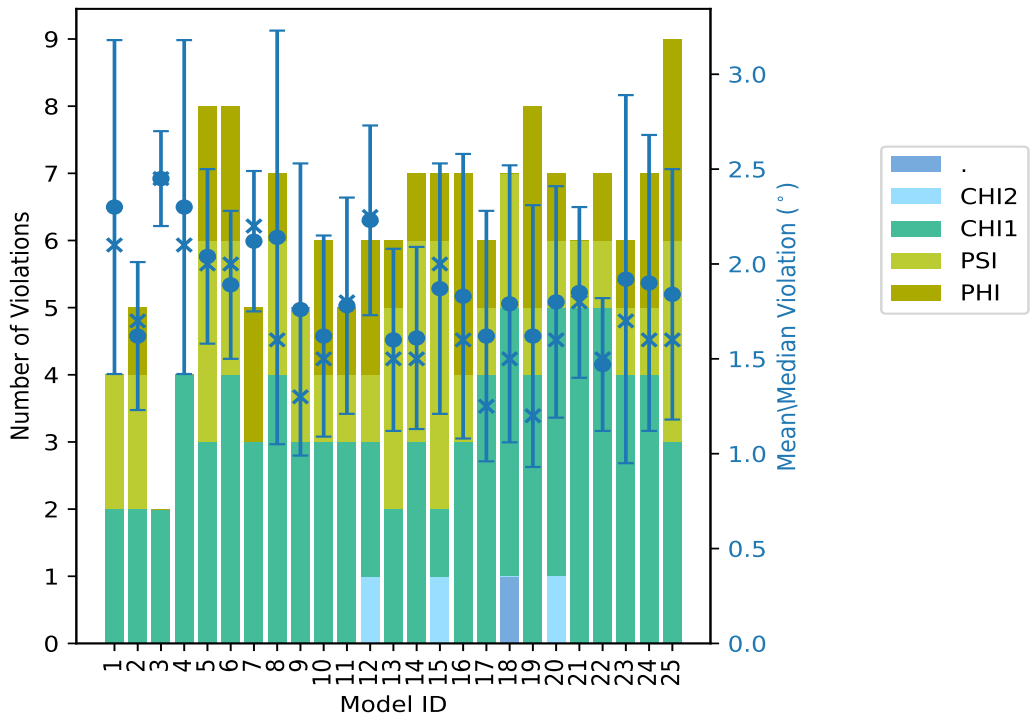
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations						Mean (°)	Max (°)	SD (°)	Median (°)
	.	CHI2	CHI1	PSI	PHI	Total				
1	0	0	2	2	0	4	2.3	3.7	0.88	2.1
2	0	0	2	2	1	5	1.62	2.2	0.39	1.7
3	0	0	2	0	0	2	2.45	2.7	0.25	2.45
4	0	0	4	0	0	4	2.3	3.6	0.88	2.1
5	0	0	3	3	2	8	2.04	2.8	0.46	2.0
6	0	0	4	2	2	8	1.89	2.5	0.39	2.0
7	0	0	3	0	2	5	2.12	2.6	0.37	2.2
8	0	0	4	2	1	7	2.14	4.3	1.09	1.6
9	0	0	3	2	0	5	1.76	3.2	0.77	1.3
10	0	0	3	1	2	6	1.62	2.3	0.53	1.5
11	0	0	3	1	1	5	1.78	2.8	0.57	1.8
12	0	1	2	1	2	6	2.23	2.9	0.5	2.25
13	0	0	2	3	1	6	1.6	2.4	0.48	1.5
14	0	0	3	3	1	7	1.61	2.6	0.48	1.5
15	0	1	1	4	1	7	1.87	3.0	0.66	2.0
16	0	0	3	1	3	7	1.83	3.6	0.75	1.6
17	0	0	4	1	1	6	1.62	2.8	0.66	1.25
18	1	0	4	2	0	7	1.79	3.1	0.73	1.5
19	0	0	4	1	3	8	1.62	3.0	0.69	1.2
20	0	1	4	1	1	7	1.8	3.0	0.61	1.6
21	0	0	5	1	0	6	1.85	2.7	0.45	1.8
22	0	0	5	1	1	7	1.47	2.1	0.35	1.5
23	0	0	4	1	1	6	1.92	4.0	0.97	1.7
24	0	0	4	1	2	7	1.9	3.4	0.78	1.6
25	0	0	3	3	3	9	1.84	2.7	0.66	1.6

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	
.	CHI2	CHI1	PSI	PHI	Total	Count[1]	%
1	0	5	3	0	9	1	4.0
0	0	2	3	2	7	2	8.0
0	1	1	0	0	2	3	12.0
0	0	1	0	1	2	4	16.0
0	0	1	1	2	4	5	20.0
0	0	0	0	0	0	6	24.0
0	0	0	1	0	1	7	28.0
0	0	1	0	0	1	8	32.0
0	0	1	0	0	1	9	36.0
0	0	0	0	0	0	10	40.0
0	0	0	0	0	0	11	44.0

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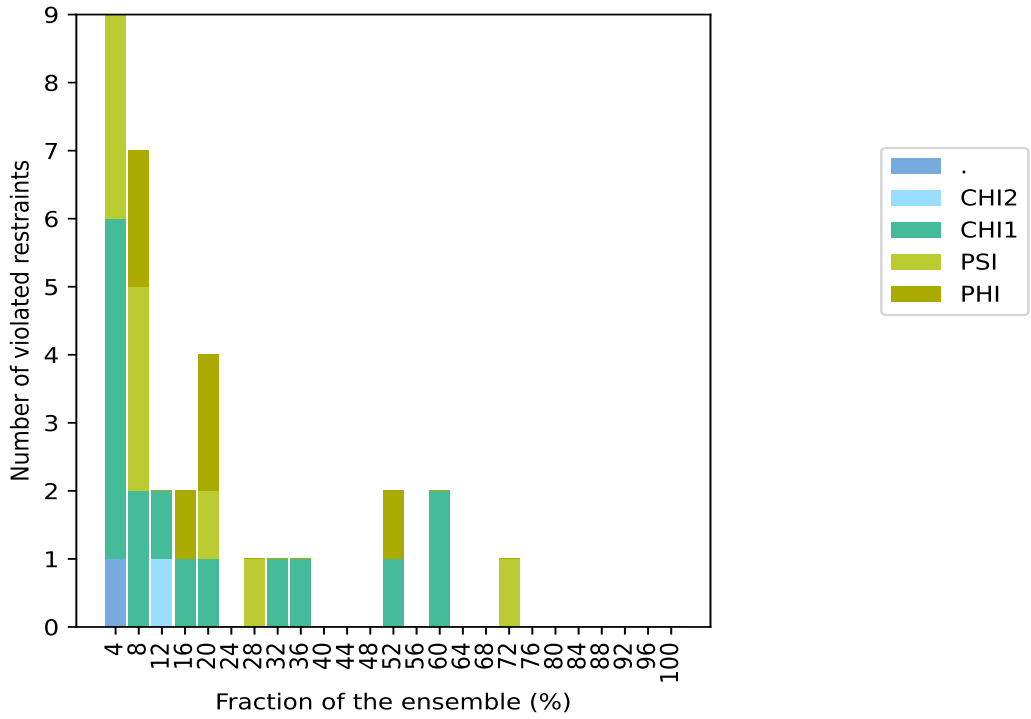
Number of violated restraints						Fraction of the ensemble	
.	CHI2	CHI1	PSI	PHI	Total	Count[1]	%
0	0	0	0	0	0	12	48.0
0	0	1	0	1	2	13	52.0
0	0	0	0	0	0	14	56.0
0	0	2	0	0	2	15	60.0
0	0	0	0	0	0	16	64.0
0	0	0	0	0	0	17	68.0
0	0	0	1	0	1	18	72.0
0	0	0	0	0	0	19	76.0
0	0	0	0	0	0	20	80.0
0	0	0	0	0	0	21	84.0
0	0	0	0	0	0	22	88.0
0	0	0	0	0	0	23	92.0
0	0	0	0	0	0	24	96.0
0	0	0	0	0	0	25	100.0

[1] Number of models with violations

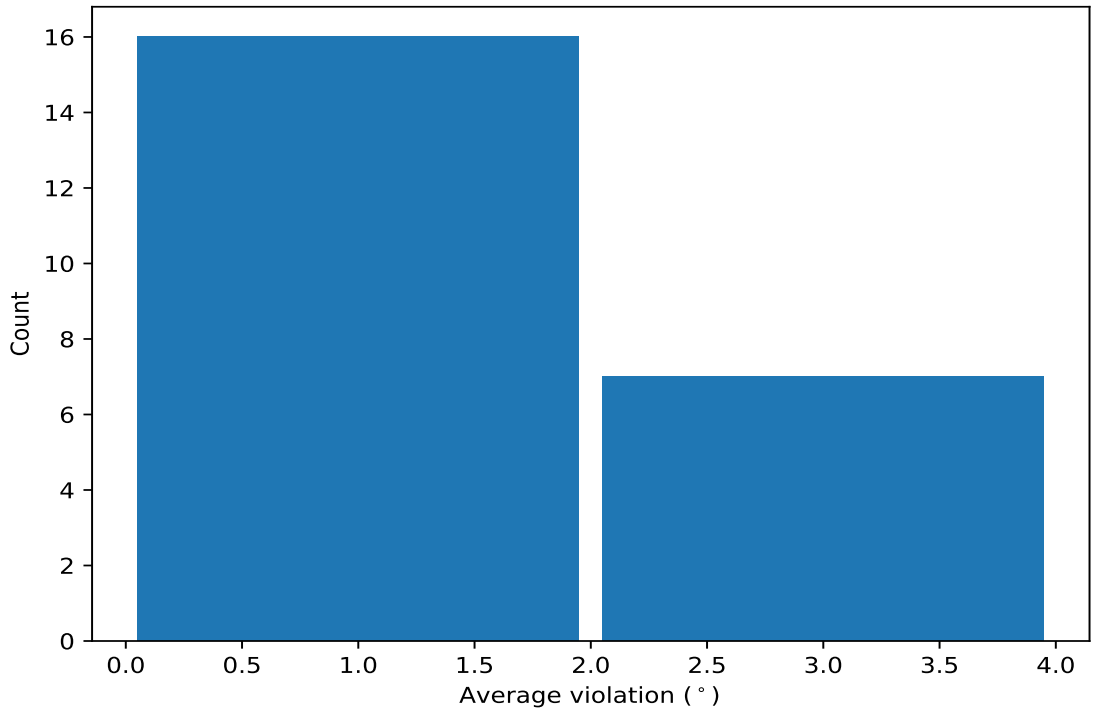
