Full wwPDB NMR Structure Validation Report (i)

Jun 5, 2023 – 06:13 PM JST

PDB ID	:	6KVG
BMRB ID	:	36286
Title	:	The solution structure of human Orc6
Authors	:	Liu, C.; Xu, N.; You, Y.; Zhu, G.
Deposited on	:	2019-09-04

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

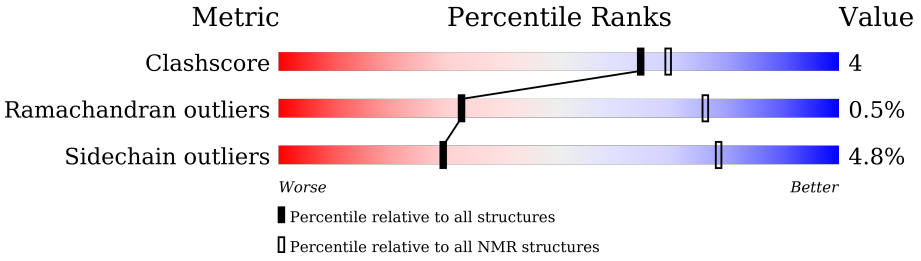
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 84%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	256	51% 6% 43%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 14 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:3-A:31, A:44-A:88 (74)	0.46	14
2	A:97-A:122, A:143-A:162, A:169-A:186 (64)	0.57	11
3	A:233-A:240 (8)	0.20	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 4 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4053 atoms, of which 2071 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	256	4053	1242	2071	346	378	16	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q9Y5N6
A	-2	PRO	-	expression tag	UNP Q9Y5N6
A	-1	GLY	-	expression tag	UNP Q9Y5N6
A	0	SER	-	expression tag	UNP Q9Y5N6

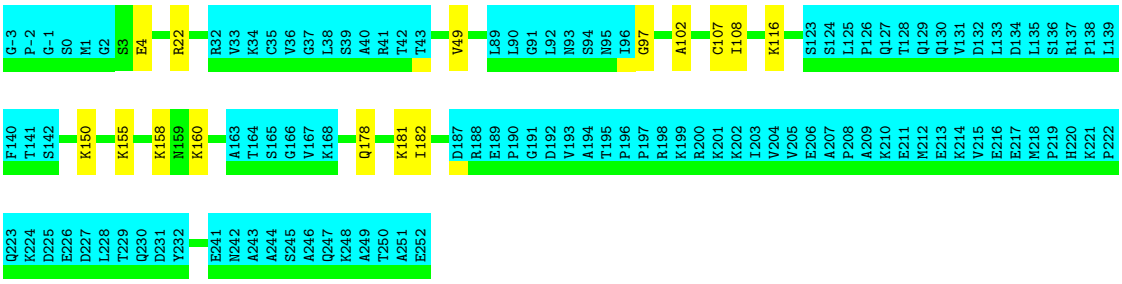
4 Residue-property plots (i)

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: Origin recognition complex subunit 6

Chain A: 51% 6% 43%



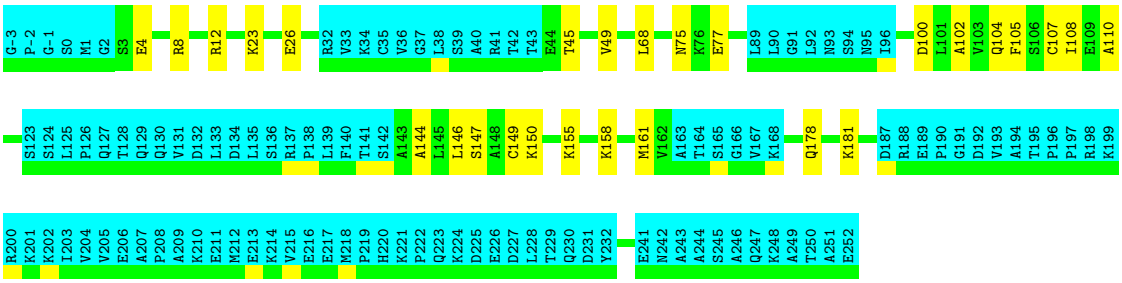
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Origin recognition complex subunit 6

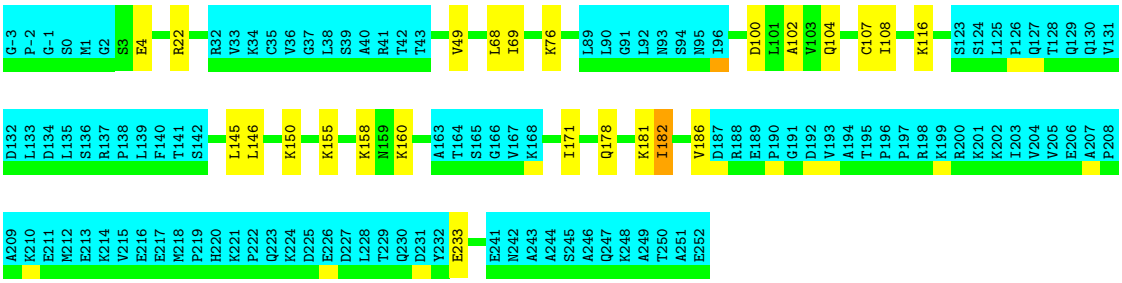
Chain A: 46% 11% 43%



4.2.2 Score per residue for model 2

- Molecule 1: Origin recognition complex subunit 6

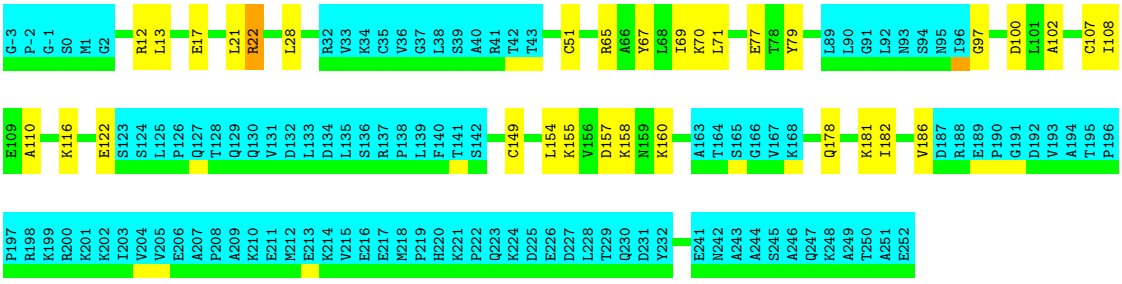
Chain A: 48% 9% 43%



4.2.3 Score per residue for model 3

- Molecule 1: Origin recognition complex subunit 6

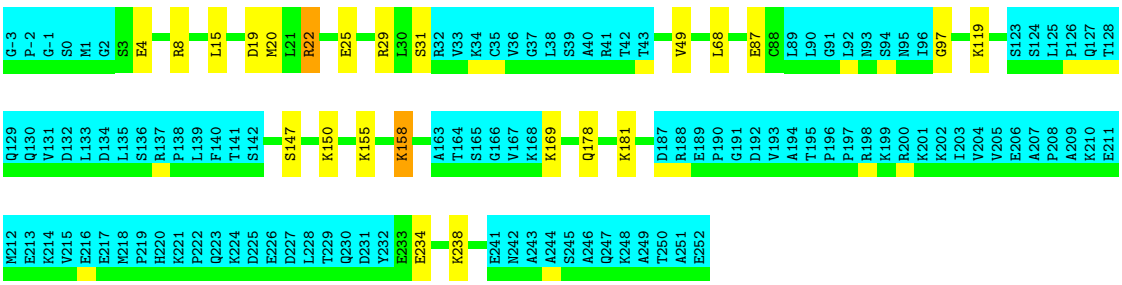
Chain A: 45% 12% 43%



4.2.4 Score per residue for model 4

- Molecule 1: Origin recognition complex subunit 6

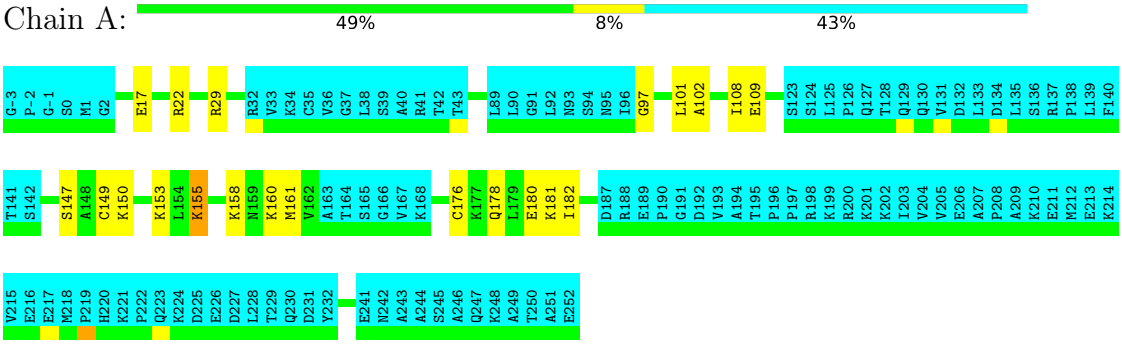
Chain A: 48% 8% • 43%



4.2.5 Score per residue for model 5

- Molecule 1: Origin recognition complex subunit 6

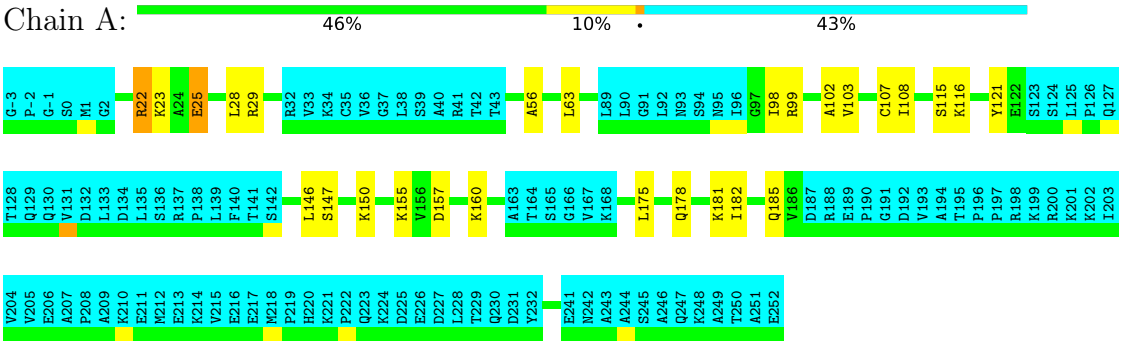
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Origin recognition complex subunit 6

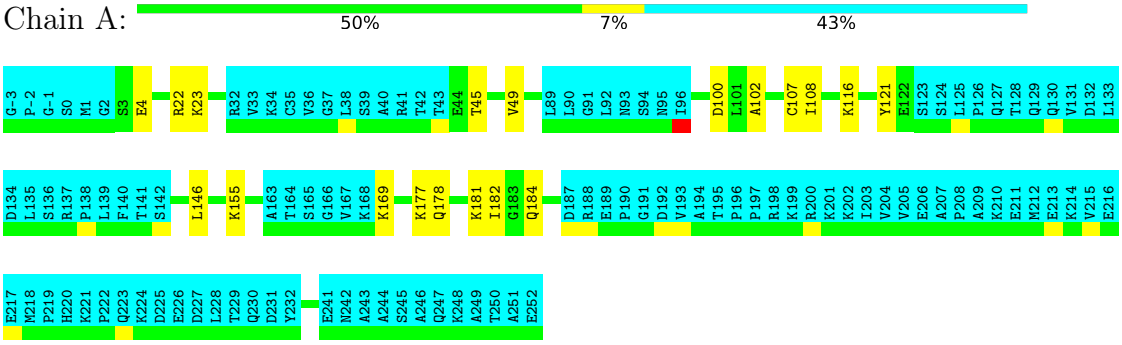
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: Origin recognition complex subunit 6

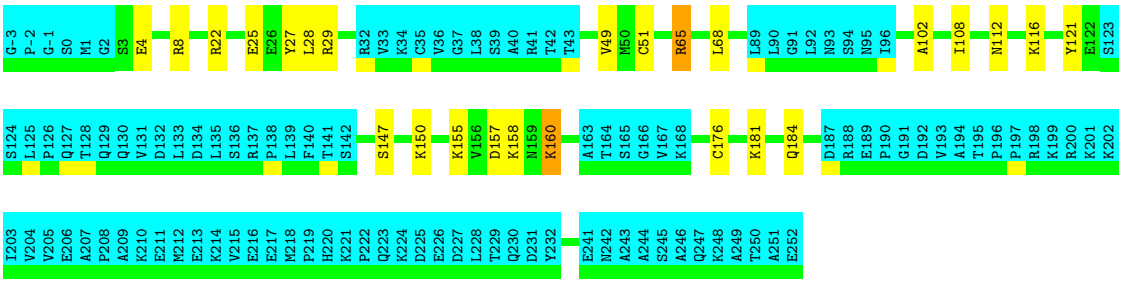
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: Origin recognition complex subunit 6

