



Full wwPDB NMR Structure Validation Report ⓘ

Mar 24, 2026 – 03:20 AM UTC

PDB ID : 9FDG / pdb_00009fdg
BMRB ID : 52384
Title : Solution structure of a de novo designed 12-stranded transmembrane beta-barrel in LDAO micelles.
Authors : Muentener, T.; Hiller, S.
Deposited on : 2024-05-17

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

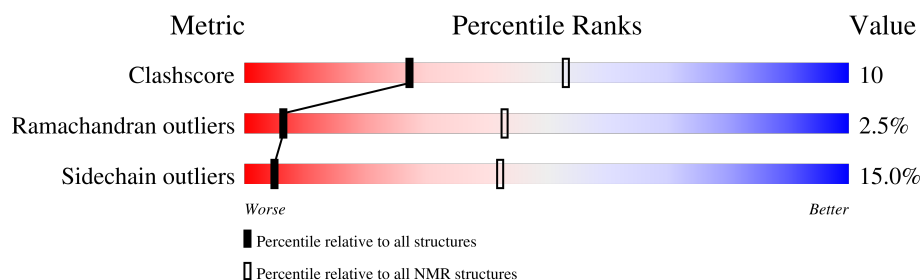
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 21%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	179	 78% 16% . .

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:4-A:133, A:139-A:179 (171)	2.50	2

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 1 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2803 atoms, of which 1361 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TMB12sol9_3.

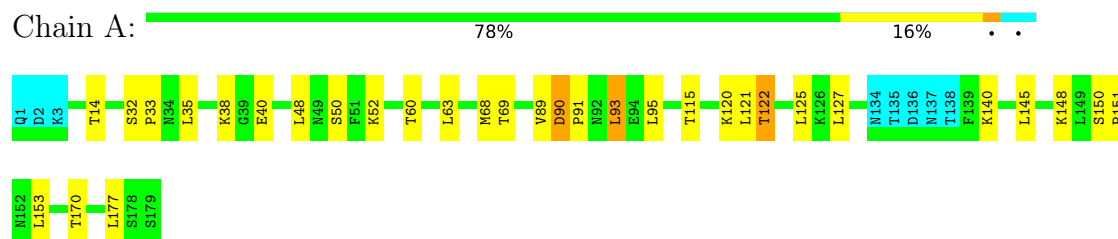
Mol	Chain	Residues	Atoms						Trace
1	A	179	Total	C	H	N	O	S	0
			2803	926	1361	228	287	1	

4 Residue-property plots

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: TMB12sol9_3

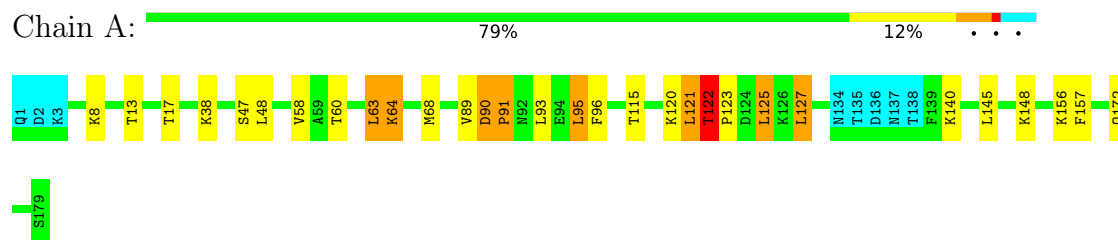


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

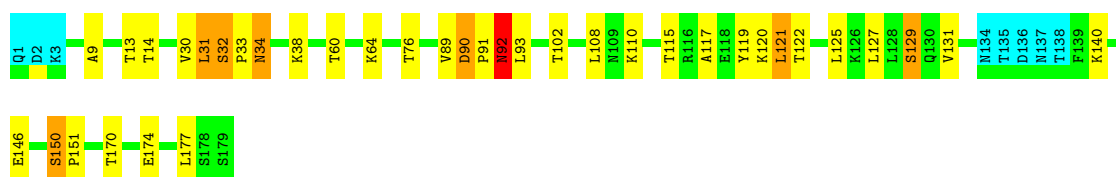
- Molecule 1: TMB12sol9_3



4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: TMB12sol9_3

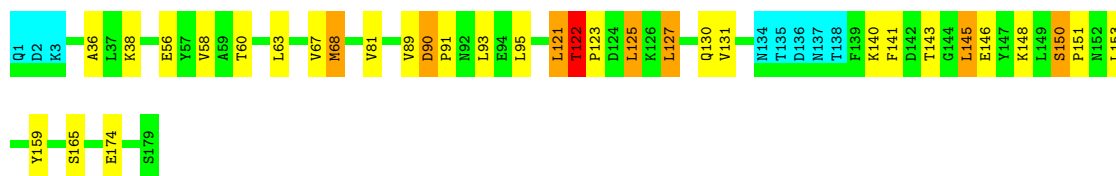




4.2.3 Score per residue for model 3

- Molecule 1: TMB12sol9_3

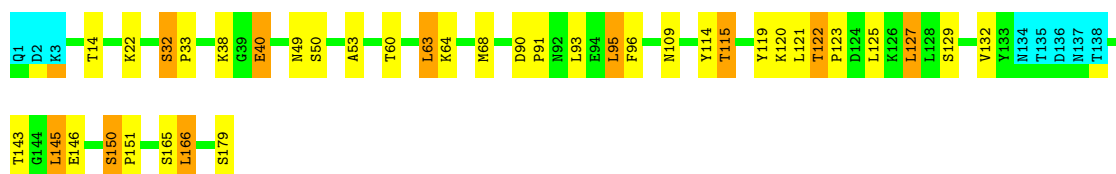
Chain A: 77% 14% . . .



4.2.4 Score per residue for model 4

- Molecule 1: TMB12sol9_3

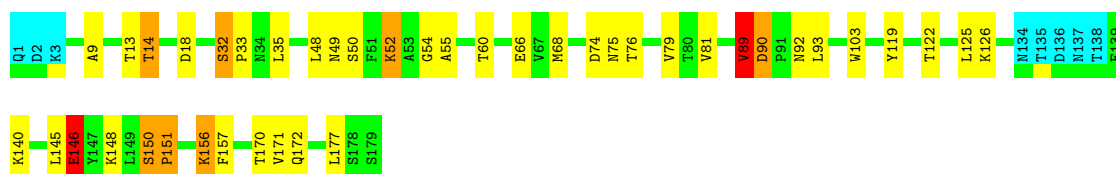
Chain A: 74% 16% 6% .



4.2.5 Score per residue for model 5

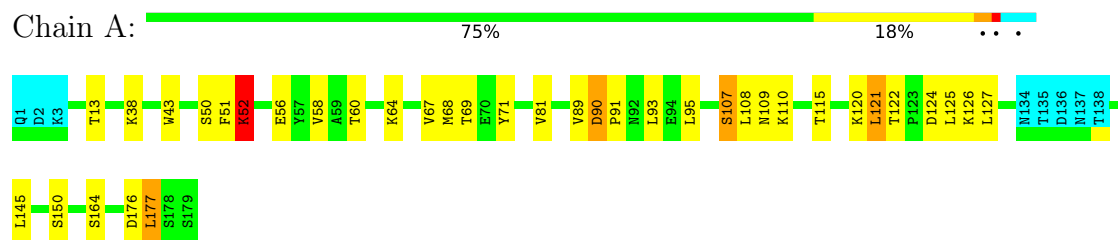
- Molecule 1: TMB12sol9_3

Chain A: 72% 18% . . .



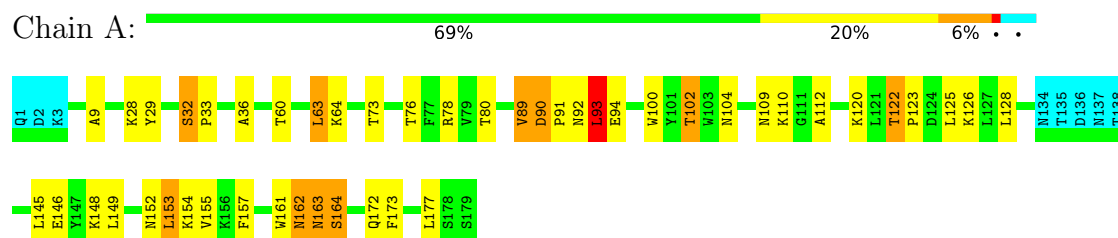
4.2.6 Score per residue for model 6

- Molecule 1: TMB12sol9_3



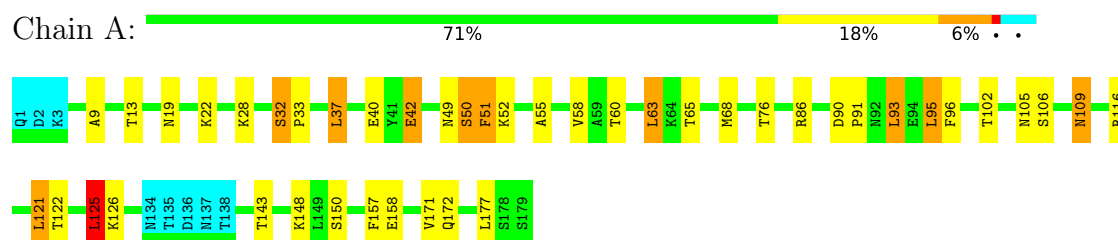
4.2.7 Score per residue for model 7

- Molecule 1: TMB12sol9_3



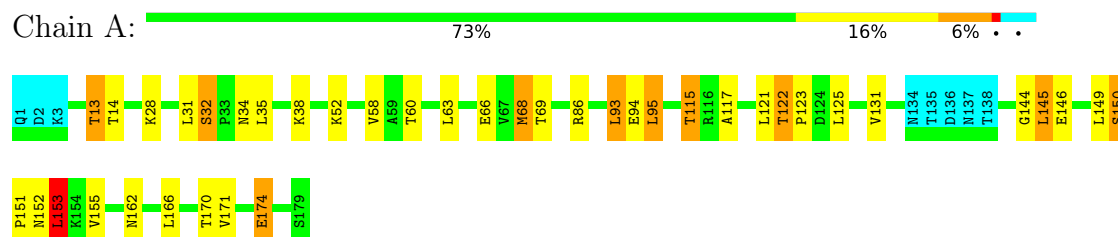
4.2.8 Score per residue for model 8

- Molecule 1: TMB12sol9_3



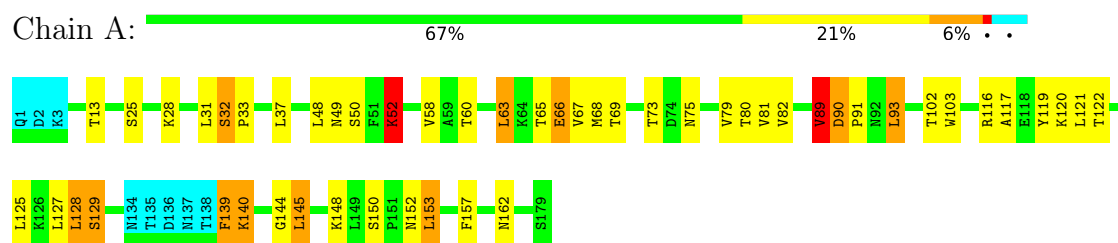
4.2.9 Score per residue for model 9

- Molecule 1: TMB12sol9_3



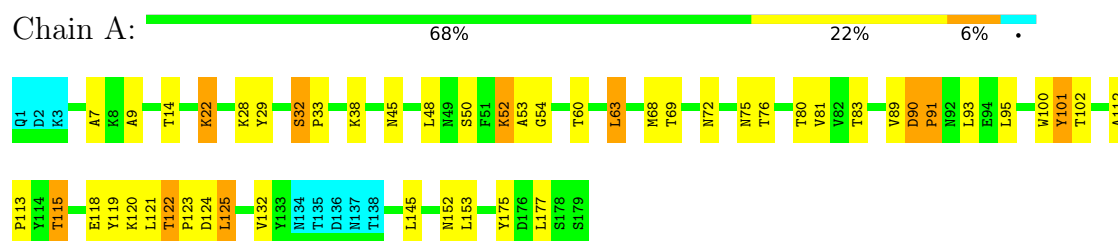
4.2.10 Score per residue for model 10

- Molecule 1: TMB12sol9_3



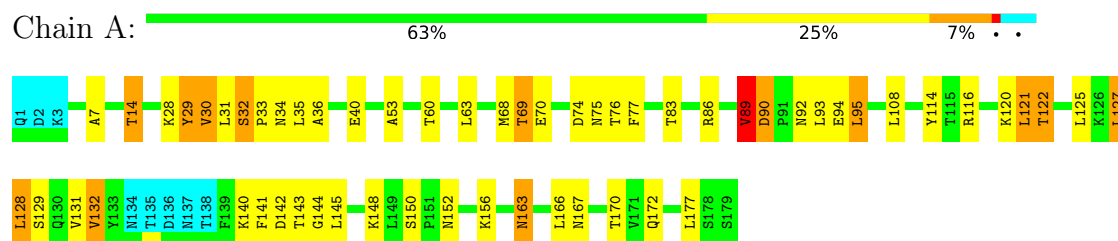
4.2.11 Score per residue for model 11

- Molecule 1: TMB12sol9_3



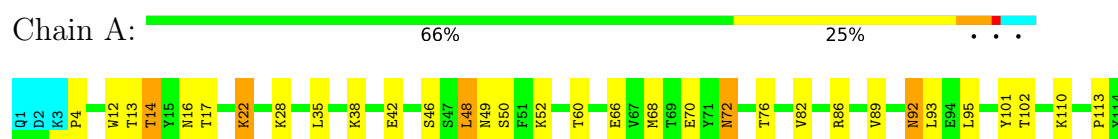
4.2.12 Score per residue for model 12

- Molecule 1: TMB12sol9_3



4.2.13 Score per residue for model 13

- Molecule 1: TMB12sol9_3





4.2.14 Score per residue for model 14

- Molecule 1: TMB12sol9_3

Chain A: 67% 22% 6% .



4.2.15 Score per residue for model 15

- Molecule 1: TMB12sol9_3

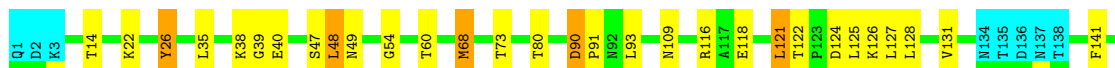
Chain A: 64% 25% 6% . .



4.2.16 Score per residue for model 16

- Molecule 1: TMB12sol9_3

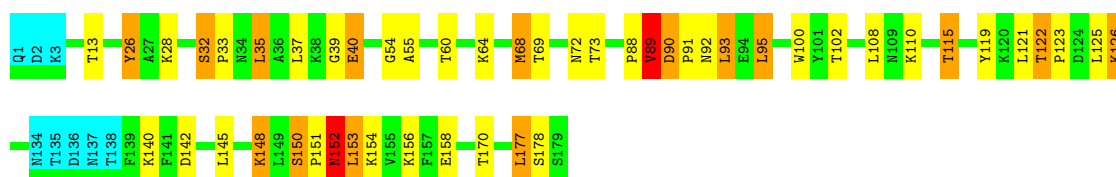
Chain A: 75% 16% . . .



4.2.17 Score per residue for model 17

- Molecule 1: TMB12sol9_3

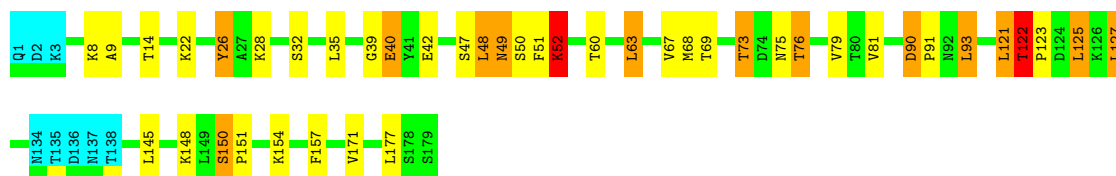
Chain A: 68% 18% 8% . .



4.2.18 Score per residue for model 18

- Molecule 1: TMB12sol9_3

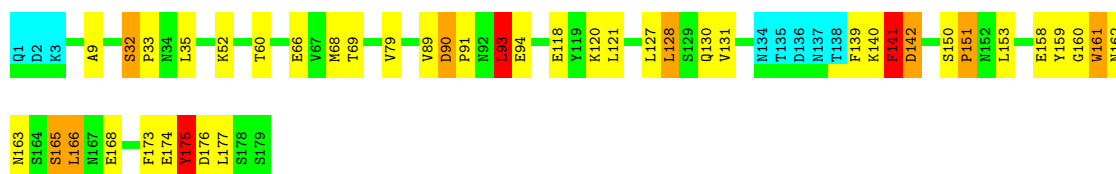
Chain A: 72% 16% 7% . .



4.2.19 Score per residue for model 19

- Molecule 1: TMB12sol9_3

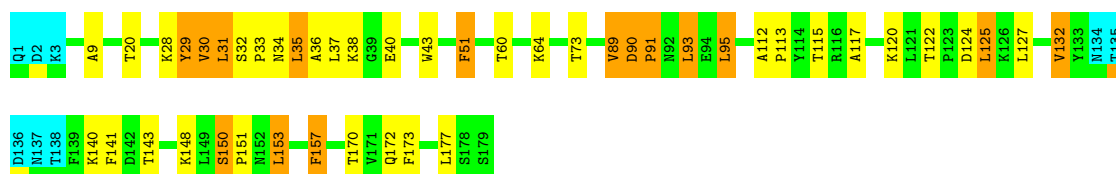
Chain A: 72% 18% . . .



4.2.20 Score per residue for model 20

- Molecule 1: TMB12sol9_3

Chain A: 70% 17% 8% .