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



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
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	18	1.81	0.6	1.75
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	15	2.55	0.82	2.2
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	15	2.13	0.47	2.1
(1,48)	1:A:112:PRO:C	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:C	13	1.88	0.59	1.8
(1,198)	1:A:115:CYS:N	1:A:115:CYS:CA	1:A:115:CYS:CB	1:A:115:CYS:SG	13	1.82	0.71	1.6
(1,176)	1:A:74:ASP:N	1:A:74:ASP:CA	1:A:74:ASP:CB	1:A:74:ASP:CG	9	1.58	0.44	1.5
(1,180)	1:A:79:GLU:N	1:A:79:GLU:CA	1:A:79:GLU:CB	1:A:79:GLU:CG	8	2.03	1.01	1.7
(1,147)	1:A:54:ASP:N	1:A:54:ASP:CA	1:A:54:ASP:C	1:A:55:VAL:N	7	1.71	0.45	1.7
(1,197)	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:CB	1:A:113:ASP:CG	5	2.06	0.62	2.1
(1,135)	1:A:72:ASP:C	1:A:73:ALA:N	1:A:73:ALA:CA	1:A:73:ALA:C	5	1.48	0.21	1.5
(1,150)	1:A:73:ALA:N	1:A:73:ALA:CA	1:A:73:ALA:C	1:A:74:ASP:N	5	1.48	0.38	1.3
(1,138)	1:A:95:ARG:C	1:A:96:CYS:N	1:A:96:CYS:CA	1:A:96:CYS:C	5	1.26	0.15	1.3
(1,166)	1:A:57:MET:N	1:A:57:MET:CA	1:A:57:MET:CB	1:A:57:MET:CG	4	1.9	1.05	1.4

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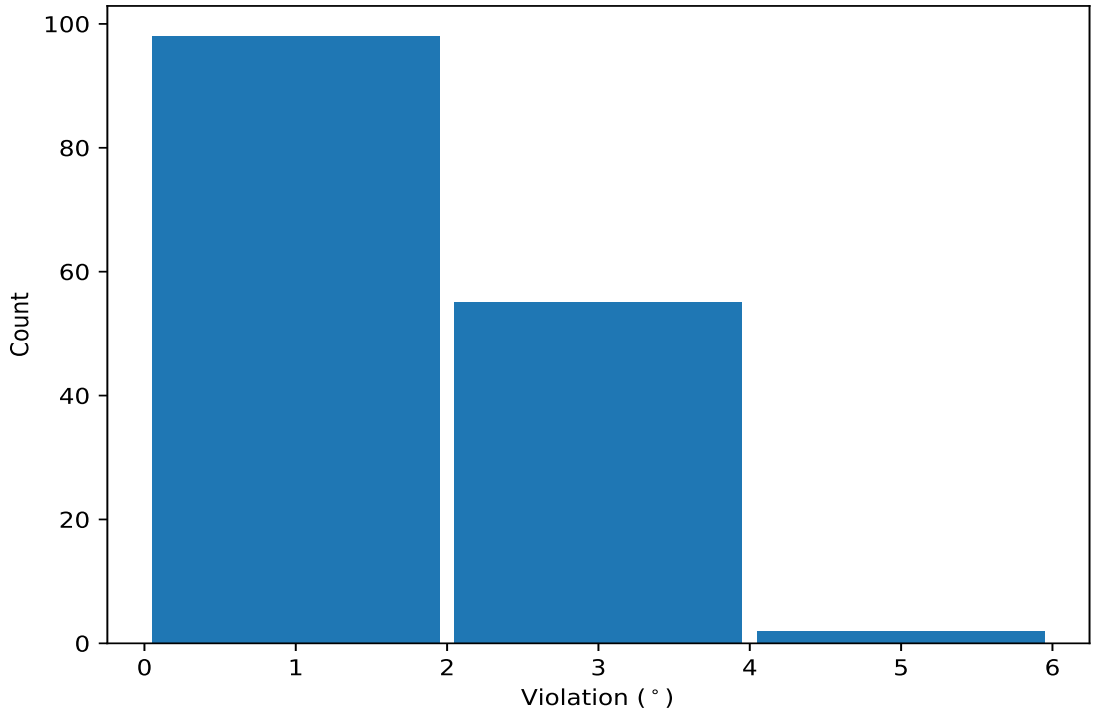
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,29)	1:A:84:TYR:C	1:A:85:LEU:N	1:A:85:LEU:CA	1:A:85:LEU:C	4	1.58	0.25	1.6
(1,223)	1:A:39:LEU:CA	1:A:39:LEU:CB	1:A:39:LEU:CG	1:A:39:LEU:CD1	3	2.0	0.49	2.0
(1,172)	1:A:67:ASP:N	1:A:67:ASP:CA	1:A:67:ASP:CB	1:A:67:ASP:CG	3	1.37	0.12	1.4
(1,109)	1:A:109:ASP:N	1:A:109:ASP:CA	1:A:109:ASP:C	1:A:110:ALA:N	2	2.5	0.0	2.5
(1,207)	1:A:131:TYR:N	1:A:131:TYR:CA	1:A:131:TYR:CB	1:A:131:TYR:CG	2	2.05	0.55	2.05
(1,53)	1:A:120:LYS:C	1:A:121:TYR:N	1:A:121:TYR:CA	1:A:121:TYR:C	2	1.85	0.45	1.85
(1,196)	1:A:111:PHE:N	1:A:111:PHE:CA	1:A:111:PHE:CB	1:A:111:PHE:CG	2	1.75	0.15	1.75