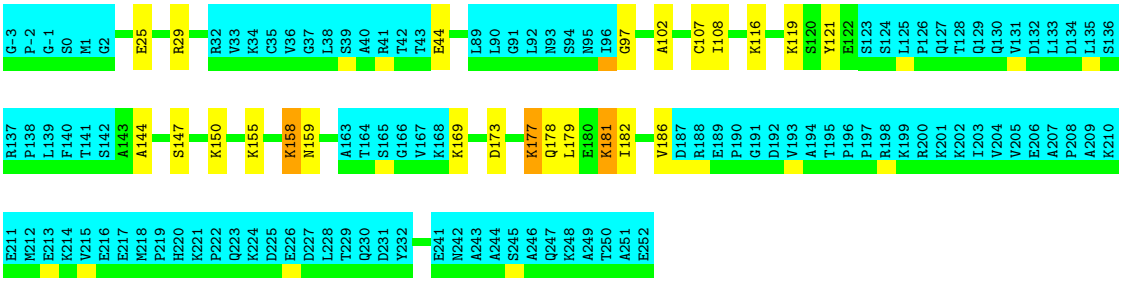
Chain A: 47% 9% • 43%



4.2.9 Score per residue for model 9

- Molecule 1: Origin recognition complex subunit 6

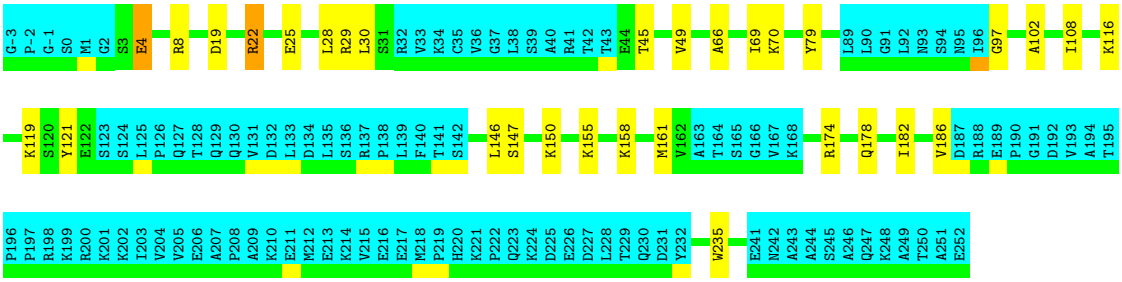
Chain A: 48% 8% • 43%



4.2.10 Score per residue for model 10

- Molecule 1: Origin recognition complex subunit 6

Chain A: 45% 11% • 43%



4.2.11 Score per residue for model 11

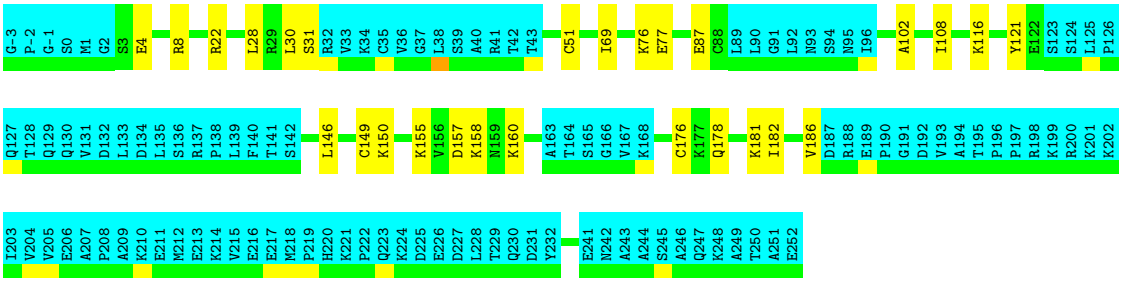
- Molecule 1: Origin recognition complex subunit 6

Chain A: 50% 7% 43%

4.2.12 Score per residue for model 12

- Molecule 1: Origin recognition complex subunit 6

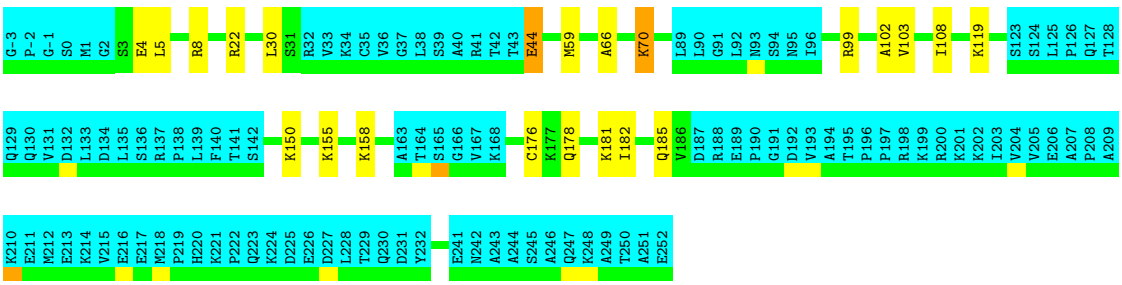
Chain A: 46% 11% 43%



4.2.13 Score per residue for model 13

- Molecule 1: Origin recognition complex subunit 6

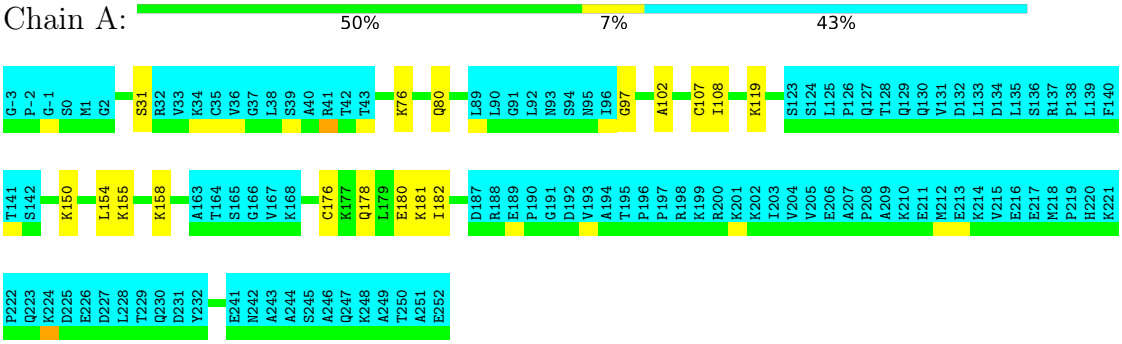
Chain A: 48% 8% • 43%



4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Origin recognition complex subunit 6

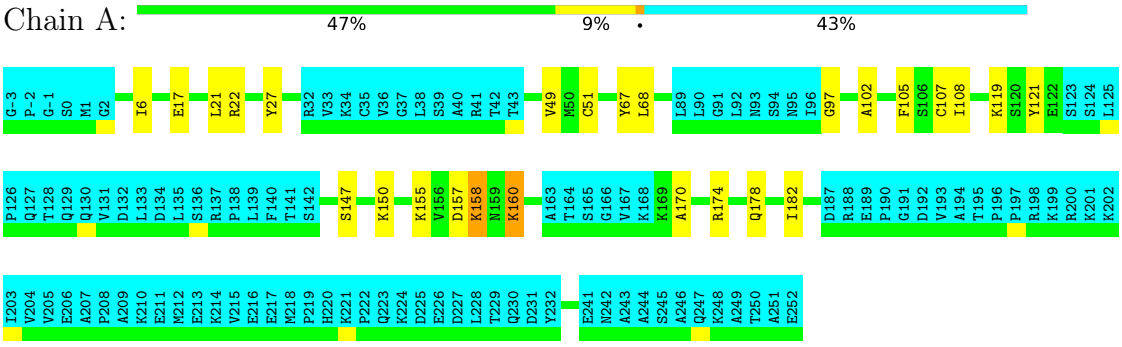
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: Origin recognition complex subunit 6

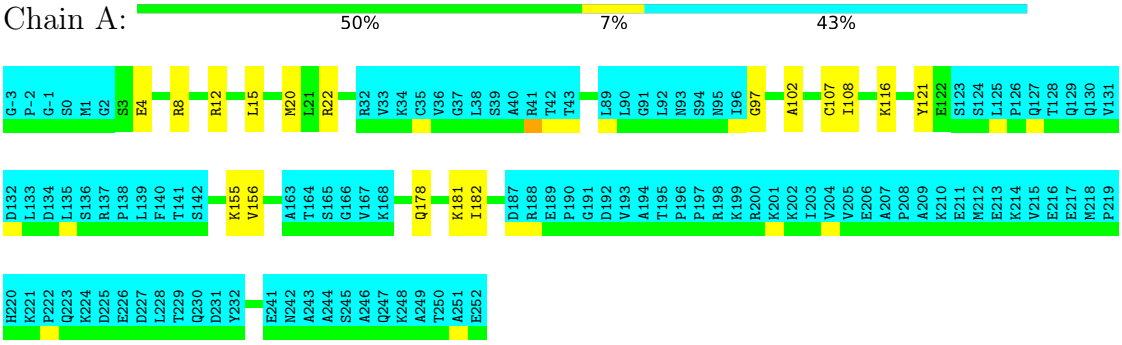
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: Origin recognition complex subunit 6

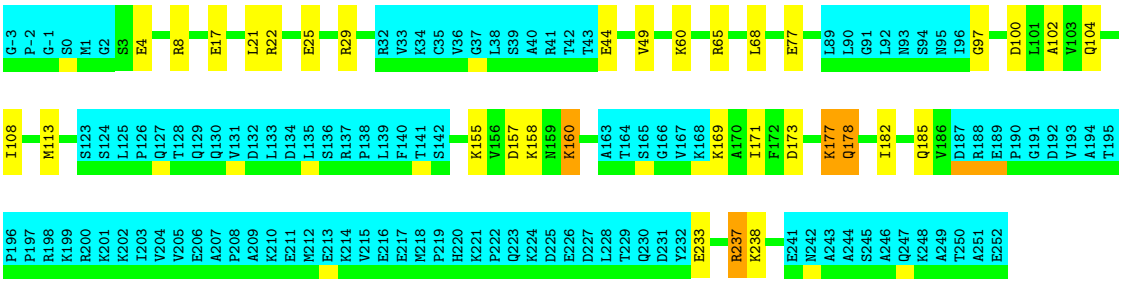
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: Origin recognition complex subunit 6

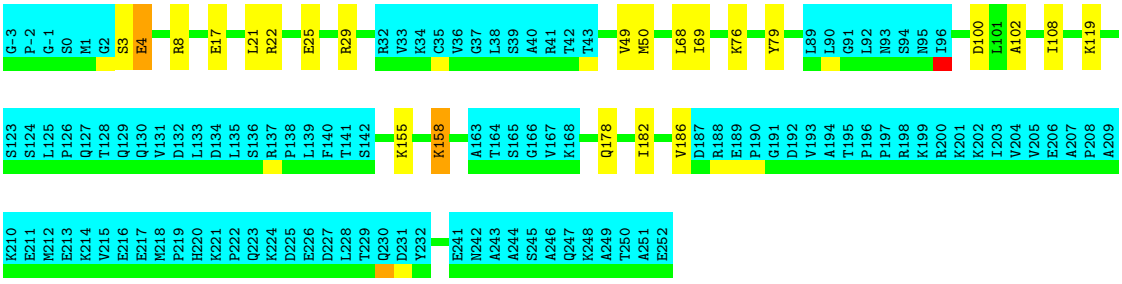
Chain A: 44% 11% • 43%



4.2.18 Score per residue for model 18

- Molecule 1: Origin recognition complex subunit 6

Chain A: 48% 8% • 43%



4.2.19 Score per residue for model 19

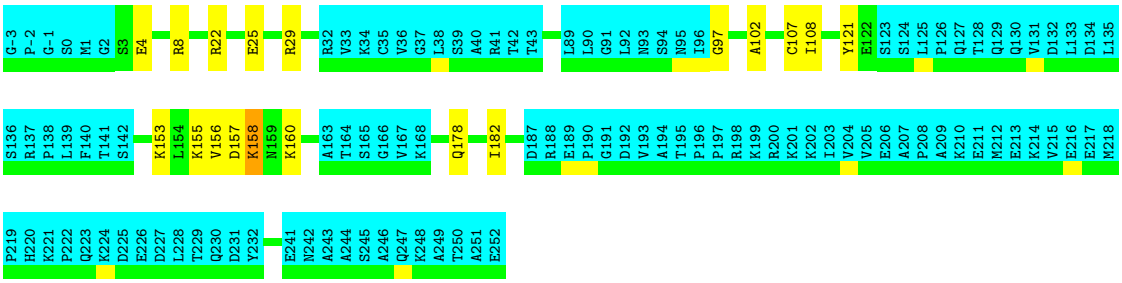
- Molecule 1: Origin recognition complex subunit 6

Chain A: 48% 9% 43%

4.2.20 Score per residue for model 20

- Molecule 1: Origin recognition complex subunit 6

Chain A: 50% 7% 43%



5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	
CYANA	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2711
Number of shifts mapped to atoms	2711
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality (i)

6.1 Standard geometry (i)

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

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
All	All	0	2

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	22	ARG	Sidechain	1
1	A	237	ARG	Sidechain	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1152	1228	1228	10±2
All	All	23040	24560	24560	199