5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	
CYANA	structure calculation	

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	478
Number of shifts mapped to atoms	478
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	21%

6 Model quality

6.1 Standard geometry

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

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	1378	1306	1306	26±8
All	All	27560	26120	26120	527

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:LEU:HD11	1:A:127:LEU:HD23	0.89	1.45	16	1
1:A:67:VAL:HG12	1:A:81:VAL:HG22	0.88	1.40	18	1
1:A:35:LEU:C	1:A:35:LEU:HD22	0.86	1.96	20	1
1:A:35:LEU:HD13	1:A:35:LEU:O	0.82	1.75	20	1
1:A:63:LEU:C	1:A:63:LEU:HD22	0.81	2.00	10	4
1:A:31:LEU:C	1:A:31:LEU:HD22	0.79	2.02	15	1
1:A:9:ALA:HB2	1:A:177:LEU:HD13	0.79	1.52	11	3
1:A:37:LEU:HD23	1:A:55:ALA:HB2	0.79	1.55	17	1
1:A:93:LEU:HD13	1:A:93:LEU:H	0.77	1.39	7	1
1:A:121:LEU:HD21	1:A:127:LEU:HD13	0.77	1.54	12	1
1:A:89:VAL:HG12	1:A:91:PRO:HD2	0.76	1.56	11	3
1:A:14:THR:HG23	1:A:170:THR:HG22	0.74	1.58	14	2
1:A:161:TRP:O	1:A:162:ASN:C	0.72	2.33	7	1
1:A:95:LEU:HD22	1:A:117:ALA:HB2	0.72	1.62	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:PHE:O	1:A:140:LYS:C	0.72	2.33	10	1
1:A:35:LEU:HD22	1:A:35:LEU:O	0.71	1.86	15	1
1:A:167:ASN:O	1:A:168:GLU:C	0.71	2.33	15	1
1:A:150:SER:N	1:A:151:PRO:CD	0.70	2.54	19	1
1:A:153:LEU:C	1:A:153:LEU:HD22	0.69	2.12	20	1
1:A:89:VAL:HG21	1:A:93:LEU:HD21	0.69	1.65	20	1
1:A:153:LEU:HD21	1:A:173:PHE:CZ	0.68	2.23	13	1
1:A:53:ALA:C	1:A:68:MET:HE3	0.67	2.14	11	2
1:A:69:THR:HG22	1:A:79:VAL:HG12	0.67	1.65	10	2
1:A:92:ASN:O	1:A:93:LEU:HD22	0.67	1.90	5	1
1:A:121:LEU:HD22	1:A:127:LEU:HD23	0.66	1.66	10	1
1:A:107:SER:O	1:A:108:LEU:HD22	0.66	1.89	15	1
1:A:34:ASN:C	1:A:35:LEU:HD22	0.66	2.15	14	1
1:A:9:ALA:HB2	1:A:177:LEU:CD1	0.66	2.20	19	2
1:A:157:PHE:HB3	1:A:170:THR:O	0.66	1.91	20	1
1:A:121:LEU:HD11	1:A:127:LEU:HB2	0.66	1.68	2	1
1:A:121:LEU:O	1:A:121:LEU:HD22	0.66	1.91	6	1
1:A:80:THR:HG22	1:A:102:THR:HG22	0.66	1.67	11	2
1:A:125:LEU:CD2	1:A:125:LEU:C	0.65	2.70	11	2
1:A:145:LEU:C	1:A:145:LEU:HD22	0.65	2.16	4	1
1:A:26:TYR:HB3	1:A:39:GLY:O	0.65	1.92	16	3
1:A:109:ASN:O	1:A:110:LYS:C	0.65	2.40	15	1
1:A:153:LEU:HD13	1:A:153:LEU:H	0.64	1.52	9	1
1:A:35:LEU:C	1:A:35:LEU:CD2	0.64	2.69	20	1
1:A:124:ASP:C	1:A:125:LEU:HD13	0.64	2.18	11	1
1:A:118:GLU:CG	1:A:128:LEU:HD12	0.64	2.23	16	1
1:A:48:LEU:HD22	1:A:73:THR:HG21	0.64	1.67	15	1
1:A:128:LEU:HD13	1:A:128:LEU:N	0.64	2.07	10	1
1:A:121:LEU:HD21	1:A:127:LEU:HD12	0.63	1.70	18	1
1:A:152:ASN:C	1:A:153:LEU:HD22	0.63	2.18	11	1
1:A:121:LEU:HD22	1:A:121:LEU:C	0.63	2.17	6	1
1:A:102:THR:HG21	1:A:108:LEU:HG	0.63	1.69	15	1
1:A:102:THR:HG22	1:A:105:ASN:ND2	0.63	2.08	15	1
1:A:174:GLU:O	1:A:175:TYR:C	0.63	2.42	19	1
1:A:100:TRP:NE1	1:A:112:ALA:HB3	0.62	2.09	7	1
1:A:66:GLU:HB2	1:A:82:VAL:HG23	0.62	1.72	13	1
1:A:93:LEU:HD12	1:A:119:TYR:CE1	0.62	2.30	17	1
1:A:166:LEU:N	1:A:166:LEU:HD13	0.62	2.09	4	1
1:A:128:LEU:HD22	1:A:156:LYS:CE	0.62	2.25	12	1
1:A:157:PHE:CE1	1:A:171:VAL:HG22	0.62	2.29	5	1
1:A:177:LEU:C	1:A:177:LEU:HD22	0.62	2.19	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:PRO:O	1:A:132:VAL:HG13	0.61	1.95	15	3
1:A:144:GLY:C	1:A:145:LEU:HD23	0.61	2.20	9	3
1:A:93:LEU:C	1:A:93:LEU:HD22	0.61	2.20	9	1
1:A:69:THR:CG2	1:A:79:VAL:HG12	0.61	2.26	14	1
1:A:80:THR:CG2	1:A:102:THR:HG22	0.61	2.24	11	1
1:A:9:ALA:CB	1:A:177:LEU:HD13	0.61	2.24	8	3
1:A:63:LEU:C	1:A:63:LEU:CD2	0.61	2.74	8	4
1:A:31:LEU:HD23	1:A:36:ALA:HB3	0.61	1.73	12	1
1:A:89:VAL:HG22	1:A:91:PRO:HD2	0.60	1.73	3	3
1:A:116:ARG:HD2	1:A:128:LEU:HD21	0.60	1.73	13	1
1:A:118:GLU:HG2	1:A:128:LEU:HD12	0.60	1.73	16	1
1:A:144:GLY:O	1:A:145:LEU:HD23	0.60	1.96	12	3
1:A:35:LEU:HD22	1:A:35:LEU:C	0.60	2.22	15	1
1:A:100:TRP:CE2	1:A:112:ALA:HB3	0.60	2.32	11	2
1:A:119:TYR:CE1	1:A:127:LEU:HD22	0.60	2.32	4	1
1:A:14:THR:HG22	1:A:170:THR:HG23	0.60	1.74	9	1
1:A:89:VAL:CG1	1:A:95:LEU:HD12	0.60	2.27	14	1
1:A:31:LEU:C	1:A:31:LEU:CD2	0.60	2.75	15	1
1:A:31:LEU:HD22	1:A:36:ALA:HB1	0.59	1.74	20	1
1:A:125:LEU:C	1:A:125:LEU:HD22	0.59	2.23	11	1
1:A:95:LEU:HD23	1:A:116:ARG:O	0.59	1.98	14	1
1:A:31:LEU:HD13	1:A:34:ASN:O	0.59	1.97	2	1
1:A:9:ALA:HB3	1:A:177:LEU:HD21	0.59	1.75	7	1
1:A:123:PRO:HG2	1:A:125:LEU:HD22	0.59	1.73	3	2
1:A:152:ASN:CB	1:A:153:LEU:HD13	0.58	2.28	10	2
1:A:161:TRP:O	1:A:164:SER:N	0.58	2.36	7	1
1:A:48:LEU:HD12	1:A:72:ASN:HB3	0.58	1.76	11	1
1:A:54:GLY:N	1:A:68:MET:HE3	0.58	2.14	17	3
1:A:121:LEU:HD22	1:A:127:LEU:HB2	0.58	1.75	19	1
1:A:117:ALA:HB3	1:A:129:SER:HB3	0.58	1.76	2	1
1:A:176:ASP:C	1:A:177:LEU:HD13	0.58	2.24	6	1
1:A:116:ARG:NE	1:A:128:LEU:HD11	0.58	2.13	13	1
1:A:67:VAL:HG12	1:A:81:VAL:CG2	0.57	2.23	18	1
1:A:14:THR:HG23	1:A:170:THR:OG1	0.57	1.99	2	1
1:A:34:ASN:O	1:A:35:LEU:HD23	0.57	1.99	9	1
1:A:31:LEU:HD22	1:A:36:ALA:CB	0.57	2.28	20	1
1:A:74:ASP:O	1:A:76:THR:HG22	0.57	1.99	12	1
1:A:66:GLU:HG2	1:A:82:VAL:HG23	0.57	1.76	10	1
1:A:121:LEU:CD2	1:A:122:THR:HG22	0.57	2.29	8	1
1:A:153:LEU:HD22	1:A:153:LEU:O	0.56	2.00	20	1
1:A:128:LEU:HB3	1:A:145:LEU:HD23	0.56	1.77	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:LEU:HD13	1:A:153:LEU:N	0.56	2.15	7	3
1:A:79:VAL:HG23	1:A:103:TRP:HB2	0.56	1.77	10	1
1:A:124:ASP:CB	1:A:125:LEU:HD13	0.56	2.31	20	1
1:A:66:GLU:CG	1:A:82:VAL:HG23	0.56	2.30	10	1
1:A:147:TYR:HB2	1:A:155:VAL:HG23	0.56	1.78	14	1
1:A:89:VAL:HG21	1:A:93:LEU:CD2	0.55	2.30	20	1
1:A:95:LEU:HD11	1:A:115:THR:CG2	0.55	2.31	4	3
1:A:67:VAL:HG22	1:A:81:VAL:HG22	0.55	1.78	10	1
1:A:69:THR:HG23	1:A:79:VAL:HG12	0.55	1.78	19	2
1:A:131:VAL:HG22	1:A:141:PHE:CD2	0.55	2.36	3	2
1:A:125:LEU:HD11	1:A:147:TYR:CE1	0.55	2.37	16	1
1:A:177:LEU:N	1:A:177:LEU:HD13	0.55	2.17	14	1
1:A:53:ALA:CA	1:A:68:MET:HE3	0.55	2.32	12	1
1:A:9:ALA:HB2	1:A:177:LEU:HD11	0.55	1.79	19	1
1:A:128:LEU:HD22	1:A:156:LYS:HE3	0.55	1.78	12	1
1:A:32:SER:CB	1:A:33:PRO:HD2	0.54	2.32	12	1
1:A:93:LEU:HD11	1:A:119:TYR:CD1	0.54	2.37	5	1
1:A:95:LEU:CD2	1:A:117:ALA:HB2	0.54	2.31	20	1
1:A:175:TYR:O	1:A:176:ASP:C	0.54	2.51	19	1
1:A:92:ASN:OD1	1:A:93:LEU:HD12	0.54	2.03	15	1
1:A:31:LEU:HD12	1:A:32:SER:HB3	0.54	1.78	9	1
1:A:121:LEU:HD22	1:A:125:LEU:HD21	0.54	1.80	18	1
1:A:35:LEU:HD22	1:A:36:ALA:N	0.54	2.18	20	1
1:A:107:SER:C	1:A:108:LEU:HD23	0.53	2.28	6	1
1:A:93:LEU:HD12	1:A:94:GLU:N	0.53	2.18	14	2
1:A:131:VAL:HG12	1:A:141:PHE:CD2	0.53	2.39	12	1
1:A:16:ASN:ND2	1:A:17:THR:HG22	0.53	2.18	13	1
1:A:149:LEU:HD11	1:A:155:VAL:CG1	0.53	2.34	9	1
1:A:125:LEU:HD11	1:A:147:TYR:CD1	0.53	2.39	16	1
1:A:125:LEU:HD12	1:A:146:GLU:O	0.53	2.04	9	2
1:A:31:LEU:HD23	1:A:36:ALA:CB	0.53	2.33	12	1
1:A:125:LEU:HD12	1:A:125:LEU:C	0.53	2.29	4	3
1:A:14:THR:HG23	1:A:170:THR:HG23	0.53	1.80	16	1
1:A:131:VAL:HG22	1:A:141:PHE:CE2	0.53	2.38	3	2
1:A:121:LEU:HD22	1:A:127:LEU:CD2	0.53	2.33	10	1
1:A:160:GLY:O	1:A:161:TRP:CB	0.53	2.57	19	1
1:A:52:LYS:HG2	1:A:68:MET:HE2	0.52	1.81	8	2
1:A:121:LEU:H	1:A:121:LEU:HD13	0.52	1.62	8	1
1:A:95:LEU:HD11	1:A:115:THR:HG23	0.52	1.81	20	1
1:A:121:LEU:HD22	1:A:127:LEU:HD13	0.52	1.80	1	1
1:A:37:LEU:HD13	1:A:38:LYS:N	0.52	2.19	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:PRO:O	1:A:89:VAL:HG13	0.52	2.05	17	1
1:A:89:VAL:HG12	1:A:90:ASP:H	0.52	1.64	12	1
1:A:28:LYS:HB3	1:A:31:LEU:HD23	0.52	1.81	20	1
1:A:52:LYS:HB3	1:A:69:THR:O	0.52	2.03	10	5
1:A:125:LEU:HD13	1:A:125:LEU:N	0.52	2.19	20	2
1:A:100:TRP:CZ2	1:A:112:ALA:HB3	0.52	2.40	11	1
1:A:35:LEU:N	1:A:35:LEU:CD1	0.52	2.73	15	1
1:A:152:ASN:HB2	1:A:153:LEU:HD13	0.52	1.81	17	1
1:A:121:LEU:HD21	1:A:127:LEU:CD1	0.52	2.33	12	1
1:A:121:LEU:HD11	1:A:127:LEU:CB	0.52	2.33	2	1
1:A:93:LEU:HD22	1:A:93:LEU:N	0.52	2.20	7	1
1:A:69:THR:HG21	1:A:77:PHE:CE2	0.52	2.40	12	1
1:A:115:THR:OG1	1:A:131:VAL:HG13	0.52	2.05	9	1
1:A:9:ALA:HB2	1:A:177:LEU:HD21	0.52	1.81	15	1
1:A:177:LEU:HD13	1:A:177:LEU:N	0.51	2.19	6	1
1:A:92:ASN:C	1:A:93:LEU:HD22	0.51	2.30	5	2
1:A:40:GLU:O	1:A:51:PHE:HB3	0.51	2.05	20	2
1:A:150:SER:N	1:A:151:PRO:HD3	0.51	2.19	19	1
1:A:93:LEU:HD23	1:A:119:TYR:CE1	0.51	2.41	10	1
1:A:72:ASN:ND2	1:A:76:THR:HG23	0.51	2.19	13	1
1:A:47:SER:O	1:A:48:LEU:C	0.51	2.52	18	1
1:A:37:LEU:HD12	1:A:55:ALA:HB2	0.51	1.81	8	1
1:A:14:THR:HG23	1:A:22:LYS:HG2	0.51	1.82	11	1
1:A:42:GLU:HB3	1:A:48:LEU:HD22	0.51	1.81	13	1
1:A:63:LEU:HD13	1:A:64:LYS:N	0.51	2.21	1	3
1:A:121:LEU:HD11	1:A:127:LEU:HD12	0.51	1.81	18	1
1:A:48:LEU:HD12	1:A:49:ASN:N	0.50	2.21	16	1
1:A:165:SER:O	1:A:166:LEU:C	0.50	2.53	19	1
1:A:118:GLU:HB3	1:A:127:LEU:O	0.50	2.06	14	2
1:A:127:LEU:HD12	1:A:128:LEU:N	0.50	2.22	13	1
1:A:126:LYS:O	1:A:145:LEU:HB3	0.50	2.06	16	1
1:A:90:ASP:CB	1:A:91:PRO:CD	0.50	2.89	17	15
1:A:32:SER:CB	1:A:33:PRO:CD	0.50	2.90	2	11
1:A:125:LEU:HD12	1:A:126:LYS:N	0.50	2.21	8	1
1:A:140:LYS:O	1:A:141:PHE:HB2	0.50	2.06	19	1
1:A:32:SER:N	1:A:33:PRO:HD2	0.50	2.22	20	10
1:A:14:THR:HG23	1:A:170:THR:CG2	0.50	2.36	14	2
1:A:153:LEU:HD11	1:A:173:PHE:CD2	0.50	2.41	19	1
1:A:121:LEU:CD2	1:A:127:LEU:HD13	0.50	2.32	12	1
1:A:92:ASN:O	1:A:93:LEU:C	0.49	2.53	7	1
1:A:52:LYS:O	1:A:68:MET:HE1	0.49	2.07	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:TRP:CE2	1:A:170:THR:HG21	0.49	2.41	15	1
1:A:89:VAL:HG12	1:A:95:LEU:HD12	0.49	1.82	14	1
1:A:67:VAL:HG13	1:A:81:VAL:HG22	0.49	1.85	3	1
1:A:90:ASP:N	1:A:91:PRO:HD2	0.49	2.22	14	12
1:A:63:LEU:HD22	1:A:63:LEU:O	0.49	2.08	11	4
1:A:7:ALA:HB3	1:A:177:LEU:HD22	0.49	1.83	12	1
1:A:153:LEU:C	1:A:153:LEU:CD2	0.49	2.84	20	2
1:A:125:LEU:C	1:A:125:LEU:HD13	0.49	2.33	12	3
1:A:153:LEU:CD2	1:A:153:LEU:C	0.49	2.85	17	3
1:A:9:ALA:O	1:A:175:TYR:HA	0.49	2.07	19	1
1:A:177:LEU:HD22	1:A:178:SER:N	0.49	2.23	17	1
1:A:122:THR:N	1:A:123:PRO:HD2	0.48	2.22	11	6
1:A:125:LEU:HD23	1:A:125:LEU:O	0.48	2.08	18	1
1:A:81:VAL:HG13	1:A:101:TYR:CD2	0.48	2.43	11	1
1:A:29:TYR:O	1:A:30:VAL:C	0.48	2.57	20	3
1:A:151:PRO:O	1:A:152:ASN:C	0.48	2.56	13	1
1:A:121:LEU:CD2	1:A:127:LEU:HD23	0.48	2.38	3	2
1:A:162:ASN:O	1:A:163:ASN:C	0.48	2.56	7	1
1:A:123:PRO:HG2	1:A:125:LEU:HD11	0.48	1.86	11	1
1:A:125:LEU:C	1:A:125:LEU:HD23	0.48	2.33	16	1
1:A:150:SER:N	1:A:151:PRO:HD2	0.48	2.23	20	9
1:A:114:TYR:CD1	1:A:132:VAL:HG22	0.48	2.43	4	2
1:A:72:ASN:HD22	1:A:76:THR:HG23	0.48	1.68	13	1
1:A:117:ALA:O	1:A:118:GLU:CB	0.48	2.61	13	2
1:A:150:SER:CB	1:A:151:PRO:CD	0.48	2.91	13	9
1:A:125:LEU:HD21	1:A:145:LEU:HB3	0.48	1.85	12	1
1:A:35:LEU:O	1:A:35:LEU:HD23	0.48	2.08	18	1
1:A:122:THR:HG22	1:A:123:PRO:HD2	0.48	1.86	7	1
1:A:35:LEU:HD12	1:A:35:LEU:O	0.48	2.09	17	2
1:A:31:LEU:HD11	1:A:37:LEU:HG	0.48	1.85	10	1
1:A:128:LEU:HD22	1:A:128:LEU:O	0.48	2.09	10	1
1:A:42:GLU:CB	1:A:48:LEU:HD22	0.47	2.39	13	1
1:A:121:LEU:HD21	1:A:127:LEU:HD22	0.47	1.84	15	1
1:A:67:VAL:HG22	1:A:81:VAL:HG13	0.47	1.86	10	1
1:A:26:TYR:HB3	1:A:39:GLY:C	0.47	2.34	17	3
1:A:49:ASN:O	1:A:50:SER:C	0.47	2.57	5	2
1:A:93:LEU:CD2	1:A:93:LEU:O	0.47	2.62	7	1
1:A:118:GLU:CG	1:A:121:LEU:HD11	0.47	2.39	11	1
1:A:41:TYR:HB3	1:A:50:SER:O	0.47	2.09	14	1
1:A:122:THR:CB	1:A:123:PRO:CD	0.47	2.93	3	6
1:A:13:THR:OG1	1:A:171:VAL:HG23	0.47	2.10	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:ASN:C	1:A:93:LEU:HD12	0.47	2.35	13	2
1:A:107:SER:C	1:A:108:LEU:HD22	0.47	2.34	15	1
1:A:145:LEU:HD22	1:A:146:GLU:N	0.47	2.25	4	1
1:A:145:LEU:C	1:A:145:LEU:HD13	0.47	2.35	5	1
1:A:93:LEU:O	1:A:93:LEU:HD23	0.47	2.10	7	1
1:A:93:LEU:HD12	1:A:119:TYR:CD1	0.47	2.45	17	1
1:A:14:THR:HG23	1:A:22:LYS:HB2	0.46	1.86	4	1
1:A:93:LEU:HD22	1:A:94:GLU:N	0.46	2.25	9	1
1:A:67:VAL:HA	1:A:81:VAL:HG22	0.46	1.87	6	1
1:A:53:ALA:HA	1:A:68:MET:HE3	0.46	1.86	12	1
1:A:26:TYR:HB2	1:A:40:GLU:HA	0.46	1.86	16	3
1:A:121:LEU:C	1:A:121:LEU:CD2	0.46	2.88	6	1
1:A:89:VAL:HG21	1:A:93:LEU:HG	0.46	1.87	14	2
1:A:48:LEU:HD12	1:A:49:ASN:H	0.46	1.71	16	1
1:A:118:GLU:HA	1:A:128:LEU:HD22	0.46	1.88	19	1
1:A:63:LEU:C	1:A:63:LEU:HD13	0.46	2.35	14	1
1:A:158:GLU:HB2	1:A:170:THR:HG23	0.46	1.86	17	1
1:A:121:LEU:CD1	1:A:127:LEU:HD23	0.46	2.28	16	1
1:A:22:LYS:HZ1	1:A:48:LEU:HD13	0.46	1.70	13	1
1:A:95:LEU:C	1:A:95:LEU:HD13	0.46	2.36	13	1
1:A:95:LEU:HD11	1:A:115:THR:HG22	0.46	1.88	17	2
1:A:9:ALA:HB3	1:A:177:LEU:HD13	0.46	1.87	2	1
1:A:115:THR:HB	1:A:131:VAL:HG13	0.46	1.87	2	1
1:A:102:THR:HG21	1:A:108:LEU:CG	0.46	2.41	15	1
1:A:127:LEU:C	1:A:127:LEU:HD13	0.46	2.36	20	1
1:A:79:VAL:HG13	1:A:103:TRP:HB2	0.45	1.87	5	1
1:A:123:PRO:HG2	1:A:125:LEU:HD21	0.45	1.86	11	1
1:A:35:LEU:N	1:A:35:LEU:HD13	0.45	2.25	15	1
1:A:9:ALA:HB2	1:A:177:LEU:CD2	0.45	2.41	15	2
1:A:121:LEU:HD13	1:A:121:LEU:N	0.45	2.25	8	1
1:A:117:ALA:HB3	1:A:129:SER:O	0.45	2.11	10	1
1:A:37:LEU:HD13	1:A:38:LYS:H	0.45	1.71	14	1
1:A:121:LEU:HD21	1:A:125:LEU:HD11	0.45	1.87	1	1
1:A:72:ASN:O	1:A:73:THR:C	0.45	2.59	17	1
1:A:9:ALA:HB2	1:A:177:LEU:HD12	0.45	1.88	20	1
1:A:66:GLU:O	1:A:81:VAL:HG13	0.45	2.12	5	1
1:A:123:PRO:CG	1:A:125:LEU:HD11	0.45	2.42	11	1
1:A:124:ASP:C	1:A:125:LEU:CD1	0.45	2.89	11	1
1:A:121:LEU:HD21	1:A:126:LYS:HG2	0.45	1.87	17	1
1:A:121:LEU:CD2	1:A:121:LEU:C	0.45	2.90	8	1
1:A:153:LEU:N	1:A:153:LEU:CD1	0.45	2.80	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:LEU:HD13	1:A:95:LEU:C	0.45	2.37	6	1
1:A:163:ASN:CG	1:A:164:SER:N	0.45	2.73	7	1
1:A:125:LEU:HD22	1:A:146:GLU:O	0.44	2.12	7	1
1:A:153:LEU:HD12	1:A:175:TYR:HA	0.44	1.88	11	1
1:A:47:SER:C	1:A:48:LEU:HD22	0.44	2.38	1	1
1:A:125:LEU:HD11	1:A:145:LEU:HD11	0.44	1.88	5	1
1:A:121:LEU:HD21	1:A:125:LEU:HD23	0.44	1.89	10	1
1:A:128:LEU:HD13	1:A:128:LEU:H	0.44	1.70	10	1
1:A:140:LYS:O	1:A:141:PHE:CB	0.44	2.65	19	1
1:A:89:VAL:HG21	1:A:93:LEU:CG	0.44	2.42	20	1
1:A:48:LEU:HD22	1:A:52:LYS:HD2	0.44	1.90	5	1
1:A:38:LYS:O	1:A:53:ALA:HB1	0.44	2.11	11	1
1:A:37:LEU:HD23	1:A:55:ALA:CB	0.44	2.37	17	1
1:A:131:VAL:HG13	1:A:139:PHE:CD1	0.44	2.47	19	1
1:A:95:LEU:HD13	1:A:96:PHE:N	0.44	2.27	4	3
1:A:145:LEU:C	1:A:145:LEU:CD2	0.44	2.88	4	1
1:A:52:LYS:HG3	1:A:68:MET:HE2	0.44	1.90	14	1
1:A:118:GLU:CB	1:A:128:LEU:HA	0.44	2.43	13	1
1:A:145:LEU:HD12	1:A:147:TYR:CE1	0.44	2.48	14	1
1:A:9:ALA:O	1:A:175:TYR:CA	0.44	2.65	19	1
1:A:29:TYR:O	1:A:36:ALA:HB1	0.43	2.13	7	1
1:A:145:LEU:HD12	1:A:157:PHE:CZ	0.43	2.48	10	1
1:A:37:LEU:CD2	1:A:55:ALA:HB2	0.43	2.36	17	1
1:A:146:GLU:CB	1:A:156:LYS:HA	0.43	2.43	5	1
1:A:149:LEU:HD13	1:A:153:LEU:C	0.43	2.38	13	1
1:A:145:LEU:HD23	1:A:157:PHE:CZ	0.43	2.48	1	1
1:A:30:VAL:HG22	1:A:32:SER:OG	0.43	2.13	12	1
1:A:177:LEU:CD2	1:A:177:LEU:C	0.43	2.91	14	1
1:A:157:PHE:CD1	1:A:171:VAL:HG13	0.43	2.48	18	1
1:A:35:LEU:HD11	1:A:55:ALA:HB1	0.43	1.89	5	1
1:A:55:ALA:HB3	1:A:67:VAL:HG13	0.43	1.91	15	1
1:A:125:LEU:HD23	1:A:126:LYS:N	0.43	2.29	16	1
1:A:36:ALA:HB3	1:A:56:GLU:HB3	0.43	1.91	14	2
1:A:75:ASN:O	1:A:76:THR:HG23	0.43	2.12	18	1
1:A:119:TYR:HB3	1:A:127:LEU:HD22	0.43	1.91	2	1
1:A:163:ASN:O	1:A:164:SER:C	0.43	2.62	7	1
1:A:157:PHE:CE1	1:A:171:VAL:HG13	0.43	2.48	8	1
1:A:121:LEU:O	1:A:122:THR:HG23	0.43	2.13	12	1
1:A:66:GLU:CB	1:A:82:VAL:HG23	0.43	2.40	13	1
1:A:40:GLU:O	1:A:41:TYR:HB2	0.43	2.14	14	1
1:A:69:THR:HG23	1:A:79:VAL:HG22	0.43	1.89	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:VAL:O	1:A:30:VAL:HG22	0.43	2.13	20	1
1:A:31:LEU:HB2	1:A:36:ALA:HB2	0.43	1.89	14	1
1:A:63:LEU:HD21	1:A:83:THR:HB	0.43	1.90	14	1
1:A:58:VAL:HG22	1:A:64:LYS:HE3	0.43	1.90	6	1
1:A:48:LEU:O	1:A:73:THR:HG22	0.43	2.14	10	1
1:A:91:PRO:HB2	1:A:93:LEU:HD12	0.43	1.90	18	1
1:A:93:LEU:CD1	1:A:93:LEU:N	0.43	2.82	9	1
1:A:129:SER:OG	1:A:143:THR:HG22	0.43	2.14	13	1
1:A:29:TYR:C	1:A:30:VAL:CG2	0.43	2.91	15	1
1:A:31:LEU:HD22	1:A:32:SER:N	0.43	2.29	15	1
1:A:155:VAL:HG22	1:A:173:PHE:HD1	0.43	1.74	7	1
1:A:145:LEU:HD12	1:A:145:LEU:O	0.43	2.13	18	1
1:A:130:GLN:O	1:A:141:PHE:HB3	0.43	2.14	19	1
1:A:67:VAL:CG2	1:A:81:VAL:HG22	0.42	2.44	10	1
1:A:119:TYR:O	1:A:120:LYS:CG	0.42	2.67	11	1
1:A:26:TYR:CB	1:A:39:GLY:O	0.42	2.67	17	1
1:A:58:VAL:O	1:A:58:VAL:HG13	0.42	2.14	15	5
1:A:90:ASP:C	1:A:92:ASN:H	0.42	2.22	17	1
1:A:67:VAL:HG13	1:A:67:VAL:O	0.42	2.14	15	1
1:A:67:VAL:HA	1:A:81:VAL:HG13	0.42	1.90	15	1
1:A:141:PHE:O	1:A:142:ASP:HB2	0.42	2.15	19	1
1:A:51:PHE:O	1:A:52:LYS:HB2	0.42	2.13	15	3
1:A:122:THR:HG22	1:A:123:PRO:N	0.42	2.29	9	1
1:A:125:LEU:HD22	1:A:125:LEU:O	0.42	2.14	11	1
1:A:86:ARG:HG3	1:A:95:LEU:HD12	0.42	1.91	12	1
1:A:149:LEU:HD23	1:A:149:LEU:O	0.42	2.15	14	1
1:A:121:LEU:HD21	1:A:126:LYS:CG	0.42	2.44	17	1
1:A:47:SER:C	1:A:48:LEU:HG	0.42	2.40	18	1
1:A:38:LYS:HE2	1:A:68:MET:HE3	0.42	1.91	3	1
1:A:53:ALA:C	1:A:68:MET:HE2	0.42	2.39	15	1
1:A:35:LEU:O	1:A:35:LEU:CD1	0.42	2.60	20	1
1:A:7:ALA:HB2	1:A:29:TYR:CD2	0.42	2.50	11	1
1:A:143:THR:HG23	1:A:159:TYR:CE1	0.42	2.50	3	1
1:A:48:LEU:HD12	1:A:72:ASN:CB	0.42	2.44	11	1
1:A:116:ARG:NH1	1:A:128:LEU:HD21	0.41	2.30	12	1
1:A:165:SER:C	1:A:166:LEU:HG	0.41	2.40	19	1
1:A:119:TYR:CE1	1:A:127:LEU:HD13	0.41	2.50	4	1
1:A:89:VAL:HG22	1:A:90:ASP:H	0.41	1.75	5	1
1:A:42:GLU:C	1:A:50:SER:HA	0.41	2.41	13	1
1:A:26:TYR:CB	1:A:39:GLY:C	0.41	2.93	17	1
1:A:26:TYR:HB2	1:A:40:GLU:CA	0.41	2.45	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:LEU:C	1:A:177:LEU:CD2	0.41	2.90	17	1
1:A:153:LEU:N	1:A:153:LEU:HD13	0.41	2.30	20	1
1:A:145:LEU:HD23	1:A:157:PHE:O	0.41	2.14	7	1
1:A:37:LEU:CD1	1:A:55:ALA:HB2	0.41	2.45	8	1
1:A:49:ASN:O	1:A:73:THR:HG23	0.41	2.15	10	1
1:A:69:THR:HG23	1:A:79:VAL:CG1	0.41	2.43	19	1
1:A:50:SER:O	1:A:51:PHE:HB2	0.41	2.14	8	1
1:A:58:VAL:HG13	1:A:58:VAL:O	0.41	2.16	10	2
1:A:9:ALA:H	1:A:175:TYR:HA	0.41	1.74	19	1
1:A:166:LEU:N	1:A:166:LEU:CD1	0.41	2.80	4	1
1:A:14:THR:HG23	1:A:170:THR:HB	0.41	1.91	5	1
1:A:152:ASN:HB3	1:A:153:LEU:HD13	0.41	1.92	10	1
1:A:118:GLU:HB2	1:A:121:LEU:HD11	0.41	1.93	11	1
1:A:128:LEU:CB	1:A:145:LEU:HD23	0.41	2.46	16	1
1:A:177:LEU:N	1:A:177:LEU:CD1	0.41	2.83	17	1
1:A:116:ARG:HB2	1:A:128:LEU:HD11	0.41	1.91	16	1
1:A:128:LEU:C	1:A:128:LEU:HD23	0.41	2.41	16	1
1:A:142:ASP:HB3	1:A:159:TYR:O	0.40	2.17	19	1
1:A:153:LEU:HD23	1:A:173:PHE:CE1	0.40	2.51	20	1
1:A:119:TYR:O	1:A:121:LEU:HD23	0.40	2.16	11	1
1:A:102:THR:HG22	1:A:105:ASN:CG	0.40	2.42	15	1
1:A:116:ARG:HB2	1:A:128:LEU:HD21	0.40	1.93	16	1
1:A:54:GLY:HA3	1:A:68:MET:HA	0.40	1.93	5	1
1:A:125:LEU:HD12	1:A:145:LEU:HB2	0.40	1.92	3	1
1:A:30:VAL:HG22	1:A:30:VAL:O	0.40	2.15	12	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	170/179 (95%)	147±5 (86±3%)	19±4 (11±2%)	4±2 (2±1%)	6	43
All	All	3400/3580 (95%)	2934 (86%)	382 (11%)	84 (2%)	6	43