(1,81)	1:A:59:GLU:N	1:A:59:GLU:CA	1:A:59:GLU:C	1:A:60:ASN:N	2	1.6	0.5	1.6
(1,144)	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	1:A:34:LEU:N	2	1.6	0.1	1.6
(1,62)	1:A:129:VAL:C	1:A:130:PRO:N	1:A:130:PRO:CA	1:A:130:PRO:C	2	1.35	0.15	1.35

[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 (°)
(1,180)	1:A:79:GLU:N	1:A:79:GLU:CA	1:A:79:GLU:CB	1:A:79:GLU:CG	8	4.3
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	23	4.0
(1,166)	1:A:57:MET:N	1:A:57:MET:CA	1:A:57:MET:CB	1:A:57:MET:CG	1	3.7
(1,198)	1:A:115:CYS:N	1:A:115:CYS:CA	1:A:115:CYS:CB	1:A:115:CYS:SG	16	3.6
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	4	3.6
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	24	3.4
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	8	3.2
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	9	3.2
(1,224)	1:A:85:LEU:CA	1:A:85:LEU:CB	1:A:85:LEU:CG	1:A:85:LEU:CD2	18	3.1
(1,48)	1:A:112:PRO:C	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:C	20	3.0
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	15	3.0
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	19	3.0
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	12	2.9
(1,48)	1:A:112:PRO:C	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:C	5	2.8
(1,197)	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:CB	1:A:113:ASP:CG	17	2.8
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	11	2.8
(1,198)	1:A:115:CYS:N	1:A:115:CYS:CA	1:A:115:CYS:CB	1:A:115:CYS:SG	3	2.7
(1,180)	1:A:79:GLU:N	1:A:79:GLU:CA	1:A:79:GLU:CB	1:A:79:GLU:CG	21	2.7
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	18	2.7
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	24	2.7
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	25	2.7
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	25	2.7
(1,223)	1:A:39:LEU:CA	1:A:39:LEU:CB	1:A:39:LEU:CG	1:A:39:LEU:CD1	12	2.6