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ALA:HA	1:A:107:CYS:SG	0.68	2.28	6	6
1:A:28:LEU:HB2	1:A:51:CYS:SG	0.63	2.32	12	2
1:A:4:GLU:O	1:A:8:ARG:HG3	0.61	1.95	16	8
1:A:102:ALA:HB1	1:A:108:ILE:HA	0.59	1.74	14	18
1:A:146:LEU:O	1:A:150:LYS:HG3	0.58	1.97	2	1
1:A:147:SER:O	1:A:150:LYS:HG2	0.58	1.98	5	9
1:A:107:CYS:SG	1:A:110:ALA:HB3	0.57	2.39	3	1
1:A:100:ASP:O	1:A:104:GLN:HG2	0.55	2.01	2	3
1:A:233:GLU:O	1:A:237:ARG:HD3	0.55	2.01	17	1
1:A:178:GLN:O	1:A:181:LYS:HG2	0.54	2.03	14	12
1:A:25:GLU:O	1:A:29:ARG:HG3	0.54	2.02	10	5
1:A:66:ALA:O	1:A:70:LYS:HD3	0.53	2.03	13	2
1:A:107:CYS:SG	1:A:149:CYS:HB2	0.53	2.42	3	1
1:A:176:CYS:O	1:A:180:GLU:HB2	0.52	2.04	5	2
1:A:49:VAL:CG1	1:A:68:LEU:HB2	0.51	2.35	17	7
1:A:158:LYS:HD3	1:A:158:LYS:H	0.51	1.65	4	4
1:A:56:ALA:HB3	1:A:63:LEU:HD11	0.51	1.81	6	1
1:A:107:CYS:SG	1:A:156:VAL:HG11	0.51	2.45	20	2
1:A:19:ASP:O	1:A:22:ARG:HG3	0.51	2.05	10	2
1:A:102:ALA:HB1	1:A:108:ILE:CA	0.51	2.36	14	9
1:A:109:GLU:OE2	1:A:153:LYS:HG3	0.50	2.06	5	1
1:A:181:LYS:O	1:A:185:GLN:HG2	0.49	2.08	6	2
1:A:178:GLN:O	1:A:182:ILE:HG12	0.48	2.08	2	1
1:A:112:ASN:O	1:A:116:LYS:HG2	0.48	2.09	8	1
1:A:12:ARG:HA	1:A:12:ARG:NE	0.48	2.24	1	1
1:A:150:LYS:O	1:A:154:LEU:HB2	0.47	2.09	14	1
1:A:45:THR:O	1:A:49:VAL:HG23	0.47	2.08	1	3
1:A:69:ILE:HG12	1:A:79:TYR:CG	0.47	2.44	3	2
1:A:49:VAL:HG13	1:A:68:LEU:HB2	0.47	1.87	17	1
1:A:25:GLU:O	1:A:29:ARG:HG2	0.47	2.10	17	3
1:A:107:CYS:SG	1:A:145:LEU:HB3	0.47	2.50	2	1
1:A:150:LYS:HE2	1:A:176:CYS:SG	0.47	2.50	13	3
1:A:65:ARG:HA	1:A:68:LEU:HG	0.46	1.87	19	3
1:A:173:ASP:O	1:A:177:LYS:HD3	0.46	2.11	17	1
1:A:17:GLU:O	1:A:21:LEU:HD23	0.46	2.11	17	5
1:A:182:ILE:O	1:A:186:VAL:HG23	0.45	2.11	18	7
1:A:67:TYR:O	1:A:71:LEU:HG	0.45	2.12	3	1
1:A:50:MET:HA	1:A:79:TYR:OH	0.45	2.10	18	1
1:A:170:ALA:O	1:A:174:ARG:HG2	0.45	2.10	15	1
1:A:112:ASN:O	1:A:116:LYS:HD3	0.45	2.11	11	1
1:A:22:ARG:HD2	1:A:23:LYS:N	0.45	2.26	7	1
1:A:69:ILE:HD13	1:A:76:LYS:HA	0.45	1.87	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:PHE:HB2	1:A:107:CYS:SG	0.44	2.52	15	2
1:A:4:GLU:H	1:A:4:GLU:CD	0.44	2.16	18	2
1:A:157:ASP:O	1:A:160:LYS:HG2	0.44	2.11	6	7
1:A:234:GLU:O	1:A:238:LYS:HG3	0.44	2.13	4	1
1:A:178:GLN:O	1:A:182:ILE:HG13	0.44	2.12	10	15
1:A:98:ILE:HD13	1:A:115:SER:OG	0.44	2.12	6	1
1:A:27:TYR:HB2	1:A:51:CYS:HB2	0.44	1.90	15	2
1:A:5:LEU:CD1	1:A:44:GLU:HB2	0.43	2.43	13	1
1:A:144:ALA:N	1:A:179:LEU:HD23	0.43	2.28	9	1
1:A:4:GLU:O	1:A:8:ARG:HG2	0.43	2.13	17	2
1:A:15:LEU:HD13	1:A:20:MET:SD	0.43	2.54	16	2
1:A:55:ALA:O	1:A:59:MET:HG2	0.43	2.14	19	1
1:A:158:LYS:HD2	1:A:159:ASN:N	0.42	2.29	9	1
1:A:44:GLU:CD	1:A:44:GLU:H	0.42	2.16	11	1
1:A:75:ASN:HB3	1:A:77:GLU:OE2	0.42	2.15	1	1
1:A:49:VAL:HG11	1:A:68:LEU:O	0.42	2.15	11	2
1:A:174:ARG:O	1:A:178:GLN:HG2	0.42	2.13	10	1
1:A:69:ILE:CD1	1:A:76:LYS:HD3	0.42	2.45	2	2
1:A:65:ARG:O	1:A:69:ILE:HG13	0.42	2.14	3	1
1:A:173:ASP:O	1:A:177:LYS:HE3	0.41	2.15	9	1
1:A:157:ASP:OD2	1:A:160:LYS:HB3	0.41	2.15	17	1
1:A:146:LEU:HA	1:A:149:CYS:SG	0.41	2.55	12	1
1:A:233:GLU:CD	1:A:233:GLU:H	0.41	2.18	2	1
1:A:69:ILE:CD1	1:A:76:LYS:HG3	0.41	2.45	12	1
1:A:4:GLU:OE1	1:A:5:LEU:HG	0.41	2.15	13	1
1:A:110:ALA:HB2	1:A:149:CYS:SG	0.41	2.56	1	1
1:A:12:ARG:HG3	1:A:13:LEU:HG	0.41	1.92	3	1
1:A:149:CYS:SG	1:A:155:LYS:HE2	0.41	2.56	5	1
1:A:99:ARG:O	1:A:103:VAL:HG23	0.41	2.16	13	2
1:A:76:LYS:HG2	1:A:80:GLN:NE2	0.41	2.31	14	1
1:A:22:ARG:HD3	1:A:23:LYS:N	0.40	2.31	6	1
1:A:23:LYS:O	1:A:26:GLU:HB3	0.40	2.16	1	1
1:A:109:GLU:OE2	1:A:155:LYS:HE2	0.40	2.17	5	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	146/256 (57%)	141±2 (96±1%)	5±2 (3±1%)	1±1 (0±0%)	32 76
All	All	2920/5120 (57%)	2813 (96%)	93 (3%)	14 (0%)	32 76

All 3 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	97	GLY	12
1	A	154	LEU	1
1	A	3	SER	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	127/220 (58%)	121±2 (95±2%)	6±2 (5±2%)	29 78
All	All	2540/4400 (58%)	2417 (95%)	123 (5%)	29 78

All 32 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	155	LYS	20
1	A	158	LYS	17
1	A	22	ARG	16
1	A	116	LYS	9
1	A	119	LYS	8
1	A	160	LYS	5
1	A	169	LYS	5
1	A	161	MET	4
1	A	4	GLU	3
1	A	70	LYS	3
1	A	77	GLU	3
1	A	177	LYS	3
1	A	30	LEU	3
1	A	28	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	175	LEU	2
1	A	181	LYS	2
1	A	44	GLU	2
1	A	178	GLN	2
1	A	182	ILE	1
1	A	122	GLU	1
1	A	17	GLU	1
1	A	29	ARG	1
1	A	101	LEU	1
1	A	25	GLU	1
1	A	65	ARG	1
1	A	87	GLU	1
1	A	59	MET	1
1	A	67	TYR	1
1	A	12	ARG	1
1	A	60	LYS	1
1	A	113	MET	1
1	A	153	LYS	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

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	2711
Number of shifts mapped to atoms	2711
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	245	-0.39 ± 0.05	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	229	0.08 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	224	-0.30 ± 0.11	None needed (< 0.5 ppm)
^{15}N	234	-0.10 ± 0.21	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 84%, i.e. 1731 atoms were assigned a chemical shift out of a possible 2068. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	720/729 (99%)	292/294 (99%)	285/292 (98%)	143/143 (100%)
Sidechain	982/1249 (79%)	683/815 (84%)	299/385 (78%)	0/49 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	29/90 (32%)	29/43 (67%)	0/45 (0%)	0/2 (0%)
Overall	1731/2068 (84%)	1004/1152 (87%)	584/722 (81%)	143/194 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 2711 atoms were assigned a chemical shift out of a possible 3504. 0 out of 46 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1176/1268 (93%)	473/512 (92%)	469/512 (92%)	234/244 (96%)
Sidechain	1506/2120 (71%)	1026/1377 (75%)	480/657 (73%)	0/86 (0%)
Aromatic	29/116 (25%)	29/56 (52%)	0/57 (0%)	0/3 (0%)
Overall	2711/3504 (77%)	1528/1945 (79%)	949/1226 (77%)	234/333 (70%)

7.1.4 Statistically unusual chemical shifts (i)

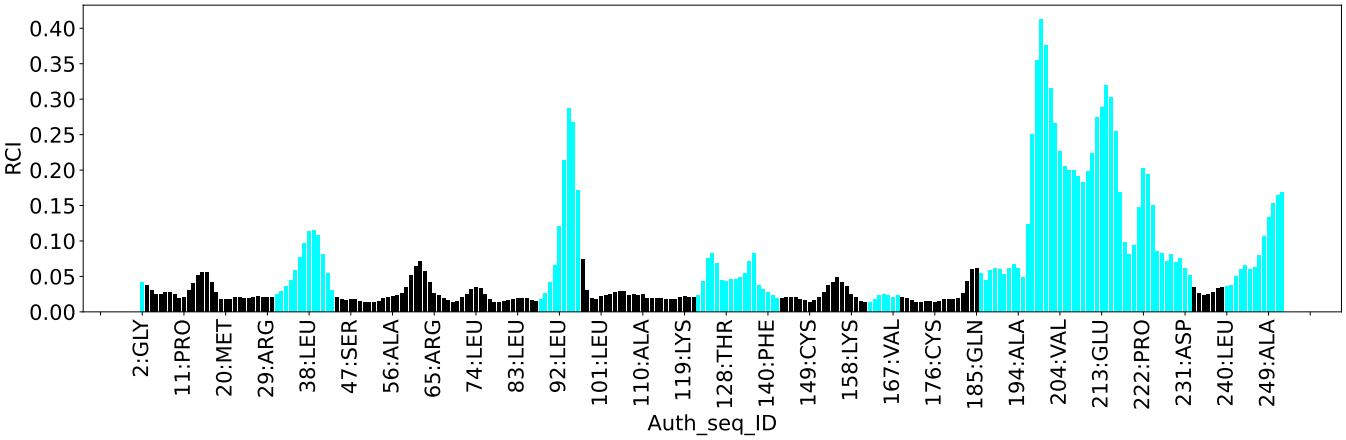
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	23	LYS	HE2	1.58	1.95 – 3.88	-6.9
1	A	23	LYS	HE3	1.58	1.92 – 3.89	-6.7

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
2:GLY
11:PRO
20:MET
29:ARG
38:LEU
47:SER
56:ALA
65:ARG
74:LEU
83:LEU
92:LEU
101:LEU
110:ALA
119:LYS
128:THR
140:PHE
149:CYS
158:LYS
167:VAL
176:CYS
185:GLN
194:ALA
204:VAL
213:GLU
222:PRO
231:ASP
240:LEU
249:ALA
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	3674
Intra-residue (|i-j|=0)	806
Sequential (|i-j|=1)	1033
Medium range (|i-j|>1 and |i-j|<5)	881
Long range (|i-j|≥5)	624
Inter-chain	0
Hydrogen bond restraints	330
Disulfide bond restraints	0
Total dihedral-angle restraints	294
Number of unmapped restraints	0
Number of restraints per residue	15.5
Number of long range restraints per residue[1]	2.4

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

8.2 Residual restraint violations (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	14.8	0.2
0.2-0.5 (Medium)	2.4	0.46
>0.5 (Large)	None	None

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	6.8	3.9
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