All 44 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	93	LEU	9
1	A	89	VAL	5
1	A	52	LYS	5
1	A	30	VAL	4
1	A	75	ASN	4
1	A	91	PRO	3
1	A	122	THR	3
1	A	34	ASN	3
1	A	42	GLU	3
1	A	152	ASN	3
1	A	92	ASN	2
1	A	49	ASN	2
1	A	151	PRO	2
1	A	109	ASN	2
1	A	51	PHE	2
1	A	174	GLU	2
1	A	140	LYS	2
1	A	118	GLU	2
1	A	40	GLU	1
1	A	165	SER	1
1	A	76	THR	1
1	A	146	GLU	1
1	A	124	ASP	1
1	A	162	ASN	1
1	A	19	ASN	1
1	A	106	SER	1
1	A	125	LEU	1
1	A	153	LEU	1
1	A	45	ASN	1
1	A	163	ASN	1
1	A	12	TRP	1
1	A	46	SER	1
1	A	33	PRO	1
1	A	41	TYR	1
1	A	47	SER	1
1	A	110	LYS	1
1	A	168	GLU	1
1	A	145	LEU	1
1	A	148	LYS	1
1	A	73	THR	1
1	A	141	PHE	1
1	A	142	ASP	1
1	A	175	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	157	PHE	1

6.3.2 Protein sidechains ⓘ

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	149/157 (95%)	127±4 (85±3%)	22±4 (15±3%)	5	42
All	All	2980/3140 (95%)	2532 (85%)	448 (15%)	5	42

All 104 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	60	THR	19
1	A	122	THR	18
1	A	90	ASP	16
1	A	150	SER	15
1	A	32	SER	13
1	A	121	LEU	12
1	A	120	LYS	11
1	A	148	LYS	11
1	A	63	LEU	10
1	A	68	MET	10
1	A	13	THR	9
1	A	38	LYS	9
1	A	93	LEU	9
1	A	145	LEU	9
1	A	28	LYS	9
1	A	95	LEU	8
1	A	50	SER	8
1	A	89	VAL	8
1	A	115	THR	7
1	A	125	LEU	7
1	A	127	LEU	7
1	A	140	LYS	7
1	A	172	GLN	7
1	A	102	THR	7

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Mol	Chain	Res	Type	Models (Total)
1	A	153	LEU	6
1	A	22	LYS	6
1	A	35	LEU	6
1	A	64	LYS	5
1	A	76	THR	5
1	A	110	LYS	5
1	A	129	SER	5
1	A	166	LEU	5
1	A	52	LYS	5
1	A	128	LEU	5
1	A	174	GLU	4
1	A	40	GLU	4
1	A	109	ASN	4
1	A	143	THR	4
1	A	14	THR	4
1	A	126	LYS	4
1	A	73	THR	4
1	A	154	LYS	4
1	A	37	LEU	4
1	A	69	THR	4
1	A	156	LYS	3
1	A	31	LEU	3
1	A	108	LEU	3
1	A	146	GLU	3
1	A	43	TRP	3
1	A	177	LEU	3
1	A	163	ASN	3
1	A	49	ASN	3
1	A	65	THR	3
1	A	86	ARG	3
1	A	66	GLU	3
1	A	162	ASN	3
1	A	80	THR	3
1	A	29	TYR	3
1	A	142	ASP	3
1	A	48	LEU	3
1	A	26	TYR	3
1	A	8	LYS	2
1	A	17	THR	2
1	A	165	SER	2
1	A	164	SER	2
1	A	78	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	94	GLU	2
1	A	149	LEU	2
1	A	42	GLU	2
1	A	116	ARG	2
1	A	158	GLU	2
1	A	83	THR	2
1	A	101	TYR	2
1	A	70	GLU	2
1	A	132	VAL	2
1	A	141	PHE	2
1	A	92	ASN	1
1	A	130	GLN	1
1	A	179	SER	1
1	A	18	ASP	1
1	A	74	ASP	1
1	A	56	GLU	1
1	A	71	TYR	1
1	A	107	SER	1
1	A	104	ASN	1
1	A	105	ASN	1
1	A	25	SER	1
1	A	139	PHE	1
1	A	167	ASN	1
1	A	72	ASN	1
1	A	118	GLU	1
1	A	82	VAL	1
1	A	30	VAL	1
1	A	44	ASN	1
1	A	103	TRP	1
1	A	47	SER	1
1	A	124	ASP	1
1	A	170	THR	1
1	A	100	TRP	1
1	A	152	ASN	1
1	A	161	TRP	1
1	A	168	GLU	1
1	A	175	TYR	1
1	A	20	THR	1

6.3.3 RNA ⓘ

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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 21% for the well-defined parts and 20% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping

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	478
Number of shifts mapped to atoms	478
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	95	-0.34 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	82	-1.41 ± 0.12	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	103	-0.54 ± 0.60	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 21%, i.e. 478 atoms were assigned a chemical shift out of a possible 2281. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	301/850 (35%)	103/346 (30%)	95/342 (28%)	103/162 (64%)
Sidechain	177/1146 (15%)	78/741 (11%)	99/365 (27%)	0/40 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/285 (0%)	0/135 (0%)	0/145 (0%)	0/5 (0%)
Overall	478/2281 (21%)	181/1222 (15%)	194/852 (23%)	103/207 (50%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 20%, i.e. 478 atoms were assigned a chemical shift out of a possible 2378. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	301/890 (34%)	103/362 (28%)	95/358 (27%)	103/170 (61%)
Sidechain	177/1203 (15%)	78/775 (10%)	99/384 (26%)	0/44 (0%)
Aromatic	0/285 (0%)	0/135 (0%)	0/145 (0%)	0/5 (0%)
Overall	478/2378 (20%)	181/1272 (14%)	194/887 (22%)	103/219 (47%)

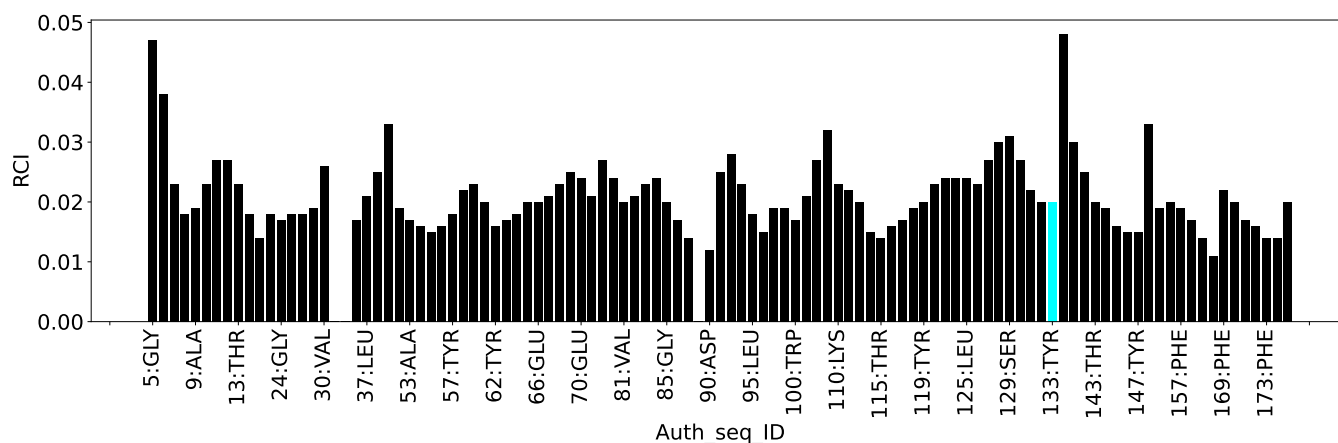
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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	392
Intra-residue ($ i-j =0$)	22
Sequential ($ i-j =1$)	61
Medium range ($ i-j >1$ and $ i-j <5$)	20
Long range ($ i-j \geq 5$)	97
Inter-chain	0
Hydrogen bond restraints	192
Disulfide bond restraints	0
Total dihedral-angle restraints	122
Number of unmapped restraints	0
Number of restraints per residue	2.9
Number of long range restraints per residue ¹	1.6

¹Long 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

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

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	6.7	0.2
0.2-0.5 (Medium)	5.6	0.48
>0.5 (Large)	1.0	1.42

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)	6.5	9.83
10.0-20.0 (Medium)	0.2	16.98
>20.0 (Large)	None	None

