



Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2023 – 05:06 pm BST

PDB ID : 6F2X
BMRB ID : 34300
Title : Structural characterization of the Mycobacterium tuberculosis Protein Tyrosine Kinase A (PtkA)
Authors : Niesteruk, A.; Jonker, H.R.A.; Sreeramulu, S.; Richter, C.; Hutchison, M.; Linhard, V.; Schwalbe, H.
Deposited on : 2017-11-27

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

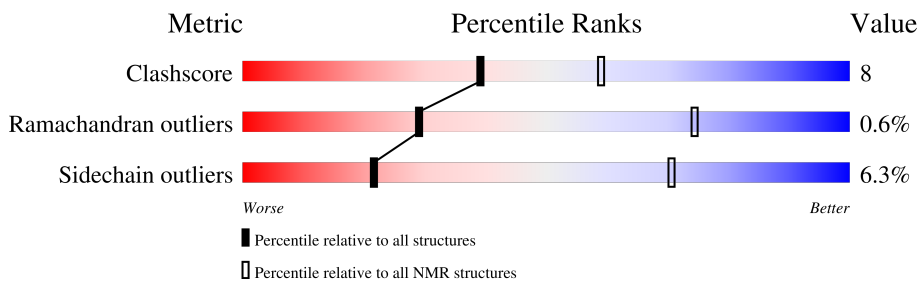
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 74%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	216	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:77-A:209, A:218-A:260, A:277-A:291 (191)	1.32	15

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 2 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3211 atoms, of which 1601 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein Tyrosine Kinase A.

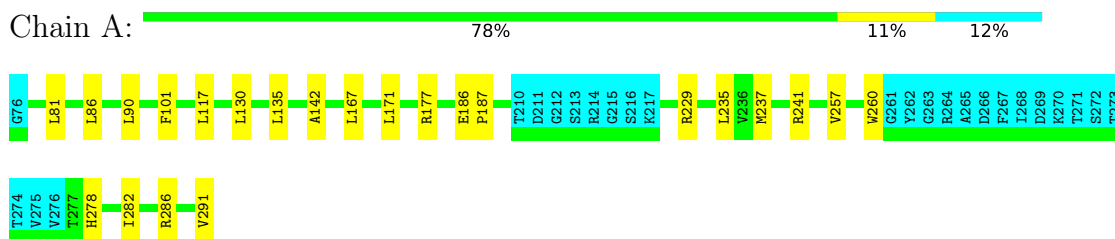
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	216	3211	1004	1601	294	308	4	0

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Protein Tyrosine Kinase A

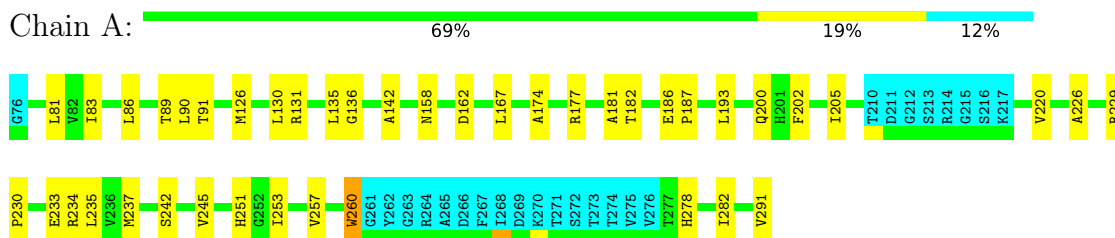


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

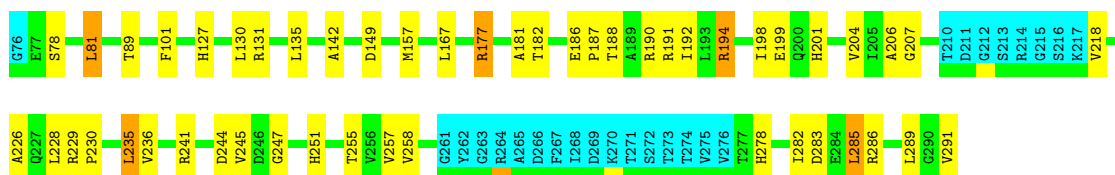
- Molecule 1: Protein Tyrosine Kinase A



4.2.2 Score per residue for model 2

- Molecule 1: Protein Tyrosine Kinase A





4.2.3 Score per residue for model 3

- Molecule 1: Protein Tyrosine Kinase A

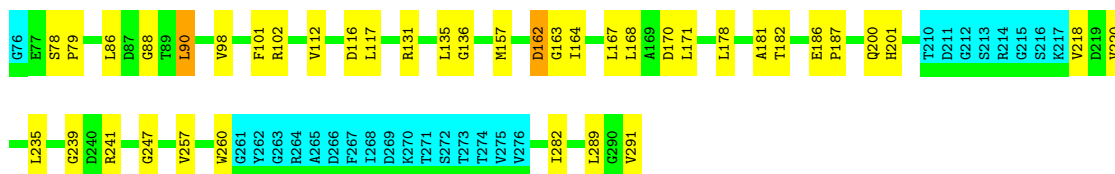
Chain A: 65% 22% 12%



4.2.4 Score per residue for model 4

- Molecule 1: Protein Tyrosine Kinase A

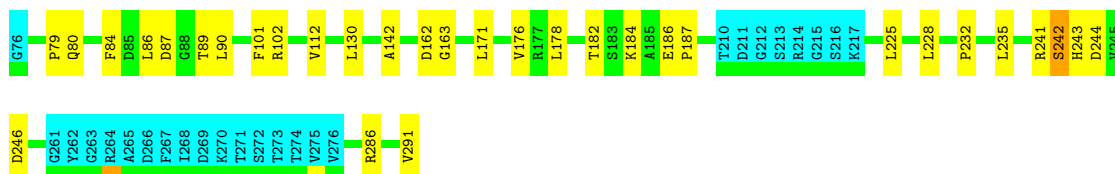
Chain A: 70% 18% 12%



4.2.5 Score per residue for model 5

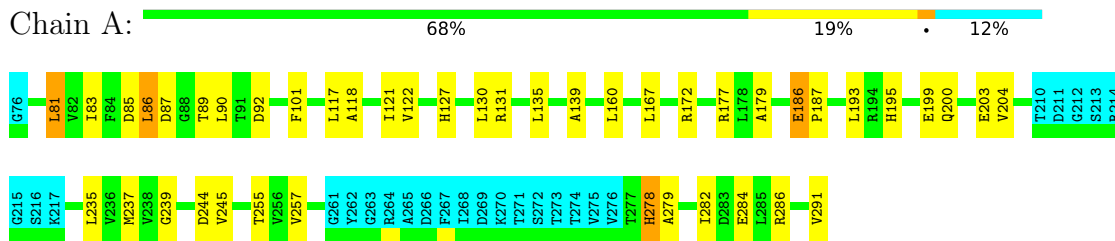
- Molecule 1: Protein Tyrosine Kinase A

Chain A: 74% 14% 12%



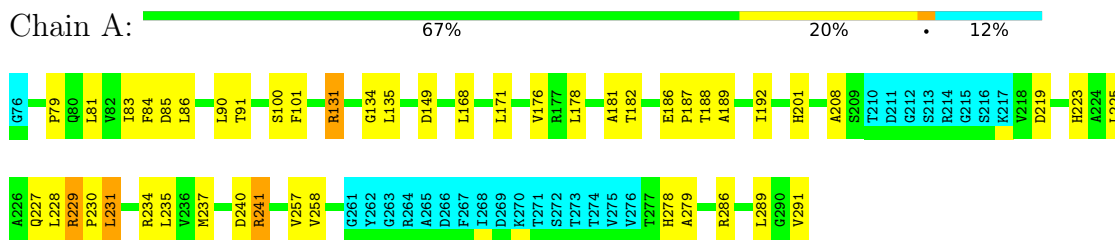
4.2.6 Score per residue for model 6

- Molecule 1: Protein Tyrosine Kinase A



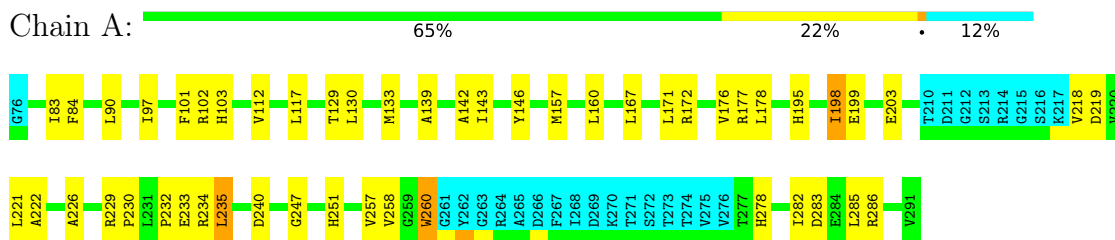
4.2.7 Score per residue for model 7

- Molecule 1: Protein Tyrosine Kinase A



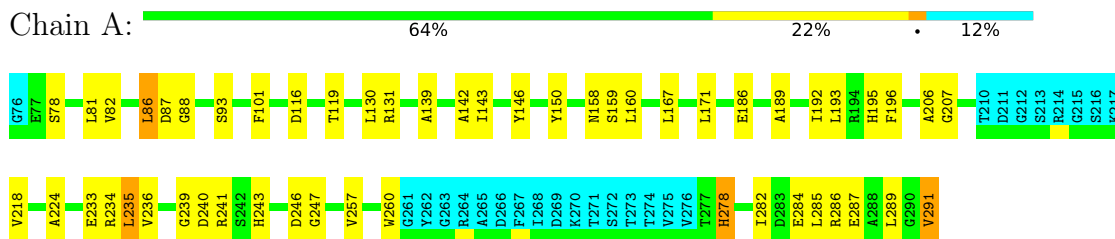
4.2.8 Score per residue for model 8

- Molecule 1: Protein Tyrosine Kinase A



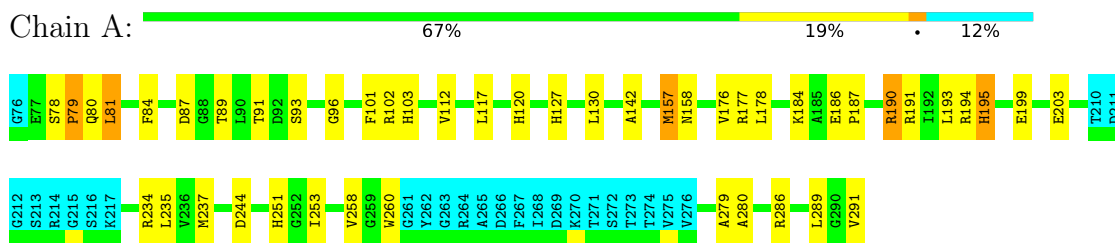
4.2.9 Score per residue for model 9

- Molecule 1: Protein Tyrosine Kinase A



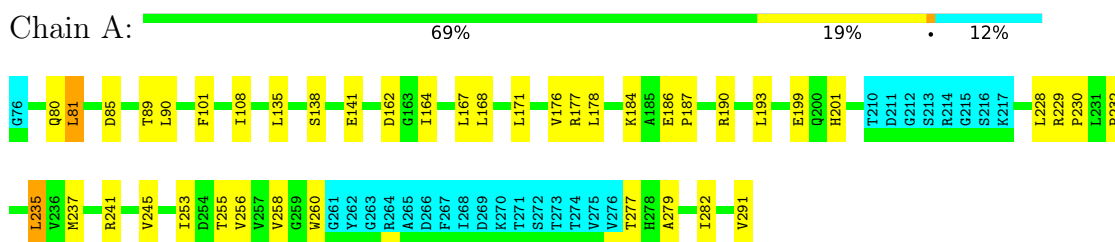
4.2.10 Score per residue for model 10

- Molecule 1: Protein Tyrosine Kinase A



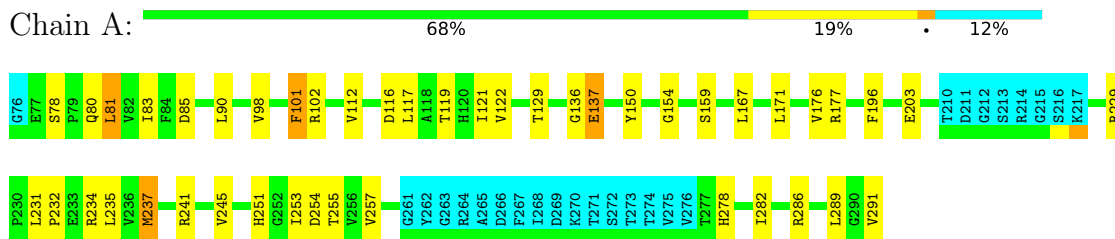
4.2.11 Score per residue for model 11

- Molecule 1: Protein Tyrosine Kinase A



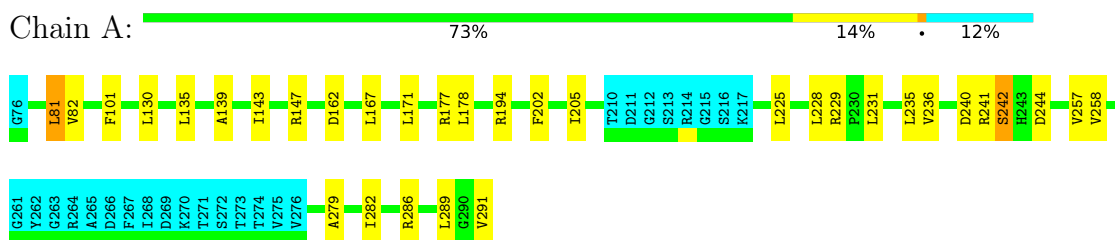
4.2.12 Score per residue for model 12

- Molecule 1: Protein Tyrosine Kinase A



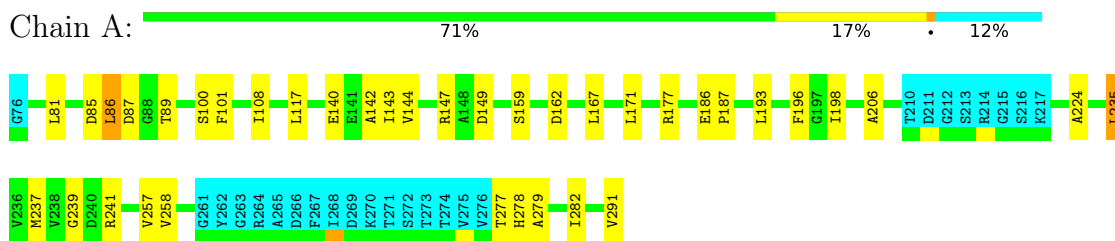
4.2.13 Score per residue for model 13

- Molecule 1: Protein Tyrosine Kinase A



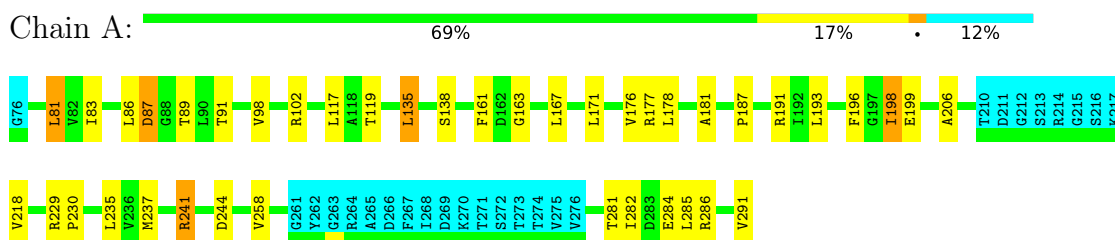
4.2.14 Score per residue for model 14

- Molecule 1: Protein Tyrosine Kinase A



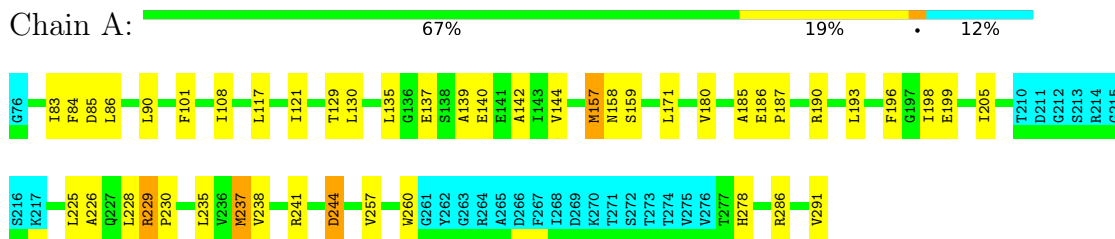
4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Protein Tyrosine Kinase A



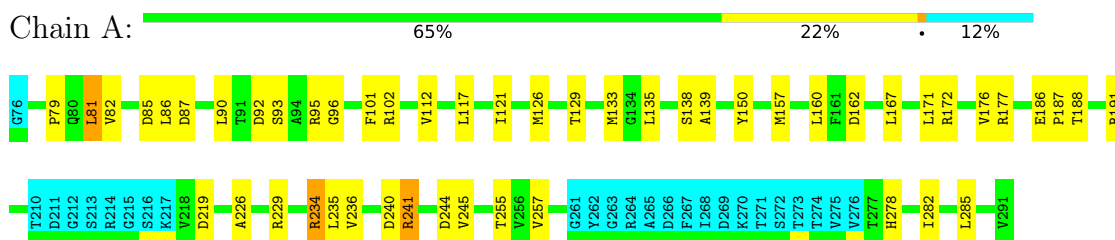
4.2.16 Score per residue for model 16

- Molecule 1: Protein Tyrosine Kinase A



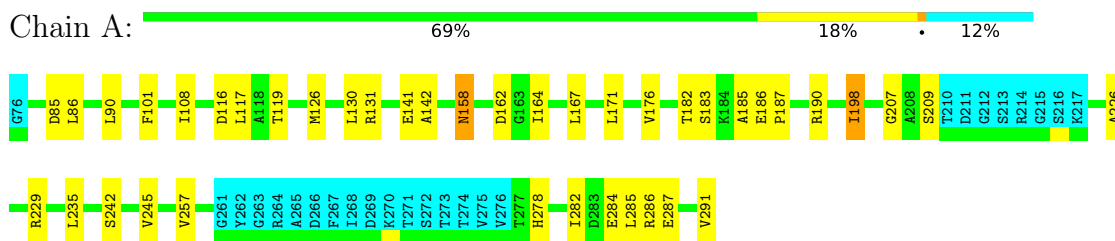
4.2.17 Score per residue for model 17

- Molecule 1: Protein Tyrosine Kinase A



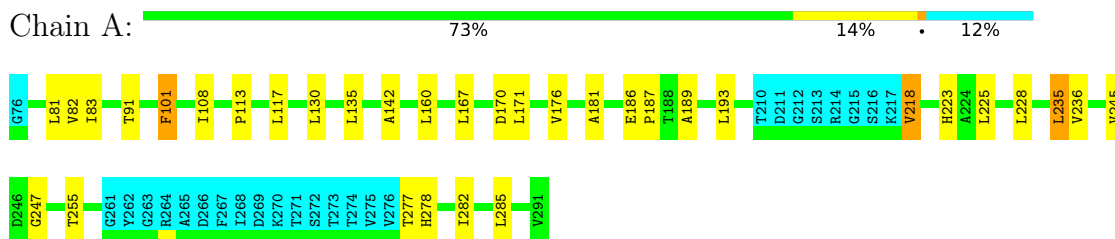
4.2.18 Score per residue for model 18

- Molecule 1: Protein Tyrosine Kinase A



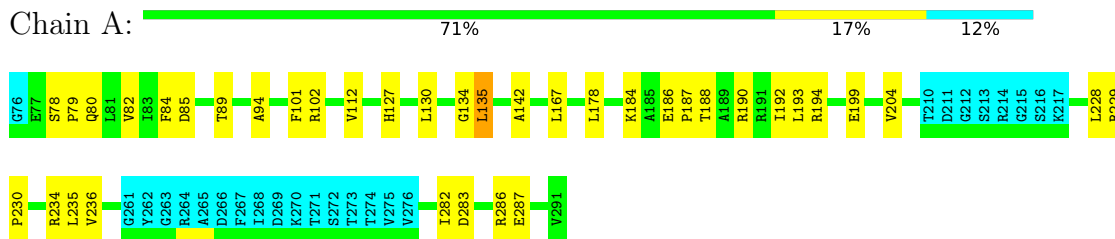
4.2.19 Score per residue for model 19

- Molecule 1: Protein Tyrosine Kinase A



4.2.20 Score per residue for model 20

- Molecule 1: Protein Tyrosine Kinase A



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure calculation	3.97
CNS	structure calculation	1.1
ARIA	refinement	1.2 HJ development version

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	1935
Number of shifts mapped to atoms	1935
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

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	1430	1425	1415	22±4
All	All	28600	28500	28300	443