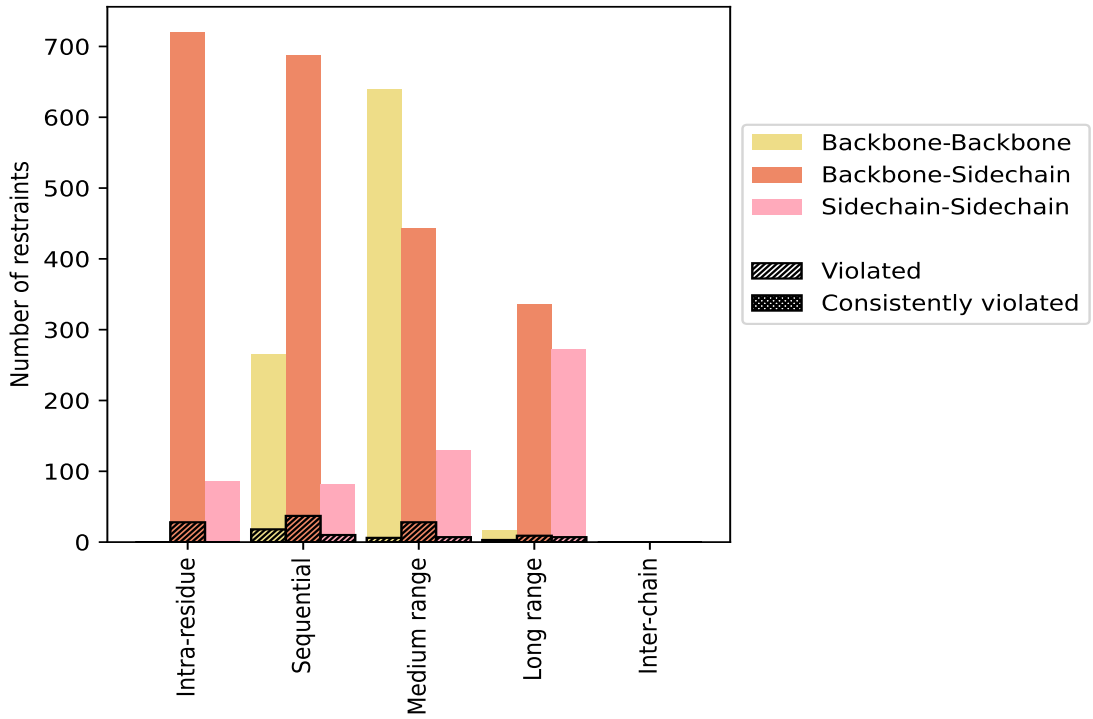
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	806	21.9	28	3.5	0.8	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	720	19.6	28	3.9	0.8	0	0.0	0.0
Sidechain-Sidechain	86	2.3	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	1033	28.1	65	6.3	1.8	0	0.0	0.0
Backbone-Backbone	265	7.2	18	6.8	0.5	0	0.0	0.0
Backbone-Sidechain	687	18.7	37	5.4	1.0	0	0.0	0.0
Sidechain-Sidechain	81	2.2	10	12.3	0.3	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	881	24.0	41	4.7	1.1	0	0.0	0.0
Backbone-Backbone	309	8.4	6	1.9	0.2	0	0.0	0.0
Backbone-Sidechain	443	12.1	28	6.3	0.8	0	0.0	0.0
Sidechain-Sidechain	129	3.5	7	5.4	0.2	0	0.0	0.0
Long range (|i-j|≥5)	624	17.0	19	3.0	0.5	0	0.0	0.0
Backbone-Backbone	17	0.5	3	17.6	0.1	0	0.0	0.0
Backbone-Sidechain	335	9.1	9	2.7	0.2	0	0.0	0.0
Sidechain-Sidechain	272	7.4	7	2.6	0.2	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	330	9.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3674	100.0	153	4.2	4.2	0	0.0	0.0
Backbone-Backbone	921	25.1	27	2.9	0.7	0	0.0	0.0
Backbone-Sidechain	2185	59.5	102	4.7	2.8	0	0.0	0.0
Sidechain-Sidechain	568	15.5	24	4.2	0.7	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 disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	3	4	3	2	0	12	0.15	0.25	0.04	0.12
2	5	6	6	1	0	18	0.15	0.35	0.06	0.12
3	5	11	4	2	0	22	0.17	0.34	0.06	0.16
4	1	10	4	1	0	16	0.15	0.41	0.07	0.12
5	2	5	8	1	0	16	0.16	0.36	0.06	0.13
6	3	9	5	4	0	21	0.15	0.34	0.06	0.13
7	2	5	4	4	0	15	0.16	0.43	0.08	0.13
8	3	6	5	1	0	15	0.15	0.38	0.07	0.12
9	4	5	6	0	0	15	0.14	0.36	0.06	0.12
10	1	6	4	3	0	14	0.14	0.33	0.06	0.12
11	1	9	7	4	0	21	0.15	0.4	0.07	0.13

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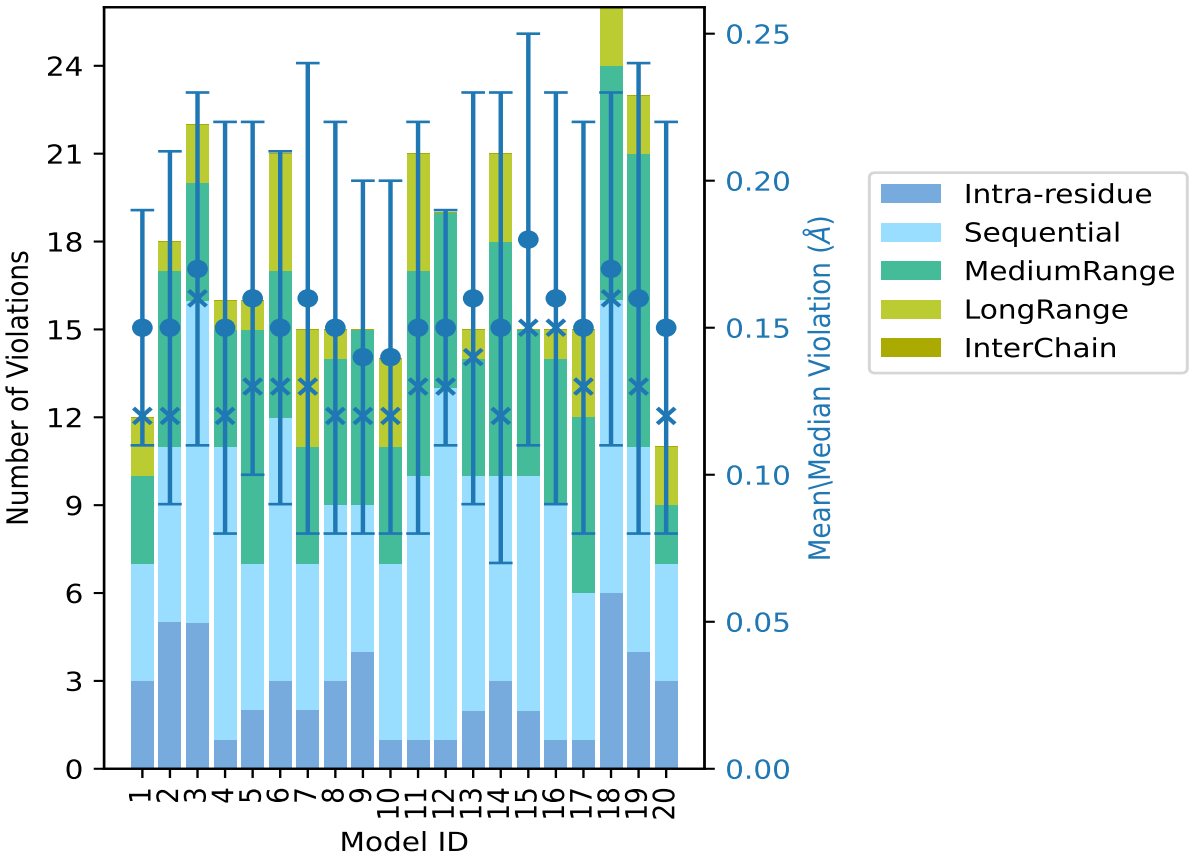
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	12	6	0	0	19	0.15	0.27	0.04	0.13
13	2	8	4	1	0	15	0.16	0.4	0.07	0.14
14	3	7	8	3	0	21	0.15	0.38	0.08	0.12
15	2	8	5	0	0	15	0.18	0.35	0.07	0.15
16	1	8	5	1	0	15	0.16	0.43	0.07	0.15
17	1	5	6	3	0	15	0.15	0.34	0.07	0.13
18	6	10	8	2	0	26	0.17	0.38	0.06	0.16
19	4	7	10	2	0	23	0.16	0.46	0.08	0.13
20	3	4	2	2	0	11	0.15	0.35	0.07	0.12

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model (i)



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

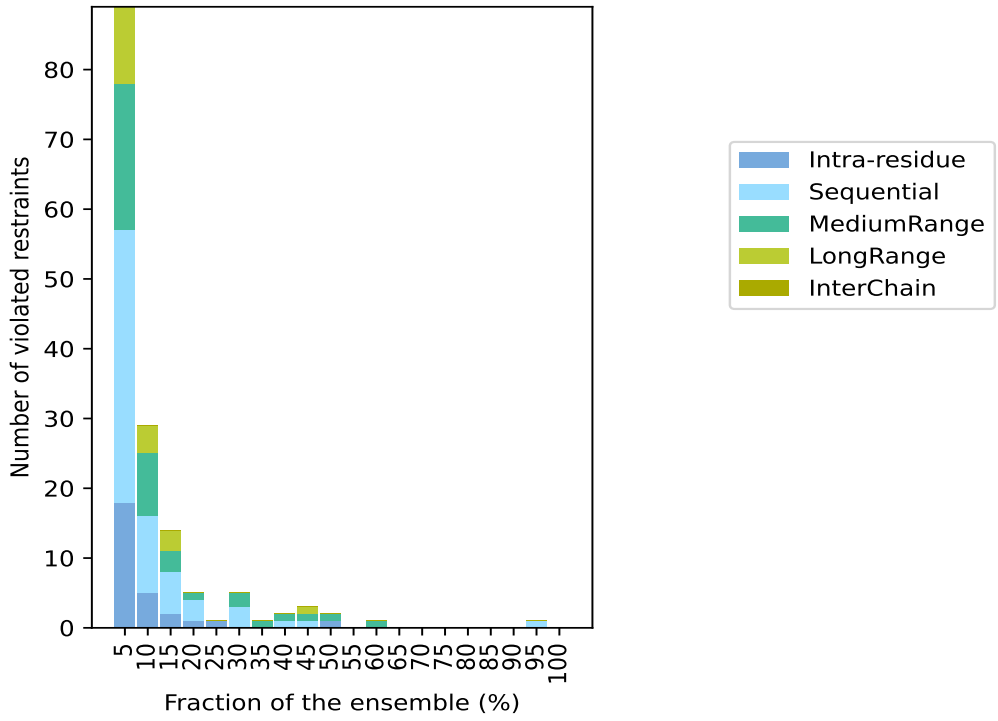
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3191(IR:778, SQ:968, MR:840, LR:605, 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]	%
18	39	21	11	0	89	1	5.0
5	11	9	4	0	29	2	10.0
2	6	3	3	0	14	3	15.0
1	3	1	0	0	5	4	20.0
1	0	0	0	0	1	5	25.0
0	3	2	0	0	5	6	30.0
0	0	1	0	0	1	7	35.0
0	1	1	0	0	2	8	40.0
0	1	1	1	0	3	9	45.0
1	0	1	0	0	2	10	50.0
0	0	0	0	0	0	11	55.0
0	0	1	0	0	1	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	1	0	0	0	1	19	95.0
0	0	0	0	0	0	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