(1,207)	1:A:131:TYR:N	1:A:131:TYR:CA	1:A:131:TYR:CB	1:A:131:TYR:CG	25	2.6
(1,198)	1:A:115:CYS:N	1:A:115:CYS:CA	1:A:115:CYS:CB	1:A:115:CYS:SG	4	2.6
(1,197)	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:CB	1:A:113:ASP:CG	7	2.6
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	14	2.6
(1,147)	1:A:54:ASP:N	1:A:54:ASP:CA	1:A:54:ASP:C	1:A:55:VAL:N	15	2.5
(1,109)	1:A:109:ASP:N	1:A:109:ASP:CA	1:A:109:ASP:C	1:A:110:ALA:N	5	2.5
(1,109)	1:A:109:ASP:N	1:A:109:ASP:CA	1:A:109:ASP:C	1:A:110:ALA:N	19	2.5
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	6	2.5
(1,48)	1:A:112:PRO:C	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:C	7	2.4
(1,176)	1:A:74:ASP:N	1:A:74:ASP:CA	1:A:74:ASP:CB	1:A:74:ASP:CG	12	2.4
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	13	2.4
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	5	2.4
(1,53)	1:A:120:LYS:C	1:A:121:TYR:N	1:A:121:TYR:CA	1:A:121:TYR:C	6	2.3
(1,180)	1:A:79:GLU:N	1:A:79:GLU:CA	1:A:79:GLU:CB	1:A:79:GLU:CG	10	2.3
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	20	2.3
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	1	2.3
(1,48)	1:A:112:PRO:C	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:C	10	2.2
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	2	2.2
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	3	2.2
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	7	2.2
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	17	2.2
(1,150)	1:A:73:ALA:N	1:A:73:ALA:CA	1:A:73:ALA:C	1:A:74:ASP:N	25	2.2
(1,81)	1:A:59:GLU:N	1:A:59:GLU:CA	1:A:59:GLU:C	1:A:60:ASN:N	5	2.1
(1,48)	1:A:112:PRO:C	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:C	12	2.1
(1,197)	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:CB	1:A:113:ASP:CG	8	2.1
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	12	2.1
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	22	2.1