9 Distance violation analysis

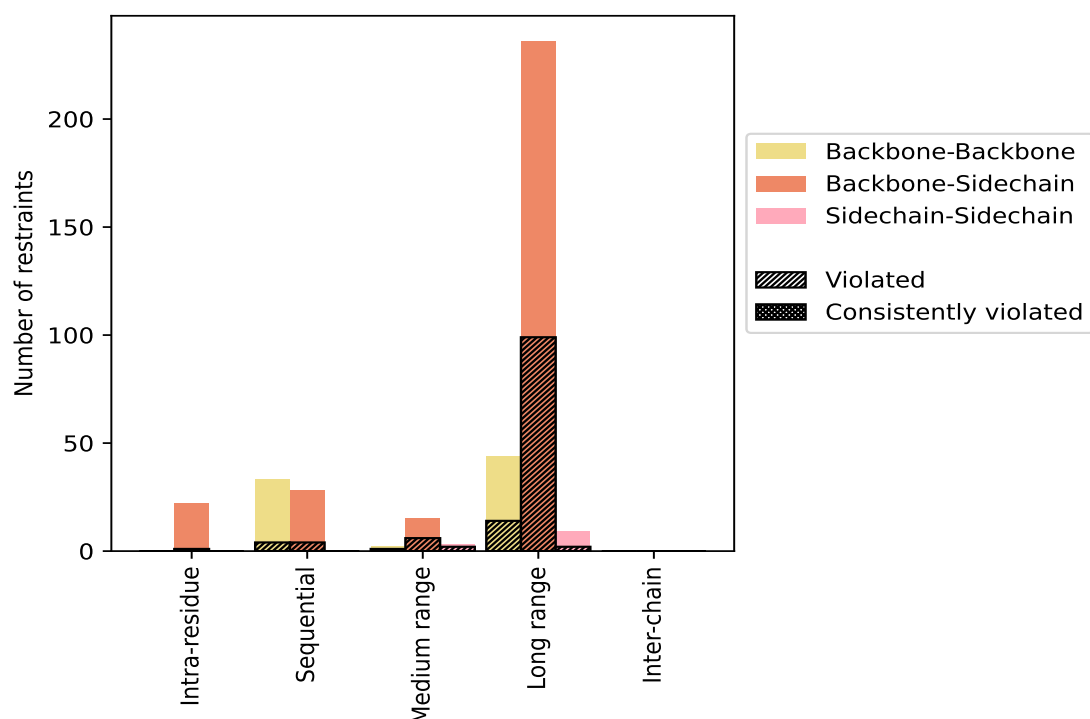
9.1 Summary of distance violations

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	22	5.6	1	4.5	0.3	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	22	5.6	1	4.5	0.3	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	61	15.6	8	13.1	2.0	0	0.0	0.0
Backbone-Backbone	33	8.4	4	12.1	1.0	0	0.0	0.0
Backbone-Sidechain	28	7.1	4	14.3	1.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	20	5.1	9	45.0	2.3	0	0.0	0.0
Backbone-Backbone	2	0.5	1	50.0	0.3	0	0.0	0.0
Backbone-Sidechain	15	3.8	6	40.0	1.5	0	0.0	0.0
Sidechain-Sidechain	3	0.8	2	66.7	0.5	0	0.0	0.0
Long range ($ i-j \geq 5$)	97	24.7	28	28.9	7.1	0	0.0	0.0
Backbone-Backbone	44	11.2	14	31.8	3.6	0	0.0	0.0
Backbone-Sidechain	44	11.2	12	27.3	3.1	0	0.0	0.0
Sidechain-Sidechain	9	2.3	2	22.2	0.5	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	192	49.0	87	45.3	22.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	392	100.0	133	33.9	33.9	0	0.0	0.0
Backbone-Backbone	79	20.2	19	24.1	4.8	0	0.0	0.0
Backbone-Sidechain	301	76.8	110	36.5	28.1	0	0.0	0.0
Sidechain-Sidechain	12	3.1	4	33.3	1.0	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	1	1	0	2	0.23	0.26	0.03	0.23
2	0	1	1	2	0	4	0.26	0.37	0.09	0.24
3	0	0	1	4	0	5	0.18	0.27	0.05	0.17
4	0	0	2	4	0	6	0.27	0.36	0.08	0.29
5	0	0	1	12	0	13	0.22	0.41	0.09	0.21
6	0	0	0	9	0	9	0.23	0.43	0.11	0.17
7	0	0	1	10	0	11	0.18	0.3	0.08	0.14
8	0	0	1	13	0	14	0.2	0.38	0.1	0.17
9	0	1	2	3	0	6	0.43	1.42	0.46	0.27
10	0	0	0	17	0	17	0.18	0.45	0.1	0.14

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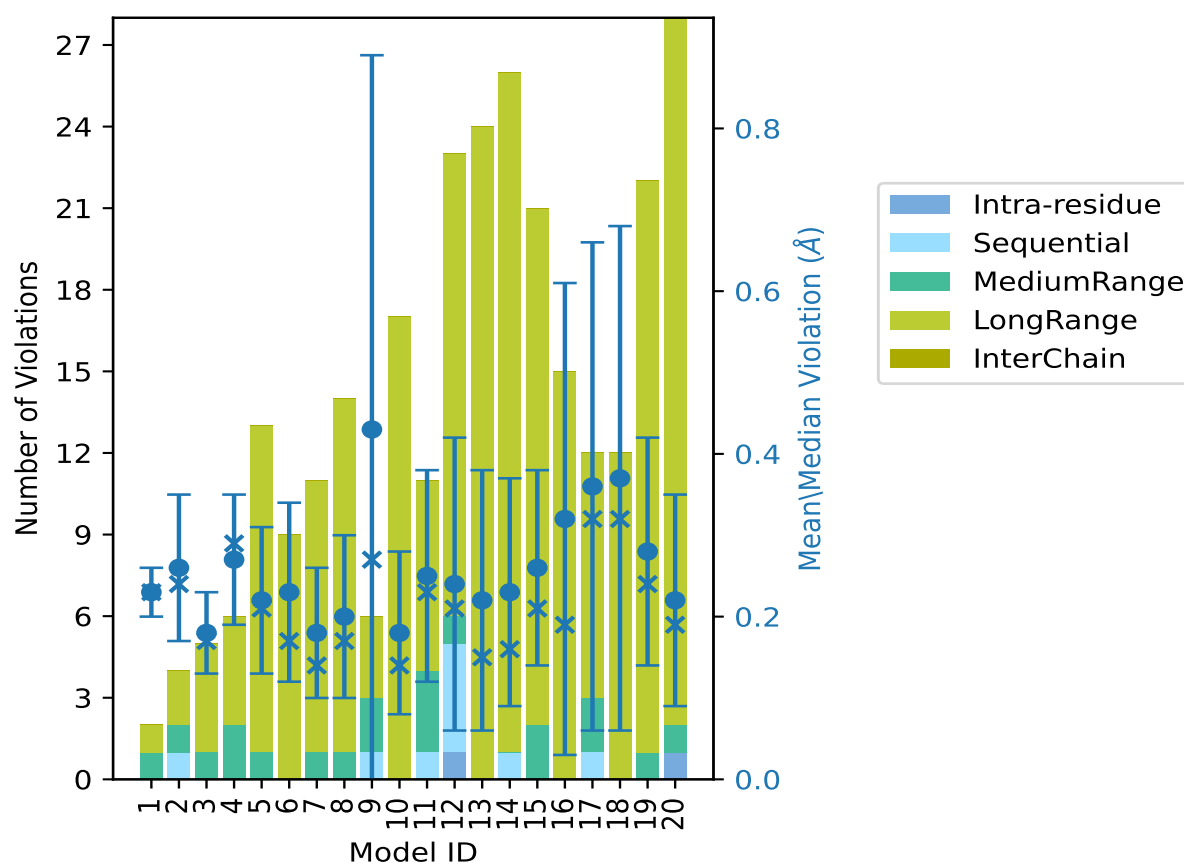
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	1	3	7	0	11	0.25	0.55	0.13	0.23
12	1	4	1	17	0	23	0.24	0.86	0.18	0.21
13	0	0	0	24	0	24	0.22	0.7	0.16	0.15
14	0	1	0	25	0	26	0.23	0.68	0.14	0.16
15	0	0	2	19	0	21	0.26	0.59	0.12	0.21
16	0	0	0	15	0	15	0.32	1.25	0.29	0.19
17	0	1	2	9	0	12	0.36	1.23	0.3	0.32
18	0	0	0	12	0	12	0.37	1.26	0.31	0.32
19	0	0	1	21	0	22	0.28	0.54	0.14	0.24
20	1	0	1	26	0	28	0.22	0.65	0.13	0.19

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

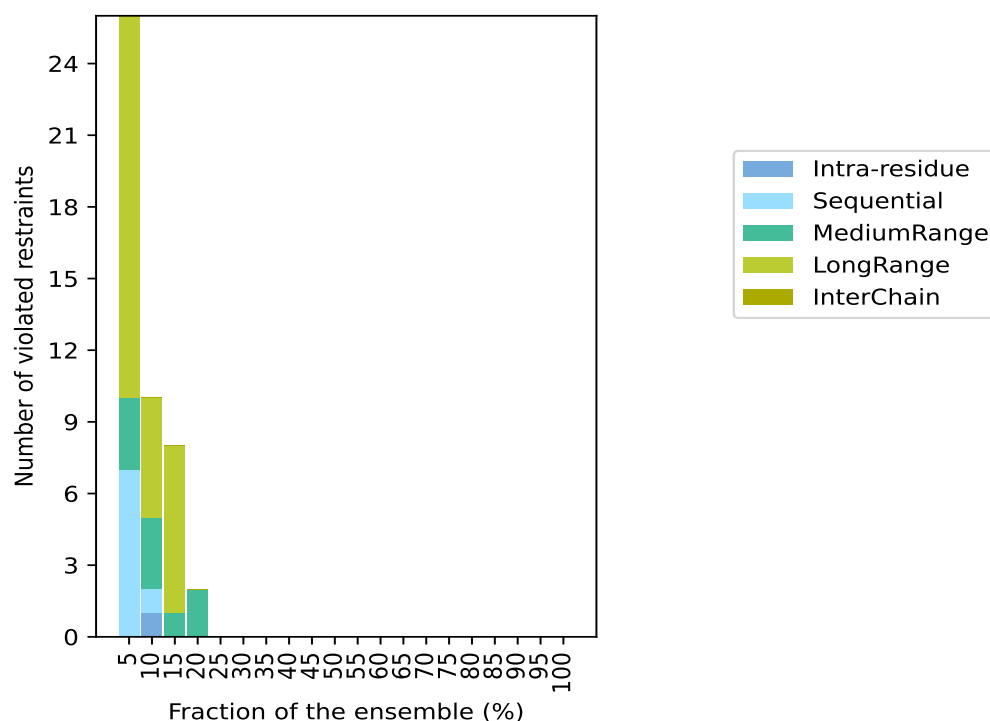
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 154(IR:21, SQ:53, MR:11, LR:69, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	7	3	16	0	26	1	5.0
1	1	3	5	0	10	2	10.0
0	0	1	7	0	8	3	15.0
0	0	2	0	0	2	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

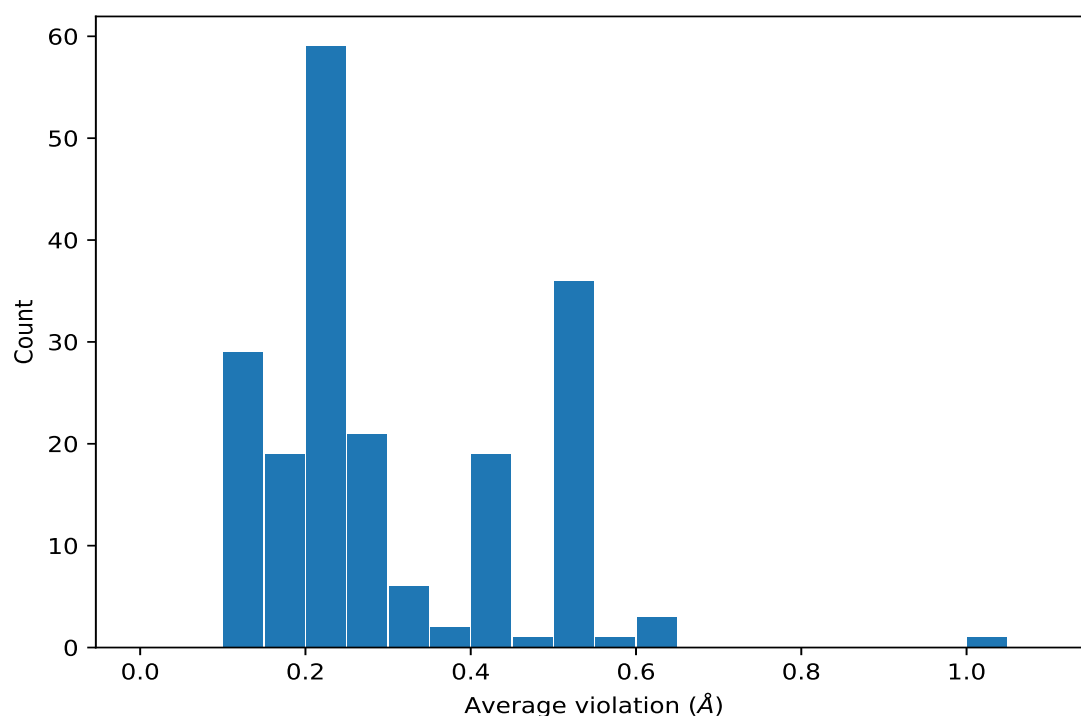
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(2,83)	1:95:A:LEU:H	1:87:A:TYR:O	11	0.18	0.03	0.19
(2,57)	1:53:A:ALA:H	1:69:A:THR:O	7	0.33	0.11	0.36
(2,43)	1:52:A:LYS:H	1:40:A:GLU:O	6	0.26	0.08	0.25
(2,115)	1:110:A:LYS:H	1:102:A:THR:O	6	0.22	0.12	0.19
(2,109)	1:100:A:TRP:H	1:112:A:ALA:O	6	0.16	0.04	0.15
(2,45)	1:42:A:GLU:H	1:50:A:SER:O	5	0.33	0.11	0.3
(2,63)	1:71:A:TYR:H	1:51:A:PHE:O	5	0.32	0.03	0.33
(2,58)	1:53:A:ALA:N	1:69:A:THR:O	5	0.14	0.04	0.12
(2,21)	1:27:A:ALA:H	1:39:A:GLY:O	4	1.02	0.39	1.24
(2,27)	1:41:A:TYR:H	1:25:A:SER:O	4	0.58	0.13	0.64
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD11	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD12	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD13	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD21	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD22	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD23	4	0.5	0.14	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD11	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD12	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD13	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD21	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD22	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD23	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD11	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD12	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD13	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD21	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD22	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD23	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD11	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD12	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD13	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD21	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD22	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD23	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD11	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD12	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD13	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD21	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD22	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD23	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD11	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD12	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD13	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD21	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD22	4	0.5	0.14	0.5
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD23	4	0.5	0.14	0.5
(2,28)	1:41:A:TYR:N	1:25:A:SER:O	4	0.33	0.11	0.39
(2,153)	1:143:A:THR:H	1:159:A:TYR:O	4	0.29	0.14	0.22
(2,183)	1:11:A:GLY:H	1:173:A:PHE:O	4	0.27	0.12	0.28
(1,154)	1:89:A:VAL:HG11	1:92:A:ASN:H	4	0.25	0.03	0.24
(1,154)	1:89:A:VAL:HG12	1:92:A:ASN:H	4	0.25	0.03	0.24
(1,154)	1:89:A:VAL:HG13	1:92:A:ASN:H	4	0.25	0.03	0.24
(1,154)	1:89:A:VAL:HG21	1:92:A:ASN:H	4	0.25	0.03	0.24
(1,154)	1:89:A:VAL:HG22	1:92:A:ASN:H	4	0.25	0.03	0.24
(1,154)	1:89:A:VAL:HG23	1:92:A:ASN:H	4	0.25	0.03	0.24
(2,151)	1:157:A:PHE:H	1:145:A:LEU:O	4	0.2	0.07	0.2
(2,143)	1:140:A:LYS:H	1:132:A:VAL:O	4	0.18	0.06	0.18
(2,105)	1:98:A:GLY:H	1:114:A:TYR:O	4	0.17	0.06	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,157)	1:141:A:PHE:H	1:161:A:TRP:O	4	0.17	0.08	0.13
(2,19)	1:37:A:LEU:H	1:29:A:TYR:O	4	0.16	0.08	0.12
(2,147)	1:155:A:VAL:H	1:147:A:TYR:O	4	0.15	0.02	0.15
(2,111)	1:112:A:ALA:H	1:100:A:TRP:O	4	0.14	0.02	0.13
(2,119)	1:127:A:LEU:H	1:119:A:TYR:O	4	0.12	0.01	0.12
(2,47)	1:50:A:SER:H	1:42:A:GLU:O	3	0.45	0.19	0.41
(2,177)	1:175:A:TYR:H	1:9:A:ALA:O	3	0.41	0.09	0.35
(1,53)	1:121:A:LEU:H	1:127:A:LEU:H	3	0.39	0.11	0.32
(1,2)	1:27:A:ALA:H	1:39:A:GLY:H	3	0.35	0.02	0.35
(1,41)	1:132:A:VAL:H	1:140:A:LYS:H	3	0.27	0.1	0.21
(1,61)	1:119:A:TYR:H	1:127:A:LEU:H	3	0.27	0.12	0.32
(1,114)	1:30:A:VAL:H	1:36:A:ALA:HB1	3	0.26	0.07	0.22
(1,114)	1:30:A:VAL:H	1:36:A:ALA:HB2	3	0.26	0.07	0.22
(1,114)	1:30:A:VAL:H	1:36:A:ALA:HB3	3	0.26	0.07	0.22
(1,116)	1:27:A:ALA:HB1	1:39:A:GLY:H	3	0.25	0.07	0.29
(1,116)	1:27:A:ALA:HB2	1:39:A:GLY:H	3	0.25	0.07	0.29
(1,116)	1:27:A:ALA:HB3	1:39:A:GLY:H	3	0.25	0.07	0.29
(2,117)	1:119:A:TYR:H	1:127:A:LEU:O	3	0.25	0.1	0.32
(1,128)	1:30:A:VAL:HG11	1:36:A:ALA:H	3	0.24	0.13	0.17
(1,128)	1:30:A:VAL:HG12	1:36:A:ALA:H	3	0.24	0.13	0.17
(1,128)	1:30:A:VAL:HG13	1:36:A:ALA:H	3	0.24	0.13	0.17
(1,128)	1:30:A:VAL:HG21	1:36:A:ALA:H	3	0.24	0.13	0.17
(1,128)	1:30:A:VAL:HG22	1:36:A:ALA:H	3	0.24	0.13	0.17
(1,128)	1:30:A:VAL:HG23	1:36:A:ALA:H	3	0.24	0.13	0.17
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD11	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD12	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD13	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD21	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD22	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD23	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD11	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD12	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD13	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD21	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD22	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD23	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD11	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD12	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD13	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD21	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD22	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD23	3	0.22	0.03	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD11	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD12	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD13	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD21	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD22	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD23	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD11	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD12	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD13	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD21	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD22	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD23	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD11	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD12	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD13	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD21	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD22	3	0.22	0.03	0.23
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD23	3	0.22	0.03	0.23
(2,175)	1:168:A:GLU:H	1:160:A:GLY:O	3	0.2	0.12	0.12
(2,159)	1:161:A:TRP:H	1:141:A:PHE:O	3	0.19	0.08	0.14
(2,64)	1:71:A:TYR:N	1:51:A:PHE:O	3	0.17	0.03	0.15
(2,161)	1:154:A:LYS:H	1:174:A:GLU:O	3	0.14	0.03	0.13
(2,51)	1:65:A:THR:H	1:57:A:TYR:O	3	0.12	0.03	0.1
(2,1)	1:8:A:LYS:H	1:28:A:LYS:O	3	0.12	0.02	0.11
(1,95)	1:117:A:ALA:HB1	1:129:A:SER:H	2	0.64	0.04	0.64
(1,95)	1:117:A:ALA:HB2	1:129:A:SER:H	2	0.64	0.04	0.64
(1,95)	1:117:A:ALA:HB3	1:129:A:SER:H	2	0.64	0.04	0.64
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD11	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD12	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD13	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD21	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD22	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD23	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD11	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD12	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD13	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD21	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD22	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD23	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD11	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD12	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD13	2	0.4	0.01	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD21	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD22	2	0.4	0.01	0.4
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD23	2	0.4	0.01	0.4
(1,54)	1:92:A:ASN:H	1:93:A:LEU:H	2	0.37	0.0	0.37
(2,141)	1:132:A:VAL:H	1:140:A:LYS:O	2	0.31	0.14	0.31
(2,61)	1:51:A:PHE:H	1:71:A:TYR:O	2	0.26	0.02	0.26
(2,123)	1:129:A:SER:H	1:117:A:ALA:O	2	0.26	0.02	0.26
(2,139)	1:142:A:ASP:H	1:130:A:GLN:O	2	0.25	0.14	0.25
(2,25)	1:25:A:SER:H	1:41:A:TYR:O	2	0.24	0.06	0.24
(2,22)	1:27:A:ALA:N	1:39:A:GLY:O	2	0.24	0.04	0.24
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD11	2	0.23	0.02	0.23
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD12	2	0.23	0.02	0.23
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD13	2	0.23	0.02	0.23
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD21	2	0.23	0.02	0.23
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD22	2	0.23	0.02	0.23
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD23	2	0.23	0.02	0.23
(1,155)	1:89:A:VAL:HG11	1:93:A:LEU:H	2	0.2	0.09	0.2
(1,155)	1:89:A:VAL:HG12	1:93:A:LEU:H	2	0.2	0.09	0.2
(1,155)	1:89:A:VAL:HG13	1:93:A:LEU:H	2	0.2	0.09	0.2
(1,155)	1:89:A:VAL:HG21	1:93:A:LEU:H	2	0.2	0.09	0.2
(1,155)	1:89:A:VAL:HG22	1:93:A:LEU:H	2	0.2	0.09	0.2
(1,155)	1:89:A:VAL:HG23	1:93:A:LEU:H	2	0.2	0.09	0.2
(2,87)	1:99:A:GLY:H	1:83:A:THR:O	2	0.18	0.04	0.18
(1,4)	1:38:A:LYS:H	1:54:A:GLY:H	2	0.18	0.06	0.18
(1,130)	1:30:A:VAL:HG11	1:37:A:LEU:H	2	0.17	0.0	0.17
(1,130)	1:30:A:VAL:HG12	1:37:A:LEU:H	2	0.17	0.0	0.17
(1,130)	1:30:A:VAL:HG13	1:37:A:LEU:H	2	0.17	0.0	0.17
(1,130)	1:30:A:VAL:HG21	1:37:A:LEU:H	2	0.17	0.0	0.17
(1,130)	1:30:A:VAL:HG22	1:37:A:LEU:H	2	0.17	0.0	0.17
(1,130)	1:30:A:VAL:HG23	1:37:A:LEU:H	2	0.17	0.0	0.17
(2,129)	1:126:A:LYS:H	1:146:A:GLU:O	2	0.16	0.01	0.16
(2,79)	1:78:A:ARG:H	1:70:A:GLU:O	2	0.16	0.04	0.16
(2,97)	1:94:A:GLU:H	1:118:A:GLU:O	2	0.16	0.03	0.16
(1,58)	1:119:A:TYR:H	1:121:A:LEU:H	2	0.15	0.05	0.15
(2,187)	1:13:A:THR:H	1:171:A:VAL:O	2	0.15	0.02	0.15
(2,118)	1:119:A:TYR:N	1:127:A:LEU:O	2	0.15	0.0	0.15
(2,46)	1:42:A:GLU:N	1:50:A:SER:O	2	0.14	0.03	0.14
(2,53)	1:55:A:ALA:H	1:67:A:VAL:O	2	0.14	0.0	0.14
(2,125)	1:115:A:THR:H	1:131:A:VAL:O	2	0.13	0.01	0.13
(2,133)	1:128:A:LEU:H	1:144:A:GLY:O	2	0.12	0.02	0.12
(1,104)	1:7:A:ALA:HB1	1:27:A:ALA:HB1	2	0.12	0.02	0.12
(1,104)	1:7:A:ALA:HB1	1:27:A:ALA:HB2	2	0.12	0.02	0.12