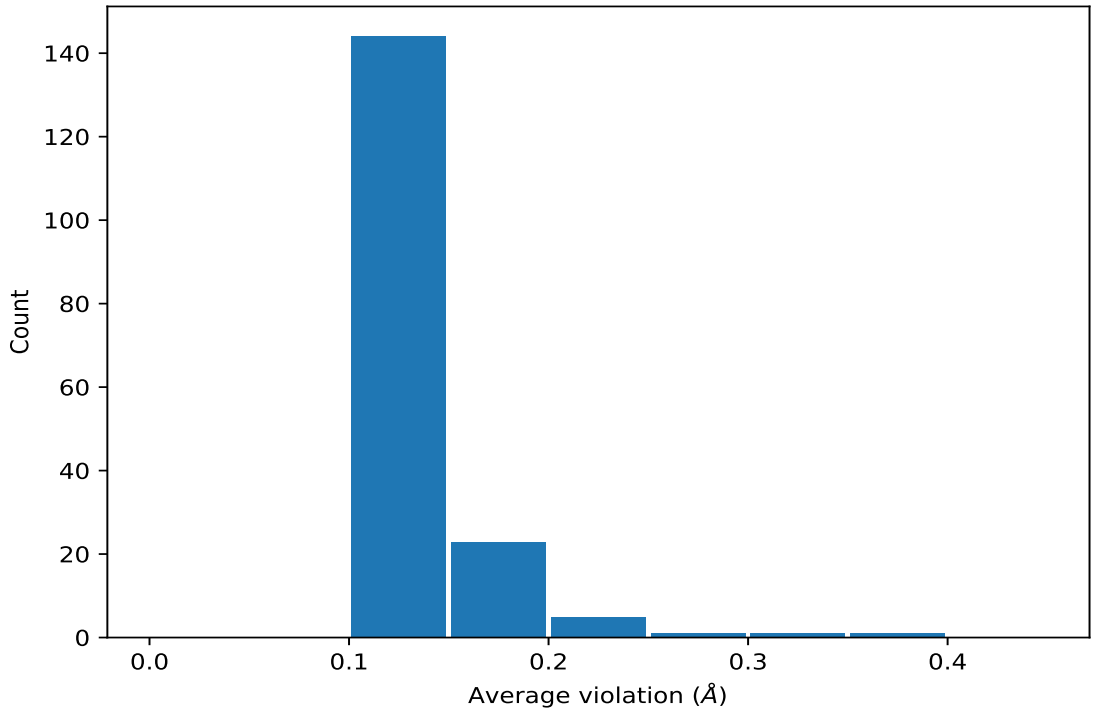
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	19	0.36	0.06	0.36
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB1	12	0.13	0.02	0.12
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB2	12	0.13	0.02	0.12
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB3	12	0.13	0.02	0.12
(1,1483)	1:A:30:LEU:H	1:A:30:LEU:HG	10	0.24	0.04	0.25
(1,972)	1:A:83:LEU:HD21	1:A:87:GLU:H	10	0.12	0.01	0.12
(1,972)	1:A:83:LEU:HD22	1:A:87:GLU:H	10	0.12	0.01	0.12
(1,972)	1:A:83:LEU:HD23	1:A:87:GLU:H	10	0.12	0.01	0.12
(1,259)	1:A:63:LEU:HG	1:A:64:ASP:H	9	0.17	0.01	0.16
(1,2548)	1:A:10:ALA:HA	1:A:49:VAL:HA	9	0.13	0.02	0.12
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB2	9	0.12	0.01	0.11
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB3	9	0.12	0.01	0.11
(1,2582)	1:A:8:ARG:HG2	1:A:9:LEU:H	8	0.2	0.02	0.2
(1,2582)	1:A:8:ARG:HG3	1:A:9:LEU:H	8	0.2	0.02	0.2
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD11	8	0.13	0.02	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD12	8	0.13	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD13	8	0.13	0.02	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD21	8	0.13	0.02	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD22	8	0.13	0.02	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD23	8	0.13	0.02	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD11	8	0.13	0.02	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD12	8	0.13	0.02	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD13	8	0.13	0.02	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD21	8	0.13	0.02	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD22	8	0.13	0.02	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD23	8	0.13	0.02	0.14
(1,832)	1:A:4:GLU:HB2	1:A:8:ARG:H	7	0.13	0.01	0.12
(1,832)	1:A:4:GLU:HB3	1:A:8:ARG:H	7	0.13	0.01	0.12
(1,969)	1:A:83:LEU:HG	1:A:87:GLU:H	6	0.16	0.03	0.18
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD11	6	0.16	0.03	0.16
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD12	6	0.16	0.03	0.16
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD13	6	0.16	0.03	0.16
(1,2489)	1:A:95:ASN:HB2	1:A:96:ILE:HB	6	0.13	0.02	0.13
(1,2489)	1:A:95:ASN:HB3	1:A:96:ILE:HB	6	0.13	0.02	0.13
(1,1451)	1:A:17:GLU:HG2	1:A:19:ASP:H	6	0.12	0.01	0.12
(1,1451)	1:A:17:GLU:HG3	1:A:19:ASP:H	6	0.12	0.01	0.12
(1,2581)	1:A:8:ARG:HB2	1:A:9:LEU:H	6	0.12	0.01	0.11
(1,2581)	1:A:8:ARG:HB3	1:A:9:LEU:H	6	0.12	0.01	0.11
(1,1176)	1:A:85:SER:H	1:A:85:SER:HB3	5	0.12	0.01	0.12
(1,609)	1:A:71:LEU:H	1:A:71:LEU:HG	4	0.2	0.01	0.2
(1,3156)	1:A:187:ASP:H	1:A:188:ARG:H	4	0.16	0.04	0.16
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD11	4	0.16	0.03	0.16
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD12	4	0.16	0.03	0.16
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD13	4	0.16	0.03	0.16
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD21	4	0.16	0.03	0.16
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD22	4	0.16	0.03	0.16
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD23	4	0.16	0.03	0.16
(1,2453)	1:A:116:LYS:HE2	1:A:119:LYS:HG2	4	0.15	0.04	0.14
(1,2453)	1:A:116:LYS:HE2	1:A:119:LYS:HG3	4	0.15	0.04	0.14
(1,2453)	1:A:116:LYS:HE3	1:A:119:LYS:HG2	4	0.15	0.04	0.14
(1,2453)	1:A:116:LYS:HE3	1:A:119:LYS:HG3	4	0.15	0.04	0.14
(1,876)	1:A:181:LYS:H	1:A:182:ILE:HG21	4	0.12	0.01	0.12
(1,876)	1:A:181:LYS:H	1:A:182:ILE:HG22	4	0.12	0.01	0.12
(1,876)	1:A:181:LYS:H	1:A:182:ILE:HG23	4	0.12	0.01	0.12
(1,3279)	1:A:222:PRO:HA	1:A:223:GLN:H	3	0.21	0.04	0.23
(1,2699)	1:A:48:ALA:H	1:A:50:MET:HB2	3	0.16	0.04	0.17
(1,2699)	1:A:48:ALA:H	1:A:50:MET:HB3	3	0.16	0.04	0.17
(1,3164)	1:A:188:ARG:H	1:A:189:GLU:H	3	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1153)	1:A:32:ARG:HA	1:A:39:SER:H	3	0.15	0.04	0.13
(1,1018)	1:A:41:ARG:H	1:A:41:ARG:HB3	3	0.15	0.01	0.16
(1,2433)	1:A:30:LEU:HD11	1:A:31:SER:HA	3	0.15	0.02	0.15
(1,2433)	1:A:30:LEU:HD12	1:A:31:SER:HA	3	0.15	0.02	0.15
(1,2433)	1:A:30:LEU:HD13	1:A:31:SER:HA	3	0.15	0.02	0.15
(1,2433)	1:A:30:LEU:HD21	1:A:31:SER:HA	3	0.15	0.02	0.15
(1,2433)	1:A:30:LEU:HD22	1:A:31:SER:HA	3	0.15	0.02	0.15
(1,2433)	1:A:30:LEU:HD23	1:A:31:SER:HA	3	0.15	0.02	0.15
(1,2567)	1:A:4:GLU:HA	1:A:4:GLU:HG2	3	0.15	0.0	0.15
(1,2567)	1:A:4:GLU:HA	1:A:4:GLU:HG3	3	0.15	0.0	0.15
(1,3283)	1:A:222:PRO:HG2	1:A:223:GLN:H	3	0.13	0.02	0.13
(1,3283)	1:A:222:PRO:HG3	1:A:223:GLN:H	3	0.13	0.02	0.13
(1,1765)	1:A:116:LYS:HB3	1:A:117:ILE:HD11	3	0.13	0.01	0.13
(1,1765)	1:A:116:LYS:HB3	1:A:117:ILE:HD12	3	0.13	0.01	0.13
(1,1765)	1:A:116:LYS:HB3	1:A:117:ILE:HD13	3	0.13	0.01	0.13
(1,1335)	1:A:162:VAL:HB	1:A:164:THR:H	3	0.12	0.0	0.12
(1,1252)	1:A:52:LEU:HD11	1:A:57:SER:H	3	0.12	0.01	0.11
(1,1252)	1:A:52:LEU:HD12	1:A:57:SER:H	3	0.12	0.01	0.11
(1,1252)	1:A:52:LEU:HD13	1:A:57:SER:H	3	0.12	0.01	0.11
(1,1252)	1:A:52:LEU:HD21	1:A:57:SER:H	3	0.12	0.01	0.11
(1,1252)	1:A:52:LEU:HD22	1:A:57:SER:H	3	0.12	0.01	0.11
(1,1252)	1:A:52:LEU:HD23	1:A:57:SER:H	3	0.12	0.01	0.11
(1,2523)	1:A:132:ASP:HB2	1:A:133:LEU:HB2	3	0.12	0.01	0.11
(1,2523)	1:A:132:ASP:HB2	1:A:133:LEU:HB3	3	0.12	0.01	0.11
(1,2653)	1:A:29:ARG:HG2	1:A:31:SER:H	3	0.12	0.0	0.12
(1,2653)	1:A:29:ARG:HG3	1:A:31:SER:H	3	0.12	0.0	0.12
(1,334)	1:A:114:ALA:H	1:A:148:ALA:H	3	0.11	0.0	0.11
(1,199)	1:A:96:ILE:H	1:A:96:ILE:HG13	2	0.32	0.03	0.32
(1,1347)	1:A:40:ALA:HA	1:A:42:THR:H	2	0.28	0.1	0.28
(1,673)	1:A:130:GLN:H	1:A:130:GLN:HB3	2	0.18	0.06	0.18
(1,1021)	1:A:41:ARG:H	1:A:42:THR:HG21	2	0.18	0.03	0.18
(1,1021)	1:A:41:ARG:H	1:A:42:THR:HG22	2	0.18	0.03	0.18
(1,1021)	1:A:41:ARG:H	1:A:42:THR:HG23	2	0.18	0.03	0.18
(1,3189)	1:A:192:ASP:H	1:A:193:VAL:HB	2	0.18	0.03	0.18
(1,1052)	1:A:165:SER:H	1:A:167:VAL:HG21	2	0.17	0.03	0.17
(1,1052)	1:A:165:SER:H	1:A:167:VAL:HG22	2	0.17	0.03	0.17
(1,1052)	1:A:165:SER:H	1:A:167:VAL:HG23	2	0.17	0.03	0.17
(1,3205)	1:A:199:LYS:HA	1:A:200:ARG:H	2	0.15	0.04	0.15
(1,743)	1:A:22:ARG:HG2	1:A:23:LYS:H	2	0.15	0.0	0.15
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD11	2	0.15	0.03	0.15
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD12	2	0.15	0.03	0.15
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD13	2	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD21	2	0.15	0.03	0.15
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD22	2	0.15	0.03	0.15
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD23	2	0.15	0.03	0.15
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG11	2	0.14	0.0	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG12	2	0.14	0.0	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG13	2	0.14	0.0	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG21	2	0.14	0.0	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG22	2	0.14	0.0	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG23	2	0.14	0.0	0.14
(1,2686)	1:A:39:SER:HB2	1:A:41:ARG:HB2	2	0.14	0.02	0.14
(1,2686)	1:A:39:SER:HB2	1:A:41:ARG:HB3	2	0.14	0.02	0.14
(1,2686)	1:A:39:SER:HB3	1:A:41:ARG:HB2	2	0.14	0.02	0.14
(1,2686)	1:A:39:SER:HB3	1:A:41:ARG:HB3	2	0.14	0.02	0.14
(1,1177)	1:A:151:ILE:HA	1:A:153:LYS:H	2	0.14	0.01	0.14
(1,504)	1:A:43:THR:HB	1:A:47:SER:H	2	0.13	0.01	0.13
(1,1175)	1:A:85:SER:H	1:A:85:SER:HB2	2	0.13	0.01	0.13
(1,3266)	1:A:215:VAL:H	1:A:216:GLU:H	2	0.13	0.0	0.13
(1,391)	1:A:158:LYS:HA	1:A:160:LYS:H	2	0.12	0.01	0.12
(1,929)	1:A:77:GLU:HG3	1:A:78:THR:H	2	0.12	0.01	0.12
(1,3151)	1:A:187:ASP:HB2	1:A:188:ARG:H	2	0.12	0.01	0.12
(1,3151)	1:A:187:ASP:HB3	1:A:188:ARG:H	2	0.12	0.01	0.12
(1,1551)	1:A:16:ALA:H	1:A:21:LEU:HD11	2	0.12	0.01	0.12
(1,1551)	1:A:16:ALA:H	1:A:21:LEU:HD12	2	0.12	0.01	0.12
(1,1551)	1:A:16:ALA:H	1:A:21:LEU:HD13	2	0.12	0.01	0.12
(1,475)	1:A:99:ARG:H	1:A:99:ARG:HD2	2	0.12	0.0	0.12
(1,475)	1:A:99:ARG:H	1:A:99:ARG:HD3	2	0.12	0.0	0.12
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD11	2	0.12	0.0	0.12
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD12	2	0.12	0.0	0.12
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD13	2	0.12	0.0	0.12
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD21	2	0.12	0.0	0.12
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD22	2	0.12	0.0	0.12
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD23	2	0.12	0.0	0.12
(1,1644)	1:A:167:VAL:HA	1:A:171:ILE:HD11	2	0.12	0.0	0.12
(1,1644)	1:A:167:VAL:HA	1:A:171:ILE:HD12	2	0.12	0.0	0.12
(1,1644)	1:A:167:VAL:HA	1:A:171:ILE:HD13	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD11	1:A:48:ALA:HB1	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD11	1:A:48:ALA:HB2	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD11	1:A:48:ALA:HB3	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD12	1:A:48:ALA:HB1	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD12	1:A:48:ALA:HB2	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD12	1:A:48:ALA:HB3	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD13	1:A:48:ALA:HB1	2	0.12	0.0	0.12