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:ASP:HB3	1:A:241:ARG:HH22	0.89	1.27	15	1
1:A:286:ARG:HG3	1:A:291:VAL:HG23	0.86	1.48	9	4
1:A:171:LEU:HA	1:A:291:VAL:HG11	0.85	1.46	16	5
1:A:286:ARG:HG2	1:A:291:VAL:HG23	0.84	1.50	16	1
1:A:183:SER:HB2	1:A:207:GLY:HA3	0.78	1.52	18	1
1:A:218:VAL:HG21	1:A:247:GLY:HA2	0.76	1.56	19	2
1:A:83:ILE:HB	1:A:237:MET:HG2	0.73	1.58	1	3
1:A:245:VAL:HG13	1:A:255:THR:HG21	0.73	1.61	17	4
1:A:130:LEU:HG	1:A:135:LEU:HD22	0.72	1.58	13	3
1:A:91:THR:HB	1:A:158:ASN:OD1	0.72	1.85	10	2
1:A:135:LEU:HD11	1:A:138:SER:HB2	0.71	1.62	11	1
1:A:89:THR:HG23	1:A:258:VAL:HG21	0.71	1.62	14	1
1:A:90:LEU:HG	1:A:164:ILE:HG21	0.70	1.63	3	2
1:A:171:LEU:HD23	1:A:178:LEU:HD11	0.70	1.63	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:ASP:OD1	1:A:89:THR:HB	0.69	1.87	20	1
1:A:81:LEU:HD11	1:A:228:LEU:HD11	0.68	1.63	11	1
1:A:243:HIS:HA	1:A:246:ASP:HB3	0.68	1.63	9	2
1:A:193:LEU:HB3	1:A:199:GLU:HB2	0.68	1.64	15	4
1:A:185:ALA:HA	1:A:209:SER:HA	0.68	1.64	18	1
1:A:257:VAL:O	1:A:278:HIS:HA	0.68	1.89	14	11
1:A:86:LEU:HD23	1:A:90:LEU:HD12	0.67	1.65	16	1
1:A:167:LEU:HD22	1:A:282:ILE:HD11	0.66	1.65	6	16
1:A:81:LEU:HD13	1:A:228:LEU:HD22	0.66	1.67	19	1
1:A:86:LEU:H	1:A:182:THR:HB	0.66	1.50	4	1
1:A:88:GLY:HA3	1:A:241:ARG:HH22	0.65	1.51	9	1
1:A:225:LEU:HB3	1:A:231:LEU:HD13	0.65	1.68	7	1
1:A:258:VAL:HG12	1:A:279:ALA:HB3	0.64	1.69	14	2
1:A:135:LEU:HD21	1:A:138:SER:HB2	0.63	1.71	17	1
1:A:131:ARG:HA	1:A:135:LEU:HB3	0.62	1.71	6	3
1:A:89:THR:HG23	1:A:258:VAL:HB	0.61	1.71	10	2
1:A:226:ALA:O	1:A:229:ARG:HG2	0.58	1.99	16	3
1:A:239:GLY:O	1:A:257:VAL:HA	0.57	1.99	4	4
1:A:180:VAL:HG12	1:A:205:ILE:HA	0.57	1.76	16	1
1:A:81:LEU:HD22	1:A:228:LEU:HD11	0.57	1.76	7	1
1:A:242:SER:HA	1:A:245:VAL:HG12	0.57	1.75	1	2
1:A:86:LEU:HD11	1:A:193:LEU:HD11	0.57	1.77	1	1
1:A:186:GLU:HG3	1:A:187:PRO:HD3	0.56	1.77	4	1
1:A:130:LEU:HD21	1:A:142:ALA:HB3	0.56	1.77	8	9
1:A:241:ARG:HD3	1:A:242:SER:N	0.56	2.16	13	1
1:A:171:LEU:HD12	1:A:176:VAL:HG11	0.56	1.77	19	1
1:A:286:ARG:HG2	1:A:291:VAL:HG21	0.56	1.77	18	1
1:A:79:PRO:HB3	1:A:234:ARG:HG3	0.56	1.77	10	2
1:A:258:VAL:HG22	1:A:279:ALA:HB3	0.55	1.76	10	3
1:A:78:SER:HA	1:A:289:LEU:O	0.55	2.02	12	5
1:A:87:ASP:HB3	1:A:241:ARG:HH12	0.55	1.61	5	1
1:A:80:GLN:HB3	1:A:232:PRO:HB3	0.55	1.77	11	1
1:A:159:SER:HA	1:A:196:PHE:CZ	0.55	2.37	9	3
1:A:193:LEU:HD13	1:A:198:ILE:HG13	0.55	1.79	16	1
1:A:241:ARG:HB2	1:A:244:ASP:OD1	0.55	2.01	16	2
1:A:286:ARG:HG2	1:A:291:VAL:CG2	0.54	2.32	18	1
1:A:143:ILE:O	1:A:147:ARG:HG3	0.54	2.02	13	1
1:A:218:VAL:HG12	1:A:247:GLY:HA2	0.54	1.78	2	1
1:A:258:VAL:HG11	1:A:285:LEU:HD11	0.54	1.79	8	1
1:A:285:LEU:O	1:A:289:LEU:HG	0.54	2.02	3	2
1:A:225:LEU:HA	1:A:228:LEU:HG	0.53	1.81	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:LEU:HD23	1:A:235:LEU:HD21	0.53	1.80	14	1
1:A:86:LEU:HD21	1:A:193:LEU:HD21	0.53	1.79	14	1
1:A:113:PRO:HB2	1:A:117:LEU:HD21	0.53	1.80	19	1
1:A:187:PRO:O	1:A:191:ARG:HG2	0.53	2.03	2	3
1:A:186:GLU:HG3	1:A:208:ALA:N	0.53	2.17	7	1
1:A:87:ASP:HB3	1:A:241:ARG:NH1	0.53	2.19	5	1
1:A:245:VAL:HA	1:A:255:THR:HG21	0.53	1.81	19	1
1:A:164:ILE:O	1:A:168:LEU:HG	0.53	2.04	4	1
1:A:85:ASP:O	1:A:89:THR:HB	0.53	2.04	11	1
1:A:85:ASP:O	1:A:90:LEU:HG	0.53	2.04	16	2
1:A:150:TYR:HA	1:A:154:GLY:HA3	0.53	1.80	12	1
1:A:233:GLU:HG3	1:A:234:ARG:HG3	0.52	1.80	9	2
1:A:204:VAL:HG21	1:A:228:LEU:HB3	0.52	1.80	20	2
1:A:167:LEU:O	1:A:171:LEU:HG	0.52	2.03	9	2
1:A:286:ARG:CG	1:A:291:VAL:HG13	0.52	2.35	5	1
1:A:131:ARG:HA	1:A:135:LEU:O	0.52	2.05	2	3
1:A:240:ASP:HA	1:A:257:VAL:HG13	0.52	1.80	8	4
1:A:108:ILE:HG22	1:A:141:GLU:HG3	0.51	1.82	11	1
1:A:81:LEU:HG	1:A:177:ARG:HB3	0.51	1.81	2	1
1:A:229:ARG:HB3	1:A:231:LEU:HD23	0.51	1.82	7	1
1:A:92:ASP:OD2	1:A:160:LEU:HA	0.51	2.05	6	1
1:A:190:ARG:O	1:A:194:ARG:HB2	0.51	2.05	2	2
1:A:98:VAL:O	1:A:102:ARG:HG3	0.51	2.06	15	3
1:A:229:ARG:HB2	1:A:230:PRO:HA	0.51	1.83	1	3
1:A:256:VAL:HG12	1:A:277:THR:HB	0.51	1.81	11	1
1:A:108:ILE:HD13	1:A:142:ALA:HB2	0.50	1.83	19	3
1:A:157:MET:HA	1:A:157:MET:CE	0.50	2.36	16	4
1:A:130:LEU:HG	1:A:135:LEU:HD12	0.50	1.83	19	1
1:A:229:ARG:HB3	1:A:230:PRO:HA	0.50	1.83	11	1
1:A:186:GLU:N	1:A:187:PRO:HD2	0.50	2.22	16	12
1:A:242:SER:HA	1:A:245:VAL:CG1	0.50	2.37	1	1
1:A:188:THR:O	1:A:192:ILE:HG12	0.50	2.06	7	3
1:A:229:ARG:HG2	1:A:231:LEU:HD12	0.50	1.83	12	1
1:A:286:ARG:HG3	1:A:291:VAL:CG2	0.50	2.32	9	1
1:A:168:LEU:HD13	1:A:201:HIS:HE1	0.50	1.67	11	1
1:A:245:VAL:HG23	1:A:255:THR:HG21	0.50	1.83	11	1
1:A:87:ASP:HB3	1:A:241:ARG:NH2	0.50	2.09	15	1
1:A:235:LEU:HB3	1:A:253:ILE:HG23	0.49	1.84	11	1
1:A:159:SER:HA	1:A:196:PHE:CE2	0.49	2.42	16	3
1:A:85:ASP:HA	1:A:182:THR:OG1	0.49	2.06	18	1
1:A:118:ALA:O	1:A:122:VAL:HG23	0.49	2.07	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:GLY:HA2	1:A:157:MET:HE3	0.49	1.84	17	1
1:A:80:GLN:HG2	1:A:232:PRO:HB3	0.49	1.85	5	1
1:A:186:GLU:HB2	1:A:187:PRO:HD3	0.49	1.84	5	2
1:A:81:LEU:HD12	1:A:177:ARG:HB2	0.49	1.85	10	2
1:A:121:ILE:HG22	1:A:129:THR:HG21	0.49	1.85	16	1
1:A:182:THR:HG22	1:A:207:GLY:HA2	0.49	1.83	2	1
1:A:218:VAL:HG22	1:A:247:GLY:HA2	0.49	1.84	4	2
1:A:171:LEU:HB3	1:A:176:VAL:HB	0.49	1.84	7	1
1:A:158:ASN:HD22	1:A:158:ASN:N	0.49	2.05	18	1
1:A:135:LEU:O	1:A:139:ALA:HB2	0.49	2.08	16	1
1:A:87:ASP:HB2	1:A:184:LYS:NZ	0.48	2.23	10	1
1:A:87:ASP:OD1	1:A:93:SER:HB2	0.48	2.08	17	1
1:A:81:LEU:HA	1:A:177:ARG:O	0.48	2.08	1	2
1:A:171:LEU:O	1:A:176:VAL:HG12	0.48	2.09	18	7
1:A:146:TYR:O	1:A:150:TYR:HB2	0.48	2.09	9	1
1:A:80:GLN:HG2	1:A:234:ARG:HB3	0.48	1.85	10	1
1:A:162:ASP:OD2	1:A:282:ILE:HB	0.48	2.08	13	1
1:A:291:VAL:HG13	1:A:291:VAL:OXT	0.48	2.09	3	1
1:A:171:LEU:HD22	1:A:178:LEU:HD11	0.48	1.84	7	1
1:A:188:THR:O	1:A:191:ARG:HG2	0.48	2.08	17	1
1:A:193:LEU:HD13	1:A:199:GLU:HG3	0.48	1.86	20	1
1:A:202:PHE:HB2	1:A:205:ILE:HD11	0.48	1.86	1	2
1:A:86:LEU:HG	1:A:189:ALA:HB1	0.47	1.84	9	1
1:A:191:ARG:O	1:A:195:HIS:HB2	0.47	2.09	10	1
1:A:171:LEU:HD12	1:A:291:VAL:HG11	0.47	1.84	11	1
1:A:92:ASP:OD1	1:A:95:ARG:HG2	0.47	2.09	17	1
1:A:82:VAL:HG13	1:A:236:VAL:HG13	0.47	1.86	19	5
1:A:86:LEU:O	1:A:90:LEU:HB2	0.47	2.09	17	1
1:A:186:GLU:HB3	1:A:187:PRO:HD3	0.47	1.85	2	1
1:A:84:PHE:HE1	1:A:178:LEU:HD12	0.47	1.69	10	5
1:A:226:ALA:O	1:A:229:ARG:HG3	0.47	2.08	17	3
1:A:192:ILE:HA	1:A:195:HIS:CD2	0.47	2.44	3	1
1:A:218:VAL:HG21	1:A:247:GLY:CA	0.47	2.37	19	1
1:A:218:VAL:HG12	1:A:247:GLY:CA	0.47	2.39	2	1
1:A:258:VAL:HG21	1:A:285:LEU:HG	0.47	1.86	2	1
1:A:86:LEU:HD21	1:A:193:LEU:HD13	0.47	1.87	9	1
1:A:260:TRP:CE3	1:A:260:TRP:HA	0.47	2.45	8	1
1:A:240:ASP:HA	1:A:257:VAL:HG23	0.47	1.87	13	1
1:A:198:ILE:HD13	1:A:198:ILE:H	0.47	1.70	18	2
1:A:91:THR:HG22	1:A:160:LEU:HB3	0.47	1.86	19	1
1:A:198:ILE:HA	1:A:201:HIS:HD2	0.47	1.69	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:ASP:HB3	1:A:237:MET:CE	0.47	2.39	6	1
1:A:257:VAL:HB	1:A:278:HIS:HB3	0.47	1.87	3	1
1:A:83:ILE:HG23	1:A:181:ALA:HB3	0.47	1.86	7	1
1:A:90:LEU:HD23	1:A:90:LEU:H	0.47	1.69	7	1
1:A:100:SER:HA	1:A:149:ASP:OD2	0.47	2.10	14	2
1:A:140:GLU:HA	1:A:143:ILE:HG22	0.47	1.87	14	1
1:A:102:ARG:HG2	1:A:112:VAL:HG11	0.46	1.87	8	5
1:A:140:GLU:O	1:A:144:VAL:HG23	0.46	2.10	16	1
1:A:229:ARG:HA	1:A:230:PRO:C	0.46	2.31	1	6
1:A:88:GLY:HA3	1:A:241:ARG:NH2	0.46	2.24	9	1
1:A:135:LEU:HD12	1:A:137:GLU:HB3	0.46	1.86	16	1
1:A:283:ASP:OD2	1:A:286:ARG:HD3	0.46	2.10	20	1
1:A:125:PRO:HB2	1:A:128:GLU:OE2	0.46	2.10	3	1
1:A:135:LEU:HD11	1:A:139:ALA:HA	0.46	1.86	6	1
1:A:84:PHE:HB3	1:A:90:LEU:HD11	0.46	1.88	8	1
1:A:81:LEU:HB3	1:A:235:LEU:HD22	0.46	1.87	9	1
1:A:182:THR:CG2	1:A:207:GLY:HA2	0.46	2.40	2	1
1:A:139:ALA:O	1:A:143:ILE:HG12	0.46	2.11	9	2
1:A:119:THR:O	1:A:122:VAL:HG12	0.46	2.10	12	1
1:A:86:LEU:HA	1:A:90:LEU:CB	0.46	2.41	18	1
1:A:135:LEU:HD13	1:A:138:SER:H	0.46	1.70	15	1
1:A:86:LEU:HB3	1:A:182:THR:O	0.45	2.11	1	1
1:A:170:ASP:HB3	1:A:291:VAL:HG11	0.45	1.88	4	1
1:A:186:GLU:CG	1:A:187:PRO:HD3	0.45	2.40	4	1
1:A:182:THR:HG21	1:A:189:ALA:HB2	0.45	1.89	7	1
1:A:284:GLU:HA	1:A:287:GLU:HG2	0.45	1.87	9	2
1:A:83:ILE:CG2	1:A:181:ALA:HB3	0.45	2.42	19	2
1:A:135:LEU:HD11	1:A:139:ALA:N	0.45	2.27	17	1
1:A:83:ILE:HB	1:A:237:MET:HA	0.45	1.88	12	1
1:A:137:GLU:H	1:A:137:GLU:CD	0.45	2.15	12	1
1:A:80:GLN:HA	1:A:80:GLN:OE1	0.45	2.12	20	1
1:A:286:ARG:O	1:A:291:VAL:HG12	0.45	2.11	15	2
1:A:85:ASP:OD2	1:A:182:THR:HA	0.45	2.11	7	1
1:A:167:LEU:O	1:A:171:LEU:HB2	0.45	2.12	8	1
1:A:225:LEU:HA	1:A:228:LEU:CG	0.45	2.42	19	1
1:A:81:LEU:HD22	1:A:177:ARG:HB2	0.45	1.87	17	2
1:A:101:PHE:CZ	1:A:112:VAL:HG23	0.45	2.47	12	1
1:A:171:LEU:HD21	1:A:289:LEU:CD1	0.45	2.42	7	1
1:A:102:ARG:HA	1:A:112:VAL:HG21	0.44	1.88	12	3
1:A:85:ASP:O	1:A:86:LEU:HB2	0.44	2.12	6	1
1:A:186:GLU:HA	1:A:207:GLY:HA3	0.44	1.89	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:234:ARG:HA	1:A:234:ARG:HE	0.44	1.70	17	1
1:A:189:ALA:O	1:A:193:LEU:HG	0.44	2.12	19	1
1:A:181:ALA:HB1	1:A:220:VAL:HG12	0.44	1.88	4	2
1:A:181:ALA:HA	1:A:206:ALA:HB3	0.44	1.89	2	2
1:A:81:LEU:O	1:A:235:LEU:HD13	0.44	2.13	19	1
1:A:203:GLU:HG3	1:A:204:VAL:HG23	0.44	1.89	6	1
1:A:283:ASP:O	1:A:286:ARG:HG2	0.44	2.12	20	1
1:A:98:VAL:HG12	1:A:102:ARG:HE	0.44	1.73	4	1
1:A:86:LEU:HB3	1:A:182:THR:HG21	0.44	1.90	18	1
1:A:135:LEU:HD13	1:A:135:LEU:N	0.44	2.27	20	1
1:A:87:ASP:HB3	1:A:93:SER:CB	0.44	2.43	3	1
1:A:86:LEU:O	1:A:87:ASP:HB2	0.44	2.12	15	1
1:A:81:LEU:HB3	1:A:235:LEU:CD2	0.44	2.43	3	1
1:A:192:ILE:O	1:A:195:HIS:HB2	0.44	2.13	9	1
1:A:84:PHE:CD2	1:A:238:VAL:HG21	0.44	2.48	16	1
1:A:218:VAL:HG12	1:A:251:HIS:CD2	0.43	2.47	8	1
1:A:171:LEU:HD23	1:A:291:VAL:CG1	0.43	2.43	14	2
1:A:229:ARG:HG2	1:A:231:LEU:CD1	0.43	2.43	12	2
1:A:196:PHE:HB2	1:A:198:ILE:HD12	0.43	1.90	15	1
1:A:79:PRO:HA	1:A:234:ARG:HB3	0.43	1.88	7	1
1:A:233:GLU:HB3	1:A:234:ARG:HH11	0.43	1.72	8	1
1:A:78:SER:HB2	1:A:176:VAL:HB	0.43	1.90	10	1
1:A:78:SER:HB3	1:A:79:PRO:HD2	0.43	1.89	20	1
1:A:260:TRP:N	1:A:260:TRP:HE3	0.43	2.11	3	1
1:A:162:ASP:OD2	1:A:164:ILE:HG12	0.43	2.14	18	1
1:A:144:VAL:HA	1:A:147:ARG:HD3	0.43	1.90	14	1
1:A:89:THR:HA	1:A:260:TRP:CD1	0.43	2.47	1	1
1:A:83:ILE:HG13	1:A:221:LEU:HD11	0.43	1.91	8	2
1:A:286:ARG:HB2	1:A:291:VAL:HG11	0.43	1.89	3	1
1:A:279:ALA:HB1	1:A:284:GLU:HB2	0.43	1.90	6	1
1:A:87:ASP:OD1	1:A:93:SER:HB3	0.43	2.13	9	1
1:A:91:THR:HG21	1:A:196:PHE:CE1	0.43	2.48	15	1
1:A:186:GLU:HG3	1:A:208:ALA:O	0.43	2.13	3	1
1:A:177:ARG:HD2	1:A:203:GLU:OE1	0.43	2.14	12	1
1:A:235:LEU:HD13	1:A:236:VAL:N	0.43	2.29	2	1
1:A:86:LEU:O	1:A:86:LEU:HG	0.43	2.13	4	1
1:A:206:ALA:HB2	1:A:224:ALA:HB2	0.43	1.91	14	2
1:A:85:ASP:OD1	1:A:86:LEU:N	0.43	2.52	3	1
1:A:97:ILE:HG23	1:A:146:TYR:OH	0.43	2.14	8	1
1:A:116:ASP:O	1:A:119:THR:HG22	0.43	2.14	18	3
1:A:160:LEU:HD12	1:A:160:LEU:O	0.42	2.12	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:281:THR:CG2	1:A:284:GLU:HG3	0.42	2.44	15	1
1:A:286:ARG:HG2	1:A:291:VAL:HG13	0.42	1.91	5	1
1:A:241:ARG:NE	1:A:241:ARG:HA	0.42	2.29	7	1
1:A:171:LEU:HD23	1:A:178:LEU:HD21	0.42	1.89	13	2
1:A:232:PRO:HG2	1:A:235:LEU:CD2	0.42	2.44	8	1
1:A:135:LEU:HD21	1:A:139:ALA:HA	0.42	1.91	13	1
1:A:131:ARG:HA	1:A:135:LEU:CB	0.42	2.44	7	1
1:A:177:ARG:HD3	1:A:203:GLU:HG2	0.42	1.90	8	1
1:A:84:PHE:HA	1:A:238:VAL:CG2	0.42	2.44	16	1
1:A:89:THR:HG22	1:A:90:LEU:HD12	0.42	1.92	5	1
1:A:129:THR:O	1:A:133:MET:HG2	0.42	2.14	8	1
1:A:81:LEU:HD12	1:A:177:ARG:O	0.42	2.14	14	1
1:A:108:ILE:HG22	1:A:141:GLU:OE1	0.42	2.14	18	1
1:A:286:ARG:HB2	1:A:291:VAL:CG1	0.42	2.44	10	2
1:A:186:GLU:O	1:A:190:ARG:HG2	0.42	2.15	16	3
1:A:86:LEU:HB2	1:A:182:THR:HG21	0.42	1.92	5	1
1:A:168:LEU:HB3	1:A:201:HIS:CD2	0.42	2.50	7	1
1:A:283:ASP:O	1:A:286:ARG:HB3	0.42	2.15	8	1
1:A:251:HIS:HB3	1:A:253:ILE:HD12	0.42	1.91	12	3
1:A:121:ILE:HB	1:A:129:THR:HG21	0.42	1.92	12	1
1:A:101:PHE:CZ	1:A:117:LEU:HG	0.42	2.50	19	1
1:A:80:GLN:HB3	1:A:232:PRO:HB2	0.41	1.92	12	1
1:A:129:THR:O	1:A:133:MET:HG3	0.41	2.15	17	1
1:A:193:LEU:HD12	1:A:199:GLU:HA	0.41	1.91	6	2
1:A:171:LEU:HA	1:A:291:VAL:CG1	0.41	2.46	12	1
1:A:193:LEU:HD22	1:A:198:ILE:HD11	0.41	1.90	14	1
1:A:177:ARG:HD3	1:A:203:GLU:OE1	0.41	2.15	6	1
1:A:90:LEU:HA	1:A:164:ILE:HG13	0.41	1.91	4	1
1:A:241:ARG:HD3	1:A:242:SER:H	0.41	1.76	13	1
1:A:186:GLU:HB2	1:A:187:PRO:CD	0.41	2.46	17	1
1:A:96:GLY:HA3	1:A:157:MET:CE	0.41	2.45	10	1
1:A:260:TRP:HA	1:A:280:ALA:O	0.41	2.16	10	1
1:A:171:LEU:HD21	1:A:289:LEU:HD13	0.41	1.92	13	1
1:A:86:LEU:H	1:A:182:THR:CB	0.41	2.26	4	1
1:A:85:ASP:CG	1:A:86:LEU:H	0.41	2.18	17	1
1:A:90:LEU:HG	1:A:91:THR:HG23	0.41	1.92	7	1
1:A:192:ILE:HA	1:A:195:HIS:HD2	0.41	1.76	3	1
1:A:83:ILE:HD13	1:A:179:ALA:HB3	0.41	1.91	6	1
1:A:286:ARG:HB2	1:A:291:VAL:HG13	0.41	1.92	6	1
1:A:222:ALA:HB2	1:A:251:HIS:CD2	0.41	2.50	8	1
1:A:260:TRP:HA	1:A:260:TRP:HE3	0.41	1.75	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:162:ASP:HB3	1:A:164:ILE:CD1	0.41	2.46	11	1
1:A:81:LEU:HG	1:A:177:ARG:HB2	0.41	1.92	15	1
1:A:89:THR:HG23	1:A:258:VAL:HG11	0.41	1.92	15	1
1:A:163:GLY:HA3	1:A:282:ILE:HG21	0.41	1.93	15	1
1:A:286:ARG:HB2	1:A:291:VAL:CG2	0.40	2.46	2	1
1:A:86:LEU:HB3	1:A:89:THR:HB	0.40	1.92	6	1
1:A:117:LEU:O	1:A:121:ILE:HG12	0.40	2.16	6	1
1:A:223:HIS:O	1:A:227:GLN:HG2	0.40	2.16	7	1
1:A:174:ALA:HB2	1:A:291:VAL:HG23	0.40	1.91	1	1
1:A:198:ILE:H	1:A:198:ILE:HD13	0.40	1.75	8	1
1:A:160:LEU:O	1:A:160:LEU:HD12	0.40	2.16	3	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	190/216 (88%)	175±3 (92±2%)	14±3 (7±2%)	1±1 (1±1%)	29	74
All	All	3800/4320 (88%)	3500 (92%)	276 (7%)	24 (1%)	29	74

All 14 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	79	PRO	4
1	A	136	GLY	3
1	A	134	GLY	3
1	A	162	ASP	2
1	A	163	GLY	2
1	A	218	VAL	2
1	A	88	GLY	1
1	A	242	SER	1
1	A	86	LEU	1
1	A	90	LEU	1
1	A	87	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	185	ALA	1
1	A	121	ILE	1
1	A	94	ALA	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	145/164 (88%)	136±2 (94±2%)	9±2 (6±2%)	21 70
All	All	2900/3280 (88%)	2716 (94%)	184 (6%)	21 70