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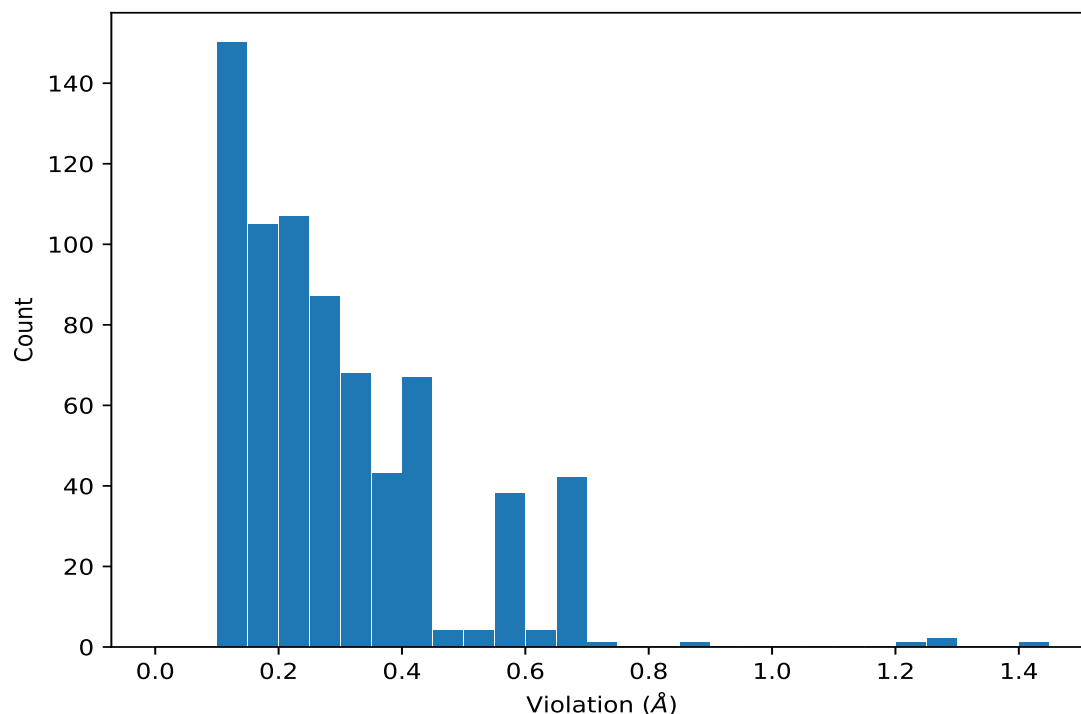
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,104)	1:7:A:ALA:HB1	1:27:A:ALA:HB3	2	0.12	0.02	0.12
(1,104)	1:7:A:ALA:HB2	1:27:A:ALA:HB1	2	0.12	0.02	0.12
(1,104)	1:7:A:ALA:HB2	1:27:A:ALA:HB2	2	0.12	0.02	0.12
(1,104)	1:7:A:ALA:HB2	1:27:A:ALA:HB3	2	0.12	0.02	0.12
(1,104)	1:7:A:ALA:HB3	1:27:A:ALA:HB1	2	0.12	0.02	0.12
(1,104)	1:7:A:ALA:HB3	1:27:A:ALA:HB2	2	0.12	0.02	0.12
(1,104)	1:7:A:ALA:HB3	1:27:A:ALA:HB3	2	0.12	0.02	0.12
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD11	2	0.1	0.0	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD12	2	0.1	0.0	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD13	2	0.1	0.0	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD21	2	0.1	0.0	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD22	2	0.1	0.0	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD23	2	0.1	0.0	0.1

¹Number of violated models, ²Standard 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