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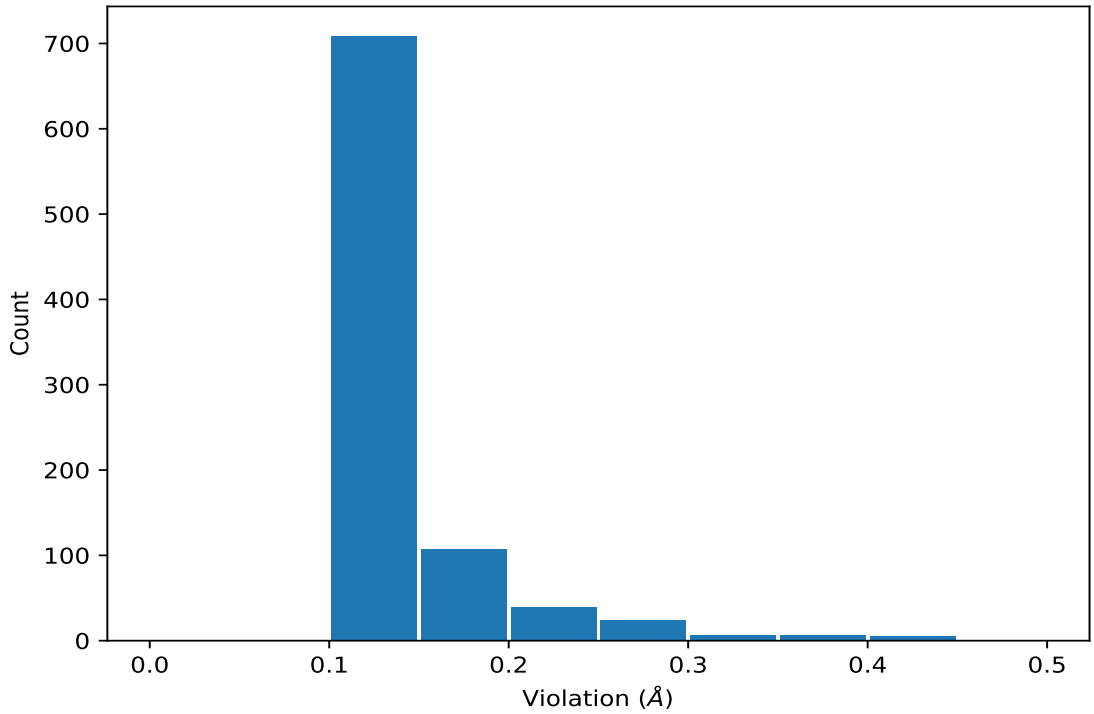
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1736)	1:A:5:LEU:HD13	1:A:48:ALA:HB2	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD13	1:A:48:ALA:HB3	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD21	1:A:48:ALA:HB1	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD21	1:A:48:ALA:HB2	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD21	1:A:48:ALA:HB3	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD22	1:A:48:ALA:HB1	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD22	1:A:48:ALA:HB2	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD22	1:A:48:ALA:HB3	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD23	1:A:48:ALA:HB1	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD23	1:A:48:ALA:HB2	2	0.12	0.0	0.12
(1,1736)	1:A:5:LEU:HD23	1:A:48:ALA:HB3	2	0.12	0.0	0.12
(1,2188)	1:A:62:PRO:HA	1:A:63:LEU:HG	2	0.12	0.0	0.12
(1,2587)	1:A:10:ALA:HB1	1:A:20:MET:HB2	2	0.12	0.0	0.12
(1,2587)	1:A:10:ALA:HB1	1:A:20:MET:HB3	2	0.12	0.0	0.12
(1,2587)	1:A:10:ALA:HB2	1:A:20:MET:HB2	2	0.12	0.0	0.12
(1,2587)	1:A:10:ALA:HB2	1:A:20:MET:HB3	2	0.12	0.0	0.12
(1,2587)	1:A:10:ALA:HB3	1:A:20:MET:HB2	2	0.12	0.0	0.12
(1,2587)	1:A:10:ALA:HB3	1:A:20:MET:HB3	2	0.12	0.0	0.12
(1,3105)	1:A:175:LEU:HD11	1:A:178:GLN:HA	2	0.12	0.0	0.12
(1,3105)	1:A:175:LEU:HD12	1:A:178:GLN:HA	2	0.12	0.0	0.12
(1,3105)	1:A:175:LEU:HD13	1:A:178:GLN:HA	2	0.12	0.0	0.12
(1,3105)	1:A:175:LEU:HD21	1:A:178:GLN:HA	2	0.12	0.0	0.12
(1,3105)	1:A:175:LEU:HD22	1:A:178:GLN:HA	2	0.12	0.0	0.12
(1,3105)	1:A:175:LEU:HD23	1:A:178:GLN:HA	2	0.12	0.0	0.12
(1,3145)	1:A:185:GLN:HB2	1:A:186:VAL:H	2	0.12	0.0	0.12
(1,3145)	1:A:185:GLN:HB3	1:A:186:VAL:H	2	0.12	0.0	0.12
(1,3294)	1:A:225:ASP:HA	1:A:226:GLU:H	2	0.12	0.0	0.12
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD11	2	0.11	0.0	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD12	2	0.11	0.0	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD13	2	0.11	0.0	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD21	2	0.11	0.0	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD22	2	0.11	0.0	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD23	2	0.11	0.0	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	19	0.46
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	7	0.43
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	16	0.43
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	4	0.41
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	11	0.4
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	13	0.4
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	8	0.38
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	18	0.38
(1,1347)	1:A:40:ALA:HA	1:A:42:THR:H	14	0.38
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	14	0.37
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	5	0.36
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	9	0.36
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	15	0.35
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	20	0.35
(1,199)	1:A:96:ILE:H	1:A:96:ILE:HG13	2	0.35
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	6	0.34
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	17	0.34
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	10	0.33
(1,2847)	1:A:92:LEU:HA	1:A:92:LEU:HD11	15	0.3
(1,2847)	1:A:92:LEU:HA	1:A:92:LEU:HD12	15	0.3
(1,2847)	1:A:92:LEU:HA	1:A:92:LEU:HD13	15	0.3
(1,2847)	1:A:92:LEU:HA	1:A:92:LEU:HD21	15	0.3
(1,2847)	1:A:92:LEU:HA	1:A:92:LEU:HD22	15	0.3
(1,2847)	1:A:92:LEU:HA	1:A:92:LEU:HD23	15	0.3
(1,199)	1:A:96:ILE:H	1:A:96:ILE:HG13	7	0.29
(1,1483)	1:A:30:LEU:H	1:A:30:LEU:HG	2	0.29
(1,1483)	1:A:30:LEU:H	1:A:30:LEU:HG	17	0.29
(1,665)	1:A:162:VAL:H	1:A:162:VAL:HB	3	0.27
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	12	0.27
(1,3148)	1:A:186:VAL:H	1:A:189:GLU:HB2	19	0.27
(1,3148)	1:A:186:VAL:H	1:A:189:GLU:HB3	19	0.27
(1,2758)	1:A:65:ARG:HG2	1:A:66:ALA:HA	18	0.26
(1,2758)	1:A:65:ARG:HG3	1:A:66:ALA:HA	18	0.26
(1,1483)	1:A:30:LEU:H	1:A:30:LEU:HG	3	0.26
(1,1483)	1:A:30:LEU:H	1:A:30:LEU:HG	11	0.26
(1,673)	1:A:130:GLN:H	1:A:130:GLN:HB3	19	0.25
(1,3279)	1:A:222:PRO:HA	1:A:223:GLN:H	15	0.25
(1,2582)	1:A:8:ARG:HG2	1:A:9:LEU:H	18	0.25
(1,2582)	1:A:8:ARG:HG3	1:A:9:LEU:H	18	0.25
(1,1483)	1:A:30:LEU:H	1:A:30:LEU:HG	1	0.25
(1,1483)	1:A:30:LEU:H	1:A:30:LEU:HG	6	0.25
(1,1483)	1:A:30:LEU:H	1:A:30:LEU:HG	15	0.25
(1,1483)	1:A:30:LEU:H	1:A:30:LEU:HG	18	0.24
(1,3279)	1:A:222:PRO:HA	1:A:223:GLN:H	5	0.23
(1,1483)	1:A:30:LEU:H	1:A:30:LEU:HG	19	0.23
(1,3156)	1:A:187:ASP:H	1:A:188:ARG:H	3	0.22
(1,2582)	1:A:8:ARG:HG2	1:A:9:LEU:H	1	0.22
(1,2582)	1:A:8:ARG:HG3	1:A:9:LEU:H	1	0.22
(1,609)	1:A:71:LEU:H	1:A:71:LEU:HG	9	0.21
(1,609)	1:A:71:LEU:H	1:A:71:LEU:HG	18	0.21
(1,3164)	1:A:188:ARG:H	1:A:189:GLU:H	3	0.21
(1,2699)	1:A:48:ALA:H	1:A:50:MET:HB2	19	0.21
(1,2699)	1:A:48:ALA:H	1:A:50:MET:HB3	19	0.21
(1,2491)	1:A:95:ASN:HB2	1:A:96:ILE:HD11	11	0.21
(1,2491)	1:A:95:ASN:HB2	1:A:96:ILE:HD12	11	0.21
(1,2491)	1:A:95:ASN:HB2	1:A:96:ILE:HD13	11	0.21
(1,2491)	1:A:95:ASN:HB3	1:A:96:ILE:HD11	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2491)	1:A:95:ASN:HB3	1:A:96:ILE:HD12	11	0.21
(1,2491)	1:A:95:ASN:HB3	1:A:96:ILE:HD13	11	0.21
(1,2453)	1:A:116:LYS:HE2	1:A:119:LYS:HG2	8	0.21
(1,2453)	1:A:116:LYS:HE2	1:A:119:LYS:HG3	8	0.21
(1,2453)	1:A:116:LYS:HE3	1:A:119:LYS:HG2	8	0.21
(1,2453)	1:A:116:LYS:HE3	1:A:119:LYS:HG3	8	0.21
(1,1153)	1:A:32:ARG:HA	1:A:39:SER:H	3	0.21
(1,1021)	1:A:41:ARG:H	1:A:42:THR:HG21	18	0.21
(1,1021)	1:A:41:ARG:H	1:A:42:THR:HG22	18	0.21
(1,1021)	1:A:41:ARG:H	1:A:42:THR:HG23	18	0.21
(1,969)	1:A:83:LEU:HG	1:A:87:GLU:H	15	0.2
(1,3189)	1:A:192:ASP:H	1:A:193:VAL:HB	14	0.2
(1,2582)	1:A:8:ARG:HG2	1:A:9:LEU:H	10	0.2
(1,2582)	1:A:8:ARG:HG3	1:A:9:LEU:H	10	0.2
(1,2582)	1:A:8:ARG:HG2	1:A:9:LEU:H	12	0.2
(1,2582)	1:A:8:ARG:HG3	1:A:9:LEU:H	12	0.2
(1,2535)	1:A:12:ARG:HA	1:A:12:ARG:HD2	3	0.2
(1,2535)	1:A:12:ARG:HA	1:A:12:ARG:HD3	3	0.2
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD11	5	0.2
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD12	5	0.2
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD13	5	0.2
(1,1052)	1:A:165:SER:H	1:A:167:VAL:HG21	6	0.2
(1,1052)	1:A:165:SER:H	1:A:167:VAL:HG22	6	0.2
(1,1052)	1:A:165:SER:H	1:A:167:VAL:HG23	6	0.2
(1,969)	1:A:83:LEU:HG	1:A:87:GLU:H	13	0.19
(1,609)	1:A:71:LEU:H	1:A:71:LEU:HG	20	0.19
(1,3263)	1:A:215:VAL:HA	1:A:216:GLU:H	12	0.19
(1,3205)	1:A:199:LYS:HA	1:A:200:ARG:H	3	0.19
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD11	20	0.19
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD12	20	0.19
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD13	20	0.19
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD21	20	0.19
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD22	20	0.19
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD23	20	0.19
(1,259)	1:A:63:LEU:HG	1:A:64:ASP:H	12	0.19
(1,2582)	1:A:8:ARG:HG2	1:A:9:LEU:H	4	0.19
(1,2582)	1:A:8:ARG:HG3	1:A:9:LEU:H	4	0.19
(1,2582)	1:A:8:ARG:HG2	1:A:9:LEU:H	8	0.19
(1,2582)	1:A:8:ARG:HG3	1:A:9:LEU:H	8	0.19
(1,2582)	1:A:8:ARG:HG2	1:A:9:LEU:H	13	0.19
(1,2582)	1:A:8:ARG:HG3	1:A:9:LEU:H	13	0.19
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD11	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD12	12	0.19
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD13	12	0.19
(1,1669)	1:A:93:ASN:HA	1:A:96:ILE:HD11	13	0.19
(1,1669)	1:A:93:ASN:HA	1:A:96:ILE:HD12	13	0.19
(1,1669)	1:A:93:ASN:HA	1:A:96:ILE:HD13	13	0.19
(1,969)	1:A:83:LEU:HG	1:A:87:GLU:H	18	0.18
(1,668)	1:A:129:GLN:HG2	1:A:130:GLN:H	18	0.18
(1,668)	1:A:129:GLN:HG3	1:A:130:GLN:H	18	0.18
(1,609)	1:A:71:LEU:H	1:A:71:LEU:HG	6	0.18
(1,259)	1:A:63:LEU:HG	1:A:64:ASP:H	11	0.18
(1,259)	1:A:63:LEU:HG	1:A:64:ASP:H	13	0.18
(1,2582)	1:A:8:ARG:HG2	1:A:9:LEU:H	16	0.18
(1,2582)	1:A:8:ARG:HG3	1:A:9:LEU:H	16	0.18
(1,2433)	1:A:30:LEU:HD11	1:A:31:SER:HA	4	0.18
(1,2433)	1:A:30:LEU:HD12	1:A:31:SER:HA	4	0.18
(1,2433)	1:A:30:LEU:HD13	1:A:31:SER:HA	4	0.18
(1,2433)	1:A:30:LEU:HD21	1:A:31:SER:HA	4	0.18
(1,2433)	1:A:30:LEU:HD22	1:A:31:SER:HA	4	0.18
(1,2433)	1:A:30:LEU:HD23	1:A:31:SER:HA	4	0.18
(1,1347)	1:A:40:ALA:HA	1:A:42:THR:H	18	0.18
(1,969)	1:A:83:LEU:HG	1:A:87:GLU:H	7	0.17
(1,3156)	1:A:187:ASP:H	1:A:188:ARG:H	12	0.17
(1,3150)	1:A:187:ASP:HB2	1:A:188:ARG:H	1	0.17
(1,3020)	1:A:153:LYS:HA	1:A:153:LYS:HD2	14	0.17
(1,3020)	1:A:153:LYS:HA	1:A:153:LYS:HD3	14	0.17
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD11	18	0.17
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD12	18	0.17
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD13	18	0.17
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD21	18	0.17
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD22	18	0.17
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD23	18	0.17
(1,2699)	1:A:48:ALA:H	1:A:50:MET:HB2	18	0.17
(1,2699)	1:A:48:ALA:H	1:A:50:MET:HB3	18	0.17
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD11	18	0.17
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD12	18	0.17
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD13	18	0.17
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD21	18	0.17
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD22	18	0.17
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD23	18	0.17
(1,259)	1:A:63:LEU:HG	1:A:64:ASP:H	5	0.17
(1,2548)	1:A:10:ALA:HA	1:A:49:VAL:HA	7	0.17
(1,1984)	1:A:41:ARG:HA	1:A:41:ARG:HD2	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1984)	1:A:41:ARG:HA	1:A:41:ARG:HD3	19	0.17
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD11	15	0.17
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD12	15	0.17
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD13	15	0.17
(1,1269)	1:A:32:ARG:HG3	1:A:33:VAL:H	11	0.17
(1,928)	1:A:77:GLU:HG2	1:A:78:THR:H	7	0.16
(1,888)	1:A:150:LYS:HG2	1:A:152:LEU:H	2	0.16
(1,888)	1:A:150:LYS:HG3	1:A:152:LEU:H	2	0.16
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB1	16	0.16
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB2	16	0.16
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB3	16	0.16
(1,832)	1:A:4:GLU:HB2	1:A:8:ARG:H	16	0.16