All 57 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	235	LEU	20
1	A	101	PHE	18
1	A	117	LEU	10
1	A	241	ARG	9
1	A	81	LEU	8
1	A	260	TRP	7
1	A	244	ASP	7
1	A	237	MET	7
1	A	285	LEU	6
1	A	127	HIS	5
1	A	194	ARG	4
1	A	172	ARG	4
1	A	162	ASP	4
1	A	126	MET	3
1	A	200	GLN	3
1	A	234	ARG	3
1	A	184	LYS	3
1	A	195	HIS	3
1	A	278	HIS	3
1	A	86	LEU	3
1	A	131	ARG	3
1	A	198	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	158	ASN	3
1	A	90	LEU	2
1	A	177	ARG	2
1	A	199	GLU	2
1	A	87	ASP	2
1	A	219	ASP	2
1	A	229	ARG	2
1	A	103	HIS	2
1	A	157	MET	2
1	A	190	ARG	2
1	A	277	THR	2
1	A	135	LEU	2
1	A	149	ASP	1
1	A	251	HIS	1
1	A	283	ASP	1
1	A	78	SER	1
1	A	140	GLU	1
1	A	116	ASP	1
1	A	201	HIS	1
1	A	186	GLU	1
1	A	231	LEU	1
1	A	240	ASP	1
1	A	291	VAL	1
1	A	93	SER	1
1	A	120	HIS	1
1	A	203	GLU	1
1	A	137	GLU	1
1	A	254	ASP	1
1	A	242	SER	1
1	A	85	ASP	1
1	A	161	PHE	1
1	A	150	TYR	1
1	A	170	ASP	1
1	A	223	HIS	1
1	A	287	GLU	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 monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 74% for the well-defined parts and 69% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *PtkA-bmrb.tbl*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1935
Number of shifts mapped to atoms	1935
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	183	-0.46 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	161	0.08 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	151	-0.21 ± 0.06	None needed (< 0.5 ppm)
^{15}N	165	0.10 ± 0.28	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 74%, i.e. 1860 atoms were assigned a chemical shift out of a possible 2525. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	823/955 (86%)	344/391 (88%)	320/382 (84%)	159/182 (87%)
Sidechain	951/1398 (68%)	651/924 (70%)	300/426 (70%)	0/48 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	86/172 (50%)	43/85 (51%)	41/65 (63%)	2/22 (9%)
Overall	1860/2525 (74%)	1038/1400 (74%)	661/873 (76%)	161/252 (64%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 1935 atoms were assigned a chemical shift out of a possible 2824. 0 out of 39 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	858/1085 (79%)	359/446 (80%)	334/432 (77%)	165/207 (80%)
Sidechain	973/1548 (63%)	666/1020 (65%)	307/472 (65%)	0/56 (0%)
Aromatic	104/191 (54%)	52/94 (55%)	50/75 (67%)	2/22 (9%)
Overall	1935/2824 (69%)	1077/1560 (69%)	691/979 (71%)	167/285 (59%)

7.1.4 Statistically unusual chemical shifts [i](#)

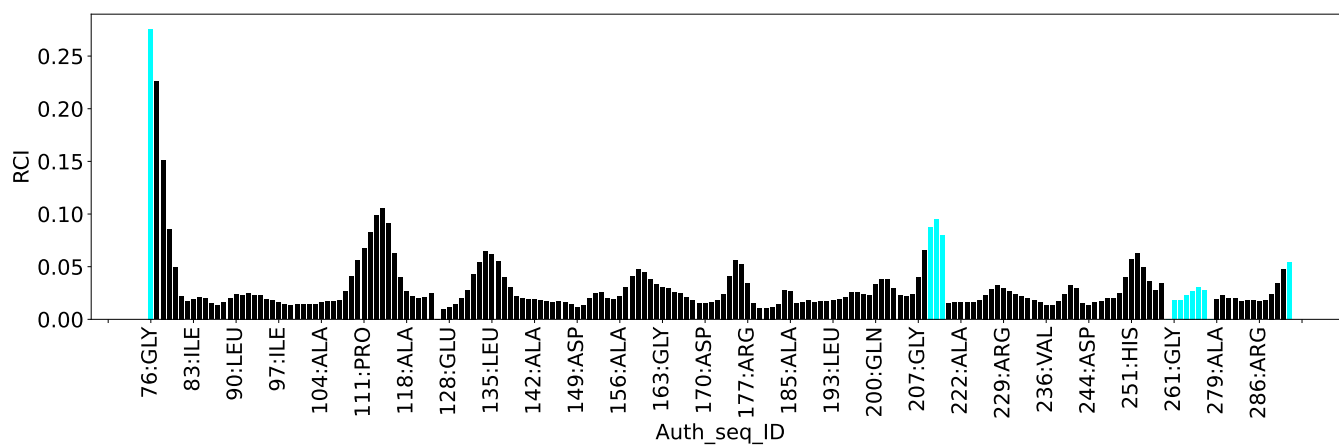
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	156	ALA	HB1	-0.24	0.14 – 2.58	-6.5
1	A	156	ALA	HB2	-0.24	0.14 – 2.58	-6.5
1	A	156	ALA	HB3	-0.24	0.14 – 2.58	-6.5

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

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

Random coil index (RCI) for chain A:



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	1810
Intra-residue ($ i-j =0$)	411
Sequential ($ i-j =1$)	459
Medium range ($ i-j >1$ and $ i-j <5$)	292
Long range ($ i-j \geq 5$)	484
Inter-chain	0
Hydrogen bond restraints	164
Disulfide bond restraints	0
Total dihedral-angle restraints	202
Number of unmapped restraints	0
Number of restraints per residue	9.3
Number of long range restraints per residue ¹	2.4

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)	14.2	0.2
0.2-0.5 (Medium)	1.1	0.3
>0.5 (Large)	None	None

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.2	9.5
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis [i](#)

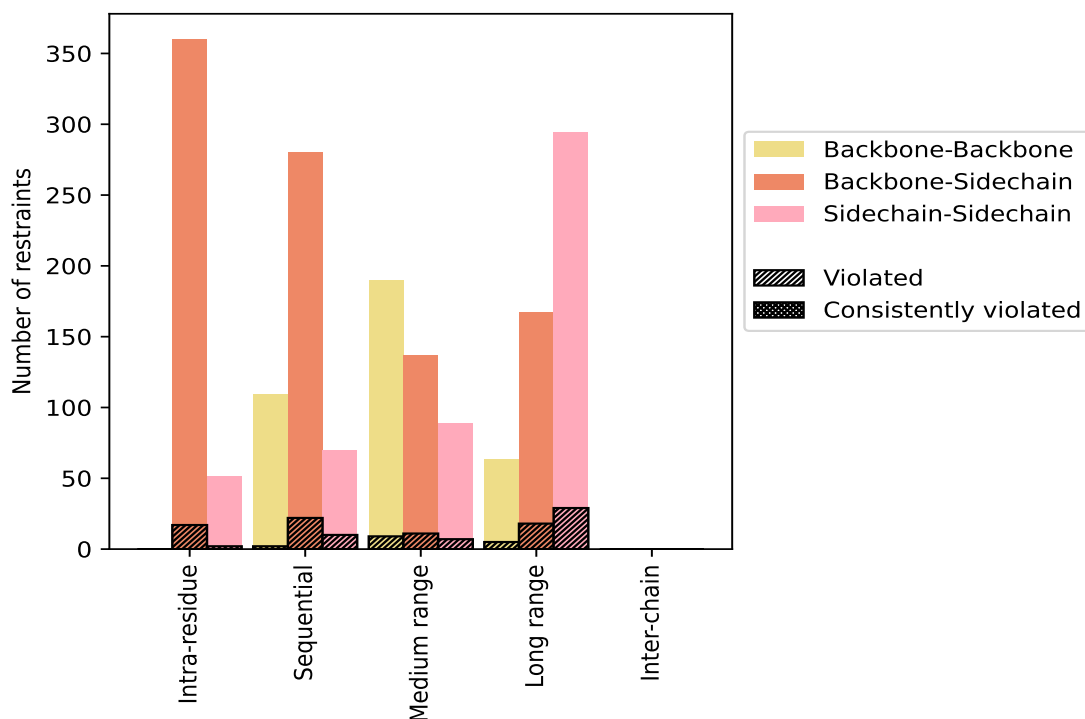
9.1 Summary of distance violations [i](#)

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	411	22.7	19	4.6	1.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	360	19.9	17	4.7	0.9	0	0.0	0.0
Sidechain-Sidechain	51	2.8	2	3.9	0.1	0	0.0	0.0
Sequential ($i-j =1$)	459	25.4	34	7.4	1.9	0	0.0	0.0
Backbone-Backbone	109	6.0	2	1.8	0.1	0	0.0	0.0
Backbone-Sidechain	280	15.5	22	7.9	1.2	0	0.0	0.0
Sidechain-Sidechain	70	3.9	10	14.3	0.6	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	292	16.1	18	6.2	1.0	0	0.0	0.0
Backbone-Backbone	66	3.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	137	7.6	11	8.0	0.6	0	0.0	0.0
Sidechain-Sidechain	89	4.9	7	7.9	0.4	0	0.0	0.0
Long range ($i-j \geq 5$)	484	26.7	48	9.9	2.7	0	0.0	0.0
Backbone-Backbone	23	1.3	1	4.3	0.1	0	0.0	0.0
Backbone-Sidechain	167	9.2	18	10.8	1.0	0	0.0	0.0
Sidechain-Sidechain	294	16.2	29	9.9	1.6	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	164	9.1	13	7.9	0.7	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1810	100.0	132	7.3	7.3	0	0.0	0.0
Backbone-Backbone	362	20.0	16	4.4	0.9	0	0.0	0.0
Backbone-Sidechain	944	52.2	68	7.2	3.8	0	0.0	0.0
Sidechain-Sidechain	504	27.8	48	9.5	2.7	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 disulfid bonds are counted in their appropriate category on the x-axis

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	3	5	5	10	0	23	0.14	0.22	0.03	0.12
2	1	6	6	3	0	16	0.13	0.19	0.03	0.12
3	2	2	4	8	0	16	0.14	0.25	0.03	0.13
4	3	6	0	5	0	14	0.14	0.24	0.04	0.13
5	3	6	3	3	0	15	0.16	0.28	0.05	0.13
6	2	5	1	9	0	17	0.15	0.27	0.04	0.14
7	4	6	4	2	0	16	0.15	0.21	0.03	0.14
8	1	4	4	7	0	16	0.13	0.19	0.02	0.12
9	4	3	6	9	0	22	0.15	0.24	0.03	0.15
10	2	4	3	6	0	15	0.14	0.22	0.03	0.13
11	2	5	2	6	0	15	0.13	0.19	0.03	0.12

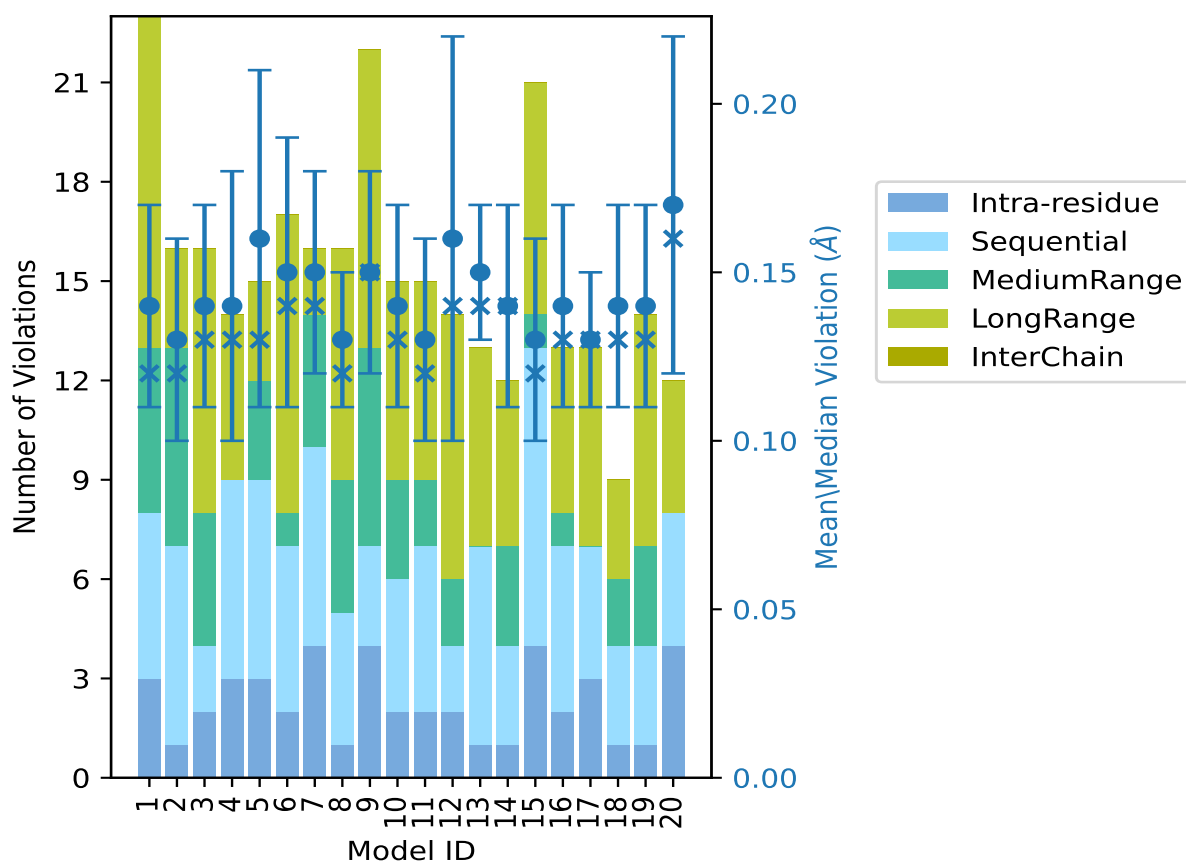
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
12	2	2	2	8	0	14	0.16	0.3	0.06	0.14
13	1	6	0	6	0	13	0.15	0.2	0.02	0.14
14	1	3	3	5	0	12	0.14	0.21	0.03	0.14
15	4	9	1	7	0	21	0.13	0.21	0.03	0.12
16	2	5	1	5	0	13	0.14	0.2	0.03	0.13
17	3	4	0	6	0	13	0.13	0.19	0.02	0.13
18	1	3	2	3	0	9	0.14	0.2	0.03	0.13
19	1	3	3	7	0	14	0.14	0.2	0.03	0.13
20	4	4	0	4	0	12	0.17	0.28	0.05	0.16

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 [\(i\)](#)



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

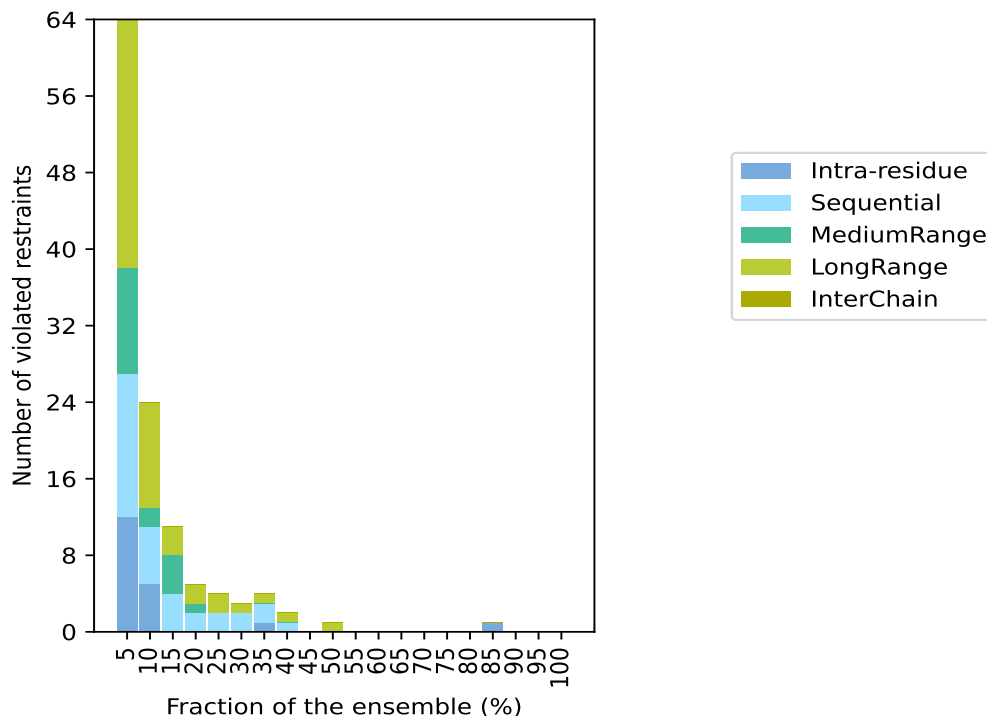
9.3 Distance violation statistics for the ensemble

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, 1527(IR:392, SQ:425, MR:274, LR:436, 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	%
12	15	11	26	0	64	1	5.0
5	6	2	11	0	24	2	10.0
0	4	4	3	0	11	3	15.0
0	2	1	2	0	5	4	20.0
0	2	0	2	0	4	5	25.0
0	2	0	1	0	3	6	30.0
1	2	0	1	0	4	7	35.0
0	1	0	1	0	2	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	1	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	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
1	0	0	0	0	1	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