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)
(1,59)	1:121:A:LEU:H	1:122:A:THR:H	9	1.42
(2,21)	1:27:A:ALA:H	1:39:A:GLY:O	18	1.26
(2,21)	1:27:A:ALA:H	1:39:A:GLY:O	16	1.25
(2,21)	1:27:A:ALA:H	1:39:A:GLY:O	17	1.23
(2,81)	1:87:A:TYR:H	1:95:A:LEU:O	12	0.86
(2,47)	1:50:A:SER:H	1:42:A:GLU:O	13	0.7
(2,27)	1:41:A:TYR:H	1:25:A:SER:O	16	0.68
(2,27)	1:41:A:TYR:H	1:25:A:SER:O	18	0.68
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD11	12	0.68
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD12	12	0.68
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD13	12	0.68
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD21	12	0.68
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD22	12	0.68
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD23	12	0.68
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD11	12	0.68
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD12	12	0.68
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD13	12	0.68
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD21	12	0.68
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD22	12	0.68
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD23	12	0.68
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD11	12	0.68
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD12	12	0.68
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD13	12	0.68
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD21	12	0.68
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD22	12	0.68
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD23	12	0.68
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD11	12	0.68
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD12	12	0.68
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD13	12	0.68
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD21	12	0.68
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD22	12	0.68
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD23	12	0.68
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD11	12	0.68
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD12	12	0.68
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD13	12	0.68
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD21	12	0.68
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD22	12	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD23	12	0.68
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD11	12	0.68
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD12	12	0.68
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD13	12	0.68
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD21	12	0.68
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD22	12	0.68
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD23	12	0.68
(1,95)	1:117:A:ALA:HB1	1:129:A:SER:H	14	0.68
(1,95)	1:117:A:ALA:HB2	1:129:A:SER:H	14	0.68
(1,95)	1:117:A:ALA:HB3	1:129:A:SER:H	14	0.68
(2,169)	1:158:A:GLU:H	1:170:A:THR:O	20	0.65
(2,27)	1:41:A:TYR:H	1:25:A:SER:O	17	0.6
(1,95)	1:117:A:ALA:HB1	1:129:A:SER:H	13	0.6
(1,95)	1:117:A:ALA:HB2	1:129:A:SER:H	13	0.6
(1,95)	1:117:A:ALA:HB3	1:129:A:SER:H	13	0.6
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD11	15	0.59
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD12	15	0.59
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD13	15	0.59
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD21	15	0.59
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD22	15	0.59
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD23	15	0.59
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD11	15	0.59
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD12	15	0.59
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD13	15	0.59
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD21	15	0.59
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD22	15	0.59
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD23	15	0.59
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD11	15	0.59
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD12	15	0.59
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD13	15	0.59
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD21	15	0.59
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD22	15	0.59
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD23	15	0.59
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD11	15	0.59
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD12	15	0.59
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD13	15	0.59
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD21	15	0.59
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD22	15	0.59
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD23	15	0.59
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD11	15	0.59
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD12	15	0.59
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD13	15	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD21	15	0.59
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD22	15	0.59
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD23	15	0.59
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD11	15	0.59
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD12	15	0.59
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD13	15	0.59
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD21	15	0.59
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD22	15	0.59
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD23	15	0.59
(1,27)	1:158:A:GLU:H	1:170:A:THR:H	20	0.58
(1,53)	1:121:A:LEU:H	1:127:A:LEU:H	11	0.55
(2,179)	1:9:A:ALA:H	1:175:A:TYR:O	19	0.54
(2,177)	1:175:A:TYR:H	1:9:A:ALA:O	19	0.54
(2,153)	1:143:A:THR:H	1:159:A:TYR:O	19	0.53
(2,45)	1:42:A:GLU:H	1:50:A:SER:O	14	0.52
(2,131)	1:146:A:GLU:H	1:126:A:LYS:O	16	0.48
(2,180)	1:9:A:ALA:N	1:175:A:TYR:O	19	0.45
(2,141)	1:132:A:VAL:H	1:140:A:LYS:O	19	0.45
(2,57)	1:53:A:ALA:H	1:69:A:THR:O	10	0.45
(2,57)	1:53:A:ALA:H	1:69:A:THR:O	11	0.44
(2,115)	1:110:A:LYS:H	1:102:A:THR:O	6	0.43
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD11	20	0.42
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD12	20	0.42
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD13	20	0.42
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD21	20	0.42
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD22	20	0.42
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD23	20	0.42
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD11	20	0.42
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD12	20	0.42
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD13	20	0.42
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD21	20	0.42
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD22	20	0.42
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD23	20	0.42
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD11	20	0.42
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD12	20	0.42
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD13	20	0.42
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD21	20	0.42
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD22	20	0.42
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD23	20	0.42
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD11	20	0.42
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD12	20	0.42
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD13	20	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD21	20	0.42
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD22	20	0.42
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD23	20	0.42
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD11	20	0.42
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD12	20	0.42
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD13	20	0.42
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD21	20	0.42
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD22	20	0.42
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD23	20	0.42
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD11	20	0.42
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD12	20	0.42
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD13	20	0.42
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD21	20	0.42
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD22	20	0.42
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD23	20	0.42
(1,128)	1:30:A:VAL:HG11	1:36:A:ALA:H	14	0.42
(1,128)	1:30:A:VAL:HG12	1:36:A:ALA:H	14	0.42
(1,128)	1:30:A:VAL:HG13	1:36:A:ALA:H	14	0.42
(1,128)	1:30:A:VAL:HG21	1:36:A:ALA:H	14	0.42
(1,128)	1:30:A:VAL:HG22	1:36:A:ALA:H	14	0.42
(1,128)	1:30:A:VAL:HG23	1:36:A:ALA:H	14	0.42
(2,183)	1:11:A:GLY:H	1:173:A:PHE:O	15	0.41
(2,47)	1:50:A:SER:H	1:42:A:GLU:O	5	0.41
(2,28)	1:41:A:TYR:N	1:25:A:SER:O	16	0.41
(1,41)	1:132:A:VAL:H	1:140:A:LYS:H	10	0.41
(2,154)	1:143:A:THR:N	1:159:A:TYR:O	19	0.4
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD11	13	0.4
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD12	13	0.4
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD13	13	0.4
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD21	13	0.4
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD22	13	0.4
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD23	13	0.4
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD11	13	0.4
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD12	13	0.4
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD13	13	0.4
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD21	13	0.4
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD22	13	0.4
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD23	13	0.4
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD11	13	0.4
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD12	13	0.4
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD13	13	0.4
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD21	13	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD22	13	0.4
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD23	13	0.4
(2,139)	1:142:A:ASP:H	1:130:A:GLN:O	19	0.39
(2,28)	1:41:A:TYR:N	1:25:A:SER:O	17	0.39
(2,28)	1:41:A:TYR:N	1:25:A:SER:O	18	0.39
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD11	14	0.39
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD12	14	0.39
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD13	14	0.39
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD21	14	0.39
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD22	14	0.39
(1,170)	1:117:A:ALA:HB1	1:127:A:LEU:HD23	14	0.39
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD11	14	0.39
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD12	14	0.39
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD13	14	0.39
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD21	14	0.39
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD22	14	0.39
(1,170)	1:117:A:ALA:HB2	1:127:A:LEU:HD23	14	0.39
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD11	14	0.39
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD12	14	0.39
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD13	14	0.39
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD21	14	0.39
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD22	14	0.39
(1,170)	1:117:A:ALA:HB3	1:127:A:LEU:HD23	14	0.39
(2,57)	1:53:A:ALA:H	1:69:A:THR:O	18	0.38
(2,43)	1:52:A:LYS:H	1:40:A:GLU:O	8	0.38
(1,61)	1:119:A:TYR:H	1:127:A:LEU:H	13	0.38
(2,183)	1:11:A:GLY:H	1:173:A:PHE:O	9	0.37
(2,175)	1:168:A:GLU:H	1:160:A:GLY:O	15	0.37
(2,31)	1:43:A:TRP:H	1:23:A:GLY:O	8	0.37
(1,54)	1:92:A:ASN:H	1:93:A:LEU:H	2	0.37
(1,54)	1:92:A:ASN:H	1:93:A:LEU:H	17	0.37
(1,2)	1:27:A:ALA:H	1:39:A:GLY:H	17	0.37
(2,63)	1:71:A:TYR:H	1:51:A:PHE:O	15	0.36
(2,63)	1:71:A:TYR:H	1:51:A:PHE:O	18	0.36
(2,57)	1:53:A:ALA:H	1:69:A:THR:O	6	0.36
(2,27)	1:41:A:TYR:H	1:25:A:SER:O	4	0.36
(1,67)	1:102:A:THR:H	1:110:A:LYS:H	15	0.36
(2,177)	1:175:A:TYR:H	1:9:A:ALA:O	15	0.35
(2,145)	1:147:A:TYR:H	1:155:A:VAL:O	5	0.35
(2,57)	1:53:A:ALA:H	1:69:A:THR:O	15	0.35
(2,45)	1:42:A:GLU:H	1:50:A:SER:O	8	0.35
(1,114)	1:30:A:VAL:H	1:36:A:ALA:HB1	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:30:A:VAL:H	1:36:A:ALA:HB2	15	0.35
(1,114)	1:30:A:VAL:H	1:36:A:ALA:HB3	15	0.35
(1,2)	1:27:A:ALA:H	1:39:A:GLY:H	18	0.35
(2,177)	1:175:A:TYR:H	1:9:A:ALA:O	9	0.34
(2,21)	1:27:A:ALA:H	1:39:A:GLY:O	4	0.34
(1,11)	1:8:A:LYS:H	1:177:A:LEU:H	19	0.34
(2,117)	1:119:A:TYR:H	1:127:A:LEU:O	14	0.33
(2,115)	1:110:A:LYS:H	1:102:A:THR:O	15	0.33
(2,63)	1:71:A:TYR:H	1:51:A:PHE:O	6	0.33
(2,43)	1:52:A:LYS:H	1:40:A:GLU:O	14	0.33
(1,2)	1:27:A:ALA:H	1:39:A:GLY:H	16	0.33
(2,117)	1:119:A:TYR:H	1:127:A:LEU:O	13	0.32
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD11	2	0.32
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD12	2	0.32
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD13	2	0.32
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD21	2	0.32
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD22	2	0.32
(1,131)	1:31:A:LEU:HD11	1:35:A:LEU:HD23	2	0.32
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD11	2	0.32
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD12	2	0.32
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD13	2	0.32
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD21	2	0.32
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD22	2	0.32
(1,131)	1:31:A:LEU:HD12	1:35:A:LEU:HD23	2	0.32
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD11	2	0.32
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD12	2	0.32
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD13	2	0.32
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD21	2	0.32
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD22	2	0.32
(1,131)	1:31:A:LEU:HD13	1:35:A:LEU:HD23	2	0.32
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD11	2	0.32
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD12	2	0.32
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD13	2	0.32
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD21	2	0.32
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD22	2	0.32
(1,131)	1:31:A:LEU:HD21	1:35:A:LEU:HD23	2	0.32
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD11	2	0.32
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD12	2	0.32
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD13	2	0.32
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD21	2	0.32
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD22	2	0.32
(1,131)	1:31:A:LEU:HD22	1:35:A:LEU:HD23	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD11	2	0.32
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD12	2	0.32
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD13	2	0.32
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD21	2	0.32
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD22	2	0.32
(1,131)	1:31:A:LEU:HD23	1:35:A:LEU:HD23	2	0.32
(1,61)	1:119:A:TYR:H	1:127:A:LEU:H	14	0.32
(1,53)	1:121:A:LEU:H	1:127:A:LEU:H	17	0.32
(2,151)	1:157:A:PHE:H	1:145:A:LEU:O	5	0.31
(2,25)	1:25:A:SER:H	1:41:A:TYR:O	8	0.31
(1,116)	1:27:A:ALA:HB1	1:39:A:GLY:H	17	0.31
(1,116)	1:27:A:ALA:HB2	1:39:A:GLY:H	17	0.31
(1,116)	1:27:A:ALA:HB3	1:39:A:GLY:H	17	0.31
(1,53)	1:121:A:LEU:H	1:127:A:LEU:H	4	0.31
(2,159)	1:161:A:TRP:H	1:141:A:PHE:O	19	0.3
(2,157)	1:141:A:PHE:H	1:161:A:TRP:O	7	0.3
(2,45)	1:42:A:GLU:H	1:50:A:SER:O	20	0.3
(1,161)	1:93:A:LEU:HD11	1:118:A:GLU:H	12	0.3
(1,161)	1:93:A:LEU:HD12	1:118:A:GLU:H	12	0.3
(1,161)	1:93:A:LEU:HD13	1:118:A:GLU:H	12	0.3
(1,161)	1:93:A:LEU:HD21	1:118:A:GLU:H	12	0.3
(1,161)	1:93:A:LEU:HD22	1:118:A:GLU:H	12	0.3
(1,161)	1:93:A:LEU:HD23	1:118:A:GLU:H	12	0.3
(1,154)	1:89:A:VAL:HG11	1:92:A:ASN:H	11	0.3
(1,154)	1:89:A:VAL:HG12	1:92:A:ASN:H	11	0.3
(1,154)	1:89:A:VAL:HG13	1:92:A:ASN:H	11	0.3
(1,154)	1:89:A:VAL:HG21	1:92:A:ASN:H	11	0.3
(1,154)	1:89:A:VAL:HG22	1:92:A:ASN:H	11	0.3
(1,154)	1:89:A:VAL:HG23	1:92:A:ASN:H	11	0.3
(2,63)	1:71:A:TYR:H	1:51:A:PHE:O	10	0.29
(2,61)	1:51:A:PHE:H	1:71:A:TYR:O	5	0.29
(2,45)	1:42:A:GLU:H	1:50:A:SER:O	13	0.29
(2,43)	1:52:A:LYS:H	1:40:A:GLU:O	20	0.29
(2,19)	1:37:A:LEU:H	1:29:A:TYR:O	12	0.29
(1,116)	1:27:A:ALA:HB1	1:39:A:GLY:H	18	0.29
(1,116)	1:27:A:ALA:HB2	1:39:A:GLY:H	18	0.29
(1,116)	1:27:A:ALA:HB3	1:39:A:GLY:H	18	0.29
(2,158)	1:141:A:PHE:N	1:161:A:TRP:O	7	0.28
(2,123)	1:129:A:SER:H	1:117:A:ALA:O	14	0.28
(2,63)	1:71:A:TYR:H	1:51:A:PHE:O	11	0.28
(2,22)	1:27:A:ALA:N	1:39:A:GLY:O	16	0.28
(1,155)	1:89:A:VAL:HG11	1:93:A:LEU:H	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,155)	1:89:A:VAL:HG12	1:93:A:LEU:H	7	0.28
(1,155)	1:89:A:VAL:HG13	1:93:A:LEU:H	7	0.28
(1,155)	1:89:A:VAL:HG21	1:93:A:LEU:H	7	0.28
(1,155)	1:89:A:VAL:HG22	1:93:A:LEU:H	7	0.28
(1,155)	1:89:A:VAL:HG23	1:93:A:LEU:H	7	0.28
(2,142)	1:132:A:VAL:N	1:140:A:LYS:O	19	0.27
(1,94)	1:59:A:ALA:HB1	1:63:A:LEU:H	3	0.27
(1,94)	1:59:A:ALA:HB2	1:63:A:LEU:H	3	0.27
(1,94)	1:59:A:ALA:HB3	1:63:A:LEU:H	3	0.27
(2,153)	1:143:A:THR:H	1:159:A:TYR:O	7	0.26
(2,143)	1:140:A:LYS:H	1:132:A:VAL:O	10	0.26
(2,105)	1:98:A:GLY:H	1:114:A:TYR:O	12	0.26
(1,199)	1:175:A:TYR:H	1:177:A:LEU:HD11	19	0.26
(1,199)	1:175:A:TYR:H	1:177:A:LEU:HD12	19	0.26
(1,199)	1:175:A:TYR:H	1:177:A:LEU:HD13	19	0.26
(1,199)	1:175:A:TYR:H	1:177:A:LEU:HD21	19	0.26
(1,199)	1:175:A:TYR:H	1:177:A:LEU:HD22	19	0.26
(1,199)	1:175:A:TYR:H	1:177:A:LEU:HD23	19	0.26
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD11	4	0.26
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD12	4	0.26
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD13	4	0.26
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD21	4	0.26
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD22	4	0.26
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD23	4	0.26
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD11	4	0.26
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD12	4	0.26
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD13	4	0.26
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD21	4	0.26
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD22	4	0.26
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD23	4	0.26
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD11	4	0.26
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD12	4	0.26
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD13	4	0.26
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD21	4	0.26
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD22	4	0.26
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD23	4	0.26
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD11	4	0.26
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD12	4	0.26
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD13	4	0.26
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD21	4	0.26
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD22	4	0.26
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD23	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD11	4	0.26
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD12	4	0.26
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD13	4	0.26
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD21	4	0.26
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD22	4	0.26
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD23	4	0.26
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD11	4	0.26
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD12	4	0.26
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD13	4	0.26
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD21	4	0.26
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD22	4	0.26
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD23	4	0.26
(1,154)	1:89:A:VAL:HG11	1:92:A:ASN:H	1	0.26
(1,154)	1:89:A:VAL:HG12	1:92:A:ASN:H	1	0.26
(1,154)	1:89:A:VAL:HG13	1:92:A:ASN:H	1	0.26
(1,154)	1:89:A:VAL:HG21	1:92:A:ASN:H	1	0.26
(1,154)	1:89:A:VAL:HG22	1:92:A:ASN:H	1	0.26
(1,154)	1:89:A:VAL:HG23	1:92:A:ASN:H	1	0.26
(2,123)	1:129:A:SER:H	1:117:A:ALA:O	13	0.25
(2,115)	1:110:A:LYS:H	1:102:A:THR:O	8	0.25
(1,160)	1:93:A:LEU:HD11	1:94:A:GLU:H	12	0.25
(1,160)	1:93:A:LEU:HD12	1:94:A:GLU:H	12	0.25
(1,160)	1:93:A:LEU:HD13	1:94:A:GLU:H	12	0.25
(1,160)	1:93:A:LEU:HD21	1:94:A:GLU:H	12	0.25
(1,160)	1:93:A:LEU:HD22	1:94:A:GLU:H	12	0.25
(1,160)	1:93:A:LEU:HD23	1:94:A:GLU:H	12	0.25
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD11	20	0.25
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD12	20	0.25
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD13	20	0.25
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD21	20	0.25
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD22	20	0.25
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD23	20	0.25
(2,83)	1:95:A:LEU:H	1:87:A:TYR:O	11	0.24
(2,61)	1:51:A:PHE:H	1:71:A:TYR:O	13	0.24
(2,41)	1:40:A:GLU:H	1:52:A:LYS:O	20	0.24
(1,157)	1:89:A:VAL:HG11	1:95:A:LEU:H	20	0.24
(1,157)	1:89:A:VAL:HG12	1:95:A:LEU:H	20	0.24
(1,157)	1:89:A:VAL:HG13	1:95:A:LEU:H	20	0.24
(1,157)	1:89:A:VAL:HG21	1:95:A:LEU:H	20	0.24
(1,157)	1:89:A:VAL:HG22	1:95:A:LEU:H	20	0.24
(1,157)	1:89:A:VAL:HG23	1:95:A:LEU:H	20	0.24
(1,86)	1:126:A:LYS:H	1:146:A:GLU:H	16	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,143)	1:140:A:LYS:H	1:132:A:VAL:O	12	0.23
(2,47)	1:50:A:SER:H	1:42:A:GLU:O	14	0.23
(2,44)	1:52:A:LYS:N	1:40:A:GLU:O	14	0.23
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD11	17	0.23
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD12	17	0.23
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD13	17	0.23
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD21	17	0.23
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD22	17	0.23
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD23	17	0.23
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD11	17	0.23
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD12	17	0.23
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD13	17	0.23
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD21	17	0.23
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD22	17	0.23
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD23	17	0.23
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD11	17	0.23
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD12	17	0.23
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD13	17	0.23
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD21	17	0.23
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD22	17	0.23
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD23	17	0.23
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD11	17	0.23
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD12	17	0.23
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD13	17	0.23
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD21	17	0.23
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD22	17	0.23
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD23	17	0.23
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD11	17	0.23
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD12	17	0.23
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD13	17	0.23
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD21	17	0.23
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD22	17	0.23
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD23	17	0.23
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD11	17	0.23
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD12	17	0.23
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD13	17	0.23
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD21	17	0.23
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD22	17	0.23
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD23	17	0.23
(1,176)	1:121:A:LEU:HD11	1:122:A:THR:H	11	0.23
(1,176)	1:121:A:LEU:HD12	1:122:A:THR:H	11	0.23
(1,176)	1:121:A:LEU:HD13	1:122:A:THR:H	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,176)	1:121:A:LEU:HD21	1:122:A:THR:H	11	0.23
(1,176)	1:121:A:LEU:HD22	1:122:A:THR:H	11	0.23
(1,176)	1:121:A:LEU:HD23	1:122:A:THR:H	11	0.23
(1,107)	1:7:A:ALA:HB1	1:177:A:LEU:H	19	0.23
(1,107)	1:7:A:ALA:HB2	1:177:A:LEU:H	19	0.23
(1,107)	1:7:A:ALA:HB3	1:177:A:LEU:H	19	0.23
(1,4)	1:38:A:LYS:H	1:54:A:GLY:H	20	0.23
(2,137)	1:130:A:GLN:H	1:142:A:ASP:O	19	0.22
(2,109)	1:100:A:TRP:H	1:112:A:ALA:O	12	0.22
(2,87)	1:99:A:GLY:H	1:83:A:THR:O	12	0.22
(2,57)	1:53:A:ALA:H	1:69:A:THR:O	5	0.22
(1,177)	1:121:A:LEU:HD11	1:125:A:LEU:H	4	0.22
(1,177)	1:121:A:LEU:HD12	1:125:A:LEU:H	4	0.22
(1,177)	1:121:A:LEU:HD13	1:125:A:LEU:H	4	0.22
(1,177)	1:121:A:LEU:HD21	1:125:A:LEU:H	4	0.22
(1,177)	1:121:A:LEU:HD22	1:125:A:LEU:H	4	0.22
(1,177)	1:121:A:LEU:HD23	1:125:A:LEU:H	4	0.22
(1,154)	1:89:A:VAL:HG11	1:92:A:ASN:H	5	0.22
(1,154)	1:89:A:VAL:HG12	1:92:A:ASN:H	5	0.22
(1,154)	1:89:A:VAL:HG13	1:92:A:ASN:H	5	0.22
(1,154)	1:89:A:VAL:HG21	1:92:A:ASN:H	5	0.22
(1,154)	1:89:A:VAL:HG22	1:92:A:ASN:H	5	0.22
(1,154)	1:89:A:VAL:HG23	1:92:A:ASN:H	5	0.22
(1,154)	1:89:A:VAL:HG11	1:92:A:ASN:H	15	0.22
(1,154)	1:89:A:VAL:HG12	1:92:A:ASN:H	15	0.22
(1,154)	1:89:A:VAL:HG13	1:92:A:ASN:H	15	0.22
(1,154)	1:89:A:VAL:HG21	1:92:A:ASN:H	15	0.22
(1,154)	1:89:A:VAL:HG22	1:92:A:ASN:H	15	0.22
(1,154)	1:89:A:VAL:HG23	1:92:A:ASN:H	15	0.22
(1,114)	1:30:A:VAL:H	1:36:A:ALA:HB1	20	0.22
(1,114)	1:30:A:VAL:H	1:36:A:ALA:HB2	20	0.22
(1,114)	1:30:A:VAL:H	1:36:A:ALA:HB3	20	0.22
(1,57)	1:86:A:ARG:H	1:87:A:TYR:H	12	0.22
(2,167)	1:172:A:GLN:H	1:156:A:LYS:O	20	0.21
(2,151)	1:157:A:PHE:H	1:145:A:LEU:O	20	0.21
(2,83)	1:95:A:LEU:H	1:87:A:TYR:O	13	0.21
(2,83)	1:95:A:LEU:H	1:87:A:TYR:O	20	0.21
(2,64)	1:71:A:TYR:N	1:51:A:PHE:O	15	0.21
(2,58)	1:53:A:ALA:N	1:69:A:THR:O	11	0.21
(2,43)	1:52:A:LYS:H	1:40:A:GLU:O	5	0.21
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD11	12	0.21
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD12	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD13	12	0.21
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD21	12	0.21
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD22	12	0.21
(1,159)	1:93:A:LEU:H	1:93:A:LEU:HD23	12	0.21
(1,41)	1:132:A:VAL:H	1:140:A:LYS:H	12	0.21
(2,83)	1:95:A:LEU:H	1:87:A:TYR:O	1	0.2
(2,79)	1:78:A:ARG:H	1:70:A:GLU:O	3	0.2
(2,43)	1:52:A:LYS:H	1:40:A:GLU:O	13	0.2
(2,22)	1:27:A:ALA:N	1:39:A:GLY:O	18	0.2
(1,114)	1:30:A:VAL:H	1:36:A:ALA:HB1	12	0.2
(1,114)	1:30:A:VAL:H	1:36:A:ALA:HB2	12	0.2
(1,114)	1:30:A:VAL:H	1:36:A:ALA:HB3	12	0.2
(1,58)	1:119:A:TYR:H	1:121:A:LEU:H	9	0.2
(2,165)	1:156:A:LYS:H	1:172:A:GLN:O	20	0.19
(2,153)	1:143:A:THR:H	1:159:A:TYR:O	10	0.19
(2,151)	1:157:A:PHE:H	1:145:A:LEU:O	16	0.19
(2,97)	1:94:A:GLU:H	1:118:A:GLU:O	12	0.19
(2,83)	1:95:A:LEU:H	1:87:A:TYR:O	6	0.19
(2,83)	1:95:A:LEU:H	1:87:A:TYR:O	14	0.19
(2,83)	1:95:A:LEU:H	1:87:A:TYR:O	15	0.19
(1,41)	1:132:A:VAL:H	1:140:A:LYS:H	20	0.19
(2,183)	1:11:A:GLY:H	1:173:A:PHE:O	19	0.18
(2,161)	1:154:A:LYS:H	1:174:A:GLU:O	19	0.18
(2,153)	1:143:A:THR:H	1:159:A:TYR:O	20	0.18
(2,147)	1:155:A:VAL:H	1:147:A:TYR:O	19	0.18
(2,132)	1:146:A:GLU:N	1:126:A:LYS:O	16	0.18
(2,107)	1:114:A:TYR:H	1:98:A:GLY:O	15	0.18
(2,46)	1:42:A:GLU:N	1:50:A:SER:O	8	0.18
(2,32)	1:43:A:TRP:N	1:23:A:GLY:O	8	0.18
(2,25)	1:25:A:SER:H	1:41:A:TYR:O	14	0.18
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD11	11	0.18
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD12	11	0.18
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD13	11	0.18
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD21	11	0.18
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD22	11	0.18
(1,178)	1:121:A:LEU:HD11	1:125:A:LEU:HD23	11	0.18
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD11	11	0.18
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD12	11	0.18
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD13	11	0.18
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD21	11	0.18
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD22	11	0.18
(1,178)	1:121:A:LEU:HD12	1:125:A:LEU:HD23	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD11	11	0.18
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD12	11	0.18
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD13	11	0.18
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD21	11	0.18
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD22	11	0.18
(1,178)	1:121:A:LEU:HD13	1:125:A:LEU:HD23	11	0.18
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD11	11	0.18
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD12	11	0.18
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD13	11	0.18
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD21	11	0.18
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD22	11	0.18
(1,178)	1:121:A:LEU:HD21	1:125:A:LEU:HD23	11	0.18
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD11	11	0.18
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD12	11	0.18
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD13	11	0.18
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD21	11	0.18
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD22	11	0.18
(1,178)	1:121:A:LEU:HD22	1:125:A:LEU:HD23	11	0.18
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD11	11	0.18
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD12	11	0.18
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD13	11	0.18
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD21	11	0.18
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD22	11	0.18
(1,178)	1:121:A:LEU:HD23	1:125:A:LEU:HD23	11	0.18
(2,187)	1:13:A:THR:H	1:171:A:VAL:O	15	0.17
(2,141)	1:132:A:VAL:H	1:140:A:LYS:O	10	0.17
(2,129)	1:126:A:LYS:H	1:146:A:GLU:O	20	0.17
(2,111)	1:112:A:ALA:H	1:100:A:TRP:O	13	0.17
(2,109)	1:100:A:TRP:H	1:112:A:ALA:O	6	0.17
(2,105)	1:98:A:GLY:H	1:114:A:TYR:O	6	0.17
(2,93)	1:79:A:VAL:H	1:103:A:TRP:O	15	0.17
(2,51)	1:65:A:THR:H	1:57:A:TYR:O	3	0.17
(2,45)	1:42:A:GLU:H	1:50:A:SER:O	18	0.17
(1,130)	1:30:A:VAL:HG11	1:37:A:LEU:H	2	0.17
(1,130)	1:30:A:VAL:HG12	1:37:A:LEU:H	2	0.17
(1,130)	1:30:A:VAL:HG13	1:37:A:LEU:H	2	0.17
(1,130)	1:30:A:VAL:HG21	1:37:A:LEU:H	2	0.17
(1,130)	1:30:A:VAL:HG22	1:37:A:LEU:H	2	0.17
(1,130)	1:30:A:VAL:HG23	1:37:A:LEU:H	2	0.17
(1,130)	1:30:A:VAL:HG11	1:37:A:LEU:H	14	0.17
(1,130)	1:30:A:VAL:HG12	1:37:A:LEU:H	14	0.17
(1,130)	1:30:A:VAL:HG13	1:37:A:LEU:H	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,130)	1:30:A:VAL:HG21	1:37:A:LEU:H	14	0.17
(1,130)	1:30:A:VAL:HG22	1:37:A:LEU:H	14	0.17
(1,130)	1:30:A:VAL:HG23	1:37:A:LEU:H	14	0.17
(1,128)	1:30:A:VAL:HG11	1:36:A:ALA:H	2	0.17
(1,128)	1:30:A:VAL:HG12	1:36:A:ALA:H	2	0.17
(1,128)	1:30:A:VAL:HG13	1:36:A:ALA:H	2	0.17
(1,128)	1:30:A:VAL:HG21	1:36:A:ALA:H	2	0.17
(1,128)	1:30:A:VAL:HG22	1:36:A:ALA:H	2	0.17
(1,128)	1:30:A:VAL:HG23	1:36:A:ALA:H	2	0.17
(2,129)	1:126:A:LYS:H	1:146:A:GLU:O	16	0.16
(2,109)	1:100:A:TRP:H	1:112:A:ALA:O	8	0.16
(2,83)	1:95:A:LEU:H	1:87:A:TYR:O	5	0.16
(2,59)	1:69:A:THR:H	1:53:A:ALA:O	10	0.16
(1,116)	1:27:A:ALA:HB1	1:39:A:GLY:H	16	0.16
(1,116)	1:27:A:ALA:HB2	1:39:A:GLY:H	16	0.16
(1,116)	1:27:A:ALA:HB3	1:39:A:GLY:H	16	0.16
(1,100)	1:53:A:ALA:H	1:68:A:MET:HE1	14	0.16
(1,100)	1:53:A:ALA:H	1:68:A:MET:HE2	14	0.16
(1,100)	1:53:A:ALA:H	1:68:A:MET:HE3	14	0.16
(1,62)	1:119:A:TYR:H	1:120:A:LYS:H	12	0.16
(2,170)	1:158:A:GLU:N	1:170:A:THR:O	20	0.15
(2,152)	1:157:A:PHE:N	1:145:A:LEU:O	5	0.15
(2,147)	1:155:A:VAL:H	1:147:A:TYR:O	16	0.15
(2,133)	1:128:A:LEU:H	1:144:A:GLY:O	16	0.15
(2,118)	1:119:A:TYR:N	1:127:A:LEU:O	13	0.15
(2,118)	1:119:A:TYR:N	1:127:A:LEU:O	14	0.15
(2,87)	1:99:A:GLY:H	1:83:A:THR:O	15	0.15
(2,83)	1:95:A:LEU:H	1:87:A:TYR:O	12	0.15
(2,80)	1:78:A:ARG:N	1:70:A:GLU:O	3	0.15
(2,64)	1:71:A:TYR:N	1:51:A:PHE:O	6	0.15
(2,58)	1:53:A:ALA:N	1:69:A:THR:O	10	0.15
(2,43)	1:52:A:LYS:H	1:40:A:GLU:O	18	0.15
(2,15)	1:22:A:LYS:H	1:14:A:THR:O	13	0.15
(2,1)	1:8:A:LYS:H	1:28:A:LYS:O	19	0.15
(2,184)	1:11:A:GLY:N	1:173:A:PHE:O	19	0.14
(2,159)	1:161:A:TRP:H	1:141:A:PHE:O	7	0.14
(2,159)	1:161:A:TRP:H	1:141:A:PHE:O	20	0.14
(2,157)	1:141:A:PHE:H	1:161:A:TRP:O	10	0.14
(2,147)	1:155:A:VAL:H	1:147:A:TYR:O	15	0.14
(2,147)	1:155:A:VAL:H	1:147:A:TYR:O	20	0.14
(2,140)	1:142:A:ASP:N	1:130:A:GLN:O	19	0.14
(2,125)	1:115:A:THR:H	1:131:A:VAL:O	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,109)	1:100:A:TRP:H	1:112:A:ALA:O	15	0.14
(2,109)	1:100:A:TRP:H	1:112:A:ALA:O	20	0.14
(2,94)	1:79:A:VAL:N	1:103:A:TRP:O	15	0.14
(2,83)	1:95:A:LEU:H	1:87:A:TYR:O	7	0.14
(2,64)	1:71:A:TYR:N	1:51:A:PHE:O	18	0.14
(2,53)	1:55:A:ALA:H	1:67:A:VAL:O	5	0.14
(2,53)	1:55:A:ALA:H	1:67:A:VAL:O	14	0.14
(2,28)	1:41:A:TYR:N	1:25:A:SER:O	4	0.14
(2,19)	1:37:A:LEU:H	1:29:A:TYR:O	19	0.14
(1,147)	1:81:A:VAL:H	1:82:A:VAL:HG11	14	0.14
(1,147)	1:81:A:VAL:H	1:82:A:VAL:HG12	14	0.14
(1,147)	1:81:A:VAL:H	1:82:A:VAL:HG13	14	0.14
(1,147)	1:81:A:VAL:H	1:82:A:VAL:HG21	14	0.14
(1,147)	1:81:A:VAL:H	1:82:A:VAL:HG22	14	0.14
(1,147)	1:81:A:VAL:H	1:82:A:VAL:HG23	14	0.14
(2,187)	1:13:A:THR:H	1:171:A:VAL:O	13	0.13
(2,183)	1:11:A:GLY:H	1:173:A:PHE:O	13	0.13
(2,171)	1:170:A:THR:H	1:158:A:GLU:O	20	0.13
(2,161)	1:154:A:LYS:H	1:174:A:GLU:O	13	0.13
(2,146)	1:147:A:TYR:N	1:155:A:VAL:O	5	0.13
(2,143)	1:140:A:LYS:H	1:132:A:VAL:O	7	0.13
(2,119)	1:127:A:LEU:H	1:119:A:TYR:O	7	0.13
(2,119)	1:127:A:LEU:H	1:119:A:TYR:O	13	0.13
(2,115)	1:110:A:LYS:H	1:102:A:THR:O	7	0.13
(2,111)	1:112:A:ALA:H	1:100:A:TRP:O	8	0.13
(2,111)	1:112:A:ALA:H	1:100:A:TRP:O	11	0.13
(2,105)	1:98:A:GLY:H	1:114:A:TYR:O	8	0.13
(2,97)	1:94:A:GLU:H	1:118:A:GLU:O	17	0.13
(2,57)	1:53:A:ALA:H	1:69:A:THR:O	14	0.13
(1,158)	1:92:A:ASN:H	1:93:A:LEU:HD11	12	0.13
(1,158)	1:92:A:ASN:H	1:93:A:LEU:HD12	12	0.13
(1,158)	1:92:A:ASN:H	1:93:A:LEU:HD13	12	0.13
(1,158)	1:92:A:ASN:H	1:93:A:LEU:HD21	12	0.13
(1,158)	1:92:A:ASN:H	1:93:A:LEU:HD22	12	0.13
(1,158)	1:92:A:ASN:H	1:93:A:LEU:HD23	12	0.13
(1,128)	1:30:A:VAL:HG11	1:36:A:ALA:H	12	0.13
(1,128)	1:30:A:VAL:HG12	1:36:A:ALA:H	12	0.13
(1,128)	1:30:A:VAL:HG13	1:36:A:ALA:H	12	0.13
(1,128)	1:30:A:VAL:HG21	1:36:A:ALA:H	12	0.13
(1,128)	1:30:A:VAL:HG22	1:36:A:ALA:H	12	0.13
(1,128)	1:30:A:VAL:HG23	1:36:A:ALA:H	12	0.13
(1,104)	1:7:A:ALA:HB1	1:27:A:ALA:HB1	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:7:A:ALA:HB1	1:27:A:ALA:HB2	14	0.13
(1,104)	1:7:A:ALA:HB1	1:27:A:ALA:HB3	14	0.13
(1,104)	1:7:A:ALA:HB2	1:27:A:ALA:HB1	14	0.13
(1,104)	1:7:A:ALA:HB2	1:27:A:ALA:HB2	14	0.13
(1,104)	1:7:A:ALA:HB2	1:27:A:ALA:HB3	14	0.13
(1,104)	1:7:A:ALA:HB3	1:27:A:ALA:HB1	14	0.13
(1,104)	1:7:A:ALA:HB3	1:27:A:ALA:HB2	14	0.13
(1,104)	1:7:A:ALA:HB3	1:27:A:ALA:HB3	14	0.13
(1,69)	1:51:A:PHE:H	1:71:A:TYR:H	13	0.13
(2,178)	1:175:A:TYR:N	1:9:A:ALA:O	9	0.12
(2,175)	1:168:A:GLU:H	1:160:A:GLY:O	19	0.12
(2,161)	1:154:A:LYS:H	1:174:A:GLU:O	15	0.12
(2,157)	1:141:A:PHE:H	1:161:A:TRP:O	12	0.12
(2,143)	1:140:A:LYS:H	1:132:A:VAL:O	20	0.12
(2,125)	1:115:A:THR:H	1:131:A:VAL:O	13	0.12
(2,119)	1:127:A:LEU:H	1:119:A:TYR:O	14	0.12
(2,110)	1:100:A:TRP:N	1:112:A:ALA:O	12	0.12
(2,105)	1:98:A:GLY:H	1:114:A:TYR:O	20	0.12
(2,83)	1:95:A:LEU:H	1:87:A:TYR:O	10	0.12
(2,79)	1:78:A:ARG:H	1:70:A:GLU:O	5	0.12
(2,58)	1:53:A:ALA:N	1:69:A:THR:O	6	0.12
(2,55)	1:67:A:VAL:H	1:55:A:ALA:O	14	0.12
(1,13)	1:10:A:GLY:H	1:26:A:TYR:H	17	0.12
(1,4)	1:38:A:LYS:H	1:54:A:GLY:H	8	0.12
(1,3)	1:53:A:ALA:H	1:69:A:THR:H	10	0.12
(1,1)	1:83:A:THR:H	1:99:A:GLY:H	12	0.12
(2,191)	1:15:A:TYR:H	1:169:A:PHE:O	13	0.11
(2,175)	1:168:A:GLU:H	1:160:A:GLY:O	20	0.11
(2,157)	1:141:A:PHE:H	1:161:A:TRP:O	20	0.11
(2,151)	1:157:A:PHE:H	1:145:A:LEU:O	10	0.11
(2,139)	1:142:A:ASP:H	1:130:A:GLN:O	10	0.11
(2,135)	1:144:A:GLY:H	1:128:A:LEU:O	10	0.11
(2,119)	1:127:A:LEU:H	1:119:A:TYR:O	15	0.11
(2,117)	1:119:A:TYR:H	1:127:A:LEU:O	3	0.11
(2,115)	1:110:A:LYS:H	1:102:A:THR:O	11	0.11
(2,111)	1:112:A:ALA:H	1:100:A:TRP:O	20	0.11
(2,103)	1:116:A:ARG:H	1:96:A:PHE:O	6	0.11
(2,67)	1:84:A:GLU:H	1:64:A:LYS:O	12	0.11
(2,58)	1:53:A:ALA:N	1:69:A:THR:O	5	0.11
(2,46)	1:42:A:GLU:N	1:50:A:SER:O	13	0.11
(2,33)	1:36:A:ALA:H	1:56:A:GLU:O	14	0.11
(2,26)	1:25:A:SER:N	1:41:A:TYR:O	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:37:A:LEU:H	1:29:A:TYR:O	14	0.11
(2,1)	1:8:A:LYS:H	1:28:A:LYS:O	17	0.11
(1,186)	1:125:A:LEU:HD11	1:146:A:GLU:H	16	0.11
(1,186)	1:125:A:LEU:HD12	1:146:A:GLU:H	16	0.11
(1,186)	1:125:A:LEU:HD13	1:146:A:GLU:H	16	0.11
(1,186)	1:125:A:LEU:HD21	1:146:A:GLU:H	16	0.11
(1,186)	1:125:A:LEU:HD22	1:146:A:GLU:H	16	0.11
(1,186)	1:125:A:LEU:HD23	1:146:A:GLU:H	16	0.11
(1,168)	1:114:A:TYR:H	1:132:A:VAL:HG11	20	0.11
(1,168)	1:114:A:TYR:H	1:132:A:VAL:HG12	20	0.11
(1,168)	1:114:A:TYR:H	1:132:A:VAL:HG13	20	0.11
(1,168)	1:114:A:TYR:H	1:132:A:VAL:HG21	20	0.11
(1,168)	1:114:A:TYR:H	1:132:A:VAL:HG22	20	0.11
(1,168)	1:114:A:TYR:H	1:132:A:VAL:HG23	20	0.11
(1,155)	1:89:A:VAL:HG11	1:93:A:LEU:H	11	0.11
(1,155)	1:89:A:VAL:HG12	1:93:A:LEU:H	11	0.11
(1,155)	1:89:A:VAL:HG13	1:93:A:LEU:H	11	0.11
(1,155)	1:89:A:VAL:HG21	1:93:A:LEU:H	11	0.11
(1,155)	1:89:A:VAL:HG22	1:93:A:LEU:H	11	0.11
(1,155)	1:89:A:VAL:HG23	1:93:A:LEU:H	11	0.11
(1,117)	1:8:A:LYS:H	1:27:A:ALA:HB1	14	0.11
(1,117)	1:8:A:LYS:H	1:27:A:ALA:HB2	14	0.11
(1,117)	1:8:A:LYS:H	1:27:A:ALA:HB3	14	0.11
(1,61)	1:119:A:TYR:H	1:127:A:LEU:H	7	0.11
(1,38)	1:98:A:GLY:H	1:115:A:THR:H	12	0.11
(2,133)	1:128:A:LEU:H	1:144:A:GLY:O	10	0.1
(2,115)	1:110:A:LYS:H	1:102:A:THR:O	13	0.1
(2,109)	1:100:A:TRP:H	1:112:A:ALA:O	7	0.1
(2,99)	1:118:A:GLU:H	1:94:A:GLU:O	14	0.1
(2,58)	1:53:A:ALA:N	1:69:A:THR:O	18	0.1
(2,51)	1:65:A:THR:H	1:57:A:TYR:O	8	0.1
(2,51)	1:65:A:THR:H	1:57:A:TYR:O	10	0.1
(2,23)	1:39:A:GLY:H	1:27:A:ALA:O	14	0.1
(2,19)	1:37:A:LEU:H	1:29:A:TYR:O	16	0.1
(2,3)	1:28:A:LYS:H	1:8:A:LYS:O	13	0.1
(2,1)	1:8:A:LYS:H	1:28:A:LYS:O	13	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD11	9	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD12	9	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD13	9	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD21	9	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD22	9	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD23	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD11	17	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD12	17	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD13	17	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD21	17	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD22	17	0.1
(1,182)	1:122:A:THR:H	1:125:A:LEU:HD23	17	0.1
(1,104)	1:7:A:ALA:HB1	1:27:A:ALA:HB1	19	0.1
(1,104)	1:7:A:ALA:HB1	1:27:A:ALA:HB2	19	0.1
(1,104)	1:7:A:ALA:HB1	1:27:A:ALA:HB3	19	0.1
(1,104)	1:7:A:ALA:HB2	1:27:A:ALA:HB1	19	0.1
(1,104)	1:7:A:ALA:HB2	1:27:A:ALA:HB2	19	0.1
(1,104)	1:7:A:ALA:HB2	1:27:A:ALA:HB3	19	0.1
(1,104)	1:7:A:ALA:HB3	1:27:A:ALA:HB1	19	0.1
(1,104)	1:7:A:ALA:HB3	1:27:A:ALA:HB2	19	0.1
(1,104)	1:7:A:ALA:HB3	1:27:A:ALA:HB3	19	0.1
(1,58)	1:119:A:TYR:H	1:121:A:LEU:H	8	0.1