(1,832)	1:A:4:GLU:HB3	1:A:8:ARG:H	16	0.16
(1,641)	1:A:129:GLN:H	1:A:129:GLN:HG2	2	0.16
(1,641)	1:A:129:GLN:H	1:A:129:GLN:HG3	2	0.16
(1,3267)	1:A:216:GLU:HA	1:A:217:GLU:H	16	0.16
(1,3191)	1:A:193:VAL:HA	1:A:194:ALA:H	9	0.16
(1,3165)	1:A:189:GLU:HB3	1:A:192:ASP:H	3	0.16
(1,3164)	1:A:188:ARG:H	1:A:189:GLU:H	19	0.16
(1,2686)	1:A:39:SER:HB2	1:A:41:ARG:HB2	18	0.16
(1,2686)	1:A:39:SER:HB2	1:A:41:ARG:HB3	18	0.16
(1,2686)	1:A:39:SER:HB3	1:A:41:ARG:HB2	18	0.16
(1,2686)	1:A:39:SER:HB3	1:A:41:ARG:HB3	18	0.16
(1,259)	1:A:63:LEU:HG	1:A:64:ASP:H	3	0.16
(1,259)	1:A:63:LEU:HG	1:A:64:ASP:H	15	0.16
(1,259)	1:A:63:LEU:HG	1:A:64:ASP:H	16	0.16
(1,2548)	1:A:10:ALA:HA	1:A:49:VAL:HA	16	0.16
(1,2489)	1:A:95:ASN:HB2	1:A:96:ILE:HB	14	0.16
(1,2489)	1:A:95:ASN:HB3	1:A:96:ILE:HB	14	0.16
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD11	5	0.16
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD12	5	0.16
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD13	5	0.16
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD21	5	0.16
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD22	5	0.16
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD23	5	0.16
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD11	5	0.16
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD12	5	0.16
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD13	5	0.16
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD21	5	0.16
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD22	5	0.16
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD23	5	0.16
(1,2113)	1:A:70:LYS:HA	1:A:70:LYS:HD2	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2113)	1:A:70:LYS:HA	1:A:70:LYS:HD3	12	0.16
(1,2071)	1:A:0:SER:HA	1:A:4:GLU:HB2	14	0.16
(1,2071)	1:A:0:SER:HA	1:A:4:GLU:HB3	14	0.16
(1,1018)	1:A:41:ARG:H	1:A:41:ARG:HB3	3	0.16
(1,1018)	1:A:41:ARG:H	1:A:41:ARG:HB3	14	0.16
(1,997)	1:A:92:LEU:HB2	1:A:93:ASN:H	15	0.15
(1,997)	1:A:92:LEU:HB3	1:A:93:ASN:H	15	0.15
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB1	1	0.15
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB2	1	0.15
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB3	1	0.15
(1,743)	1:A:22:ARG:HG2	1:A:23:LYS:H	18	0.15
(1,3283)	1:A:222:PRO:HG2	1:A:223:GLN:H	14	0.15
(1,3283)	1:A:222:PRO:HG3	1:A:223:GLN:H	14	0.15
(1,3279)	1:A:222:PRO:HA	1:A:223:GLN:H	3	0.15
(1,3218)	1:A:203:ILE:HA	1:A:204:VAL:H	13	0.15
(1,3189)	1:A:192:ASP:H	1:A:193:VAL:HB	12	0.15
(1,3156)	1:A:187:ASP:H	1:A:188:ARG:H	17	0.15
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD11	19	0.15
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD12	19	0.15
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD13	19	0.15
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD21	19	0.15
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD22	19	0.15
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD23	19	0.15
(1,259)	1:A:63:LEU:HG	1:A:64:ASP:H	2	0.15
(1,2567)	1:A:4:GLU:HA	1:A:4:GLU:HG2	13	0.15
(1,2567)	1:A:4:GLU:HA	1:A:4:GLU:HG3	13	0.15
(1,2567)	1:A:4:GLU:HA	1:A:4:GLU:HG2	18	0.15
(1,2567)	1:A:4:GLU:HA	1:A:4:GLU:HG3	18	0.15
(1,2489)	1:A:95:ASN:HB2	1:A:96:ILE:HB	6	0.15
(1,2489)	1:A:95:ASN:HB3	1:A:96:ILE:HB	6	0.15
(1,2433)	1:A:30:LEU:HD11	1:A:31:SER:HA	5	0.15
(1,2433)	1:A:30:LEU:HD12	1:A:31:SER:HA	5	0.15
(1,2433)	1:A:30:LEU:HD13	1:A:31:SER:HA	5	0.15
(1,2433)	1:A:30:LEU:HD21	1:A:31:SER:HA	5	0.15
(1,2433)	1:A:30:LEU:HD22	1:A:31:SER:HA	5	0.15
(1,2433)	1:A:30:LEU:HD23	1:A:31:SER:HA	5	0.15
(1,2098)	1:A:67:TYR:HA	1:A:70:LYS:HD2	2	0.15
(1,2098)	1:A:67:TYR:HA	1:A:70:LYS:HD3	2	0.15
(1,1458)	1:A:153:LYS:HG2	1:A:154:LEU:H	16	0.15
(1,1458)	1:A:153:LYS:HG3	1:A:154:LEU:H	16	0.15
(1,1451)	1:A:17:GLU:HG2	1:A:19:ASP:H	5	0.15
(1,1451)	1:A:17:GLU:HG3	1:A:19:ASP:H	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,972)	1:A:83:LEU:HD21	1:A:87:GLU:H	3	0.14
(1,972)	1:A:83:LEU:HD22	1:A:87:GLU:H	3	0.14
(1,972)	1:A:83:LEU:HD23	1:A:87:GLU:H	3	0.14
(1,972)	1:A:83:LEU:HD21	1:A:87:GLU:H	17	0.14
(1,972)	1:A:83:LEU:HD22	1:A:87:GLU:H	17	0.14
(1,972)	1:A:83:LEU:HD23	1:A:87:GLU:H	17	0.14
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB1	8	0.14
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB2	8	0.14
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB3	8	0.14
(1,743)	1:A:22:ARG:HG2	1:A:23:LYS:H	6	0.14
(1,504)	1:A:43:THR:HB	1:A:47:SER:H	11	0.14
(1,3274)	1:A:217:GLU:HB2	1:A:218:MET:H	4	0.14
(1,3274)	1:A:217:GLU:HB3	1:A:218:MET:H	4	0.14
(1,3273)	1:A:217:GLU:HB2	1:A:218:MET:H	16	0.14
(1,3241)	1:A:209:ALA:HA	1:A:210:LYS:H	18	0.14
(1,3240)	1:A:208:PRO:HA	1:A:209:ALA:H	2	0.14
(1,259)	1:A:63:LEU:HG	1:A:64:ASP:H	10	0.14
(1,2567)	1:A:4:GLU:HA	1:A:4:GLU:HG2	10	0.14
(1,2567)	1:A:4:GLU:HA	1:A:4:GLU:HG3	10	0.14
(1,2548)	1:A:10:ALA:HA	1:A:49:VAL:HA	2	0.14
(1,2548)	1:A:10:ALA:HA	1:A:49:VAL:HA	11	0.14
(1,2493)	1:A:122:GLU:HA	1:A:123:SER:HA	13	0.14
(1,2453)	1:A:116:LYS:HE2	1:A:119:LYS:HG2	17	0.14
(1,2453)	1:A:116:LYS:HE2	1:A:119:LYS:HG3	17	0.14
(1,2453)	1:A:116:LYS:HE3	1:A:119:LYS:HG2	17	0.14
(1,2453)	1:A:116:LYS:HE3	1:A:119:LYS:HG3	17	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG11	1	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG12	1	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG13	1	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG21	1	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG22	1	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG23	1	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG11	11	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG12	11	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG13	11	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG21	11	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG22	11	0.14
(1,2332)	1:A:129:GLN:HA	1:A:131:VAL:HG23	11	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD11	10	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD12	10	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD13	10	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD21	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD22	10	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD23	10	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD11	10	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD12	10	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD13	10	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD21	10	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD22	10	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD23	10	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD11	15	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD12	15	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD13	15	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD21	15	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD22	15	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD23	15	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD11	15	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD12	15	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD13	15	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD21	15	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD22	15	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD23	15	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD11	16	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD12	16	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD13	16	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD21	16	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD22	16	0.14
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD23	16	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD11	16	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD12	16	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD13	16	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD21	16	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD22	16	0.14
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD23	16	0.14
(1,1988)	1:A:22:ARG:HD2	1:A:23:LYS:HG2	7	0.14
(1,1988)	1:A:22:ARG:HD2	1:A:23:LYS:HG3	7	0.14
(1,1988)	1:A:22:ARG:HD3	1:A:23:LYS:HG2	7	0.14
(1,1988)	1:A:22:ARG:HD3	1:A:23:LYS:HG3	7	0.14
(1,1953)	1:A:68:LEU:HD11	1:A:79:TYR:HB3	19	0.14
(1,1953)	1:A:68:LEU:HD12	1:A:79:TYR:HB3	19	0.14
(1,1953)	1:A:68:LEU:HD13	1:A:79:TYR:HB3	19	0.14
(1,1765)	1:A:116:LYS:HB3	1:A:117:ILE:HD11	6	0.14
(1,1765)	1:A:116:LYS:HB3	1:A:117:ILE:HD12	6	0.14
(1,1765)	1:A:116:LYS:HB3	1:A:117:ILE:HD13	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD11	17	0.14
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD12	17	0.14
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD13	17	0.14
(1,1607)	1:A:52:LEU:HD11	1:A:53:ASP:H	3	0.14
(1,1607)	1:A:52:LEU:HD12	1:A:53:ASP:H	3	0.14
(1,1607)	1:A:52:LEU:HD13	1:A:53:ASP:H	3	0.14
(1,1607)	1:A:52:LEU:HD21	1:A:53:ASP:H	3	0.14
(1,1607)	1:A:52:LEU:HD22	1:A:53:ASP:H	3	0.14
(1,1607)	1:A:52:LEU:HD23	1:A:53:ASP:H	3	0.14
(1,1177)	1:A:151:ILE:HA	1:A:153:LYS:H	11	0.14
(1,1175)	1:A:85:SER:H	1:A:85:SER:HB2	9	0.14
(1,1052)	1:A:165:SER:H	1:A:167:VAL:HG21	11	0.14
(1,1052)	1:A:165:SER:H	1:A:167:VAL:HG22	11	0.14
(1,1052)	1:A:165:SER:H	1:A:167:VAL:HG23	11	0.14
(1,1021)	1:A:41:ARG:H	1:A:42:THR:HG21	3	0.14
(1,1021)	1:A:41:ARG:H	1:A:42:THR:HG22	3	0.14
(1,1021)	1:A:41:ARG:H	1:A:42:THR:HG23	3	0.14
(1,972)	1:A:83:LEU:HD21	1:A:87:GLU:H	6	0.13
(1,972)	1:A:83:LEU:HD22	1:A:87:GLU:H	6	0.13
(1,972)	1:A:83:LEU:HD23	1:A:87:GLU:H	6	0.13
(1,972)	1:A:83:LEU:HD21	1:A:87:GLU:H	9	0.13
(1,972)	1:A:83:LEU:HD22	1:A:87:GLU:H	9	0.13
(1,972)	1:A:83:LEU:HD23	1:A:87:GLU:H	9	0.13
(1,929)	1:A:77:GLU:HG3	1:A:78:THR:H	19	0.13
(1,876)	1:A:181:LYS:H	1:A:182:ILE:HG21	4	0.13
(1,876)	1:A:181:LYS:H	1:A:182:ILE:HG22	4	0.13
(1,876)	1:A:181:LYS:H	1:A:182:ILE:HG23	4	0.13
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB1	6	0.13
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB2	6	0.13
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB3	6	0.13
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB1	7	0.13
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB2	7	0.13
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB3	7	0.13
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB1	14	0.13