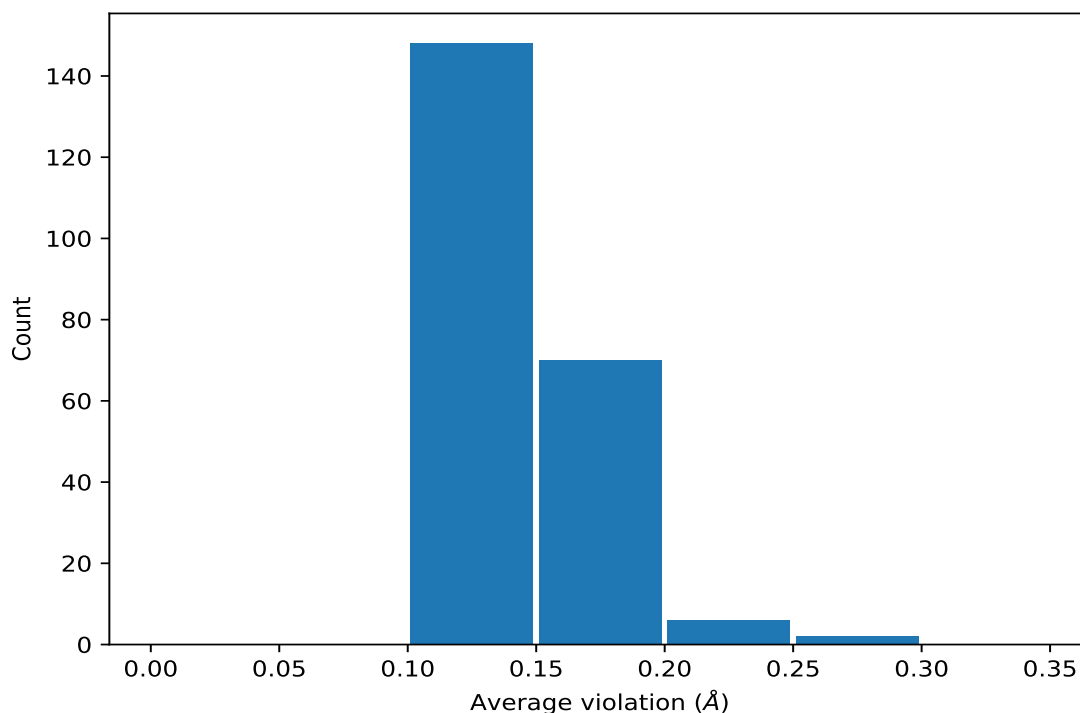
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	17	0.2	0.03	0.2
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	17	0.2	0.03	0.2
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	17	0.2	0.03	0.2
(1,1458)	1:A:167:LEU:HD11	1:A:282:ILE:HB	10	0.12	0.01	0.11
(1,1458)	1:A:167:LEU:HD12	1:A:282:ILE:HB	10	0.12	0.01	0.11
(1,1458)	1:A:167:LEU:HD13	1:A:282:ILE:HB	10	0.12	0.01	0.11
(1,1458)	1:A:167:LEU:HD21	1:A:282:ILE:HB	10	0.12	0.01	0.11
(1,1458)	1:A:167:LEU:HD22	1:A:282:ILE:HB	10	0.12	0.01	0.11
(1,1458)	1:A:167:LEU:HD23	1:A:282:ILE:HB	10	0.12	0.01	0.11
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB1	8	0.15	0.02	0.15
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB2	8	0.15	0.02	0.15
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB3	8	0.15	0.02	0.15
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB1	8	0.15	0.02	0.15
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB2	8	0.15	0.02	0.15
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB3	8	0.15	0.02	0.15
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD11	8	0.15	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD12	8	0.15	0.03	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD13	8	0.15	0.03	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD21	8	0.15	0.03	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD22	8	0.15	0.03	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD23	8	0.15	0.03	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD11	8	0.15	0.03	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD12	8	0.15	0.03	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD13	8	0.15	0.03	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD21	8	0.15	0.03	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD22	8	0.15	0.03	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD23	8	0.15	0.03	0.16
(1,1523)	1:A:180:VAL:HG11	1:A:205:ILE:HB	7	0.15	0.02	0.14
(1,1523)	1:A:180:VAL:HG12	1:A:205:ILE:HB	7	0.15	0.02	0.14
(1,1523)	1:A:180:VAL:HG13	1:A:205:ILE:HB	7	0.15	0.02	0.14
(1,1523)	1:A:180:VAL:HG21	1:A:205:ILE:HB	7	0.15	0.02	0.14
(1,1523)	1:A:180:VAL:HG22	1:A:205:ILE:HB	7	0.15	0.02	0.14
(1,1523)	1:A:180:VAL:HG23	1:A:205:ILE:HB	7	0.15	0.02	0.14
(1,641)	1:A:164:ILE:HG12	1:A:165:GLY:H	7	0.15	0.02	0.14
(1,641)	1:A:164:ILE:HG13	1:A:165:GLY:H	7	0.15	0.02	0.14
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD11	7	0.14	0.01	0.14
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD12	7	0.14	0.01	0.14
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD13	7	0.14	0.01	0.14
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG2	7	0.13	0.01	0.13
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG3	7	0.13	0.01	0.13
(1,802)	1:A:244:ASP:HB2	1:A:245:VAL:HB	6	0.18	0.04	0.18
(1,802)	1:A:244:ASP:HB3	1:A:245:VAL:HB	6	0.18	0.04	0.18
(1,1475)	1:A:171:LEU:HA	1:A:291:VAL:HA	6	0.16	0.02	0.16
(2,19)	1:A:85:ASP:H	1:A:238:VAL:O	6	0.13	0.02	0.12
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG11	6	0.12	0.02	0.12
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG12	6	0.12	0.02	0.12
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG13	6	0.12	0.02	0.12
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG21	6	0.12	0.02	0.12
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG22	6	0.12	0.02	0.12
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG23	6	0.12	0.02	0.12
(1,1432)	1:A:160:LEU:HB2	1:A:196:PHE:HD1	5	0.14	0.02	0.13
(1,1432)	1:A:160:LEU:HB2	1:A:196:PHE:HD2	5	0.14	0.02	0.13
(1,1432)	1:A:160:LEU:HB3	1:A:196:PHE:HD1	5	0.14	0.02	0.13
(1,1432)	1:A:160:LEU:HB3	1:A:196:PHE:HD2	5	0.14	0.02	0.13
(1,502)	1:A:111:PRO:HB2	1:A:112:VAL:HA	5	0.14	0.03	0.13
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB1	5	0.13	0.02	0.14
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB2	5	0.13	0.02	0.14
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB3	5	0.13	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB1	5	0.13	0.02	0.14
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB2	5	0.13	0.02	0.14
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB3	5	0.13	0.02	0.14
(1,1238)	1:A:83:ILE:HG12	1:A:221:LEU:HA	5	0.12	0.02	0.11
(1,1238)	1:A:83:ILE:HG13	1:A:221:LEU:HA	5	0.12	0.02	0.11
(1,451)	1:A:98:VAL:HB	1:A:99:SER:H	4	0.21	0.02	0.2
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG11	4	0.18	0.03	0.18
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG12	4	0.18	0.03	0.18
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG13	4	0.18	0.03	0.18
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG21	4	0.18	0.03	0.18
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG22	4	0.18	0.03	0.18
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG23	4	0.18	0.03	0.18
(1,777)	1:A:229:ARG:HD2	1:A:230:PRO:HA	4	0.17	0.03	0.16
(1,777)	1:A:229:ARG:HD3	1:A:230:PRO:HA	4	0.17	0.03	0.16
(1,1507)	1:A:179:ALA:HB1	1:A:204:VAL:HB	4	0.14	0.01	0.15
(1,1507)	1:A:179:ALA:HB2	1:A:204:VAL:HB	4	0.14	0.01	0.15
(1,1507)	1:A:179:ALA:HB3	1:A:204:VAL:HB	4	0.14	0.01	0.15
(1,1234)	1:A:83:ILE:HD11	1:A:221:LEU:HG	4	0.13	0.02	0.13
(1,1234)	1:A:83:ILE:HD12	1:A:221:LEU:HG	4	0.13	0.02	0.13
(1,1234)	1:A:83:ILE:HD13	1:A:221:LEU:HG	4	0.13	0.02	0.13
(2,157)	1:A:251:HIS:H	1:A:247:GLY:O	4	0.13	0.02	0.13
(2,39)	1:A:259:GLY:H	1:A:279:ALA:O	4	0.12	0.01	0.12
(2,69)	1:A:131:ARG:H	1:A:127:HIS:O	4	0.12	0.01	0.11
(1,828)	1:A:264:ARG:HB2	1:A:265:ALA:HB1	3	0.16	0.04	0.13
(1,828)	1:A:264:ARG:HB2	1:A:265:ALA:HB2	3	0.16	0.04	0.13
(1,828)	1:A:264:ARG:HB2	1:A:265:ALA:HB3	3	0.16	0.04	0.13
(1,828)	1:A:264:ARG:HB3	1:A:265:ALA:HB1	3	0.16	0.04	0.13
(1,828)	1:A:264:ARG:HB3	1:A:265:ALA:HB2	3	0.16	0.04	0.13
(1,828)	1:A:264:ARG:HB3	1:A:265:ALA:HB3	3	0.16	0.04	0.13
(1,1103)	1:A:226:ALA:HB1	1:A:229:ARG:HG2	3	0.15	0.03	0.16
(1,1103)	1:A:226:ALA:HB1	1:A:229:ARG:HG3	3	0.15	0.03	0.16
(1,1103)	1:A:226:ALA:HB2	1:A:229:ARG:HG2	3	0.15	0.03	0.16
(1,1103)	1:A:226:ALA:HB2	1:A:229:ARG:HG3	3	0.15	0.03	0.16
(1,1103)	1:A:226:ALA:HB3	1:A:229:ARG:HG2	3	0.15	0.03	0.16
(1,1103)	1:A:226:ALA:HB3	1:A:229:ARG:HG3	3	0.15	0.03	0.16
(1,1284)	1:A:85:ASP:HA	1:A:237:MET:HE1	3	0.15	0.03	0.14
(1,1284)	1:A:85:ASP:HA	1:A:237:MET:HE2	3	0.15	0.03	0.14
(1,1284)	1:A:85:ASP:HA	1:A:237:MET:HE3	3	0.15	0.03	0.14
(1,1431)	1:A:159:SER:H	1:A:196:PHE:HE1	3	0.14	0.0	0.14
(1,1431)	1:A:159:SER:H	1:A:196:PHE:HE2	3	0.14	0.0	0.14
(1,430)	1:A:83:ILE:HD11	1:A:84:PHE:H	3	0.14	0.02	0.13
(1,430)	1:A:83:ILE:HD12	1:A:84:PHE:H	3	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,430)	1:A:83:ILE:HD13	1:A:84:PHE:H	3	0.14	0.02	0.13
(1,501)	1:A:111:PRO:HB3	1:A:112:VAL:H	3	0.13	0.03	0.12
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG11	3	0.13	0.01	0.13
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG12	3	0.13	0.01	0.13
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG13	3	0.13	0.01	0.13
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG21	3	0.13	0.01	0.13
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG22	3	0.13	0.01	0.13
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG23	3	0.13	0.01	0.13
(1,1151)	1:A:285:LEU:HB2	1:A:289:LEU:HG	3	0.13	0.02	0.13
(1,1151)	1:A:285:LEU:HB3	1:A:289:LEU:HG	3	0.13	0.02	0.13
(2,73)	1:A:133:MET:H	1:A:129:THR:O	3	0.13	0.01	0.12
(1,883)	1:A:92:ASP:HB2	1:A:94:ALA:H	3	0.12	0.0	0.12
(1,883)	1:A:92:ASP:HB3	1:A:94:ALA:H	3	0.12	0.0	0.12
(1,547)	1:A:132:ALA:HB1	1:A:133:MET:HG3	3	0.12	0.01	0.11
(1,547)	1:A:132:ALA:HB2	1:A:133:MET:HG3	3	0.12	0.01	0.11
(1,547)	1:A:132:ALA:HB3	1:A:133:MET:HG3	3	0.12	0.01	0.11
(1,1231)	1:A:83:ILE:HD11	1:A:180:VAL:HA	3	0.12	0.0	0.12
(1,1231)	1:A:83:ILE:HD12	1:A:180:VAL:HA	3	0.12	0.0	0.12
(1,1231)	1:A:83:ILE:HD13	1:A:180:VAL:HA	3	0.12	0.0	0.12
(1,384)	1:A:284:GLU:H	1:A:284:GLU:HG2	2	0.28	0.0	0.28
(1,384)	1:A:284:GLU:H	1:A:284:GLU:HG3	2	0.28	0.0	0.28
(1,182)	1:A:161:PHE:H	1:A:161:PHE:HD1	2	0.2	0.02	0.2
(1,182)	1:A:161:PHE:H	1:A:161:PHE:HD2	2	0.2	0.02	0.2
(1,838)	1:A:266:ASP:H	1:A:267:PHE:HD1	2	0.16	0.02	0.16
(1,838)	1:A:266:ASP:H	1:A:267:PHE:HD2	2	0.16	0.02	0.16
(1,891)	1:A:95:ARG:HA	1:A:98:VAL:HG21	2	0.15	0.01	0.15
(1,891)	1:A:95:ARG:HA	1:A:98:VAL:HG22	2	0.15	0.01	0.15
(1,891)	1:A:95:ARG:HA	1:A:98:VAL:HG23	2	0.15	0.01	0.15
(2,145)	1:A:245:VAL:H	1:A:241:ARG:O	2	0.15	0.02	0.15
(1,1584)	1:A:225:LEU:HD11	1:A:251:HIS:HB2	2	0.15	0.03	0.15
(1,1584)	1:A:225:LEU:HD11	1:A:251:HIS:HB3	2	0.15	0.03	0.15
(1,1584)	1:A:225:LEU:HD12	1:A:251:HIS:HB2	2	0.15	0.03	0.15
(1,1584)	1:A:225:LEU:HD12	1:A:251:HIS:HB3	2	0.15	0.03	0.15
(1,1584)	1:A:225:LEU:HD13	1:A:251:HIS:HB2	2	0.15	0.03	0.15
(1,1584)	1:A:225:LEU:HD13	1:A:251:HIS:HB3	2	0.15	0.03	0.15
(1,1584)	1:A:225:LEU:HD21	1:A:251:HIS:HB2	2	0.15	0.03	0.15
(1,1584)	1:A:225:LEU:HD21	1:A:251:HIS:HB3	2	0.15	0.03	0.15
(1,1584)	1:A:225:LEU:HD22	1:A:251:HIS:HB2	2	0.15	0.03	0.15
(1,1584)	1:A:225:LEU:HD22	1:A:251:HIS:HB3	2	0.15	0.03	0.15
(1,1584)	1:A:225:LEU:HD23	1:A:251:HIS:HB2	2	0.15	0.03	0.15
(1,1584)	1:A:225:LEU:HD23	1:A:251:HIS:HB3	2	0.15	0.03	0.15
(1,50)	1:A:101:PHE:H	1:A:101:PHE:HD1	2	0.13	0.0	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,50)	1:A:101:PHE:H	1:A:101:PHE:HD2	2	0.13	0.0	0.13
(1,1371)	1:A:105:LEU:HD11	1:A:133:MET:HA	2	0.13	0.0	0.13
(1,1371)	1:A:105:LEU:HD12	1:A:133:MET:HA	2	0.13	0.0	0.13
(1,1371)	1:A:105:LEU:HD13	1:A:133:MET:HA	2	0.13	0.0	0.13
(1,1371)	1:A:105:LEU:HD21	1:A:133:MET:HA	2	0.13	0.0	0.13
(1,1371)	1:A:105:LEU:HD22	1:A:133:MET:HA	2	0.13	0.0	0.13
(1,1371)	1:A:105:LEU:HD23	1:A:133:MET:HA	2	0.13	0.0	0.13
(1,1395)	1:A:112:VAL:HA	1:A:133:MET:HE1	2	0.13	0.01	0.13
(1,1395)	1:A:112:VAL:HA	1:A:133:MET:HE2	2	0.13	0.01	0.13
(1,1395)	1:A:112:VAL:HA	1:A:133:MET:HE3	2	0.13	0.01	0.13
(1,1645)	1:A:286:ARG:HA	1:A:291:VAL:HG21	2	0.13	0.0	0.13
(1,1645)	1:A:286:ARG:HA	1:A:291:VAL:HG22	2	0.13	0.0	0.13
(1,1645)	1:A:286:ARG:HA	1:A:291:VAL:HG23	2	0.13	0.0	0.13
(2,129)	1:A:196:PHE:H	1:A:192:ILE:O	2	0.13	0.0	0.13
(1,950)	1:A:116:ASP:HB2	1:A:119:THR:HG21	2	0.12	0.01	0.12
(1,950)	1:A:116:ASP:HB2	1:A:119:THR:HG22	2	0.12	0.01	0.12
(1,950)	1:A:116:ASP:HB2	1:A:119:THR:HG23	2	0.12	0.01	0.12
(1,1515)	1:A:180:VAL:HB	1:A:205:ILE:HD11	2	0.12	0.02	0.12
(1,1515)	1:A:180:VAL:HB	1:A:205:ILE:HD12	2	0.12	0.02	0.12
(1,1515)	1:A:180:VAL:HB	1:A:205:ILE:HD13	2	0.12	0.02	0.12
(1,722)	1:A:202:PHE:HA	1:A:203:GLU:HB3	2	0.12	0.01	0.12
(1,1415)	1:A:130:LEU:HD11	1:A:142:ALA:HA	2	0.12	0.01	0.12
(1,1415)	1:A:130:LEU:HD12	1:A:142:ALA:HA	2	0.12	0.01	0.12
(1,1415)	1:A:130:LEU:HD13	1:A:142:ALA:HA	2	0.12	0.01	0.12
(1,1415)	1:A:130:LEU:HD21	1:A:142:ALA:HA	2	0.12	0.01	0.12
(1,1415)	1:A:130:LEU:HD22	1:A:142:ALA:HA	2	0.12	0.01	0.12
(1,1415)	1:A:130:LEU:HD23	1:A:142:ALA:HA	2	0.12	0.01	0.12
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG11	2	0.12	0.01	0.12
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG12	2	0.12	0.01	0.12
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG13	2	0.12	0.01	0.12
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG21	2	0.12	0.01	0.12
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG22	2	0.12	0.01	0.12
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG23	2	0.12	0.01	0.12
(1,354)	1:A:264:ARG:HA	1:A:264:ARG:HD2	2	0.12	0.0	0.12
(1,354)	1:A:264:ARG:HA	1:A:264:ARG:HD3	2	0.12	0.0	0.12
(1,682)	1:A:175:GLY:H	1:A:176:VAL:HB	2	0.12	0.0	0.12
(1,779)	1:A:229:ARG:H	1:A:230:PRO:HA	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD11	1:A:282:ILE:HD11	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD11	1:A:282:ILE:HD12	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD11	1:A:282:ILE:HD13	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD12	1:A:282:ILE:HD11	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD12	1:A:282:ILE:HD12	2	0.12	0.0	0.12

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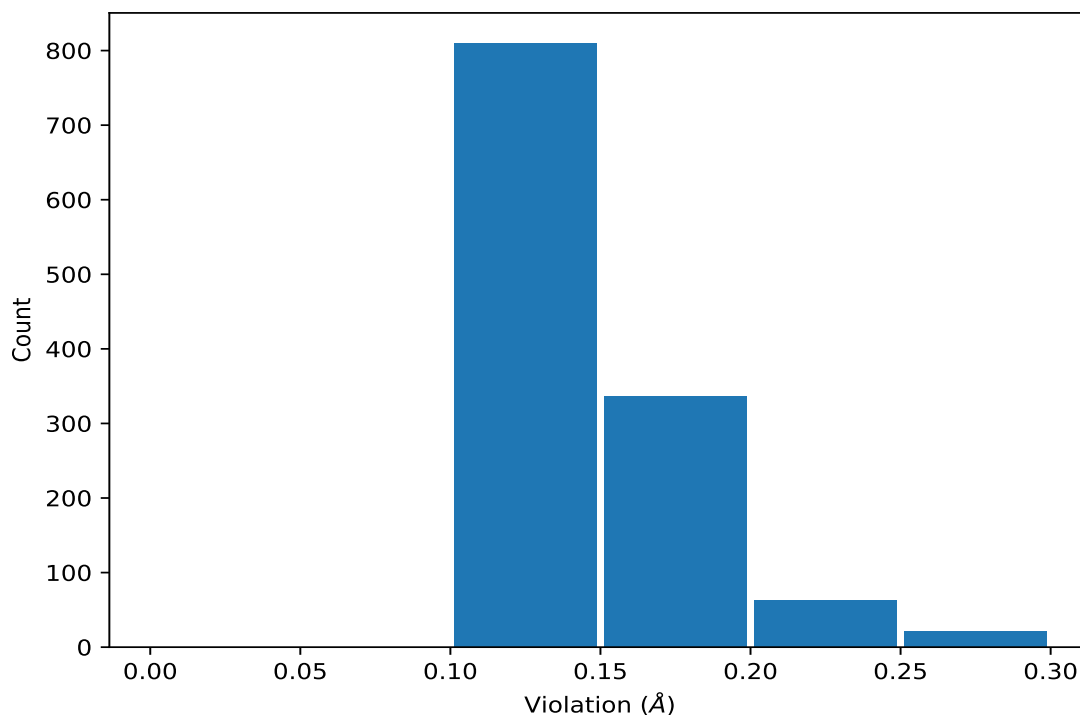
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1459)	1:A:167:LEU:HD12	1:A:282:ILE:HD13	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD13	1:A:282:ILE:HD11	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD13	1:A:282:ILE:HD12	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD13	1:A:282:ILE:HD13	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD21	1:A:282:ILE:HD11	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD21	1:A:282:ILE:HD12	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD21	1:A:282:ILE:HD13	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD22	1:A:282:ILE:HD11	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD22	1:A:282:ILE:HD12	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD22	1:A:282:ILE:HD13	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD23	1:A:282:ILE:HD11	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD23	1:A:282:ILE:HD12	2	0.12	0.0	0.12
(1,1459)	1:A:167:LEU:HD23	1:A:282:ILE:HD13	2	0.12	0.0	0.12
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG11	2	0.12	0.0	0.12
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG12	2	0.12	0.0	0.12
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG13	2	0.12	0.0	0.12
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG21	2	0.12	0.0	0.12
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG22	2	0.12	0.0	0.12
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG23	2	0.12	0.0	0.12
(1,153)	1:A:146:TYR:H	1:A:146:TYR:HD1	2	0.11	0.0	0.11
(1,153)	1:A:146:TYR:H	1:A:146:TYR:HD2	2	0.11	0.0	0.11
(1,431)	1:A:83:ILE:HG12	1:A:84:PHE:H	2	0.11	0.0	0.11
(1,431)	1:A:83:ILE:HG13	1:A:84:PHE:H	2	0.11	0.0	0.11
(1,605)	1:A:151:SER:H	1:A:152:ALA:HB1	2	0.11	0.0	0.11
(1,605)	1:A:151:SER:H	1:A:152:ALA:HB2	2	0.11	0.0	0.11
(1,605)	1:A:151:SER:H	1:A:152:ALA:HB3	2	0.11	0.0	0.11
(1,1204)	1:A:82:VAL:HG11	1:A:171:LEU:HD11	2	0.11	0.0	0.11
(1,1204)	1:A:82:VAL:HG11	1:A:171:LEU:HD12	2	0.11	0.0	0.11
(1,1204)	1:A:82:VAL:HG11	1:A:171:LEU:HD13	2	0.11	0.0	0.11
(1,1204)	1:A:82:VAL:HG12	1:A:171:LEU:HD11	2	0.11	0.0	0.11
(1,1204)	1:A:82:VAL:HG12	1:A:171:LEU:HD12	2	0.11	0.0	0.11
(1,1204)	1:A:82:VAL:HG12	1:A:171:LEU:HD13	2	0.11	0.0	0.11
(1,1204)	1:A:82:VAL:HG13	1:A:171:LEU:HD11	2	0.11	0.0	0.11
(1,1204)	1:A:82:VAL:HG13	1:A:171:LEU:HD12	2	0.11	0.0	0.11
(1,1204)	1:A:82:VAL:HG13	1:A:171:LEU:HD13	2	0.11	0.0	0.11
(1,1527)	1:A:180:VAL:HG11	1:A:202:PHE:HE1	2	0.11	0.0	0.11
(1,1527)	1:A:180:VAL:HG11	1:A:202:PHE:HE2	2	0.11	0.0	0.11
(1,1527)	1:A:180:VAL:HG12	1:A:202:PHE:HE1	2	0.11	0.0	0.11
(1,1527)	1:A:180:VAL:HG12	1:A:202:PHE:HE2	2	0.11	0.0	0.11
(1,1527)	1:A:180:VAL:HG13	1:A:202:PHE:HE1	2	0.11	0.0	0.11
(1,1527)	1:A:180:VAL:HG13	1:A:202:PHE:HE2	2	0.11	0.0	0.11
(2,11)	1:A:81:LEU:H	1:A:234:ARG:O	2	0.11	0.0	0.11