10 Dihedral-angle violation analysis [i](#)

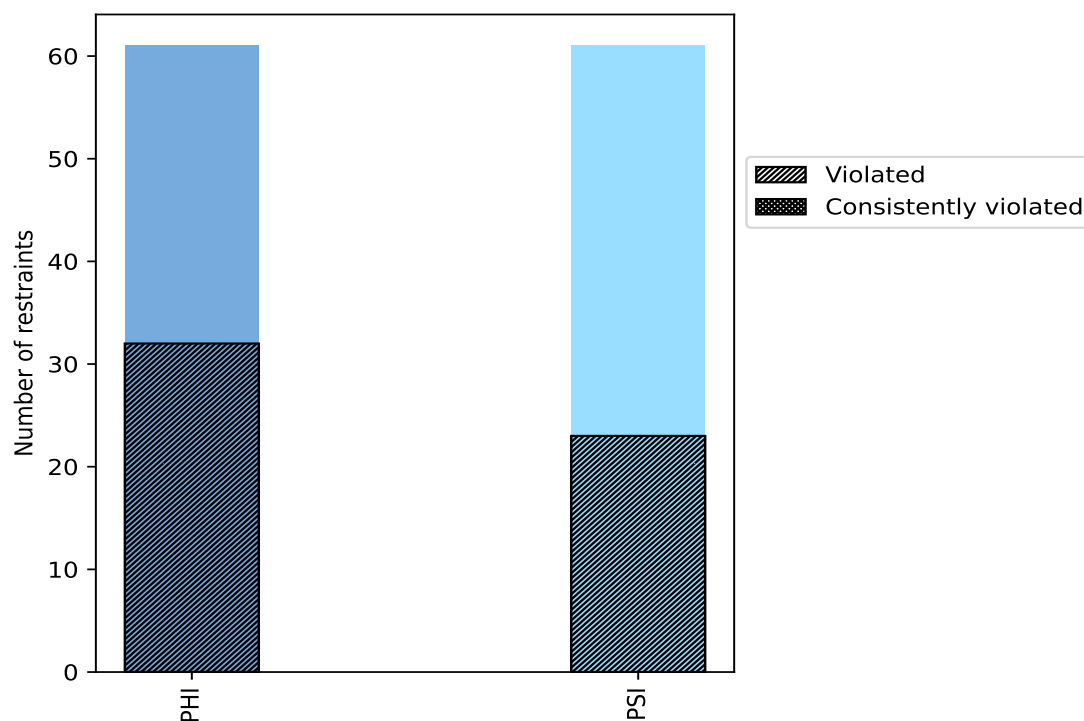
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	61	50.0	32	52.5	26.2	0	0.0	0.0
PSI	61	50.0	23	37.7	18.9	0	0.0	0.0
Total	122	100.0	55	45.1	45.1	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](#)



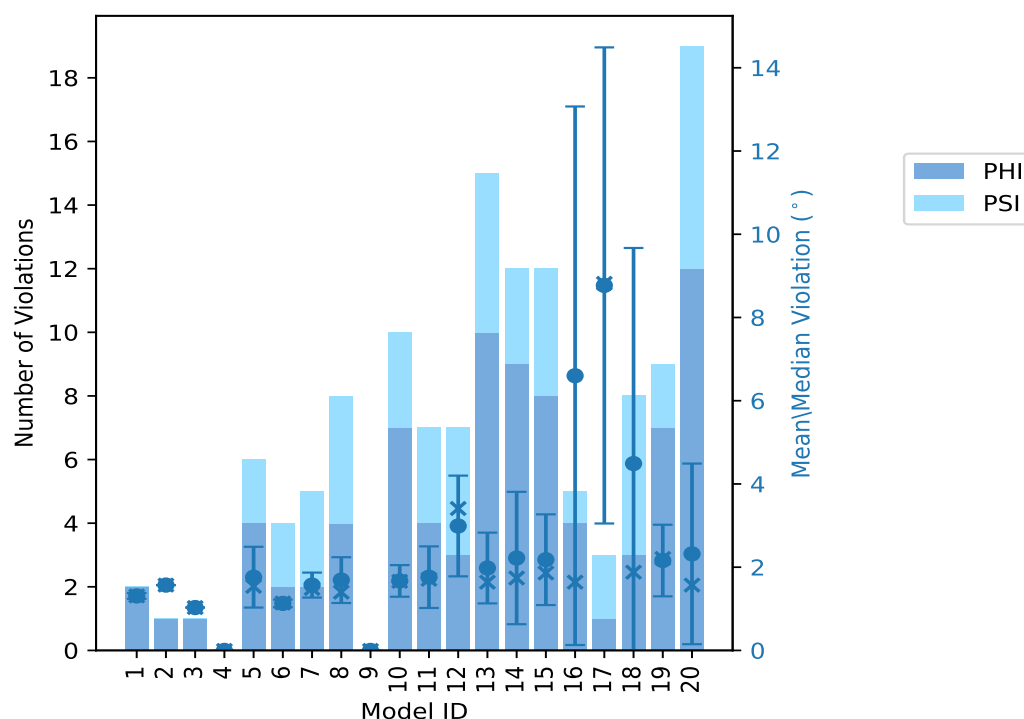
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	2	0	2	1.31	1.37	0.07	1.31
2	1	0	1	1.57	1.57	0.0	1.57
3	1	0	1	1.03	1.03	0.0	1.03
4	0	0	0	0.0	0.0	0.0	0.0
5	4	2	6	1.76	3.27	0.73	1.54
6	2	2	4	1.13	1.23	0.09	1.14
7	2	3	5	1.57	2.09	0.3	1.49
8	4	4	8	1.69	2.77	0.55	1.4
9	0	0	0	0.0	0.0	0.0	0.0
10	7	3	10	1.67	2.4	0.38	1.66
11	4	3	7	1.76	3.44	0.74	1.71
12	3	4	7	2.99	4.78	1.21	3.41
13	10	5	15	1.98	3.43	0.85	1.64
14	9	3	12	2.22	7.11	1.59	1.74
15	8	4	12	2.18	5.51	1.09	1.86
16	4	1	5	6.6	16.98	6.47	1.64
17	1	2	3	8.77	15.75	5.72	8.82
18	3	5	8	4.49	16.18	5.18	1.88
19	7	2	9	2.16	3.94	0.86	2.21
20	12	7	19	2.32	10.82	2.17	1.57

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
13	12	25	1	5.0
7	6	13	2	10.0
2	0	2	3	15.0
5	3	8	4	20.0
2	0	2	5	25.0
1	1	2	6	30.0
1	0	1	7	35.0
1	1	2	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

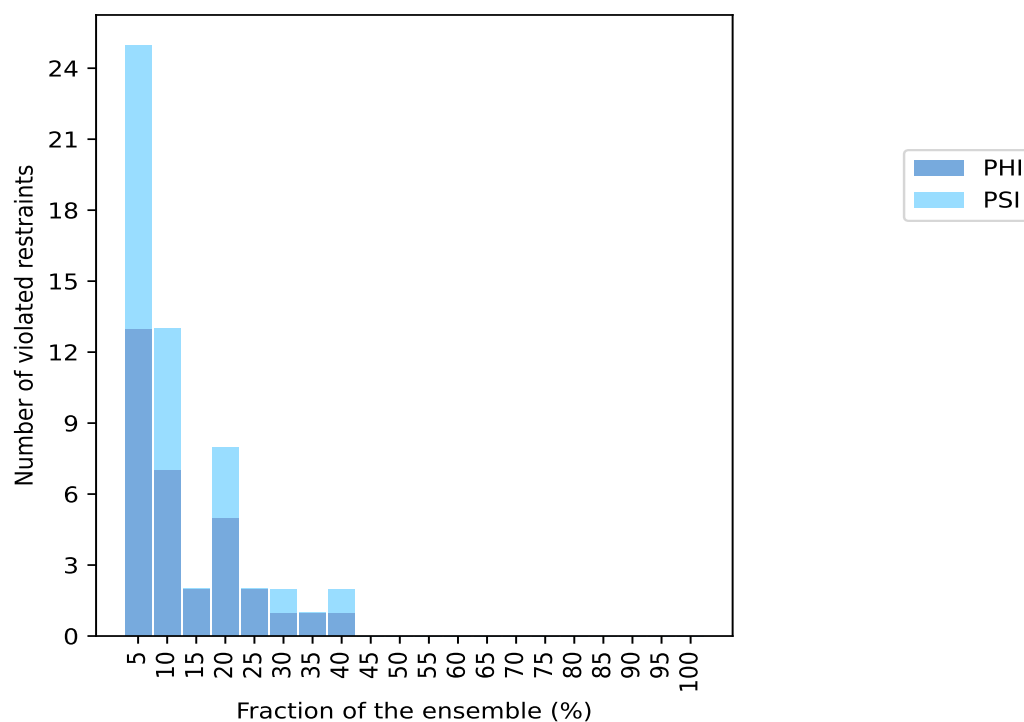
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