(1,48)	1:A:112:PRO:C	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:C	15	2.0
(1,223)	1:A:39:LEU:CA	1:A:39:LEU:CB	1:A:39:LEU:CG	1:A:39:LEU:CD1	15	2.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	6	2.0
(1,176)	1:A:74:ASP:N	1:A:74:ASP:CA	1:A:74:ASP:CB	1:A:74:ASP:CG	21	2.0
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	6	2.0
(1,147)	1:A:54:ASP:N	1:A:54:ASP:CA	1:A:54:ASP:C	1:A:55:VAL:N	6	2.0
(1,147)	1:A:54:ASP:N	1:A:54:ASP:CA	1:A:54:ASP:C	1:A:55:VAL:N	13	2.0
(1,29)	1:A:84:TYR:C	1:A:85:LEU:N	1:A:85:LEU:CA	1:A:85:LEU:C	10	1.9
(1,198)	1:A:115:CYS:N	1:A:115:CYS:CA	1:A:115:CYS:CB	1:A:115:CYS:SG	1	1.9
(1,196)	1:A:111:PHE:N	1:A:111:PHE:CA	1:A:111:PHE:CB	1:A:111:PHE:CG	5	1.9
(1,176)	1:A:74:ASP:N	1:A:74:ASP:CA	1:A:74:ASP:CB	1:A:74:ASP:CG	14	1.9
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	9	1.9
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	20	1.9
(1,48)	1:A:112:PRO:C	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:C	23	1.8
(1,48)	1:A:112:PRO:C	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:C	24	1.8
(1,198)	1:A:115:CYS:N	1:A:115:CYS:CA	1:A:115:CYS:CB	1:A:115:CYS:SG	11	1.8
(1,198)	1:A:115:CYS:N	1:A:115:CYS:CA	1:A:115:CYS:CB	1:A:115:CYS:SG	22	1.8
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	21	1.8
(1,180)	1:A:79:GLU:N	1:A:79:GLU:CA	1:A:79:GLU:CB	1:A:79:GLU:CG	23	1.8
(1,176)	1:A:74:ASP:N	1:A:74:ASP:CA	1:A:74:ASP:CB	1:A:74:ASP:CG	16	1.8
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	11	1.8
(1,135)	1:A:72:ASP:C	1:A:73:ALA:N	1:A:73:ALA:CA	1:A:73:ALA:C	7	1.8
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	2	1.8
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	21	1.8
(1,197)	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:CB	1:A:113:ASP:CG	19	1.7
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	14	1.7