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 [i](#)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1596)	1:A:235:LEU:HB2	1:A:253:ILE:HG21	12	0.3
(1,1596)	1:A:235:LEU:HB2	1:A:253:ILE:HG22	12	0.3
(1,1596)	1:A:235:LEU:HB2	1:A:253:ILE:HG23	12	0.3
(1,1596)	1:A:235:LEU:HB3	1:A:253:ILE:HG21	12	0.3
(1,1596)	1:A:235:LEU:HB3	1:A:253:ILE:HG22	12	0.3
(1,1596)	1:A:235:LEU:HB3	1:A:253:ILE:HG23	12	0.3
(1,384)	1:A:284:GLU:H	1:A:284:GLU:HG2	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,384)	1:A:284:GLU:H	1:A:284:GLU:HG3	5	0.28
(1,384)	1:A:284:GLU:H	1:A:284:GLU:HG2	20	0.28
(1,384)	1:A:284:GLU:H	1:A:284:GLU:HG3	20	0.28
(1,802)	1:A:244:ASP:HB2	1:A:245:VAL:HB	6	0.27
(1,802)	1:A:244:ASP:HB3	1:A:245:VAL:HB	6	0.27
(1,1191)	1:A:81:LEU:H	1:A:235:LEU:HD11	12	0.27
(1,1191)	1:A:81:LEU:H	1:A:235:LEU:HD12	12	0.27
(1,1191)	1:A:81:LEU:H	1:A:235:LEU:HD13	12	0.27
(1,1191)	1:A:81:LEU:H	1:A:235:LEU:HD21	12	0.27
(1,1191)	1:A:81:LEU:H	1:A:235:LEU:HD22	12	0.27
(1,1191)	1:A:81:LEU:H	1:A:235:LEU:HD23	12	0.27
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	3	0.25
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	3	0.25
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	3	0.25
(1,451)	1:A:98:VAL:HB	1:A:99:SER:H	9	0.24
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	4	0.24
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	4	0.24
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	4	0.24
(1,1063)	1:A:191:ARG:H	1:A:194:ARG:HB2	5	0.23
(1,1063)	1:A:191:ARG:H	1:A:194:ARG:HB3	5	0.23
(1,828)	1:A:264:ARG:HB2	1:A:265:ALA:HB1	4	0.22
(1,828)	1:A:264:ARG:HB2	1:A:265:ALA:HB2	4	0.22
(1,828)	1:A:264:ARG:HB2	1:A:265:ALA:HB3	4	0.22
(1,828)	1:A:264:ARG:HB3	1:A:265:ALA:HB1	4	0.22
(1,828)	1:A:264:ARG:HB3	1:A:265:ALA:HB2	4	0.22
(1,828)	1:A:264:ARG:HB3	1:A:265:ALA:HB3	4	0.22
(1,777)	1:A:229:ARG:HD2	1:A:230:PRO:HA	20	0.22
(1,777)	1:A:229:ARG:HD3	1:A:230:PRO:HA	20	0.22
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	10	0.22
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	10	0.22
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	10	0.22
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	20	0.22
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	20	0.22
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	20	0.22
(1,182)	1:A:161:PHE:H	1:A:161:PHE:HD1	1	0.22
(1,182)	1:A:161:PHE:H	1:A:161:PHE:HD2	1	0.22
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG11	6	0.22
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG12	6	0.22
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG13	6	0.22
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG21	6	0.22
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG22	6	0.22
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG23	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,451)	1:A:98:VAL:HB	1:A:99:SER:H	15	0.21
(1,386)	1:A:284:GLU:H	1:A:284:GLU:HG2	5	0.21
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	5	0.21
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	5	0.21
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	5	0.21
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	7	0.21
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	7	0.21
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	7	0.21
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	9	0.21
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	9	0.21
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	9	0.21
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	14	0.21
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	14	0.21
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	14	0.21
(1,1314)	1:A:101:PHE:HD1	1:A:117:LEU:HB2	9	0.21
(1,1314)	1:A:101:PHE:HD1	1:A:117:LEU:HB3	9	0.21
(1,1314)	1:A:101:PHE:HD2	1:A:117:LEU:HB2	9	0.21
(1,1314)	1:A:101:PHE:HD2	1:A:117:LEU:HB3	9	0.21
(1,609)	1:A:152:ALA:H	1:A:153:ARG:HB2	1	0.2
(1,609)	1:A:152:ALA:H	1:A:153:ARG:HB3	1	0.2
(1,451)	1:A:98:VAL:HB	1:A:99:SER:H	19	0.2
(1,385)	1:A:284:GLU:H	1:A:284:GLU:HG3	20	0.2
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	13	0.2
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	13	0.2
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	13	0.2
(1,1546)	1:A:185:ALA:HB1	1:A:208:ALA:HB1	18	0.2
(1,1546)	1:A:185:ALA:HB1	1:A:208:ALA:HB2	18	0.2
(1,1546)	1:A:185:ALA:HB1	1:A:208:ALA:HB3	18	0.2
(1,1546)	1:A:185:ALA:HB2	1:A:208:ALA:HB1	18	0.2
(1,1546)	1:A:185:ALA:HB2	1:A:208:ALA:HB2	18	0.2
(1,1546)	1:A:185:ALA:HB2	1:A:208:ALA:HB3	18	0.2
(1,1546)	1:A:185:ALA:HB3	1:A:208:ALA:HB1	18	0.2
(1,1546)	1:A:185:ALA:HB3	1:A:208:ALA:HB2	18	0.2
(1,1546)	1:A:185:ALA:HB3	1:A:208:ALA:HB3	18	0.2
(1,1475)	1:A:171:LEU:HA	1:A:291:VAL:HA	16	0.2
(1,641)	1:A:164:ILE:HG12	1:A:165:GLY:H	20	0.19
(1,641)	1:A:164:ILE:HG13	1:A:165:GLY:H	20	0.19
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB1	17	0.19
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB2	17	0.19
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB3	17	0.19
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB1	17	0.19
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB2	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB3	17	0.19
(1,502)	1:A:111:PRO:HB2	1:A:112:VAL:HA	11	0.19
(1,451)	1:A:98:VAL:HB	1:A:99:SER:H	2	0.19
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	6	0.19
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	6	0.19
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	6	0.19
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	8	0.19
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	8	0.19
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	8	0.19
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	18	0.19
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	18	0.19
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	18	0.19
(1,1523)	1:A:180:VAL:HG11	1:A:205:ILE:HB	10	0.19
(1,1523)	1:A:180:VAL:HG12	1:A:205:ILE:HB	10	0.19
(1,1523)	1:A:180:VAL:HG13	1:A:205:ILE:HB	10	0.19
(1,1523)	1:A:180:VAL:HG21	1:A:205:ILE:HB	10	0.19
(1,1523)	1:A:180:VAL:HG22	1:A:205:ILE:HB	10	0.19
(1,1523)	1:A:180:VAL:HG23	1:A:205:ILE:HB	10	0.19
(1,1284)	1:A:85:ASP:HA	1:A:237:MET:HE1	6	0.19
(1,1284)	1:A:85:ASP:HA	1:A:237:MET:HE2	6	0.19
(1,1284)	1:A:85:ASP:HA	1:A:237:MET:HE3	6	0.19
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD11	12	0.19
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD12	12	0.19
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD13	12	0.19
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD21	12	0.19
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD22	12	0.19
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD23	12	0.19
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD11	12	0.19
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD12	12	0.19
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD13	12	0.19
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD21	12	0.19
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD22	12	0.19
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD23	12	0.19
(1,1103)	1:A:226:ALA:HB1	1:A:229:ARG:HG2	1	0.19
(1,1103)	1:A:226:ALA:HB1	1:A:229:ARG:HG3	1	0.19
(1,1103)	1:A:226:ALA:HB2	1:A:229:ARG:HG2	1	0.19
(1,1103)	1:A:226:ALA:HB2	1:A:229:ARG:HG3	1	0.19
(1,1103)	1:A:226:ALA:HB3	1:A:229:ARG:HG2	1	0.19
(1,1103)	1:A:226:ALA:HB3	1:A:229:ARG:HG3	1	0.19
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG11	7	0.19
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG12	7	0.19
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG13	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG21	7	0.19
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG22	7	0.19
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG23	7	0.19
(2,19)	1:A:85:ASP:H	1:A:238:VAL:O	9	0.18
(1,838)	1:A:266:ASP:H	1:A:267:PHE:HD1	16	0.18
(1,838)	1:A:266:ASP:H	1:A:267:PHE:HD2	16	0.18
(1,831)	1:A:264:ARG:HG2	1:A:265:ALA:HB1	13	0.18
(1,831)	1:A:264:ARG:HG2	1:A:265:ALA:HB2	13	0.18
(1,831)	1:A:264:ARG:HG2	1:A:265:ALA:HB3	13	0.18
(1,831)	1:A:264:ARG:HG3	1:A:265:ALA:HB1	13	0.18
(1,831)	1:A:264:ARG:HG3	1:A:265:ALA:HB2	13	0.18
(1,831)	1:A:264:ARG:HG3	1:A:265:ALA:HB3	13	0.18
(1,802)	1:A:244:ASP:HB2	1:A:245:VAL:HB	2	0.18
(1,802)	1:A:244:ASP:HB3	1:A:245:VAL:HB	2	0.18
(1,802)	1:A:244:ASP:HB2	1:A:245:VAL:HB	13	0.18
(1,802)	1:A:244:ASP:HB3	1:A:245:VAL:HB	13	0.18
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	11	0.18
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	11	0.18
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	11	0.18
(1,1584)	1:A:225:LEU:HD11	1:A:251:HIS:HB2	7	0.18
(1,1584)	1:A:225:LEU:HD11	1:A:251:HIS:HB3	7	0.18
(1,1584)	1:A:225:LEU:HD12	1:A:251:HIS:HB2	7	0.18
(1,1584)	1:A:225:LEU:HD12	1:A:251:HIS:HB3	7	0.18
(1,1584)	1:A:225:LEU:HD13	1:A:251:HIS:HB2	7	0.18
(1,1584)	1:A:225:LEU:HD13	1:A:251:HIS:HB3	7	0.18
(1,1584)	1:A:225:LEU:HD21	1:A:251:HIS:HB2	7	0.18
(1,1584)	1:A:225:LEU:HD21	1:A:251:HIS:HB3	7	0.18
(1,1584)	1:A:225:LEU:HD22	1:A:251:HIS:HB2	7	0.18
(1,1584)	1:A:225:LEU:HD22	1:A:251:HIS:HB3	7	0.18
(1,1584)	1:A:225:LEU:HD23	1:A:251:HIS:HB2	7	0.18
(1,1584)	1:A:225:LEU:HD23	1:A:251:HIS:HB3	7	0.18
(1,1432)	1:A:160:LEU:HB2	1:A:196:PHE:HD1	12	0.18
(1,1432)	1:A:160:LEU:HB2	1:A:196:PHE:HD2	12	0.18
(1,1432)	1:A:160:LEU:HB3	1:A:196:PHE:HD1	12	0.18
(1,1432)	1:A:160:LEU:HB3	1:A:196:PHE:HD2	12	0.18
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG11	14	0.18
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG12	14	0.18
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG13	14	0.18
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG21	14	0.18
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG22	14	0.18
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG23	14	0.18
(2,145)	1:A:245:VAL:H	1:A:241:ARG:O	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,802)	1:A:244:ASP:HB2	1:A:245:VAL:HB	4	0.17
(1,802)	1:A:244:ASP:HB3	1:A:245:VAL:HB	4	0.17
(1,802)	1:A:244:ASP:HB2	1:A:245:VAL:HB	15	0.17
(1,802)	1:A:244:ASP:HB3	1:A:245:VAL:HB	15	0.17
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB1	19	0.17
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB2	19	0.17
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB3	19	0.17
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB1	19	0.17
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB2	19	0.17
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB3	19	0.17
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB1	20	0.17
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB2	20	0.17
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB3	20	0.17
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB1	20	0.17
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB2	20	0.17
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB3	20	0.17
(1,501)	1:A:111:PRO:HB3	1:A:112:VAL:H	14	0.17
(1,430)	1:A:83:ILE:HD11	1:A:84:PHE:H	5	0.17
(1,430)	1:A:83:ILE:HD12	1:A:84:PHE:H	5	0.17
(1,430)	1:A:83:ILE:HD13	1:A:84:PHE:H	5	0.17
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	2	0.17
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	2	0.17
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	2	0.17
(1,28)	1:A:95:ARG:HA	1:A:95:ARG:HD2	7	0.17
(1,28)	1:A:95:ARG:HA	1:A:95:ARG:HD3	7	0.17
(1,182)	1:A:161:PHE:H	1:A:161:PHE:HD1	17	0.17
(1,182)	1:A:161:PHE:H	1:A:161:PHE:HD2	17	0.17
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD11	11	0.17
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD12	11	0.17
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD13	11	0.17
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD21	11	0.17
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD22	11	0.17
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD23	11	0.17
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD11	11	0.17
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD12	11	0.17
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD13	11	0.17
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD21	11	0.17
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD22	11	0.17
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD23	11	0.17
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD11	16	0.17
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD12	16	0.17
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD13	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD21	16	0.17
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD22	16	0.17
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD23	16	0.17
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD11	16	0.17
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD12	16	0.17
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD13	16	0.17
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD21	16	0.17
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD22	16	0.17
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD23	16	0.17
(1,891)	1:A:95:ARG:HA	1:A:98:VAL:HG21	2	0.16
(1,891)	1:A:95:ARG:HA	1:A:98:VAL:HG22	2	0.16
(1,891)	1:A:95:ARG:HA	1:A:98:VAL:HG23	2	0.16
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD11	18	0.16
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD12	18	0.16
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD13	18	0.16
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG11	2	0.16
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG12	2	0.16
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG13	2	0.16
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG21	2	0.16
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG22	2	0.16
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG23	2	0.16
(1,781)	1:A:230:PRO:HB2	1:A:231:LEU:HD11	15	0.16
(1,781)	1:A:230:PRO:HB2	1:A:231:LEU:HD12	15	0.16
(1,781)	1:A:230:PRO:HB2	1:A:231:LEU:HD13	15	0.16
(1,781)	1:A:230:PRO:HB2	1:A:231:LEU:HD21	15	0.16
(1,781)	1:A:230:PRO:HB2	1:A:231:LEU:HD22	15	0.16
(1,781)	1:A:230:PRO:HB2	1:A:231:LEU:HD23	15	0.16
(1,781)	1:A:230:PRO:HB3	1:A:231:LEU:HD11	15	0.16
(1,781)	1:A:230:PRO:HB3	1:A:231:LEU:HD12	15	0.16
(1,781)	1:A:230:PRO:HB3	1:A:231:LEU:HD13	15	0.16
(1,781)	1:A:230:PRO:HB3	1:A:231:LEU:HD21	15	0.16
(1,781)	1:A:230:PRO:HB3	1:A:231:LEU:HD22	15	0.16
(1,781)	1:A:230:PRO:HB3	1:A:231:LEU:HD23	15	0.16
(1,777)	1:A:229:ARG:HD2	1:A:230:PRO:HA	1	0.16
(1,777)	1:A:229:ARG:HD3	1:A:230:PRO:HA	1	0.16
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB1	9	0.16
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB2	9	0.16
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB3	9	0.16
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB1	9	0.16
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB2	9	0.16
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB3	9	0.16
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB1	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB2	3	0.16
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB3	3	0.16
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB1	3	0.16
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB2	3	0.16
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB3	3	0.16
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	17	0.16
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	17	0.16
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	17	0.16
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	19	0.16
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	19	0.16
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	19	0.16
(1,156)	1:A:147:ARG:H	1:A:147:ARG:HD2	10	0.16
(1,156)	1:A:147:ARG:H	1:A:147:ARG:HD3	10	0.16
(1,1523)	1:A:180:VAL:HG11	1:A:205:ILE:HB	8	0.16
(1,1523)	1:A:180:VAL:HG12	1:A:205:ILE:HB	8	0.16
(1,1523)	1:A:180:VAL:HG13	1:A:205:ILE:HB	8	0.16
(1,1523)	1:A:180:VAL:HG21	1:A:205:ILE:HB	8	0.16
(1,1523)	1:A:180:VAL:HG22	1:A:205:ILE:HB	8	0.16
(1,1523)	1:A:180:VAL:HG23	1:A:205:ILE:HB	8	0.16
(1,1523)	1:A:180:VAL:HG11	1:A:205:ILE:HB	13	0.16
(1,1523)	1:A:180:VAL:HG12	1:A:205:ILE:HB	13	0.16
(1,1523)	1:A:180:VAL:HG13	1:A:205:ILE:HB	13	0.16
(1,1523)	1:A:180:VAL:HG21	1:A:205:ILE:HB	13	0.16
(1,1523)	1:A:180:VAL:HG22	1:A:205:ILE:HB	13	0.16
(1,1523)	1:A:180:VAL:HG23	1:A:205:ILE:HB	13	0.16
(1,1507)	1:A:179:ALA:HB1	1:A:204:VAL:HB	8	0.16
(1,1507)	1:A:179:ALA:HB2	1:A:204:VAL:HB	8	0.16
(1,1507)	1:A:179:ALA:HB3	1:A:204:VAL:HB	8	0.16
(1,1475)	1:A:171:LEU:HA	1:A:291:VAL:HA	6	0.16
(1,1475)	1:A:171:LEU:HA	1:A:291:VAL:HA	9	0.16
(1,1421)	1:A:130:LEU:HD11	1:A:146:TYR:HD1	9	0.16
(1,1421)	1:A:130:LEU:HD11	1:A:146:TYR:HD2	9	0.16
(1,1421)	1:A:130:LEU:HD12	1:A:146:TYR:HD1	9	0.16
(1,1421)	1:A:130:LEU:HD12	1:A:146:TYR:HD2	9	0.16
(1,1421)	1:A:130:LEU:HD13	1:A:146:TYR:HD1	9	0.16
(1,1421)	1:A:130:LEU:HD13	1:A:146:TYR:HD2	9	0.16
(1,1421)	1:A:130:LEU:HD21	1:A:146:TYR:HD1	9	0.16
(1,1421)	1:A:130:LEU:HD21	1:A:146:TYR:HD2	9	0.16
(1,1421)	1:A:130:LEU:HD22	1:A:146:TYR:HD1	9	0.16
(1,1421)	1:A:130:LEU:HD22	1:A:146:TYR:HD2	9	0.16
(1,1421)	1:A:130:LEU:HD23	1:A:146:TYR:HD1	9	0.16
(1,1421)	1:A:130:LEU:HD23	1:A:146:TYR:HD2	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1304)	1:A:98:VAL:HG11	1:A:117:LEU:HB2	13	0.16
(1,1304)	1:A:98:VAL:HG11	1:A:117:LEU:HB3	13	0.16
(1,1304)	1:A:98:VAL:HG12	1:A:117:LEU:HB2	13	0.16
(1,1304)	1:A:98:VAL:HG12	1:A:117:LEU:HB3	13	0.16
(1,1304)	1:A:98:VAL:HG13	1:A:117:LEU:HB2	13	0.16
(1,1304)	1:A:98:VAL:HG13	1:A:117:LEU:HB3	13	0.16
(1,1304)	1:A:98:VAL:HG21	1:A:117:LEU:HB2	13	0.16
(1,1304)	1:A:98:VAL:HG21	1:A:117:LEU:HB3	13	0.16
(1,1304)	1:A:98:VAL:HG22	1:A:117:LEU:HB2	13	0.16
(1,1304)	1:A:98:VAL:HG22	1:A:117:LEU:HB3	13	0.16
(1,1304)	1:A:98:VAL:HG23	1:A:117:LEU:HB2	13	0.16
(1,1304)	1:A:98:VAL:HG23	1:A:117:LEU:HB3	13	0.16
(1,1254)	1:A:84:PHE:HB2	1:A:89:THR:HG21	20	0.16
(1,1254)	1:A:84:PHE:HB2	1:A:89:THR:HG22	20	0.16
(1,1254)	1:A:84:PHE:HB2	1:A:89:THR:HG23	20	0.16
(1,1254)	1:A:84:PHE:HB3	1:A:89:THR:HG21	20	0.16
(1,1254)	1:A:84:PHE:HB3	1:A:89:THR:HG22	20	0.16
(1,1254)	1:A:84:PHE:HB3	1:A:89:THR:HG23	20	0.16
(1,1238)	1:A:83:ILE:HG12	1:A:221:LEU:HA	1	0.16
(1,1238)	1:A:83:ILE:HG13	1:A:221:LEU:HA	1	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD11	3	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD12	3	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD13	3	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD21	3	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD22	3	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD23	3	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD11	3	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD12	3	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD13	3	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD21	3	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD22	3	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD23	3	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD11	14	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD12	14	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD13	14	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD21	14	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD22	14	0.16
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD23	14	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD11	14	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD12	14	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD13	14	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD21	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD22	14	0.16
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD23	14	0.16
(1,1103)	1:A:226:ALA:HB1	1:A:229:ARG:HG2	16	0.16
(1,1103)	1:A:226:ALA:HB1	1:A:229:ARG:HG3	16	0.16
(1,1103)	1:A:226:ALA:HB2	1:A:229:ARG:HG2	16	0.16
(1,1103)	1:A:226:ALA:HB2	1:A:229:ARG:HG3	16	0.16
(1,1103)	1:A:226:ALA:HB3	1:A:229:ARG:HG2	16	0.16
(1,1103)	1:A:226:ALA:HB3	1:A:229:ARG:HG3	16	0.16
(1,1078)	1:A:203:GLU:H	1:A:205:ILE:HD11	8	0.16
(1,1078)	1:A:203:GLU:H	1:A:205:ILE:HD12	8	0.16
(1,1078)	1:A:203:GLU:H	1:A:205:ILE:HD13	8	0.16
(2,157)	1:A:251:HIS:H	1:A:247:GLY:O	1	0.15
(1,949)	1:A:116:ASP:HB3	1:A:119:THR:HG21	7	0.15
(1,949)	1:A:116:ASP:HB3	1:A:119:THR:HG22	7	0.15
(1,949)	1:A:116:ASP:HB3	1:A:119:THR:HG23	7	0.15
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG11	9	0.15
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG12	9	0.15
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG13	9	0.15
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG21	9	0.15
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG22	9	0.15
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG23	9	0.15
(1,84)	1:A:114:GLU:HA	1:A:114:GLU:HG3	15	0.15
(1,838)	1:A:266:ASP:H	1:A:267:PHE:HD1	14	0.15
(1,838)	1:A:266:ASP:H	1:A:267:PHE:HD2	14	0.15
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD11	17	0.15
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD12	17	0.15
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD13	17	0.15
(1,777)	1:A:229:ARG:HD2	1:A:230:PRO:HA	11	0.15
(1,777)	1:A:229:ARG:HD3	1:A:230:PRO:HA	11	0.15
(1,641)	1:A:164:ILE:HG12	1:A:165:GLY:H	5	0.15
(1,641)	1:A:164:ILE:HG13	1:A:165:GLY:H	5	0.15
(1,641)	1:A:164:ILE:HG12	1:A:165:GLY:H	9	0.15
(1,641)	1:A:164:ILE:HG13	1:A:165:GLY:H	9	0.15
(1,502)	1:A:111:PRO:HB2	1:A:112:VAL:HA	7	0.15
(1,1542)	1:A:181:ALA:HB1	1:A:237:MET:HE1	7	0.15
(1,1542)	1:A:181:ALA:HB1	1:A:237:MET:HE2	7	0.15
(1,1542)	1:A:181:ALA:HB1	1:A:237:MET:HE3	7	0.15
(1,1542)	1:A:181:ALA:HB2	1:A:237:MET:HE1	7	0.15
(1,1542)	1:A:181:ALA:HB2	1:A:237:MET:HE2	7	0.15
(1,1542)	1:A:181:ALA:HB2	1:A:237:MET:HE3	7	0.15
(1,1542)	1:A:181:ALA:HB3	1:A:237:MET:HE1	7	0.15
(1,1542)	1:A:181:ALA:HB3	1:A:237:MET:HE2	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1542)	1:A:181:ALA:HB3	1:A:237:MET:HE3	7	0.15
(1,1507)	1:A:179:ALA:HB1	1:A:204:VAL:HB	12	0.15
(1,1507)	1:A:179:ALA:HB2	1:A:204:VAL:HB	12	0.15
(1,1507)	1:A:179:ALA:HB3	1:A:204:VAL:HB	12	0.15
(1,1475)	1:A:171:LEU:HA	1:A:291:VAL:HA	13	0.15
(1,1458)	1:A:167:LEU:HD11	1:A:282:ILE:HB	15	0.15
(1,1458)	1:A:167:LEU:HD12	1:A:282:ILE:HB	15	0.15
(1,1458)	1:A:167:LEU:HD13	1:A:282:ILE:HB	15	0.15
(1,1458)	1:A:167:LEU:HD21	1:A:282:ILE:HB	15	0.15