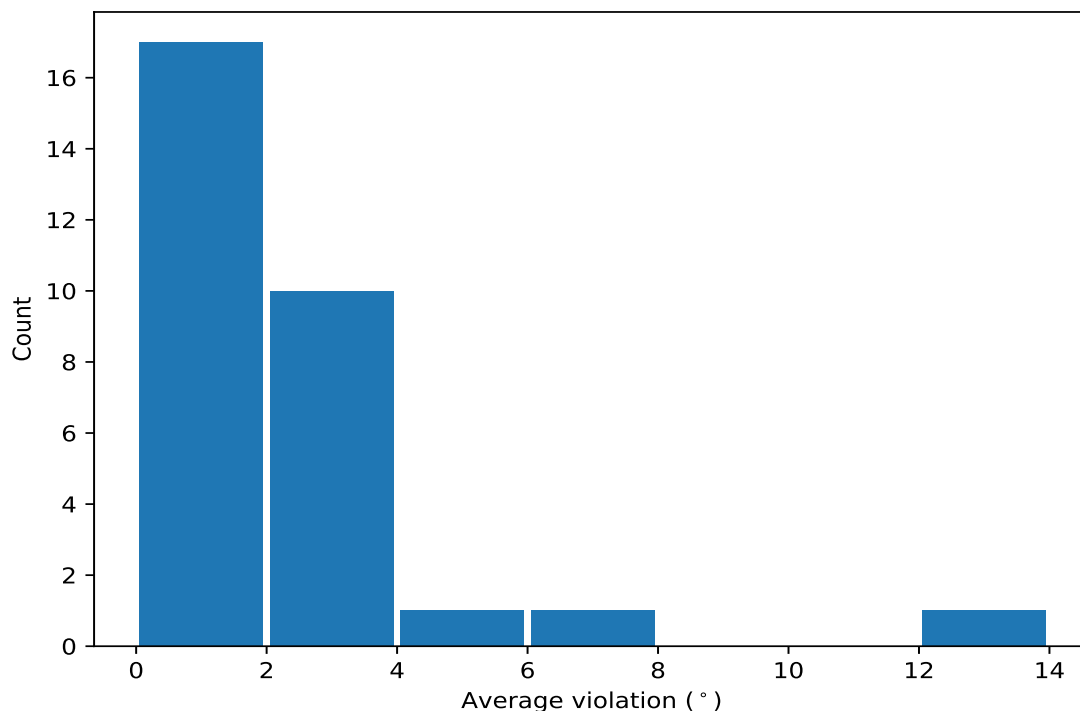


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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
(1,88)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	8	2.4	0.97	2.28
(1,87)	1:111:A:GLY:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	8	1.64	0.49	1.54
(1,121)	1:171:A:VAL:C	1:172:A:GLN:N	1:172:A:GLN:CA	1:172:A:GLN:C	7	2.01	0.74	1.68
(1,78)	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	1:97:A:PRO:N	6	2.36	0.84	2.4
(1,33)	1:52:A:LYS:C	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	6	1.73	0.29	1.76
(1,73)	1:86:A:ARG:C	1:87:A:TYR:N	1:87:A:TYR:CA	1:87:A:TYR:C	5	2.03	0.78	1.77
(1,77)	1:95:A:LEU:C	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	5	1.31	0.27	1.24
(1,20)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:ALA:N	4	12.65	6.34	15.96
(1,19)	1:25:A:SER:C	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	4	7.82	3.98	9.32
(1,97)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	4	3.58	2.14	2.78
(1,27)	1:35:A:LEU:C	1:36:A:ALA:N	1:36:A:ALA:CA	1:36:A:ALA:C	4	3.3	1.6	3.06
(1,72)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:TYR:N	4	2.21	1.51	1.5
(1,46)	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	1:64:A:LYS:N	4	1.63	0.24	1.67
(1,71)	1:85:A:GLY:C	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	4	1.46	0.29	1.38
(1,45)	1:62:A:TYR:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	4	1.21	0.13	1.19
(1,111)	1:157:A:PHE:C	1:158:A:GLU:N	1:158:A:GLU:CA	1:158:A:GLU:C	3	4.85	4.23	2.21
(1,25)	1:28:A:LYS:C	1:29:A:TYR:N	1:29:A:TYR:CA	1:29:A:TYR:C	3	1.34	0.11	1.37
(1,51)	1:67:A:VAL:C	1:68:A:MET:N	1:68:A:MET:CA	1:68:A:MET:C	2	3.01	0.26	3.01
(1,105)	1:131:A:VAL:C	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	2	2.08	0.32	2.08
(1,28)	1:36:A:ALA:N	1:36:A:ALA:CA	1:36:A:ALA:C	1:37:A:LEU:N	2	2.02	0.78	2.02

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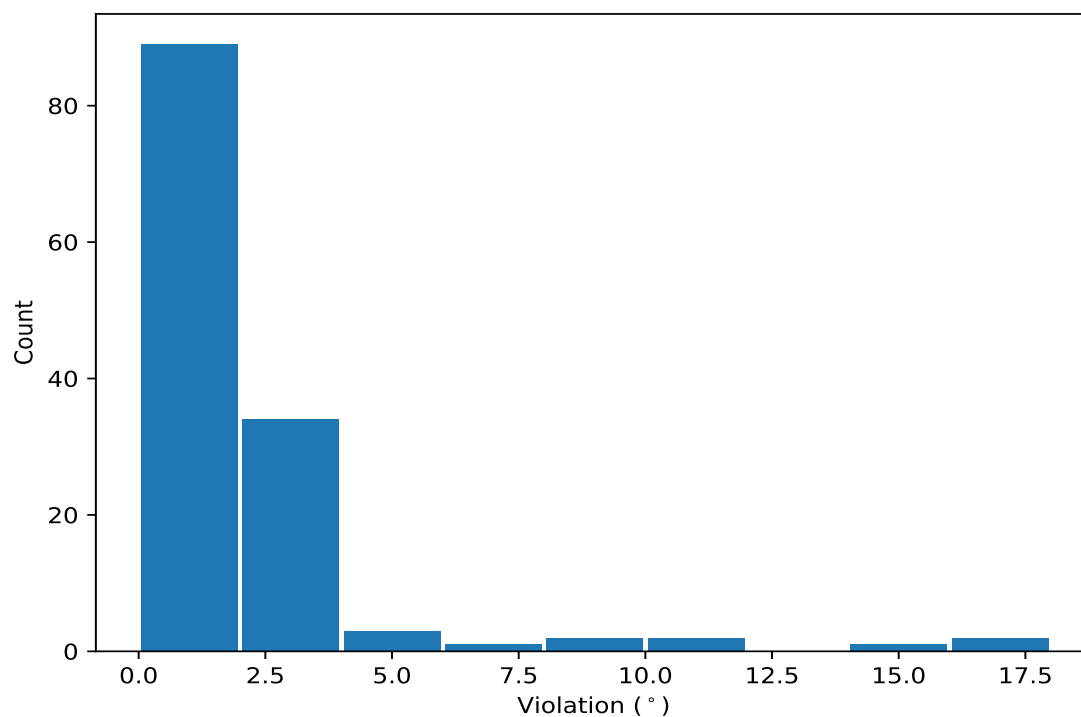
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,103)	1:130:A:GLN:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	2	1.98	0.7	1.98
(1,22)	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	1:28:A:LYS:N	2	1.84	0.11	1.84
(1,113)	1:158:A:GLU:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	2	1.82	0.24	1.82
(1,112)	1:158:A:GLU:N	1:158:A:GLU:CA	1:158:A:GLU:C	1:159:A:TYR:N	2	1.78	0.42	1.78
(1,82)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:THR:N	2	1.51	0.28	1.51
(1,107)	1:132:A:VAL:C	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	2	1.46	0.12	1.46
(1,117)	1:169:A:PHE:C	1:170:A:THR:N	1:170:A:THR:CA	1:170:A:THR:C	2	1.31	0.28	1.31
(1,79)	1:99:A:GLY:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	2	1.31	0.06	1.31
(1,74)	1:87:A:TYR:N	1:87:A:TYR:CA	1:87:A:TYR:C	1:88:A:PRO:N	2	1.22	0.19	1.22
(1,80)	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	1:101:A:TYR:N	2	1.19	0.14	1.19

¹ Number of violated models, ²Standard 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 (°)
(1,20)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:ALA:N	16	16.98
(1,20)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:ALA:N	18	16.18
(1,20)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:ALA:N	17	15.75
(1,19)	1:25:A:SER:C	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	16	11.49
(1,111)	1:157:A:PHE:C	1:158:A:GLU:N	1:158:A:GLU:CA	1:158:A:GLU:C	20	10.82
(1,19)	1:25:A:SER:C	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	18	9.83
(1,19)	1:25:A:SER:C	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	17	8.82
(1,97)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	14	7.11
(1,27)	1:35:A:LEU:C	1:36:A:ALA:N	1:36:A:ALA:CA	1:36:A:ALA:C	15	5.51
(1,72)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:TYR:N	12	4.78
(1,27)	1:35:A:LEU:C	1:36:A:ALA:N	1:36:A:ALA:CA	1:36:A:ALA:C	20	4.12
(1,9)	1:8:A:LYS:C	1:9:A:ALA:N	1:9:A:ALA:CA	1:9:A:ALA:C	19	3.94
(1,88)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	12	3.9
(1,88)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	20	3.72
(1,78)	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	1:97:A:PRO:N	11	3.44
(1,76)	1:95:A:LEU:N	1:95:A:LEU:CA	1:95:A:LEU:C	1:96:A:PHE:N	12	3.44
(1,97)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	13	3.43
(1,73)	1:86:A:ARG:C	1:87:A:TYR:N	1:87:A:TYR:CA	1:87:A:TYR:C	12	3.41
(1,120)	1:171:A:VAL:N	1:171:A:VAL:CA	1:171:A:VAL:C	1:172:A:GLN:N	13	3.3
(1,121)	1:171:A:VAL:C	1:172:A:GLN:N	1:172:A:GLN:CA	1:172:A:GLN:C	13	3.27
(1,51)	1:67:A:VAL:C	1:68:A:MET:N	1:68:A:MET:CA	1:68:A:MET:C	5	3.27
(1,78)	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	1:97:A:PRO:N	14	3.05
(1,78)	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	1:97:A:PRO:N	13	3.01
(1,10)	1:9:A:ALA:N	1:9:A:ALA:CA	1:9:A:ALA:C	1:10:A:GLY:N	19	2.89
(1,28)	1:36:A:ALA:N	1:36:A:ALA:CA	1:36:A:ALA:C	1:37:A:LEU:N	12	2.79
(1,87)	1:111:A:GLY:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	8	2.77
(1,51)	1:67:A:VAL:C	1:68:A:MET:N	1:68:A:MET:CA	1:68:A:MET:C	14	2.75
(1,121)	1:171:A:VAL:C	1:172:A:GLN:N	1:172:A:GLN:CA	1:172:A:GLN:C	20	2.69
(1,88)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	15	2.68
(1,103)	1:130:A:GLN:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	19	2.67
(1,121)	1:171:A:VAL:C	1:172:A:GLN:N	1:172:A:GLN:CA	1:172:A:GLN:C	15	2.46
(1,105)	1:131:A:VAL:C	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	10	2.4
(1,88)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	8	2.32
(1,73)	1:86:A:ARG:C	1:87:A:TYR:N	1:87:A:TYR:CA	1:87:A:TYR:C	20	2.28
(1,33)	1:52:A:LYS:C	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	18	2.26
(1,101)	1:129:A:SER:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	19	2.25
(1,88)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	13	2.24
(1,116)	1:169:A:PHE:N	1:169:A:PHE:CA	1:169:A:PHE:C	1:170:A:THR:N	15	2.21
(1,111)	1:157:A:PHE:C	1:158:A:GLU:N	1:158:A:GLU:CA	1:158:A:GLU:C	19	2.21
(1,112)	1:158:A:GLU:N	1:158:A:GLU:CA	1:158:A:GLU:C	1:159:A:TYR:N	20	2.2
(1,13)	1:13:A:THR:C	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	13	2.13
(1,97)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	10	2.12
(1,88)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	7	2.09
(1,113)	1:158:A:GLU:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	13	2.06
(1,27)	1:35:A:LEU:C	1:36:A:ALA:N	1:36:A:ALA:CA	1:36:A:ALA:C	14	2.01
(1,22)	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	1:28:A:LYS:N	18	1.95
(1,71)	1:85:A:GLY:C	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	15	1.94
(1,52)	1:68:A:MET:N	1:68:A:MET:CA	1:68:A:MET:C	1:69:A:THR:N	5	1.93
(1,46)	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	1:64:A:LYS:N	8	1.92
(1,85)	1:102:A:THR:C	1:103:A:TRP:N	1:103:A:TRP:CA	1:103:A:TRP:C	15	1.91
(1,34)	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	1:54:A:GLY:N	10	1.86
(1,72)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:TYR:N	20	1.82

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,104)	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1:132:A:VAL:N	10	1.81
(1,77)	1:95:A:LEU:C	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	11	1.81
(1,87)	1:111:A:GLY:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	15	1.8
(1,78)	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	1:97:A:PRO:N	18	1.8
(1,82)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:THR:N	15	1.79
(1,33)	1:52:A:LYS:C	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	11	1.78
(1,73)	1:86:A:ARG:C	1:87:A:TYR:N	1:87:A:TYR:CA	1:87:A:TYR:C	14	1.77
(1,33)	1:52:A:LYS:C	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	14	1.77
(1,105)	1:131:A:VAL:C	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	20	1.76
(1,33)	1:52:A:LYS:C	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	10	1.75
(1,87)	1:111:A:GLY:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	20	1.73
(1,22)	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	1:28:A:LYS:N	17	1.73
(1,21)	1:26:A:TYR:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	14	1.72
(1,46)	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	1:64:A:LYS:N	11	1.71
(1,20)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:ALA:N	14	1.69
(1,121)	1:171:A:VAL:C	1:172:A:GLN:N	1:172:A:GLN:CA	1:172:A:GLN:C	5	1.68
(1,26)	1:29:A:TYR:N	1:29:A:TYR:CA	1:29:A:TYR:C	1:30:A:VAL:N	15	1.68
(1,97)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	16	1.64
(1,87)	1:111:A:GLY:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	13	1.64
(1,78)	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	1:97:A:PRO:N	7	1.64
(1,46)	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	1:64:A:LYS:N	18	1.64
(1,7)	1:7:A:ALA:C	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	19	1.64
(1,117)	1:169:A:PHE:C	1:170:A:THR:N	1:170:A:THR:CA	1:170:A:THR:C	15	1.59
(1,107)	1:132:A:VAL:C	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	10	1.58
(1,113)	1:158:A:GLU:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	20	1.57
(1,27)	1:35:A:LEU:C	1:36:A:ALA:N	1:36:A:ALA:CA	1:36:A:ALA:C	2	1.57
(1,111)	1:157:A:PHE:C	1:158:A:GLU:N	1:158:A:GLU:CA	1:158:A:GLU:C	16	1.51
(1,121)	1:171:A:VAL:C	1:172:A:GLN:N	1:172:A:GLN:CA	1:172:A:GLN:C	19	1.5
(1,73)	1:86:A:ARG:C	1:87:A:TYR:N	1:87:A:TYR:CA	1:87:A:TYR:C	7	1.49
(1,11)	1:12:A:TRP:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	13	1.49
(1,114)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLY:N	20	1.48
(1,33)	1:52:A:LYS:C	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	15	1.47
(1,25)	1:28:A:LYS:C	1:29:A:TYR:N	1:29:A:TYR:CA	1:29:A:TYR:C	20	1.46
(1,87)	1:111:A:GLY:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	7	1.45
(1,99)	1:128:A:LEU:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	10	1.43
(1,74)	1:87:A:TYR:N	1:87:A:TYR:CA	1:87:A:TYR:C	1:88:A:PRO:N	14	1.41
(1,53)	1:68:A:MET:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	5	1.41
(1,45)	1:62:A:TYR:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	8	1.41
(1,87)	1:111:A:GLY:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	12	1.4
(1,71)	1:85:A:GLY:C	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	8	1.4
(1,121)	1:171:A:VAL:C	1:172:A:GLN:N	1:172:A:GLN:CA	1:172:A:GLN:C	16	1.39
(1,71)	1:85:A:GLY:C	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1	1.37
(1,25)	1:28:A:LYS:C	1:29:A:TYR:N	1:29:A:TYR:CA	1:29:A:TYR:C	19	1.37
(1,112)	1:158:A:GLU:N	1:158:A:GLU:CA	1:158:A:GLU:C	1:159:A:TYR:N	13	1.36
(1,79)	1:99:A:GLY:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	8	1.36
(1,107)	1:132:A:VAL:C	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	13	1.35
(1,77)	1:95:A:LEU:C	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	20	1.35
(1,33)	1:52:A:LYS:C	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	20	1.34
(1,80)	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	1:101:A:TYR:N	8	1.33
(1,87)	1:111:A:GLY:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	11	1.31
(1,103)	1:130:A:GLN:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	10	1.28

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,79)	1:99:A:GLY:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	20	1.25
(1,46)	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	1:64:A:LYS:N	10	1.25
(1,77)	1:95:A:LEU:C	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	1	1.24
(1,28)	1:36:A:ALA:N	1:36:A:ALA:CA	1:36:A:ALA:C	1:37:A:LEU:N	20	1.24
(1,88)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	11	1.23
(1,82)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:THR:N	6	1.23
(1,100)	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	1:130:A:GLN:N	13	1.22
(1,78)	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	1:97:A:PRO:N	20	1.22
(1,45)	1:62:A:TYR:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	18	1.21
(1,89)	1:113:A:PRO:C	1:114:A:TYR:N	1:114:A:TYR:CA	1:114:A:TYR:C	12	1.2
(1,73)	1:86:A:ARG:C	1:87:A:TYR:N	1:87:A:TYR:CA	1:87:A:TYR:C	6	1.2
(1,25)	1:28:A:LYS:C	1:29:A:TYR:N	1:29:A:TYR:CA	1:29:A:TYR:C	5	1.19
(1,45)	1:62:A:TYR:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	10	1.18
(1,72)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:TYR:N	7	1.17
(1,71)	1:85:A:GLY:C	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	13	1.15
(1,23)	1:27:A:ALA:C	1:28:A:LYS:N	1:28:A:LYS:CA	1:28:A:LYS:C	14	1.14
(1,19)	1:25:A:SER:C	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	14	1.13
(1,24)	1:28:A:LYS:N	1:28:A:LYS:CA	1:28:A:LYS:C	1:29:A:TYR:N	5	1.11
(1,77)	1:95:A:LEU:C	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	15	1.09
(1,121)	1:171:A:VAL:C	1:172:A:GLN:N	1:172:A:GLN:CA	1:172:A:GLN:C	14	1.08
(1,77)	1:95:A:LEU:C	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	13	1.08
(1,72)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:TYR:N	6	1.08
(1,115)	1:168:A:GLU:C	1:169:A:PHE:N	1:169:A:PHE:CA	1:169:A:PHE:C	20	1.07
(1,45)	1:62:A:TYR:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	11	1.06
(1,80)	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	1:101:A:TYR:N	20	1.05
(1,117)	1:169:A:PHE:C	1:170:A:THR:N	1:170:A:THR:CA	1:170:A:THR:C	13	1.03
(1,74)	1:87:A:TYR:N	1:87:A:TYR:CA	1:87:A:TYR:C	1:88:A:PRO:N	8	1.03
(1,43)	1:59:A:ALA:C	1:60:A:THR:N	1:60:A:THR:CA	1:60:A:THR:C	3	1.03
(1,88)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	18	1.02
(1,87)	1:111:A:GLY:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	6	1.02
(1,8)	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	1:9:A:ALA:N	19	1.01