(1,147)	1:A:54:ASP:N	1:A:54:ASP:CA	1:A:54:ASP:C	1:A:55:VAL:N	2	1.7
(1,144)	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	1:A:34:LEU:N	13	1.7
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	16	1.7
(1,29)	1:A:84:TYR:C	1:A:85:LEU:N	1:A:85:LEU:CA	1:A:85:LEU:C	16	1.6
(1,29)	1:A:84:TYR:C	1:A:85:LEU:N	1:A:85:LEU:CA	1:A:85:LEU:C	24	1.6
(1,198)	1:A:115:CYS:N	1:A:115:CYS:CA	1:A:115:CYS:CB	1:A:115:CYS:SG	5	1.6
(1,198)	1:A:115:CYS:N	1:A:115:CYS:CA	1:A:115:CYS:CB	1:A:115:CYS:SG	7	1.6
(1,198)	1:A:115:CYS:N	1:A:115:CYS:CA	1:A:115:CYS:CB	1:A:115:CYS:SG	8	1.6
(1,196)	1:A:111:PHE:N	1:A:111:PHE:CA	1:A:111:PHE:CB	1:A:111:PHE:CG	20	1.6
(1,180)	1:A:79:GLU:N	1:A:79:GLU:CA	1:A:79:GLU:CB	1:A:79:GLU:CG	4	1.6
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	21	1.6
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	23	1.6
(1,135)	1:A:72:ASP:C	1:A:73:ALA:N	1:A:73:ALA:CA	1:A:73:ALA:C	25	1.6
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	18	1.6
(1,62)	1:A:129:VAL:C	1:A:130:PRO:N	1:A:130:PRO:CA	1:A:130:PRO:C	22	1.5
(1,207)	1:A:131:TYR:N	1:A:131:TYR:CA	1:A:131:TYR:CB	1:A:131:TYR:CG	22	1.5
(1,176)	1:A:74:ASP:N	1:A:74:ASP:CA	1:A:74:ASP:CB	1:A:74:ASP:CG	6	1.5
(1,172)	1:A:67:ASP:N	1:A:67:ASP:CA	1:A:67:ASP:CB	1:A:67:ASP:CG	5	1.5
(1,166)	1:A:57:MET:N	1:A:57:MET:CA	1:A:57:MET:CB	1:A:57:MET:CG	16	1.5
(1,150)	1:A:73:ALA:N	1:A:73:ALA:CA	1:A:73:ALA:C	1:A:74:ASP:N	14	1.5
(1,144)	1:A:33:GLY:N	1:A:33:GLY:CA	1:A:33:GLY:C	1:A:34:LEU:N	18	1.5
(1,138)	1:A:95:ARG:C	1:A:96:CYS:N	1:A:96:CYS:CA	1:A:96:CYS:C	5	1.5
(1,135)	1:A:72:ASP:C	1:A:73:ALA:N	1:A:73:ALA:CA	1:A:73:ALA:C	6	1.5
(1,53)	1:A:120:LYS:C	1:A:121:TYR:N	1:A:121:TYR:CA	1:A:121:TYR:C	16	1.4
(1,223)	1:A:39:LEU:CA	1:A:39:LEU:CB	1:A:39:LEU:CG	1:A:39:LEU:CD1	20	1.4
(1,172)	1:A:67:ASP:N	1:A:67:ASP:CA	1:A:67:ASP:CB	1:A:67:ASP:CG	17	1.4
(1,163)	1:A:50:CYS:N	1:A:50:CYS:CA	1:A:50:CYS:CB	1:A:50:CYS:SG	4	1.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	24	1.4