(1,1458)	1:A:167:LEU:HD22	1:A:282:ILE:HB	15	0.15
(1,1458)	1:A:167:LEU:HD23	1:A:282:ILE:HB	15	0.15
(1,1431)	1:A:159:SER:H	1:A:196:PHE:HE1	3	0.15
(1,1431)	1:A:159:SER:H	1:A:196:PHE:HE2	3	0.15
(1,1359)	1:A:105:LEU:HA	1:A:112:VAL:HG11	9	0.15
(1,1359)	1:A:105:LEU:HA	1:A:112:VAL:HG12	9	0.15
(1,1359)	1:A:105:LEU:HA	1:A:112:VAL:HG13	9	0.15
(1,1359)	1:A:105:LEU:HA	1:A:112:VAL:HG21	9	0.15
(1,1359)	1:A:105:LEU:HA	1:A:112:VAL:HG22	9	0.15
(1,1359)	1:A:105:LEU:HA	1:A:112:VAL:HG23	9	0.15
(1,1234)	1:A:83:ILE:HD11	1:A:221:LEU:HG	1	0.15
(1,1234)	1:A:83:ILE:HD12	1:A:221:LEU:HG	1	0.15
(1,1234)	1:A:83:ILE:HD13	1:A:221:LEU:HG	1	0.15
(1,1234)	1:A:83:ILE:HD11	1:A:221:LEU:HG	19	0.15
(1,1234)	1:A:83:ILE:HD12	1:A:221:LEU:HG	19	0.15
(1,1234)	1:A:83:ILE:HD13	1:A:221:LEU:HG	19	0.15
(1,1151)	1:A:285:LEU:HB2	1:A:289:LEU:HG	18	0.15
(1,1151)	1:A:285:LEU:HB3	1:A:289:LEU:HG	18	0.15
(1,114)	1:A:133:MET:HA	1:A:133:MET:HE1	15	0.15
(1,114)	1:A:133:MET:HA	1:A:133:MET:HE2	15	0.15
(1,114)	1:A:133:MET:HA	1:A:133:MET:HE3	15	0.15
(1,110)	1:A:131:ARG:HA	1:A:131:ARG:HD2	3	0.15
(1,110)	1:A:131:ARG:HA	1:A:131:ARG:HD3	3	0.15
(1,1027)	1:A:164:ILE:HG21	1:A:167:LEU:H	8	0.15
(1,1027)	1:A:164:ILE:HG22	1:A:167:LEU:H	8	0.15
(1,1027)	1:A:164:ILE:HG23	1:A:167:LEU:H	8	0.15
(2,73)	1:A:133:MET:H	1:A:129:THR:O	9	0.14
(2,19)	1:A:85:ASP:H	1:A:238:VAL:O	20	0.14
(2,157)	1:A:251:HIS:H	1:A:247:GLY:O	12	0.14
(1,966)	1:A:135:LEU:HD11	1:A:139:ALA:HB1	10	0.14
(1,966)	1:A:135:LEU:HD11	1:A:139:ALA:HB2	10	0.14
(1,966)	1:A:135:LEU:HD11	1:A:139:ALA:HB3	10	0.14
(1,966)	1:A:135:LEU:HD12	1:A:139:ALA:HB1	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,966)	1:A:135:LEU:HD12	1:A:139:ALA:HB2	10	0.14
(1,966)	1:A:135:LEU:HD12	1:A:139:ALA:HB3	10	0.14
(1,966)	1:A:135:LEU:HD13	1:A:139:ALA:HB1	10	0.14
(1,966)	1:A:135:LEU:HD13	1:A:139:ALA:HB2	10	0.14
(1,966)	1:A:135:LEU:HD13	1:A:139:ALA:HB3	10	0.14
(1,966)	1:A:135:LEU:HD21	1:A:139:ALA:HB1	10	0.14
(1,966)	1:A:135:LEU:HD21	1:A:139:ALA:HB2	10	0.14
(1,966)	1:A:135:LEU:HD21	1:A:139:ALA:HB3	10	0.14
(1,966)	1:A:135:LEU:HD22	1:A:139:ALA:HB1	10	0.14
(1,966)	1:A:135:LEU:HD22	1:A:139:ALA:HB2	10	0.14
(1,966)	1:A:135:LEU:HD22	1:A:139:ALA:HB3	10	0.14
(1,966)	1:A:135:LEU:HD23	1:A:139:ALA:HB1	10	0.14
(1,966)	1:A:135:LEU:HD23	1:A:139:ALA:HB2	10	0.14
(1,966)	1:A:135:LEU:HD23	1:A:139:ALA:HB3	10	0.14
(1,891)	1:A:95:ARG:HA	1:A:98:VAL:HG21	19	0.14
(1,891)	1:A:95:ARG:HA	1:A:98:VAL:HG22	19	0.14
(1,891)	1:A:95:ARG:HA	1:A:98:VAL:HG23	19	0.14
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD11	10	0.14
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD12	10	0.14
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD13	10	0.14
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD11	13	0.14
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD12	13	0.14
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD13	13	0.14
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD11	15	0.14
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD12	15	0.14
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD13	15	0.14
(1,777)	1:A:229:ARG:HD2	1:A:230:PRO:HA	4	0.14
(1,777)	1:A:229:ARG:HD3	1:A:230:PRO:HA	4	0.14
(1,641)	1:A:164:ILE:HG12	1:A:165:GLY:H	6	0.14
(1,641)	1:A:164:ILE:HG13	1:A:165:GLY:H	6	0.14
(1,641)	1:A:164:ILE:HG12	1:A:165:GLY:H	11	0.14
(1,641)	1:A:164:ILE:HG13	1:A:165:GLY:H	11	0.14
(1,641)	1:A:164:ILE:HG12	1:A:165:GLY:H	13	0.14
(1,641)	1:A:164:ILE:HG13	1:A:165:GLY:H	13	0.14
(1,622)	1:A:157:MET:HA	1:A:158:ASN:H	16	0.14
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB1	8	0.14
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB2	8	0.14
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB3	8	0.14
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB1	8	0.14
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB2	8	0.14
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB3	8	0.14
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB1	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB2	15	0.14
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB3	15	0.14
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB1	15	0.14
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB2	15	0.14
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB3	15	0.14
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB1	7	0.14
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB2	7	0.14
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB3	7	0.14
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB1	7	0.14
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB2	7	0.14
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB3	7	0.14
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB1	10	0.14
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB2	10	0.14
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB3	10	0.14
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB1	10	0.14
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB2	10	0.14
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB3	10	0.14
(1,331)	1:A:237:MET:H	1:A:237:MET:HE1	12	0.14
(1,331)	1:A:237:MET:H	1:A:237:MET:HE2	12	0.14
(1,331)	1:A:237:MET:H	1:A:237:MET:HE3	12	0.14
(1,294)	1:A:231:LEU:HA	1:A:231:LEU:HD11	7	0.14
(1,294)	1:A:231:LEU:HA	1:A:231:LEU:HD12	7	0.14
(1,294)	1:A:231:LEU:HA	1:A:231:LEU:HD13	7	0.14
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG2	9	0.14
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG3	9	0.14
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG2	15	0.14
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG3	15	0.14
(1,258)	1:A:205:ILE:HG21	1:A:205:ILE:HD11	16	0.14
(1,258)	1:A:205:ILE:HG21	1:A:205:ILE:HD12	16	0.14
(1,258)	1:A:205:ILE:HG21	1:A:205:ILE:HD13	16	0.14
(1,258)	1:A:205:ILE:HG22	1:A:205:ILE:HD11	16	0.14
(1,258)	1:A:205:ILE:HG22	1:A:205:ILE:HD12	16	0.14
(1,258)	1:A:205:ILE:HG22	1:A:205:ILE:HD13	16	0.14
(1,258)	1:A:205:ILE:HG23	1:A:205:ILE:HD11	16	0.14
(1,258)	1:A:205:ILE:HG23	1:A:205:ILE:HD12	16	0.14
(1,258)	1:A:205:ILE:HG23	1:A:205:ILE:HD13	16	0.14
(1,1528)	1:A:180:VAL:HG11	1:A:205:ILE:HG21	4	0.14
(1,1528)	1:A:180:VAL:HG11	1:A:205:ILE:HG22	4	0.14
(1,1528)	1:A:180:VAL:HG11	1:A:205:ILE:HG23	4	0.14
(1,1528)	1:A:180:VAL:HG12	1:A:205:ILE:HG21	4	0.14
(1,1528)	1:A:180:VAL:HG12	1:A:205:ILE:HG22	4	0.14
(1,1528)	1:A:180:VAL:HG12	1:A:205:ILE:HG23	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1528)	1:A:180:VAL:HG13	1:A:205:ILE:HG21	4	0.14
(1,1528)	1:A:180:VAL:HG13	1:A:205:ILE:HG22	4	0.14
(1,1528)	1:A:180:VAL:HG13	1:A:205:ILE:HG23	4	0.14
(1,1523)	1:A:180:VAL:HG11	1:A:205:ILE:HB	6	0.14
(1,1523)	1:A:180:VAL:HG12	1:A:205:ILE:HB	6	0.14
(1,1523)	1:A:180:VAL:HG13	1:A:205:ILE:HB	6	0.14
(1,1523)	1:A:180:VAL:HG21	1:A:205:ILE:HB	6	0.14
(1,1523)	1:A:180:VAL:HG22	1:A:205:ILE:HB	6	0.14
(1,1523)	1:A:180:VAL:HG23	1:A:205:ILE:HB	6	0.14
(1,1523)	1:A:180:VAL:HG11	1:A:205:ILE:HB	12	0.14
(1,1523)	1:A:180:VAL:HG12	1:A:205:ILE:HB	12	0.14
(1,1523)	1:A:180:VAL:HG13	1:A:205:ILE:HB	12	0.14
(1,1523)	1:A:180:VAL:HG21	1:A:205:ILE:HB	12	0.14
(1,1523)	1:A:180:VAL:HG22	1:A:205:ILE:HB	12	0.14
(1,1523)	1:A:180:VAL:HG23	1:A:205:ILE:HB	12	0.14
(1,1523)	1:A:180:VAL:HG11	1:A:205:ILE:HB	14	0.14
(1,1523)	1:A:180:VAL:HG12	1:A:205:ILE:HB	14	0.14
(1,1523)	1:A:180:VAL:HG13	1:A:205:ILE:HB	14	0.14
(1,1523)	1:A:180:VAL:HG21	1:A:205:ILE:HB	14	0.14
(1,1523)	1:A:180:VAL:HG22	1:A:205:ILE:HB	14	0.14
(1,1523)	1:A:180:VAL:HG23	1:A:205:ILE:HB	14	0.14
(1,1515)	1:A:180:VAL:HB	1:A:205:ILE:HD11	1	0.14
(1,1515)	1:A:180:VAL:HB	1:A:205:ILE:HD12	1	0.14
(1,1515)	1:A:180:VAL:HB	1:A:205:ILE:HD13	1	0.14
(1,1507)	1:A:179:ALA:HB1	1:A:204:VAL:HB	4	0.14
(1,1507)	1:A:179:ALA:HB2	1:A:204:VAL:HB	4	0.14
(1,1507)	1:A:179:ALA:HB3	1:A:204:VAL:HB	4	0.14
(1,1482)	1:A:171:LEU:HD11	1:A:285:LEU:HD11	1	0.14
(1,1482)	1:A:171:LEU:HD11	1:A:285:LEU:HD12	1	0.14
(1,1482)	1:A:171:LEU:HD11	1:A:285:LEU:HD13	1	0.14
(1,1482)	1:A:171:LEU:HD11	1:A:285:LEU:HD21	1	0.14
(1,1482)	1:A:171:LEU:HD11	1:A:285:LEU:HD22	1	0.14
(1,1482)	1:A:171:LEU:HD11	1:A:285:LEU:HD23	1	0.14
(1,1482)	1:A:171:LEU:HD12	1:A:285:LEU:HD11	1	0.14
(1,1482)	1:A:171:LEU:HD12	1:A:285:LEU:HD12	1	0.14
(1,1482)	1:A:171:LEU:HD12	1:A:285:LEU:HD13	1	0.14
(1,1482)	1:A:171:LEU:HD12	1:A:285:LEU:HD21	1	0.14
(1,1482)	1:A:171:LEU:HD12	1:A:285:LEU:HD22	1	0.14
(1,1482)	1:A:171:LEU:HD12	1:A:285:LEU:HD23	1	0.14
(1,1482)	1:A:171:LEU:HD13	1:A:285:LEU:HD11	1	0.14
(1,1482)	1:A:171:LEU:HD13	1:A:285:LEU:HD12	1	0.14
(1,1482)	1:A:171:LEU:HD13	1:A:285:LEU:HD13	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1482)	1:A:171:LEU:HD13	1:A:285:LEU:HD21	1	0.14
(1,1482)	1:A:171:LEU:HD13	1:A:285:LEU:HD22	1	0.14
(1,1482)	1:A:171:LEU:HD13	1:A:285:LEU:HD23	1	0.14
(1,1482)	1:A:171:LEU:HD21	1:A:285:LEU:HD11	1	0.14
(1,1482)	1:A:171:LEU:HD21	1:A:285:LEU:HD12	1	0.14
(1,1482)	1:A:171:LEU:HD21	1:A:285:LEU:HD13	1	0.14
(1,1482)	1:A:171:LEU:HD21	1:A:285:LEU:HD21	1	0.14
(1,1482)	1:A:171:LEU:HD21	1:A:285:LEU:HD22	1	0.14
(1,1482)	1:A:171:LEU:HD21	1:A:285:LEU:HD23	1	0.14
(1,1482)	1:A:171:LEU:HD22	1:A:285:LEU:HD11	1	0.14
(1,1482)	1:A:171:LEU:HD22	1:A:285:LEU:HD12	1	0.14
(1,1482)	1:A:171:LEU:HD22	1:A:285:LEU:HD13	1	0.14
(1,1482)	1:A:171:LEU:HD22	1:A:285:LEU:HD21	1	0.14
(1,1482)	1:A:171:LEU:HD22	1:A:285:LEU:HD22	1	0.14
(1,1482)	1:A:171:LEU:HD22	1:A:285:LEU:HD23	1	0.14
(1,1482)	1:A:171:LEU:HD23	1:A:285:LEU:HD11	1	0.14
(1,1482)	1:A:171:LEU:HD23	1:A:285:LEU:HD12	1	0.14
(1,1482)	1:A:171:LEU:HD23	1:A:285:LEU:HD13	1	0.14
(1,1482)	1:A:171:LEU:HD23	1:A:285:LEU:HD21	1	0.14
(1,1482)	1:A:171:LEU:HD23	1:A:285:LEU:HD22	1	0.14
(1,1482)	1:A:171:LEU:HD23	1:A:285:LEU:HD23	1	0.14
(1,1475)	1:A:171:LEU:HA	1:A:291:VAL:HA	5	0.14
(1,1458)	1:A:167:LEU:HD11	1:A:282:ILE:HB	6	0.14
(1,1458)	1:A:167:LEU:HD12	1:A:282:ILE:HB	6	0.14
(1,1458)	1:A:167:LEU:HD13	1:A:282:ILE:HB	6	0.14
(1,1458)	1:A:167:LEU:HD21	1:A:282:ILE:HB	6	0.14
(1,1458)	1:A:167:LEU:HD22	1:A:282:ILE:HB	6	0.14
(1,1458)	1:A:167:LEU:HD23	1:A:282:ILE:HB	6	0.14
(1,144)	1:A:144:VAL:H	1:A:144:VAL:HB	9	0.14
(1,1432)	1:A:160:LEU:HB2	1:A:196:PHE:HD1	6	0.14
(1,1432)	1:A:160:LEU:HB2	1:A:196:PHE:HD2	6	0.14
(1,1432)	1:A:160:LEU:HB3	1:A:196:PHE:HD1	6	0.14
(1,1432)	1:A:160:LEU:HB3	1:A:196:PHE:HD2	6	0.14
(1,1431)	1:A:159:SER:H	1:A:196:PHE:HE1	9	0.14
(1,1431)	1:A:159:SER:H	1:A:196:PHE:HE2	9	0.14
(1,1431)	1:A:159:SER:H	1:A:196:PHE:HE1	14	0.14
(1,1431)	1:A:159:SER:H	1:A:196:PHE:HE2	14	0.14
(1,1395)	1:A:112:VAL:HA	1:A:133:MET:HE1	1	0.14
(1,1395)	1:A:112:VAL:HA	1:A:133:MET:HE2	1	0.14
(1,1395)	1:A:112:VAL:HA	1:A:133:MET:HE3	1	0.14
(1,1284)	1:A:85:ASP:HA	1:A:237:MET:HE1	13	0.14
(1,1284)	1:A:85:ASP:HA	1:A:237:MET:HE2	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1284)	1:A:85:ASP:HA	1:A:237:MET:HE3	13	0.14
(2,69)	1:A:131:ARG:H	1:A:127:HIS:O	10	0.13
(2,39)	1:A:259:GLY:H	1:A:279:ALA:O	10	0.13
(2,145)	1:A:245:VAL:H	1:A:241:ARG:O	8	0.13
(2,13)	1:A:236:VAL:H	1:A:81:LEU:O	19	0.13
(2,129)	1:A:196:PHE:H	1:A:192:ILE:O	3	0.13
(2,129)	1:A:196:PHE:H	1:A:192:ILE:O	9	0.13
(1,950)	1:A:116:ASP:HB2	1:A:119:THR:HG21	19	0.13
(1,950)	1:A:116:ASP:HB2	1:A:119:THR:HG22	19	0.13
(1,950)	1:A:116:ASP:HB2	1:A:119:THR:HG23	19	0.13
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG11	2	0.13
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG12	2	0.13
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG13	2	0.13
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG21	2	0.13
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG22	2	0.13
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG23	2	0.13
(1,883)	1:A:92:ASP:HB2	1:A:94:ALA:H	5	0.13
(1,883)	1:A:92:ASP:HB3	1:A:94:ALA:H	5	0.13
(1,848)	1:A:283:ASP:HB2	1:A:284:GLU:H	5	0.13
(1,848)	1:A:283:ASP:HB3	1:A:284:GLU:H	5	0.13
(1,828)	1:A:264:ARG:HB2	1:A:265:ALA:HB1	17	0.13
(1,828)	1:A:264:ARG:HB2	1:A:265:ALA:HB2	17	0.13
(1,828)	1:A:264:ARG:HB2	1:A:265:ALA:HB3	17	0.13
(1,828)	1:A:264:ARG:HB3	1:A:265:ALA:HB1	17	0.13
(1,828)	1:A:264:ARG:HB3	1:A:265:ALA:HB2	17	0.13
(1,828)	1:A:264:ARG:HB3	1:A:265:ALA:HB3	17	0.13
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG11	11	0.13
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG12	11	0.13
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG13	11	0.13
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG21	11	0.13
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG22	11	0.13
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG23	11	0.13
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG11	13	0.13
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG12	13	0.13
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG13	13	0.13
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG21	13	0.13
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG22	13	0.13
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG23	13	0.13
(1,728)	1:A:203:GLU:HG2	1:A:204:VAL:HA	4	0.13
(1,728)	1:A:203:GLU:HG3	1:A:204:VAL:HA	4	0.13
(1,722)	1:A:202:PHE:HA	1:A:203:GLU:HB3	7	0.13
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB1	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB2	15	0.13
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB3	15	0.13
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB1	15	0.13
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB2	15	0.13
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB3	15	0.13
(1,547)	1:A:132:ALA:HB1	1:A:133:MET:HG3	18	0.13
(1,547)	1:A:132:ALA:HB2	1:A:133:MET:HG3	18	0.13
(1,547)	1:A:132:ALA:HB3	1:A:133:MET:HG3	18	0.13
(1,502)	1:A:111:PRO:HB2	1:A:112:VAL:HA	6	0.13
(1,50)	1:A:101:PHE:H	1:A:101:PHE:HD1	1	0.13
(1,50)	1:A:101:PHE:H	1:A:101:PHE:HD2	1	0.13
(1,50)	1:A:101:PHE:H	1:A:101:PHE:HD1	9	0.13
(1,50)	1:A:101:PHE:H	1:A:101:PHE:HD2	9	0.13
(1,496)	1:A:110:ALA:HB1	1:A:111:PRO:HG2	19	0.13
(1,496)	1:A:110:ALA:HB1	1:A:111:PRO:HG3	19	0.13
(1,496)	1:A:110:ALA:HB2	1:A:111:PRO:HG2	19	0.13
(1,496)	1:A:110:ALA:HB2	1:A:111:PRO:HG3	19	0.13
(1,496)	1:A:110:ALA:HB3	1:A:111:PRO:HG2	19	0.13
(1,496)	1:A:110:ALA:HB3	1:A:111:PRO:HG3	19	0.13
(1,494)	1:A:110:ALA:HB1	1:A:111:PRO:HD3	7	0.13
(1,494)	1:A:110:ALA:HB2	1:A:111:PRO:HD3	7	0.13
(1,494)	1:A:110:ALA:HB3	1:A:111:PRO:HD3	7	0.13
(1,430)	1:A:83:ILE:HD11	1:A:84:PHE:H	16	0.13
(1,430)	1:A:83:ILE:HD12	1:A:84:PHE:H	16	0.13
(1,430)	1:A:83:ILE:HD13	1:A:84:PHE:H	16	0.13
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG2	4	0.13
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG3	4	0.13
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG2	20	0.13
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG3	20	0.13
(1,1645)	1:A:286:ARG:HA	1:A:291:VAL:HG21	3	0.13
(1,1645)	1:A:286:ARG:HA	1:A:291:VAL:HG22	3	0.13
(1,1645)	1:A:286:ARG:HA	1:A:291:VAL:HG23	3	0.13
(1,1645)	1:A:286:ARG:HA	1:A:291:VAL:HG21	10	0.13
(1,1645)	1:A:286:ARG:HA	1:A:291:VAL:HG22	10	0.13
(1,1645)	1:A:286:ARG:HA	1:A:291:VAL:HG23	10	0.13
(1,1523)	1:A:180:VAL:HG11	1:A:205:ILE:HB	17	0.13
(1,1523)	1:A:180:VAL:HG12	1:A:205:ILE:HB	17	0.13
(1,1523)	1:A:180:VAL:HG13	1:A:205:ILE:HB	17	0.13
(1,1523)	1:A:180:VAL:HG21	1:A:205:ILE:HB	17	0.13
(1,1523)	1:A:180:VAL:HG22	1:A:205:ILE:HB	17	0.13
(1,1523)	1:A:180:VAL:HG23	1:A:205:ILE:HB	17	0.13
(1,1458)	1:A:167:LEU:HD11	1:A:282:ILE:HB	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1458)	1:A:167:LEU:HD12	1:A:282:ILE:HB	14	0.13
(1,1458)	1:A:167:LEU:HD13	1:A:282:ILE:HB	14	0.13
(1,1458)	1:A:167:LEU:HD21	1:A:282:ILE:HB	14	0.13
(1,1458)	1:A:167:LEU:HD22	1:A:282:ILE:HB	14	0.13
(1,1458)	1:A:167:LEU:HD23	1:A:282:ILE:HB	14	0.13
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG11	3	0.13
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG12	3	0.13
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG13	3	0.13
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG21	3	0.13
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG22	3	0.13
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG23	3	0.13
(1,1432)	1:A:160:LEU:HB2	1:A:196:PHE:HD1	13	0.13
(1,1432)	1:A:160:LEU:HB2	1:A:196:PHE:HD2	13	0.13
(1,1432)	1:A:160:LEU:HB3	1:A:196:PHE:HD1	13	0.13
(1,1432)	1:A:160:LEU:HB3	1:A:196:PHE:HD2	13	0.13
(1,1432)	1:A:160:LEU:HB2	1:A:196:PHE:HD1	20	0.13
(1,1432)	1:A:160:LEU:HB2	1:A:196:PHE:HD2	20	0.13
(1,1432)	1:A:160:LEU:HB3	1:A:196:PHE:HD1	20	0.13
(1,1432)	1:A:160:LEU:HB3	1:A:196:PHE:HD2	20	0.13
(1,1415)	1:A:130:LEU:HD11	1:A:142:ALA:HA	17	0.13
(1,1415)	1:A:130:LEU:HD12	1:A:142:ALA:HA	17	0.13
(1,1415)	1:A:130:LEU:HD13	1:A:142:ALA:HA	17	0.13
(1,1415)	1:A:130:LEU:HD21	1:A:142:ALA:HA	17	0.13
(1,1415)	1:A:130:LEU:HD22	1:A:142:ALA:HA	17	0.13
(1,1415)	1:A:130:LEU:HD23	1:A:142:ALA:HA	17	0.13
(1,1400)	1:A:117:LEU:HD11	1:A:133:MET:HA	3	0.13
(1,1400)	1:A:117:LEU:HD12	1:A:133:MET:HA	3	0.13
(1,1400)	1:A:117:LEU:HD13	1:A:133:MET:HA	3	0.13
(1,1400)	1:A:117:LEU:HD21	1:A:133:MET:HA	3	0.13
(1,1400)	1:A:117:LEU:HD22	1:A:133:MET:HA	3	0.13
(1,1400)	1:A:117:LEU:HD23	1:A:133:MET:HA	3	0.13
(1,1371)	1:A:105:LEU:HD11	1:A:133:MET:HA	9	0.13
(1,1371)	1:A:105:LEU:HD12	1:A:133:MET:HA	9	0.13
(1,1371)	1:A:105:LEU:HD13	1:A:133:MET:HA	9	0.13
(1,1371)	1:A:105:LEU:HD21	1:A:133:MET:HA	9	0.13
(1,1371)	1:A:105:LEU:HD22	1:A:133:MET:HA	9	0.13
(1,1371)	1:A:105:LEU:HD23	1:A:133:MET:HA	9	0.13
(1,1371)	1:A:105:LEU:HD11	1:A:133:MET:HA	17	0.13
(1,1371)	1:A:105:LEU:HD12	1:A:133:MET:HA	17	0.13
(1,1371)	1:A:105:LEU:HD13	1:A:133:MET:HA	17	0.13
(1,1371)	1:A:105:LEU:HD21	1:A:133:MET:HA	17	0.13
(1,1371)	1:A:105:LEU:HD22	1:A:133:MET:HA	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1371)	1:A:105:LEU:HD23	1:A:133:MET:HA	17	0.13
(1,1329)	1:A:101:PHE:HZ	1:A:112:VAL:HG11	3	0.13
(1,1329)	1:A:101:PHE:HZ	1:A:112:VAL:HG12	3	0.13
(1,1329)	1:A:101:PHE:HZ	1:A:112:VAL:HG13	3	0.13
(1,1238)	1:A:83:ILE:HG12	1:A:221:LEU:HA	3	0.13
(1,1238)	1:A:83:ILE:HG13	1:A:221:LEU:HA	3	0.13
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD11	8	0.13
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD12	8	0.13
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD13	8	0.13
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD21	8	0.13
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD22	8	0.13
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD23	8	0.13
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD11	8	0.13
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD12	8	0.13
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD13	8	0.13
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD21	8	0.13
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD22	8	0.13
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD23	8	0.13
(1,1151)	1:A:285:LEU:HB2	1:A:289:LEU:HG	5	0.13
(1,1151)	1:A:285:LEU:HB3	1:A:289:LEU:HG	5	0.13
(1,1098)	1:A:224:ALA:HB1	1:A:228:LEU:HD11	11	0.13
(1,1098)	1:A:224:ALA:HB1	1:A:228:LEU:HD12	11	0.13
(1,1098)	1:A:224:ALA:HB1	1:A:228:LEU:HD13	11	0.13
(1,1098)	1:A:224:ALA:HB1	1:A:228:LEU:HD21	11	0.13
(1,1098)	1:A:224:ALA:HB1	1:A:228:LEU:HD22	11	0.13
(1,1098)	1:A:224:ALA:HB1	1:A:228:LEU:HD23	11	0.13
(1,1098)	1:A:224:ALA:HB2	1:A:228:LEU:HD11	11	0.13
(1,1098)	1:A:224:ALA:HB2	1:A:228:LEU:HD12	11	0.13
(1,1098)	1:A:224:ALA:HB2	1:A:228:LEU:HD13	11	0.13
(1,1098)	1:A:224:ALA:HB2	1:A:228:LEU:HD21	11	0.13
(1,1098)	1:A:224:ALA:HB2	1:A:228:LEU:HD22	11	0.13
(1,1098)	1:A:224:ALA:HB2	1:A:228:LEU:HD23	11	0.13
(1,1098)	1:A:224:ALA:HB3	1:A:228:LEU:HD11	11	0.13
(1,1098)	1:A:224:ALA:HB3	1:A:228:LEU:HD12	11	0.13
(1,1098)	1:A:224:ALA:HB3	1:A:228:LEU:HD13	11	0.13
(1,1098)	1:A:224:ALA:HB3	1:A:228:LEU:HD21	11	0.13
(1,1098)	1:A:224:ALA:HB3	1:A:228:LEU:HD22	11	0.13
(1,1098)	1:A:224:ALA:HB3	1:A:228:LEU:HD23	11	0.13
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG11	3	0.13
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG12	3	0.13
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG13	3	0.13
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG21	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG22	3	0.13
(1,1047)	1:A:172:ARG:H	1:A:176:VAL:HG23	3	0.13
(2,73)	1:A:133:MET:H	1:A:129:THR:O	14	0.12
(2,73)	1:A:133:MET:H	1:A:129:THR:O	18	0.12
(2,39)	1:A:259:GLY:H	1:A:279:ALA:O	19	0.12
(2,19)	1:A:85:ASP:H	1:A:238:VAL:O	2	0.12
(2,19)	1:A:85:ASP:H	1:A:238:VAL:O	16	0.12
(2,19)	1:A:85:ASP:H	1:A:238:VAL:O	19	0.12
(2,157)	1:A:251:HIS:H	1:A:247:GLY:O	7	0.12
(2,146)	1:A:245:VAL:N	1:A:241:ARG:O	9	0.12
(2,119)	1:A:191:ARG:H	1:A:187:PRO:O	10	0.12
(1,950)	1:A:116:ASP:HB2	1:A:119:THR:HG21	15	0.12
(1,950)	1:A:116:ASP:HB2	1:A:119:THR:HG22	15	0.12
(1,950)	1:A:116:ASP:HB2	1:A:119:THR:HG23	15	0.12
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG11	19	0.12
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG12	19	0.12
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG13	19	0.12
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG21	19	0.12
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG22	19	0.12
(1,886)	1:A:94:ALA:HA	1:A:98:VAL:HG23	19	0.12
(1,883)	1:A:92:ASP:HB2	1:A:94:ALA:H	1	0.12
(1,883)	1:A:92:ASP:HB3	1:A:94:ALA:H	1	0.12
(1,883)	1:A:92:ASP:HB2	1:A:94:ALA:H	2	0.12
(1,883)	1:A:92:ASP:HB3	1:A:94:ALA:H	2	0.12
(1,832)	1:A:265:ALA:HB1	1:A:266:ASP:HA	15	0.12
(1,832)	1:A:265:ALA:HB2	1:A:266:ASP:HA	15	0.12
(1,832)	1:A:265:ALA:HB3	1:A:266:ASP:HA	15	0.12
(1,828)	1:A:264:ARG:HB2	1:A:265:ALA:HB1	15	0.12
(1,828)	1:A:264:ARG:HB2	1:A:265:ALA:HB2	15	0.12
(1,828)	1:A:264:ARG:HB2	1:A:265:ALA:HB3	15	0.12
(1,828)	1:A:264:ARG:HB3	1:A:265:ALA:HB1	15	0.12
(1,828)	1:A:264:ARG:HB3	1:A:265:ALA:HB2	15	0.12
(1,828)	1:A:264:ARG:HB3	1:A:265:ALA:HB3	15	0.12
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD11	3	0.12
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD12	3	0.12
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD13	3	0.12
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD11	12	0.12
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD12	12	0.12
(1,823)	1:A:252:GLY:HA2	1:A:253:ILE:HD13	12	0.12
(1,802)	1:A:244:ASP:HB2	1:A:245:VAL:HB	5	0.12
(1,802)	1:A:244:ASP:HB3	1:A:245:VAL:HB	5	0.12
(1,791)	1:A:237:MET:HE1	1:A:238:VAL:HB	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,791)	1:A:237:MET:HE2	1:A:238:VAL:HB	16	0.12
(1,791)	1:A:237:MET:HE3	1:A:238:VAL:HB	16	0.12
(1,779)	1:A:229:ARG:H	1:A:230:PRO:HA	7	0.12
(1,682)	1:A:175:GLY:H	1:A:176:VAL:HB	12	0.12
(1,641)	1:A:164:ILE:HG12	1:A:165:GLY:H	1	0.12
(1,641)	1:A:164:ILE:HG13	1:A:165:GLY:H	1	0.12
(1,639)	1:A:161:PHE:HD1	1:A:162:ASP:H	13	0.12
(1,639)	1:A:161:PHE:HD2	1:A:162:ASP:H	13	0.12
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB1	4	0.12
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB2	4	0.12
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB3	4	0.12
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB1	4	0.12
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB2	4	0.12
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB3	4	0.12
(1,501)	1:A:111:PRO:HB3	1:A:112:VAL:H	7	0.12
(1,430)	1:A:83:ILE:HD11	1:A:84:PHE:H	18	0.12
(1,430)	1:A:83:ILE:HD12	1:A:84:PHE:H	18	0.12
(1,430)	1:A:83:ILE:HD13	1:A:84:PHE:H	18	0.12
(1,354)	1:A:264:ARG:HA	1:A:264:ARG:HD2	15	0.12
(1,354)	1:A:264:ARG:HA	1:A:264:ARG:HD3	15	0.12
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG2	16	0.12
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG3	16	0.12
(1,169)	1:A:157:MET:H	1:A:157:MET:HE1	1	0.12
(1,169)	1:A:157:MET:H	1:A:157:MET:HE2	1	0.12
(1,169)	1:A:157:MET:H	1:A:157:MET:HE3	1	0.12
(1,1607)	1:A:237:MET:HA	1:A:248:ALA:HB1	1	0.12
(1,1607)	1:A:237:MET:HA	1:A:248:ALA:HB2	1	0.12
(1,1607)	1:A:237:MET:HA	1:A:248:ALA:HB3	1	0.12
(1,1584)	1:A:225:LEU:HD11	1:A:251:HIS:HB2	12	0.12
(1,1584)	1:A:225:LEU:HD11	1:A:251:HIS:HB3	12	0.12
(1,1584)	1:A:225:LEU:HD12	1:A:251:HIS:HB2	12	0.12
(1,1584)	1:A:225:LEU:HD12	1:A:251:HIS:HB3	12	0.12
(1,1584)	1:A:225:LEU:HD13	1:A:251:HIS:HB2	12	0.12
(1,1584)	1:A:225:LEU:HD13	1:A:251:HIS:HB3	12	0.12
(1,1584)	1:A:225:LEU:HD21	1:A:251:HIS:HB2	12	0.12
(1,1584)	1:A:225:LEU:HD21	1:A:251:HIS:HB3	12	0.12
(1,1584)	1:A:225:LEU:HD22	1:A:251:HIS:HB2	12	0.12
(1,1584)	1:A:225:LEU:HD22	1:A:251:HIS:HB3	12	0.12
(1,1584)	1:A:225:LEU:HD23	1:A:251:HIS:HB2	12	0.12
(1,1584)	1:A:225:LEU:HD23	1:A:251:HIS:HB3	12	0.12
(1,1507)	1:A:179:ALA:HB1	1:A:204:VAL:HB	1	0.12
(1,1507)	1:A:179:ALA:HB2	1:A:204:VAL:HB	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1507)	1:A:179:ALA:HB3	1:A:204:VAL:HB	1	0.12
(1,1497)	1:A:174:ALA:HB1	1:A:291:VAL:HB	4	0.12
(1,1497)	1:A:174:ALA:HB2	1:A:291:VAL:HB	4	0.12
(1,1497)	1:A:174:ALA:HB3	1:A:291:VAL:HB	4	0.12
(1,1475)	1:A:171:LEU:HA	1:A:291:VAL:HA	18	0.12
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG11	11	0.12
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG12	11	0.12
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG13	11	0.12
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG21	11	0.12
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG22	11	0.12
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG23	11	0.12
(1,1459)	1:A:167:LEU:HD11	1:A:282:ILE:HD11	6	0.12
(1,1459)	1:A:167:LEU:HD11	1:A:282:ILE:HD12	6	0.12
(1,1459)	1:A:167:LEU:HD11	1:A:282:ILE:HD13	6	0.12
(1,1459)	1:A:167:LEU:HD12	1:A:282:ILE:HD11	6	0.12
(1,1459)	1:A:167:LEU:HD12	1:A:282:ILE:HD12	6	0.12
(1,1459)	1:A:167:LEU:HD12	1:A:282:ILE:HD13	6	0.12
(1,1459)	1:A:167:LEU:HD13	1:A:282:ILE:HD11	6	0.12
(1,1459)	1:A:167:LEU:HD13	1:A:282:ILE:HD12	6	0.12
(1,1459)	1:A:167:LEU:HD13	1:A:282:ILE:HD13	6	0.12
(1,1459)	1:A:167:LEU:HD21	1:A:282:ILE:HD11	6	0.12
(1,1459)	1:A:167:LEU:HD21	1:A:282:ILE:HD12	6	0.12
(1,1459)	1:A:167:LEU:HD21	1:A:282:ILE:HD13	6	0.12
(1,1459)	1:A:167:LEU:HD22	1:A:282:ILE:HD11	6	0.12
(1,1459)	1:A:167:LEU:HD22	1:A:282:ILE:HD12	6	0.12
(1,1459)	1:A:167:LEU:HD22	1:A:282:ILE:HD13	6	0.12
(1,1459)	1:A:167:LEU:HD23	1:A:282:ILE:HD11	6	0.12
(1,1459)	1:A:167:LEU:HD23	1:A:282:ILE:HD12	6	0.12
(1,1459)	1:A:167:LEU:HD23	1:A:282:ILE:HD13	6	0.12
(1,1432)	1:A:160:LEU:HB2	1:A:196:PHE:HD1	5	0.12
(1,1432)	1:A:160:LEU:HB2	1:A:196:PHE:HD2	5	0.12
(1,1432)	1:A:160:LEU:HB3	1:A:196:PHE:HD1	5	0.12
(1,1432)	1:A:160:LEU:HB3	1:A:196:PHE:HD2	5	0.12
(1,1395)	1:A:112:VAL:HA	1:A:133:MET:HE1	11	0.12
(1,1395)	1:A:112:VAL:HA	1:A:133:MET:HE2	11	0.12
(1,1395)	1:A:112:VAL:HA	1:A:133:MET:HE3	11	0.12
(1,1292)	1:A:89:THR:HG21	1:A:240:ASP:H	6	0.12
(1,1292)	1:A:89:THR:HG22	1:A:240:ASP:H	6	0.12
(1,1292)	1:A:89:THR:HG23	1:A:240:ASP:H	6	0.12
(1,1285)	1:A:85:ASP:HB2	1:A:180:VAL:HG11	4	0.12
(1,1285)	1:A:85:ASP:HB2	1:A:180:VAL:HG12	4	0.12
(1,1285)	1:A:85:ASP:HB2	1:A:180:VAL:HG13	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1285)	1:A:85:ASP:HB2	1:A:180:VAL:HG21	4	0.12
(1,1285)	1:A:85:ASP:HB2	1:A:180:VAL:HG22	4	0.12
(1,1285)	1:A:85:ASP:HB2	1:A:180:VAL:HG23	4	0.12
(1,1285)	1:A:85:ASP:HB3	1:A:180:VAL:HG11	4	0.12
(1,1285)	1:A:85:ASP:HB3	1:A:180:VAL:HG12	4	0.12
(1,1285)	1:A:85:ASP:HB3	1:A:180:VAL:HG13	4	0.12
(1,1285)	1:A:85:ASP:HB3	1:A:180:VAL:HG21	4	0.12
(1,1285)	1:A:85:ASP:HB3	1:A:180:VAL:HG22	4	0.12
(1,1285)	1:A:85:ASP:HB3	1:A:180:VAL:HG23	4	0.12
(1,1231)	1:A:83:ILE:HD11	1:A:180:VAL:HA	13	0.12
(1,1231)	1:A:83:ILE:HD12	1:A:180:VAL:HA	13	0.12
(1,1231)	1:A:83:ILE:HD13	1:A:180:VAL:HA	13	0.12
(1,1231)	1:A:83:ILE:HD11	1:A:180:VAL:HA	17	0.12
(1,1231)	1:A:83:ILE:HD12	1:A:180:VAL:HA	17	0.12
(1,1231)	1:A:83:ILE:HD13	1:A:180:VAL:HA	17	0.12
(1,1188)	1:A:81:LEU:HD11	1:A:203:GLU:HB2	20	0.12
(1,1188)	1:A:81:LEU:HD12	1:A:203:GLU:HB2	20	0.12
(1,1188)	1:A:81:LEU:HD13	1:A:203:GLU:HB2	20	0.12
(1,1188)	1:A:81:LEU:HD21	1:A:203:GLU:HB2	20	0.12
(1,1188)	1:A:81:LEU:HD22	1:A:203:GLU:HB2	20	0.12
(1,1188)	1:A:81:LEU:HD23	1:A:203:GLU:HB2	20	0.12
(1,1176)	1:A:80:GLN:HB2	1:A:234:ARG:HG2	12	0.12
(1,1176)	1:A:80:GLN:HB2	1:A:234:ARG:HG3	12	0.12
(1,1176)	1:A:80:GLN:HB3	1:A:234:ARG:HG2	12	0.12
(1,1176)	1:A:80:GLN:HB3	1:A:234:ARG:HG3	12	0.12
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD11	9	0.12
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD12	9	0.12
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD13	9	0.12
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD21	9	0.12
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD22	9	0.12
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD23	9	0.12
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD11	9	0.12
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD12	9	0.12
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD13	9	0.12
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD21	9	0.12
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD22	9	0.12
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD23	9	0.12
(1,1054)	1:A:185:ALA:HB1	1:A:187:PRO:HG3	2	0.12
(1,1054)	1:A:185:ALA:HB2	1:A:187:PRO:HG3	2	0.12
(1,1054)	1:A:185:ALA:HB3	1:A:187:PRO:HG3	2	0.12
(1,1002)	1:A:144:VAL:HG11	1:A:148:ALA:H	9	0.12
(1,1002)	1:A:144:VAL:HG12	1:A:148:ALA:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:A:144:VAL:HG13	1:A:148:ALA:H	9	0.12
(1,1002)	1:A:144:VAL:HG21	1:A:148:ALA:H	9	0.12
(1,1002)	1:A:144:VAL:HG22	1:A:148:ALA:H	9	0.12
(1,1002)	1:A:144:VAL:HG23	1:A:148:ALA:H	9	0.12
(2,95)	1:A:152:ALA:H	1:A:148:ALA:O	1	0.11
(2,69)	1:A:131:ARG:H	1:A:127:HIS:O	1	0.11
(2,69)	1:A:131:ARG:H	1:A:127:HIS:O	2	0.11
(2,69)	1:A:131:ARG:H	1:A:127:HIS:O	12	0.11
(2,39)	1:A:259:GLY:H	1:A:279:ALA:O	5	0.11
(2,39)	1:A:259:GLY:H	1:A:279:ALA:O	6	0.11
(2,19)	1:A:85:ASP:H	1:A:238:VAL:O	8	0.11
(2,159)	1:A:287:GLU:H	1:A:283:ASP:O	8	0.11
(2,157)	1:A:251:HIS:H	1:A:247:GLY:O	3	0.11
(2,11)	1:A:81:LEU:H	1:A:234:ARG:O	10	0.11
(2,11)	1:A:81:LEU:H	1:A:234:ARG:O	11	0.11
(1,869)	1:A:288:ALA:H	1:A:289:LEU:HD11	11	0.11
(1,869)	1:A:288:ALA:H	1:A:289:LEU:HD12	11	0.11
(1,869)	1:A:288:ALA:H	1:A:289:LEU:HD13	11	0.11
(1,869)	1:A:288:ALA:H	1:A:289:LEU:HD21	11	0.11
(1,869)	1:A:288:ALA:H	1:A:289:LEU:HD22	11	0.11
(1,869)	1:A:288:ALA:H	1:A:289:LEU:HD23	11	0.11
(1,849)	1:A:283:ASP:HB3	1:A:284:GLU:H	5	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG11	1	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG12	1	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG13	1	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG21	1	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG22	1	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG23	1	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG11	4	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG12	4	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG13	4	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG21	4	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG22	4	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG23	4	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG11	8	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG12	8	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG13	8	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG21	8	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG22	8	0.11
(1,794)	1:A:237:MET:H	1:A:238:VAL:HG23	8	0.11
(1,779)	1:A:229:ARG:H	1:A:230:PRO:HA	8	0.11
(1,722)	1:A:202:PHE:HA	1:A:203:GLU:HB3	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,682)	1:A:175:GLY:H	1:A:176:VAL:HB	2	0.11
(1,614)	1:A:153:ARG:HG2	1:A:154:GLY:H	6	0.11
(1,614)	1:A:153:ARG:HG3	1:A:154:GLY:H	6	0.11
(1,605)	1:A:151:SER:H	1:A:152:ALA:HB1	10	0.11
(1,605)	1:A:151:SER:H	1:A:152:ALA:HB2	10	0.11
(1,605)	1:A:151:SER:H	1:A:152:ALA:HB3	10	0.11
(1,605)	1:A:151:SER:H	1:A:152:ALA:HB1	16	0.11
(1,605)	1:A:151:SER:H	1:A:152:ALA:HB2	16	0.11
(1,605)	1:A:151:SER:H	1:A:152:ALA:HB3	16	0.11
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB1	2	0.11
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB2	2	0.11
(1,586)	1:A:147:ARG:HB2	1:A:148:ALA:HB3	2	0.11
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB1	2	0.11
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB2	2	0.11
(1,586)	1:A:147:ARG:HB3	1:A:148:ALA:HB3	2	0.11
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB1	5	0.11
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB2	5	0.11
(1,563)	1:A:141:GLU:HG2	1:A:142:ALA:HB3	5	0.11
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB1	5	0.11
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB2	5	0.11
(1,563)	1:A:141:GLU:HG3	1:A:142:ALA:HB3	5	0.11
(1,547)	1:A:132:ALA:HB1	1:A:133:MET:HG3	8	0.11
(1,547)	1:A:132:ALA:HB2	1:A:133:MET:HG3	8	0.11
(1,547)	1:A:132:ALA:HB3	1:A:133:MET:HG3	8	0.11
(1,547)	1:A:132:ALA:HB1	1:A:133:MET:HG3	14	0.11
(1,547)	1:A:132:ALA:HB2	1:A:133:MET:HG3	14	0.11
(1,547)	1:A:132:ALA:HB3	1:A:133:MET:HG3	14	0.11
(1,502)	1:A:111:PRO:HB2	1:A:112:VAL:HA	15	0.11
(1,502)	1:A:111:PRO:HB2	1:A:112:VAL:HA	17	0.11
(1,501)	1:A:111:PRO:HB3	1:A:112:VAL:H	6	0.11
(1,475)	1:A:105:LEU:HB3	1:A:106:ASN:HA	2	0.11
(1,431)	1:A:83:ILE:HG12	1:A:84:PHE:H	1	0.11
(1,431)	1:A:83:ILE:HG13	1:A:84:PHE:H	1	0.11
(1,431)	1:A:83:ILE:HG12	1:A:84:PHE:H	20	0.11
(1,431)	1:A:83:ILE:HG13	1:A:84:PHE:H	20	0.11
(1,354)	1:A:264:ARG:HA	1:A:264:ARG:HD2	4	0.11
(1,354)	1:A:264:ARG:HA	1:A:264:ARG:HD3	4	0.11
(1,32)	1:A:95:ARG:HB2	1:A:95:ARG:HD2	12	0.11
(1,32)	1:A:95:ARG:HB2	1:A:95:ARG:HD3	12	0.11
(1,32)	1:A:95:ARG:HB3	1:A:95:ARG:HD2	12	0.11
(1,32)	1:A:95:ARG:HB3	1:A:95:ARG:HD3	12	0.11
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG2	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG3	6	0.11
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG2	17	0.11
(1,280)	1:A:227:GLN:H	1:A:227:GLN:HG3	17	0.11
(1,1574)	1:A:221:LEU:HD11	1:A:248:ALA:H	10	0.11
(1,1574)	1:A:221:LEU:HD12	1:A:248:ALA:H	10	0.11
(1,1574)	1:A:221:LEU:HD13	1:A:248:ALA:H	10	0.11
(1,1574)	1:A:221:LEU:HD21	1:A:248:ALA:H	10	0.11
(1,1574)	1:A:221:LEU:HD22	1:A:248:ALA:H	10	0.11
(1,1574)	1:A:221:LEU:HD23	1:A:248:ALA:H	10	0.11
(1,1551)	1:A:199:GLU:HB2	1:A:205:ILE:HD11	1	0.11
(1,1551)	1:A:199:GLU:HB2	1:A:205:ILE:HD12	1	0.11
(1,1551)	1:A:199:GLU:HB2	1:A:205:ILE:HD13	1	0.11
(1,1551)	1:A:199:GLU:HB3	1:A:205:ILE:HD11	1	0.11
(1,1551)	1:A:199:GLU:HB3	1:A:205:ILE:HD12	1	0.11
(1,1551)	1:A:199:GLU:HB3	1:A:205:ILE:HD13	1	0.11
(1,153)	1:A:146:TYR:H	1:A:146:TYR:HD1	7	0.11
(1,153)	1:A:146:TYR:H	1:A:146:TYR:HD2	7	0.11
(1,153)	1:A:146:TYR:H	1:A:146:TYR:HD1	11	0.11
(1,153)	1:A:146:TYR:H	1:A:146:TYR:HD2	11	0.11
(1,1527)	1:A:180:VAL:HG11	1:A:202:PHE:HE1	8	0.11
(1,1527)	1:A:180:VAL:HG11	1:A:202:PHE:HE2	8	0.11
(1,1527)	1:A:180:VAL:HG12	1:A:202:PHE:HE1	8	0.11
(1,1527)	1:A:180:VAL:HG12	1:A:202:PHE:HE2	8	0.11
(1,1527)	1:A:180:VAL:HG13	1:A:202:PHE:HE1	8	0.11
(1,1527)	1:A:180:VAL:HG13	1:A:202:PHE:HE2	8	0.11
(1,1527)	1:A:180:VAL:HG11	1:A:202:PHE:HE1	19	0.11
(1,1527)	1:A:180:VAL:HG11	1:A:202:PHE:HE2	19	0.11
(1,1527)	1:A:180:VAL:HG12	1:A:202:PHE:HE1	19	0.11
(1,1527)	1:A:180:VAL:HG12	1:A:202:PHE:HE2	19	0.11
(1,1527)	1:A:180:VAL:HG13	1:A:202:PHE:HE1	19	0.11
(1,1527)	1:A:180:VAL:HG13	1:A:202:PHE:HE2	19	0.11
(1,1515)	1:A:180:VAL:HB	1:A:205:ILE:HD11	9	0.11
(1,1515)	1:A:180:VAL:HB	1:A:205:ILE:HD12	9	0.11
(1,1515)	1:A:180:VAL:HB	1:A:205:ILE:HD13	9	0.11
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG11	15	0.11
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG12	15	0.11
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG13	15	0.11
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG21	15	0.11
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG22	15	0.11
(1,1472)	1:A:170:ASP:H	1:A:291:VAL:HG23	15	0.11
(1,1459)	1:A:167:LEU:HD11	1:A:282:ILE:HD11	19	0.11
(1,1459)	1:A:167:LEU:HD11	1:A:282:ILE:HD12	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1459)	1:A:167:LEU:HD11	1:A:282:ILE:HD13	19	0.11
(1,1459)	1:A:167:LEU:HD12	1:A:282:ILE:HD11	19	0.11
(1,1459)	1:A:167:LEU:HD12	1:A:282:ILE:HD12	19	0.11
(1,1459)	1:A:167:LEU:HD12	1:A:282:ILE:HD13	19	0.11
(1,1459)	1:A:167:LEU:HD13	1:A:282:ILE:HD11	19	0.11
(1,1459)	1:A:167:LEU:HD13	1:A:282:ILE:HD12	19	0.11
(1,1459)	1:A:167:LEU:HD13	1:A:282:ILE:HD13	19	0.11
(1,1459)	1:A:167:LEU:HD21	1:A:282:ILE:HD11	19	0.11
(1,1459)	1:A:167:LEU:HD21	1:A:282:ILE:HD12	19	0.11
(1,1459)	1:A:167:LEU:HD21	1:A:282:ILE:HD13	19	0.11
(1,1459)	1:A:167:LEU:HD22	1:A:282:ILE:HD11	19	0.11
(1,1459)	1:A:167:LEU:HD22	1:A:282:ILE:HD12	19	0.11
(1,1459)	1:A:167:LEU:HD22	1:A:282:ILE:HD13	19	0.11
(1,1459)	1:A:167:LEU:HD23	1:A:282:ILE:HD11	19	0.11
(1,1459)	1:A:167:LEU:HD23	1:A:282:ILE:HD12	19	0.11
(1,1459)	1:A:167:LEU:HD23	1:A:282:ILE:HD13	19	0.11
(1,1458)	1:A:167:LEU:HD11	1:A:282:ILE:HB	1	0.11
(1,1458)	1:A:167:LEU:HD12	1:A:282:ILE:HB	1	0.11
(1,1458)	1:A:167:LEU:HD13	1:A:282:ILE:HB	1	0.11
(1,1458)	1:A:167:LEU:HD21	1:A:282:ILE:HB	1	0.11
(1,1458)	1:A:167:LEU:HD22	1:A:282:ILE:HB	1	0.11
(1,1458)	1:A:167:LEU:HD23	1:A:282:ILE:HB	1	0.11
(1,1458)	1:A:167:LEU:HD11	1:A:282:ILE:HB	2	0.11
(1,1458)	1:A:167:LEU:HD12	1:A:282:ILE:HB	2	0.11
(1,1458)	1:A:167:LEU:HD13	1:A:282:ILE:HB	2	0.11
(1,1458)	1:A:167:LEU:HD21	1:A:282:ILE:HB	2	0.11
(1,1458)	1:A:167:LEU:HD22	1:A:282:ILE:HB	2	0.11
(1,1458)	1:A:167:LEU:HD23	1:A:282:ILE:HB	2	0.11
(1,1458)	1:A:167:LEU:HD11	1:A:282:ILE:HB	4	0.11
(1,1458)	1:A:167:LEU:HD12	1:A:282:ILE:HB	4	0.11
(1,1458)	1:A:167:LEU:HD13	1:A:282:ILE:HB	4	0.11
(1,1458)	1:A:167:LEU:HD21	1:A:282:ILE:HB	4	0.11
(1,1458)	1:A:167:LEU:HD22	1:A:282:ILE:HB	4	0.11
(1,1458)	1:A:167:LEU:HD23	1:A:282:ILE:HB	4	0.11
(1,1458)	1:A:167:LEU:HD11	1:A:282:ILE:HB	8	0.11
(1,1458)	1:A:167:LEU:HD12	1:A:282:ILE:HB	8	0.11
(1,1458)	1:A:167:LEU:HD13	1:A:282:ILE:HB	8	0.11
(1,1458)	1:A:167:LEU:HD21	1:A:282:ILE:HB	8	0.11
(1,1458)	1:A:167:LEU:HD22	1:A:282:ILE:HB	8	0.11
(1,1458)	1:A:167:LEU:HD23	1:A:282:ILE:HB	8	0.11
(1,1458)	1:A:167:LEU:HD11	1:A:282:ILE:HB	16	0.11
(1,1458)	1:A:167:LEU:HD12	1:A:282:ILE:HB	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1458)	1:A:167:LEU:HD13	1:A:282:ILE:HB	16	0.11
(1,1458)	1:A:167:LEU:HD21	1:A:282:ILE:HB	16	0.11
(1,1458)	1:A:167:LEU:HD22	1:A:282:ILE:HB	16	0.11
(1,1458)	1:A:167:LEU:HD23	1:A:282:ILE:HB	16	0.11
(1,1458)	1:A:167:LEU:HD11	1:A:282:ILE:HB	17	0.11
(1,1458)	1:A:167:LEU:HD12	1:A:282:ILE:HB	17	0.11
(1,1458)	1:A:167:LEU:HD13	1:A:282:ILE:HB	17	0.11
(1,1458)	1:A:167:LEU:HD21	1:A:282:ILE:HB	17	0.11
(1,1458)	1:A:167:LEU:HD22	1:A:282:ILE:HB	17	0.11
(1,1458)	1:A:167:LEU:HD23	1:A:282:ILE:HB	17	0.11
(1,1458)	1:A:167:LEU:HD11	1:A:282:ILE:HB	18	0.11
(1,1458)	1:A:167:LEU:HD12	1:A:282:ILE:HB	18	0.11
(1,1458)	1:A:167:LEU:HD13	1:A:282:ILE:HB	18	0.11
(1,1458)	1:A:167:LEU:HD21	1:A:282:ILE:HB	18	0.11
(1,1458)	1:A:167:LEU:HD22	1:A:282:ILE:HB	18	0.11
(1,1458)	1:A:167:LEU:HD23	1:A:282:ILE:HB	18	0.11
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG11	15	0.11
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG12	15	0.11
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG13	15	0.11
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG21	15	0.11
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG22	15	0.11
(1,1457)	1:A:167:LEU:HA	1:A:291:VAL:HG23	15	0.11
(1,1438)	1:A:160:LEU:HD11	1:A:197:GLY:H	11	0.11
(1,1438)	1:A:160:LEU:HD12	1:A:197:GLY:H	11	0.11
(1,1438)	1:A:160:LEU:HD13	1:A:197:GLY:H	11	0.11
(1,1438)	1:A:160:LEU:HD21	1:A:197:GLY:H	11	0.11
(1,1438)	1:A:160:LEU:HD22	1:A:197:GLY:H	11	0.11
(1,1438)	1:A:160:LEU:HD23	1:A:197:GLY:H	11	0.11
(1,1422)	1:A:130:LEU:HG	1:A:139:ALA:HB1	6	0.11
(1,1422)	1:A:130:LEU:HG	1:A:139:ALA:HB2	6	0.11
(1,1422)	1:A:130:LEU:HG	1:A:139:ALA:HB3	6	0.11
(1,1416)	1:A:130:LEU:HD11	1:A:142:ALA:HB1	8	0.11
(1,1416)	1:A:130:LEU:HD11	1:A:142:ALA:HB2	8	0.11
(1,1416)	1:A:130:LEU:HD11	1:A:142:ALA:HB3	8	0.11
(1,1416)	1:A:130:LEU:HD12	1:A:142:ALA:HB1	8	0.11
(1,1416)	1:A:130:LEU:HD12	1:A:142:ALA:HB2	8	0.11
(1,1416)	1:A:130:LEU:HD12	1:A:142:ALA:HB3	8	0.11
(1,1416)	1:A:130:LEU:HD13	1:A:142:ALA:HB1	8	0.11
(1,1416)	1:A:130:LEU:HD13	1:A:142:ALA:HB2	8	0.11
(1,1416)	1:A:130:LEU:HD13	1:A:142:ALA:HB3	8	0.11
(1,1416)	1:A:130:LEU:HD21	1:A:142:ALA:HB1	8	0.11
(1,1416)	1:A:130:LEU:HD21	1:A:142:ALA:HB2	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1416)	1:A:130:LEU:HD21	1:A:142:ALA:HB3	8	0.11
(1,1416)	1:A:130:LEU:HD22	1:A:142:ALA:HB1	8	0.11
(1,1416)	1:A:130:LEU:HD22	1:A:142:ALA:HB2	8	0.11
(1,1416)	1:A:130:LEU:HD22	1:A:142:ALA:HB3	8	0.11
(1,1416)	1:A:130:LEU:HD23	1:A:142:ALA:HB1	8	0.11
(1,1416)	1:A:130:LEU:HD23	1:A:142:ALA:HB2	8	0.11
(1,1416)	1:A:130:LEU:HD23	1:A:142:ALA:HB3	8	0.11
(1,1415)	1:A:130:LEU:HD11	1:A:142:ALA:HA	16	0.11
(1,1415)	1:A:130:LEU:HD12	1:A:142:ALA:HA	16	0.11
(1,1415)	1:A:130:LEU:HD13	1:A:142:ALA:HA	16	0.11
(1,1415)	1:A:130:LEU:HD21	1:A:142:ALA:HA	16	0.11
(1,1415)	1:A:130:LEU:HD22	1:A:142:ALA:HA	16	0.11
(1,1415)	1:A:130:LEU:HD23	1:A:142:ALA:HA	16	0.11
(1,1411)	1:A:127:HIS:HB2	1:A:143:ILE:HD11	15	0.11
(1,1411)	1:A:127:HIS:HB2	1:A:143:ILE:HD12	15	0.11
(1,1411)	1:A:127:HIS:HB2	1:A:143:ILE:HD13	15	0.11
(1,1411)	1:A:127:HIS:HB3	1:A:143:ILE:HD11	15	0.11
(1,1411)	1:A:127:HIS:HB3	1:A:143:ILE:HD12	15	0.11
(1,1411)	1:A:127:HIS:HB3	1:A:143:ILE:HD13	15	0.11
(1,1287)	1:A:85:ASP:H	1:A:237:MET:HE1	1	0.11
(1,1287)	1:A:85:ASP:H	1:A:237:MET:HE2	1	0.11
(1,1287)	1:A:85:ASP:H	1:A:237:MET:HE3	1	0.11
(1,1284)	1:A:85:ASP:HA	1:A:237:MET:HE1	15	0.11
(1,1284)	1:A:85:ASP:HA	1:A:237:MET:HE2	15	0.11
(1,1284)	1:A:85:ASP:HA	1:A:237:MET:HE3	15	0.11
(1,1238)	1:A:83:ILE:HG12	1:A:221:LEU:HA	11	0.11
(1,1238)	1:A:83:ILE:HG13	1:A:221:LEU:HA	11	0.11
(1,1238)	1:A:83:ILE:HG12	1:A:221:LEU:HA	15	0.11
(1,1238)	1:A:83:ILE:HG13	1:A:221:LEU:HA	15	0.11
(1,1238)	1:A:83:ILE:HG12	1:A:221:LEU:HA	19	0.11
(1,1238)	1:A:83:ILE:HG13	1:A:221:LEU:HA	19	0.11
(1,1234)	1:A:83:ILE:HD11	1:A:221:LEU:HG	14	0.11
(1,1234)	1:A:83:ILE:HD12	1:A:221:LEU:HG	14	0.11
(1,1234)	1:A:83:ILE:HD13	1:A:221:LEU:HG	14	0.11
(1,1234)	1:A:83:ILE:HD11	1:A:221:LEU:HG	17	0.11
(1,1234)	1:A:83:ILE:HD12	1:A:221:LEU:HG	17	0.11
(1,1234)	1:A:83:ILE:HD13	1:A:221:LEU:HG	17	0.11
(1,1231)	1:A:83:ILE:HD11	1:A:180:VAL:HA	2	0.11
(1,1231)	1:A:83:ILE:HD12	1:A:180:VAL:HA	2	0.11
(1,1231)	1:A:83:ILE:HD13	1:A:180:VAL:HA	2	0.11
(1,1204)	1:A:82:VAL:HG11	1:A:171:LEU:HD11	3	0.11
(1,1204)	1:A:82:VAL:HG11	1:A:171:LEU:HD12	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1204)	1:A:82:VAL:HG11	1:A:171:LEU:HD13	3	0.11
(1,1204)	1:A:82:VAL:HG12	1:A:171:LEU:HD11	3	0.11
(1,1204)	1:A:82:VAL:HG12	1:A:171:LEU:HD12	3	0.11
(1,1204)	1:A:82:VAL:HG12	1:A:171:LEU:HD13	3	0.11
(1,1204)	1:A:82:VAL:HG13	1:A:171:LEU:HD11	3	0.11
(1,1204)	1:A:82:VAL:HG13	1:A:171:LEU:HD12	3	0.11
(1,1204)	1:A:82:VAL:HG13	1:A:171:LEU:HD13	3	0.11
(1,1204)	1:A:82:VAL:HG11	1:A:171:LEU:HD11	15	0.11
(1,1204)	1:A:82:VAL:HG11	1:A:171:LEU:HD12	15	0.11
(1,1204)	1:A:82:VAL:HG11	1:A:171:LEU:HD13	15	0.11
(1,1204)	1:A:82:VAL:HG12	1:A:171:LEU:HD11	15	0.11
(1,1204)	1:A:82:VAL:HG12	1:A:171:LEU:HD12	15	0.11
(1,1204)	1:A:82:VAL:HG12	1:A:171:LEU:HD13	15	0.11
(1,1204)	1:A:82:VAL:HG13	1:A:171:LEU:HD11	15	0.11
(1,1204)	1:A:82:VAL:HG13	1:A:171:LEU:HD12	15	0.11
(1,1204)	1:A:82:VAL:HG13	1:A:171:LEU:HD13	15	0.11
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD11	10	0.11
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD12	10	0.11
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD13	10	0.11
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD21	10	0.11
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD22	10	0.11
(1,1173)	1:A:79:PRO:HG2	1:A:235:LEU:HD23	10	0.11
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD11	10	0.11
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD12	10	0.11
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD13	10	0.11
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD21	10	0.11
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD22	10	0.11
(1,1173)	1:A:79:PRO:HG3	1:A:235:LEU:HD23	10	0.11
(1,1151)	1:A:285:LEU:HB2	1:A:289:LEU:HG	3	0.11
(1,1151)	1:A:285:LEU:HB3	1:A:289:LEU:HG	3	0.11
(1,1131)	1:A:251:HIS:HA	1:A:253:ILE:HD11	14	0.11
(1,1131)	1:A:251:HIS:HA	1:A:253:ILE:HD12	14	0.11
(1,1131)	1:A:251:HIS:HA	1:A:253:ILE:HD13	14	0.11
(1,1108)	1:A:228:LEU:H	1:A:231:LEU:HD11	11	0.11
(1,1108)	1:A:228:LEU:H	1:A:231:LEU:HD12	11	0.11
(1,1108)	1:A:228:LEU:H	1:A:231:LEU:HD13	11	0.11
(1,1108)	1:A:228:LEU:H	1:A:231:LEU:HD21	11	0.11
(1,1108)	1:A:228:LEU:H	1:A:231:LEU:HD22	11	0.11
(1,1108)	1:A:228:LEU:H	1:A:231:LEU:HD23	11	0.11
(1,1103)	1:A:226:ALA:HB1	1:A:229:ARG:HG2	2	0.11
(1,1103)	1:A:226:ALA:HB1	1:A:229:ARG:HG3	2	0.11
(1,1103)	1:A:226:ALA:HB2	1:A:229:ARG:HG2	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1103)	1:A:226:ALA:HB2	1:A:229:ARG:HG3	2	0.11
(1,1103)	1:A:226:ALA:HB3	1:A:229:ARG:HG2	2	0.11
(1,1103)	1:A:226:ALA:HB3	1:A:229:ARG:HG3	2	0.11
(1,1101)	1:A:226:ALA:HA	1:A:229:ARG:HD2	7	0.11
(1,1101)	1:A:226:ALA:HA	1:A:229:ARG:HD3	7	0.11