(1,93)	1:A:86:PRO:N	1:A:86:PRO:CA	1:A:86:PRO:C	1:A:87:ASP:N	15	1.3
(1,48)	1:A:112:PRO:C	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:C	8	1.3
(1,48)	1:A:112:PRO:C	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:C	13	1.3
(1,48)	1:A:112:PRO:C	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:C	14	1.3
(1,199)	1:A:119:TYR:N	1:A:119:TYR:CA	1:A:119:TYR:CB	1:A:119:TYR:CG	24	1.3
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	20	1.3
(1,180)	1:A:79:GLU:N	1:A:79:GLU:CA	1:A:79:GLU:CB	1:A:79:GLU:CG	18	1.3
(1,176)	1:A:74:ASP:N	1:A:74:ASP:CA	1:A:74:ASP:CB	1:A:74:ASP:CG	25	1.3
(1,166)	1:A:57:MET:N	1:A:57:MET:CA	1:A:57:MET:CB	1:A:57:MET:CG	6	1.3
(1,150)	1:A:73:ALA:N	1:A:73:ALA:CA	1:A:73:ALA:C	1:A:74:ASP:N	1	1.3
(1,150)	1:A:73:ALA:N	1:A:73:ALA:CA	1:A:73:ALA:C	1:A:74:ASP:N	9	1.3
(1,147)	1:A:54:ASP:N	1:A:54:ASP:CA	1:A:54:ASP:C	1:A:55:VAL:N	8	1.3
(1,147)	1:A:54:ASP:N	1:A:54:ASP:CA	1:A:54:ASP:C	1:A:55:VAL:N	9	1.3
(1,138)	1:A:95:ARG:C	1:A:96:CYS:N	1:A:96:CYS:CA	1:A:96:CYS:C	11	1.3
(1,138)	1:A:95:ARG:C	1:A:96:CYS:N	1:A:96:CYS:CA	1:A:96:CYS:C	12	1.3
(1,135)	1:A:72:ASP:C	1:A:73:ALA:N	1:A:73:ALA:CA	1:A:73:ALA:C	2	1.3
(1,89)	1:A:82:GLN:N	1:A:82:GLN:CA	1:A:82:GLN:C	1:A:83:CYS:N	25	1.2
(1,62)	1:A:129:VAL:C	1:A:130:PRO:N	1:A:130:PRO:CA	1:A:130:PRO:C	19	1.2
(1,48)	1:A:112:PRO:C	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:C	16	1.2
(1,48)	1:A:112:PRO:C	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:C	25	1.2
(1,29)	1:A:84:TYR:C	1:A:85:LEU:N	1:A:85:LEU:CA	1:A:85:LEU:C	19	1.2
(1,215)	1:A:129:VAL:N	1:A:129:VAL:CA	1:A:129:VAL:CB	1:A:129:VAL:CG1	21	1.2
(1,198)	1:A:115:CYS:N	1:A:115:CYS:CA	1:A:115:CYS:CB	1:A:115:CYS:SG	18	1.2
(1,172)	1:A:67:ASP:N	1:A:67:ASP:CA	1:A:67:ASP:CB	1:A:67:ASP:CG	22	1.2
(1,171)	1:A:65:ARG:N	1:A:65:ARG:CA	1:A:65:ARG:CB	1:A:65:ARG:CG	23	1.2
(1,147)	1:A:54:ASP:N	1:A:54:ASP:CA	1:A:54:ASP:C	1:A:55:VAL:N	14	1.2
(1,135)	1:A:72:ASP:C	1:A:73:ALA:N	1:A:73:ALA:CA	1:A:73:ALA:C	19	1.2
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	8	1.2
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	11	1.2
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	15	1.2
(1,95)	1:A:88:ALA:N	1:A:88:ALA:CA	1:A:88:ALA:C	1:A:89:PHE:N	17	1.1
(1,81)	1:A:59:GLU:N	1:A:59:GLU:CA	1:A:59:GLU:C	1:A:60:ASN:N	15	1.1
(1,198)	1:A:115:CYS:N	1:A:115:CYS:CA	1:A:115:CYS:CB	1:A:115:CYS:SG	10	1.1
(1,198)	1:A:115:CYS:N	1:A:115:CYS:CA	1:A:115:CYS:CB	1:A:115:CYS:SG	14	1.1
(1,198)	1:A:115:CYS:N	1:A:115:CYS:CA	1:A:115:CYS:CB	1:A:115:CYS:SG	17	1.1
(1,197)	1:A:113:ASP:N	1:A:113:ASP:CA	1:A:113:ASP:CB	1:A:113:ASP:CG	20	1.1
(1,187)	1:A:90:LYS:N	1:A:90:LYS:CA	1:A:90:LYS:CB	1:A:90:LYS:CG	19	1.1
(1,180)	1:A:79:GLU:N	1:A:79:GLU:CA	1:A:79:GLU:CB	1:A:79:GLU:CG	9	1.1
(1,180)	1:A:79:GLU:N	1:A:79:GLU:CA	1:A:79:GLU:CB	1:A:79:GLU:CG	24	1.1
(1,176)	1:A:74:ASP:N	1:A:74:ASP:CA	1:A:74:ASP:CB	1:A:74:ASP:CG	2	1.1
(1,176)	1:A:74:ASP:N	1:A:74:ASP:CA	1:A:74:ASP:CB	1:A:74:ASP:CG	13	1.1
(1,176)	1:A:74:ASP:N	1:A:74:ASP:CA	1:A:74:ASP:CB	1:A:74:ASP:CG	19	1.1
(1,166)	1:A:57:MET:N	1:A:57:MET:CA	1:A:57:MET:CB	1:A:57:MET:CG	22	1.1
(1,159)	1:A:44:TYR:N	1:A:44:TYR:CA	1:A:44:TYR:CB	1:A:44:TYR:CG	10	1.1
(1,157)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:CB	1:A:39:LEU:CG	18	1.1
(1,150)	1:A:73:ALA:N	1:A:73:ALA:CA	1:A:73:ALA:C	1:A:74:ASP:N	22	1.1
(1,138)	1:A:95:ARG:C	1:A:96:CYS:N	1:A:96:CYS:CA	1:A:96:CYS:C	17	1.1
(1,138)	1:A:95:ARG:C	1:A:96:CYS:N	1:A:96:CYS:CA	1:A:96:CYS:C	25	1.1
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	10	1.1
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	13	1.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,103)	1:A:98:ASN:N	1:A:98:ASN:CA	1:A:98:ASN:C	1:A:99:ARG:N	23	1.1