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

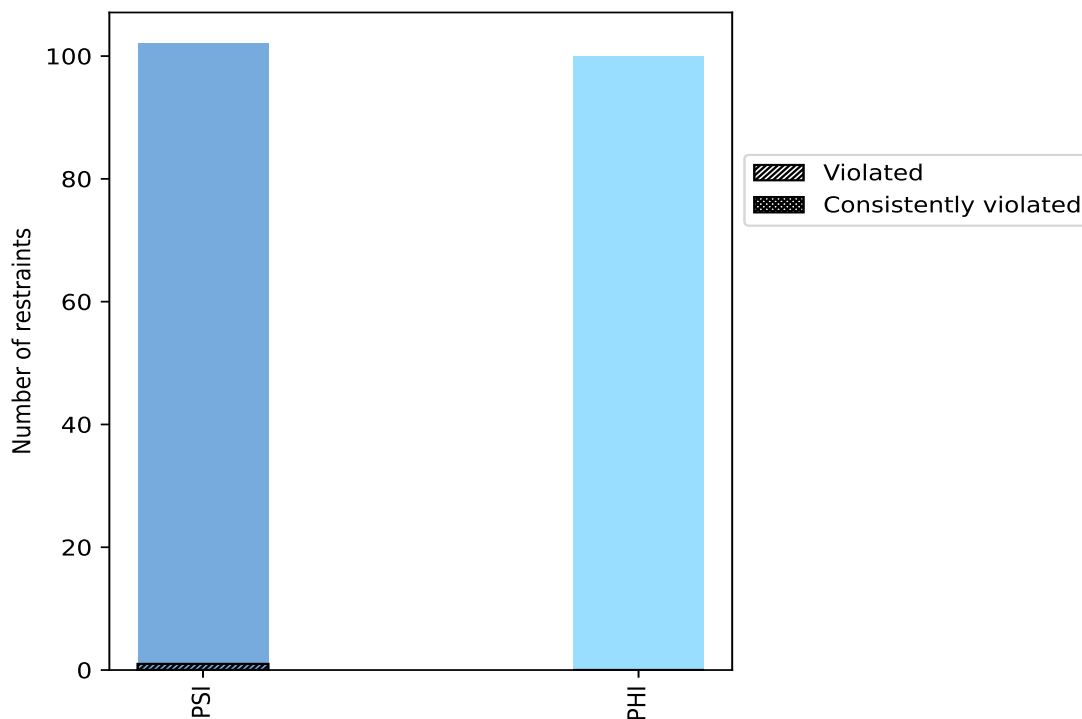
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	102	50.5	1	1.0	0.5	0	0.0	0.0
PHI	100	49.5	0	0.0	0.0	0	0.0	0.0
Total	202	100.0	1	0.5	0.5	0	0.0	0.0

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

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



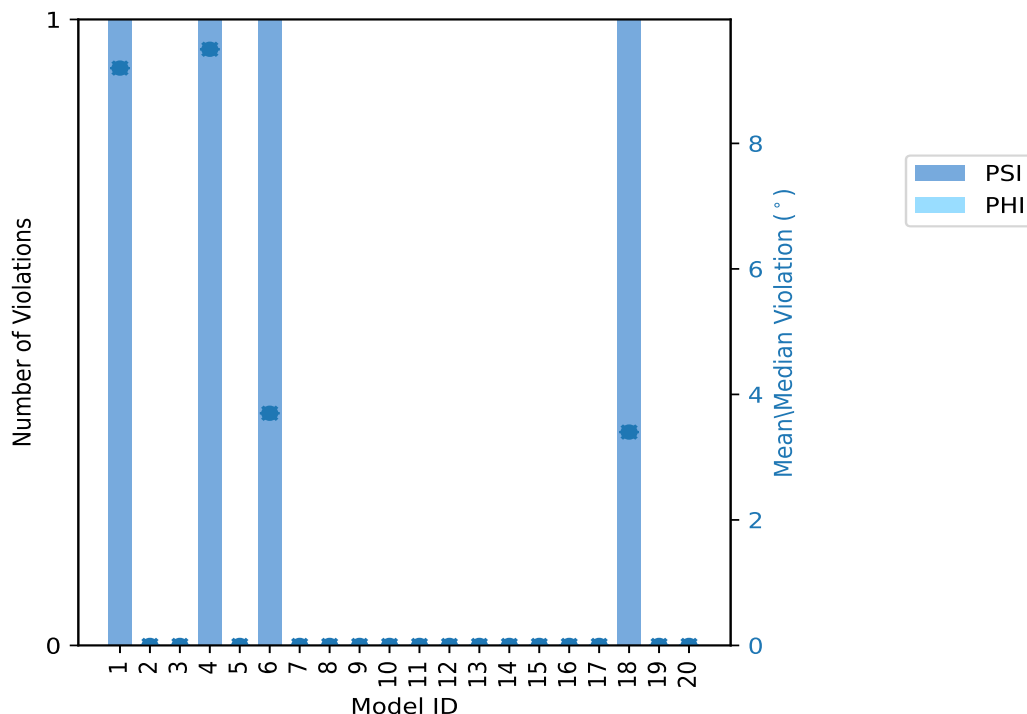
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	1	0	1	9.2	9.2	0.0	9.2
2	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0.0	0.0	0.0	0.0
4	1	0	1	9.5	9.5	0.0	9.5
5	0	0	0	0.0	0.0	0.0	0.0
6	1	0	1	3.7	3.7	0.0	3.7
7	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0.0	0.0	0.0	0.0
18	1	0	1	3.4	3.4	0.0	3.4
19	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0.0	0.0	0.0	0.0

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



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

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

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

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

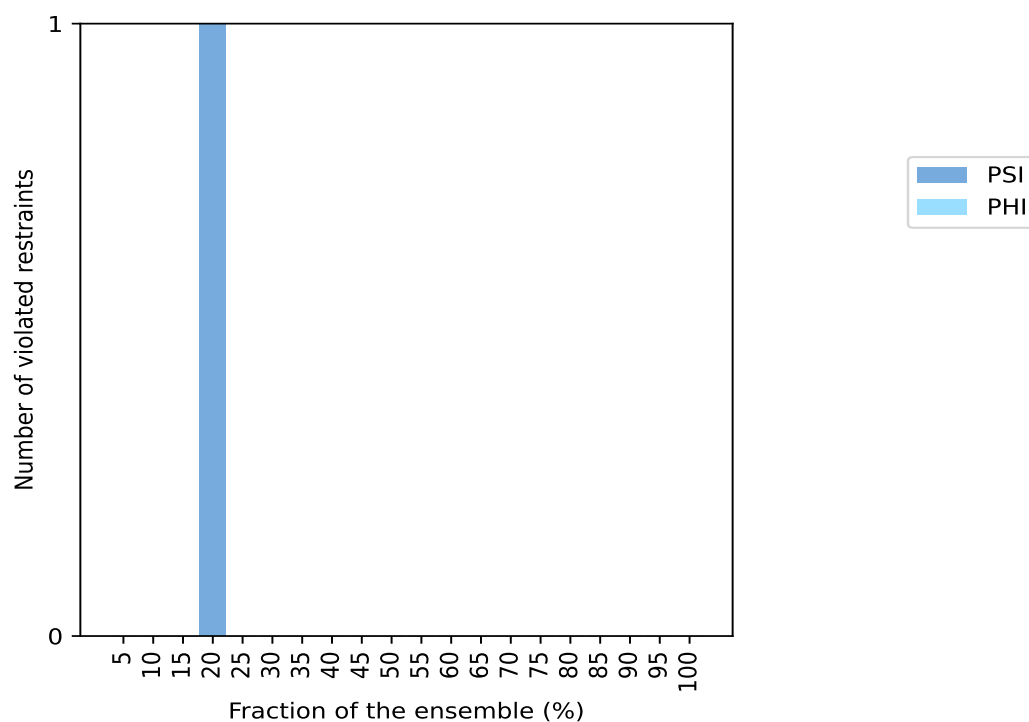
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

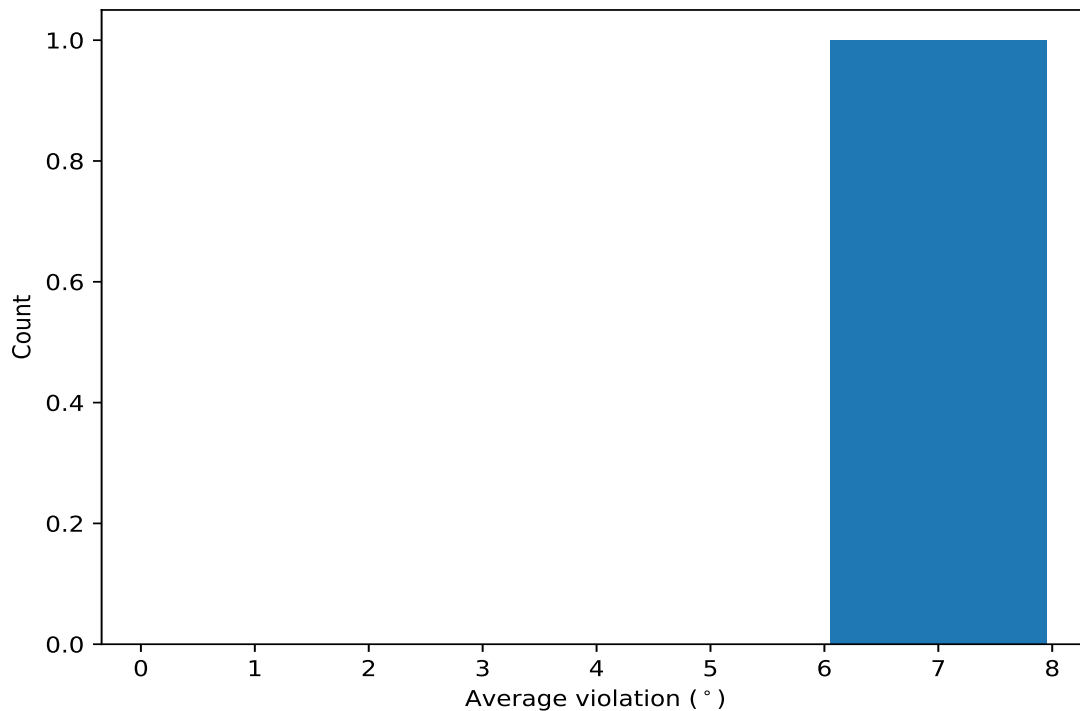


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,113)	1:A:181:ALA:N	1:A:181:ALA:CA	1:A:181:ALA:C	1:A:182:THR:N	4	6.45	2.9	6.45

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.

Data insufficient to plot histogram

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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,113)	1:A:181:ALA:N	1:A:181:ALA:CA	1:A:181:ALA:C	1:A:182:THR:N	4	9.5
(1,113)	1:A:181:ALA:N	1:A:181:ALA:CA	1:A:181:ALA:C	1:A:182:THR:N	1	9.2
(1,113)	1:A:181:ALA:N	1:A:181:ALA:CA	1:A:181:ALA:C	1:A:182:THR:N	6	3.7
(1,113)	1:A:181:ALA:N	1:A:181:ALA:CA	1:A:181:ALA:C	1:A:182:THR:N	18	3.4