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB2	14	0.13
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB3	14	0.13
(1,832)	1:A:4:GLU:HB2	1:A:8:ARG:H	17	0.13
(1,832)	1:A:4:GLU:HB3	1:A:8:ARG:H	17	0.13
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB2	8	0.13
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB3	8	0.13
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB2	13	0.13
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB3	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:A:129:GLN:HB2	1:A:130:GLN:H	19	0.13
(1,392)	1:A:157:ASP:HB2	1:A:160:LYS:H	11	0.13
(1,391)	1:A:158:LYS:HA	1:A:160:LYS:H	18	0.13
(1,344)	1:A:98:ILE:HG21	1:A:114:ALA:H	8	0.13
(1,344)	1:A:98:ILE:HG22	1:A:114:ALA:H	8	0.13
(1,344)	1:A:98:ILE:HG23	1:A:114:ALA:H	8	0.13
(1,3304)	1:A:226:GLU:H	1:A:226:GLU:HB3	2	0.13
(1,3283)	1:A:222:PRO:HG2	1:A:223:GLN:H	12	0.13
(1,3283)	1:A:222:PRO:HG3	1:A:223:GLN:H	12	0.13
(1,3266)	1:A:215:VAL:H	1:A:216:GLU:H	4	0.13
(1,3266)	1:A:215:VAL:H	1:A:216:GLU:H	16	0.13
(1,3258)	1:A:214:LYS:HA	1:A:215:VAL:H	6	0.13
(1,3151)	1:A:187:ASP:HB2	1:A:188:ARG:H	11	0.13
(1,3151)	1:A:187:ASP:HB3	1:A:188:ARG:H	11	0.13
(1,2581)	1:A:8:ARG:HB2	1:A:9:LEU:H	6	0.13
(1,2581)	1:A:8:ARG:HB3	1:A:9:LEU:H	6	0.13
(1,2523)	1:A:132:ASP:HB2	1:A:133:LEU:HB2	14	0.13
(1,2523)	1:A:132:ASP:HB2	1:A:133:LEU:HB3	14	0.13
(1,2489)	1:A:95:ASN:HB2	1:A:96:ILE:HB	3	0.13
(1,2489)	1:A:95:ASN:HB3	1:A:96:ILE:HB	3	0.13
(1,2489)	1:A:95:ASN:HB2	1:A:96:ILE:HB	7	0.13
(1,2489)	1:A:95:ASN:HB3	1:A:96:ILE:HB	7	0.13
(1,2453)	1:A:116:LYS:HE2	1:A:119:LYS:HG2	20	0.13
(1,2453)	1:A:116:LYS:HE2	1:A:119:LYS:HG3	20	0.13
(1,2453)	1:A:116:LYS:HE3	1:A:119:LYS:HG2	20	0.13
(1,2453)	1:A:116:LYS:HE3	1:A:119:LYS:HG3	20	0.13
(1,2400)	1:A:125:LEU:HD11	1:A:129:GLN:HA	5	0.13
(1,2400)	1:A:125:LEU:HD12	1:A:129:GLN:HA	5	0.13
(1,2400)	1:A:125:LEU:HD13	1:A:129:GLN:HA	5	0.13
(1,2400)	1:A:125:LEU:HD21	1:A:129:GLN:HA	5	0.13
(1,2400)	1:A:125:LEU:HD22	1:A:129:GLN:HA	5	0.13
(1,2400)	1:A:125:LEU:HD23	1:A:129:GLN:HA	5	0.13
(1,2343)	1:A:81:SER:HA	1:A:84:LYS:HD2	15	0.13
(1,2343)	1:A:81:SER:HA	1:A:84:LYS:HD3	15	0.13
(1,2194)	1:A:36:VAL:HA	1:A:42:THR:HG21	3	0.13
(1,2194)	1:A:36:VAL:HA	1:A:42:THR:HG22	3	0.13
(1,2194)	1:A:36:VAL:HA	1:A:42:THR:HG23	3	0.13
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD11	12	0.13
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD12	12	0.13
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD13	12	0.13
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD21	12	0.13
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD22	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD23	12	0.13
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD11	12	0.13
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD12	12	0.13
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD13	12	0.13
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD21	12	0.13
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD22	12	0.13
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD23	12	0.13
(1,2149)	1:A:44:GLU:HA	1:A:44:GLU:HG3	9	0.13
(1,2002)	1:A:125:LEU:HA	1:A:129:GLN:HG2	19	0.13
(1,2002)	1:A:125:LEU:HA	1:A:129:GLN:HG3	19	0.13
(1,1937)	1:A:58:TRP:HD1	1:A:59:MET:HG2	17	0.13
(1,1765)	1:A:116:LYS:HB3	1:A:117:ILE:HD11	8	0.13
(1,1765)	1:A:116:LYS:HB3	1:A:117:ILE:HD12	8	0.13
(1,1765)	1:A:116:LYS:HB3	1:A:117:ILE:HD13	8	0.13
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD11	1	0.13
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD12	1	0.13
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD13	1	0.13
(1,1551)	1:A:16:ALA:H	1:A:21:LEU:HD11	17	0.13
(1,1551)	1:A:16:ALA:H	1:A:21:LEU:HD12	17	0.13
(1,1551)	1:A:16:ALA:H	1:A:21:LEU:HD13	17	0.13
(1,1498)	1:A:21:LEU:HD11	1:A:22:ARG:H	10	0.13
(1,1498)	1:A:21:LEU:HD12	1:A:22:ARG:H	10	0.13
(1,1498)	1:A:21:LEU:HD13	1:A:22:ARG:H	10	0.13
(1,1483)	1:A:30:LEU:H	1:A:30:LEU:HG	13	0.13
(1,1380)	1:A:128:THR:H	1:A:129:GLN:HG2	19	0.13
(1,1380)	1:A:128:THR:H	1:A:129:GLN:HG3	19	0.13
(1,1252)	1:A:52:LEU:HD11	1:A:57:SER:H	11	0.13
(1,1252)	1:A:52:LEU:HD12	1:A:57:SER:H	11	0.13
(1,1252)	1:A:52:LEU:HD13	1:A:57:SER:H	11	0.13
(1,1252)	1:A:52:LEU:HD21	1:A:57:SER:H	11	0.13
(1,1252)	1:A:52:LEU:HD22	1:A:57:SER:H	11	0.13
(1,1252)	1:A:52:LEU:HD23	1:A:57:SER:H	11	0.13
(1,1177)	1:A:151:ILE:HA	1:A:153:LYS:H	12	0.13
(1,1176)	1:A:85:SER:H	1:A:85:SER:HB3	5	0.13
(1,1176)	1:A:85:SER:H	1:A:85:SER:HB3	16	0.13
(1,1153)	1:A:32:ARG:HA	1:A:39:SER:H	6	0.13
(1,1018)	1:A:41:ARG:H	1:A:41:ARG:HB3	18	0.13
(1,972)	1:A:83:LEU:HD21	1:A:87:GLU:H	10	0.12
(1,972)	1:A:83:LEU:HD22	1:A:87:GLU:H	10	0.12
(1,972)	1:A:83:LEU:HD23	1:A:87:GLU:H	10	0.12
(1,972)	1:A:83:LEU:HD21	1:A:87:GLU:H	12	0.12
(1,972)	1:A:83:LEU:HD22	1:A:87:GLU:H	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,972)	1:A:83:LEU:HD23	1:A:87:GLU:H	12	0.12
(1,972)	1:A:83:LEU:HD21	1:A:87:GLU:H	14	0.12
(1,972)	1:A:83:LEU:HD22	1:A:87:GLU:H	14	0.12
(1,972)	1:A:83:LEU:HD23	1:A:87:GLU:H	14	0.12
(1,972)	1:A:83:LEU:HD21	1:A:87:GLU:H	16	0.12
(1,972)	1:A:83:LEU:HD22	1:A:87:GLU:H	16	0.12
(1,972)	1:A:83:LEU:HD23	1:A:87:GLU:H	16	0.12
(1,969)	1:A:83:LEU:HG	1:A:87:GLU:H	19	0.12
(1,929)	1:A:77:GLU:HG3	1:A:78:THR:H	6	0.12
(1,876)	1:A:181:LYS:H	1:A:182:ILE:HG21	9	0.12
(1,876)	1:A:181:LYS:H	1:A:182:ILE:HG22	9	0.12
(1,876)	1:A:181:LYS:H	1:A:182:ILE:HG23	9	0.12
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB1	3	0.12
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB2	3	0.12
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB3	3	0.12
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB1	4	0.12
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB2	4	0.12
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB3	4	0.12
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB1	17	0.12
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB2	17	0.12
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB3	17	0.12
(1,832)	1:A:4:GLU:HB2	1:A:8:ARG:H	1	0.12
(1,832)	1:A:4:GLU:HB3	1:A:8:ARG:H	1	0.12
(1,832)	1:A:4:GLU:HB2	1:A:8:ARG:H	3	0.12
(1,832)	1:A:4:GLU:HB3	1:A:8:ARG:H	3	0.12
(1,832)	1:A:4:GLU:HB2	1:A:8:ARG:H	9	0.12
(1,832)	1:A:4:GLU:HB3	1:A:8:ARG:H	9	0.12
(1,832)	1:A:4:GLU:HB2	1:A:8:ARG:H	19	0.12
(1,832)	1:A:4:GLU:HB3	1:A:8:ARG:H	19	0.12
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB2	2	0.12
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB3	2	0.12
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB2	18	0.12
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB3	18	0.12
(1,684)	1:A:92:LEU:H	1:A:92:LEU:HD11	19	0.12
(1,684)	1:A:92:LEU:H	1:A:92:LEU:HD12	19	0.12
(1,684)	1:A:92:LEU:H	1:A:92:LEU:HD13	19	0.12
(1,673)	1:A:130:GLN:H	1:A:130:GLN:HB3	5	0.12
(1,505)	1:A:44:GLU:HA	1:A:47:SER:H	18	0.12
(1,504)	1:A:43:THR:HB	1:A:47:SER:H	16	0.12
(1,475)	1:A:99:ARG:H	1:A:99:ARG:HD2	2	0.12
(1,475)	1:A:99:ARG:H	1:A:99:ARG:HD3	2	0.12
(1,391)	1:A:158:LYS:HA	1:A:160:LYS:H	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,334)	1:A:114:ALA:H	1:A:148:ALA:H	1	0.12
(1,3308)	1:A:227:ASP:HA	1:A:228:LEU:H	11	0.12
(1,3294)	1:A:225:ASP:HA	1:A:226:GLU:H	2	0.12
(1,3225)	1:A:204:VAL:HA	1:A:205:VAL:H	2	0.12
(1,3164)	1:A:188:ARG:H	1:A:189:GLU:H	12	0.12
(1,3151)	1:A:187:ASP:HB2	1:A:188:ARG:H	3	0.12
(1,3151)	1:A:187:ASP:HB3	1:A:188:ARG:H	3	0.12
(1,3145)	1:A:185:GLN:HB2	1:A:186:VAL:H	4	0.12
(1,3145)	1:A:185:GLN:HB3	1:A:186:VAL:H	4	0.12
(1,3105)	1:A:175:LEU:HD11	1:A:178:GLN:HA	20	0.12
(1,3105)	1:A:175:LEU:HD12	1:A:178:GLN:HA	20	0.12
(1,3105)	1:A:175:LEU:HD13	1:A:178:GLN:HA	20	0.12
(1,3105)	1:A:175:LEU:HD21	1:A:178:GLN:HA	20	0.12
(1,3105)	1:A:175:LEU:HD22	1:A:178:GLN:HA	20	0.12
(1,3105)	1:A:175:LEU:HD23	1:A:178:GLN:HA	20	0.12
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD11	12	0.12
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD12	12	0.12
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD13	12	0.12
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD21	12	0.12
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD22	12	0.12
(1,2845)	1:A:91:GLY:H	1:A:92:LEU:HD23	12	0.12
(1,2686)	1:A:39:SER:HB2	1:A:41:ARG:HB2	4	0.12
(1,2686)	1:A:39:SER:HB2	1:A:41:ARG:HB3	4	0.12
(1,2686)	1:A:39:SER:HB3	1:A:41:ARG:HB2	4	0.12
(1,2686)	1:A:39:SER:HB3	1:A:41:ARG:HB3	4	0.12
(1,2682)	1:A:36:VAL:HG11	1:A:39:SER:HB2	4	0.12
(1,2682)	1:A:36:VAL:HG11	1:A:39:SER:HB3	4	0.12
(1,2682)	1:A:36:VAL:HG12	1:A:39:SER:HB2	4	0.12
(1,2682)	1:A:36:VAL:HG12	1:A:39:SER:HB3	4	0.12
(1,2682)	1:A:36:VAL:HG13	1:A:39:SER:HB2	4	0.12
(1,2682)	1:A:36:VAL:HG13	1:A:39:SER:HB3	4	0.12
(1,2682)	1:A:36:VAL:HG21	1:A:39:SER:HB2	4	0.12
(1,2682)	1:A:36:VAL:HG21	1:A:39:SER:HB3	4	0.12
(1,2682)	1:A:36:VAL:HG22	1:A:39:SER:HB2	4	0.12
(1,2682)	1:A:36:VAL:HG22	1:A:39:SER:HB3	4	0.12
(1,2682)	1:A:36:VAL:HG23	1:A:39:SER:HB2	4	0.12
(1,2682)	1:A:36:VAL:HG23	1:A:39:SER:HB3	4	0.12
(1,2677)	1:A:34:LYS:HA	1:A:34:LYS:HD2	8	0.12
(1,2677)	1:A:34:LYS:HA	1:A:34:LYS:HD3	8	0.12
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD11	5	0.12
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD12	5	0.12
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD13	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD21	5	0.12
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD22	5	0.12
(1,2676)	1:A:34:LYS:H	1:A:90:LEU:HD23	5	0.12
(1,2653)	1:A:29:ARG:HG2	1:A:31:SER:H	8	0.12
(1,2653)	1:A:29:ARG:HG3	1:A:31:SER:H	8	0.12
(1,2653)	1:A:29:ARG:HG2	1:A:31:SER:H	10	0.12
(1,2653)	1:A:29:ARG:HG3	1:A:31:SER:H	10	0.12
(1,2587)	1:A:10:ALA:HB1	1:A:20:MET:HB2	6	0.12
(1,2587)	1:A:10:ALA:HB1	1:A:20:MET:HB3	6	0.12
(1,2587)	1:A:10:ALA:HB2	1:A:20:MET:HB2	6	0.12
(1,2587)	1:A:10:ALA:HB2	1:A:20:MET:HB3	6	0.12
(1,2587)	1:A:10:ALA:HB3	1:A:20:MET:HB2	6	0.12
(1,2587)	1:A:10:ALA:HB3	1:A:20:MET:HB3	6	0.12
(1,2581)	1:A:8:ARG:HB2	1:A:9:LEU:H	20	0.12
(1,2581)	1:A:8:ARG:HB3	1:A:9:LEU:H	20	0.12
(1,2548)	1:A:10:ALA:HA	1:A:49:VAL:HA	10	0.12
(1,2548)	1:A:10:ALA:HA	1:A:49:VAL:HA	19	0.12
(1,2524)	1:A:132:ASP:HB3	1:A:133:LEU:HB2	9	0.12
(1,2524)	1:A:132:ASP:HB3	1:A:133:LEU:HB3	9	0.12
(1,2489)	1:A:95:ASN:HB2	1:A:96:ILE:HB	2	0.12
(1,2489)	1:A:95:ASN:HB3	1:A:96:ILE:HB	2	0.12
(1,2453)	1:A:116:LYS:HE2	1:A:119:LYS:HG2	7	0.12
(1,2453)	1:A:116:LYS:HE2	1:A:119:LYS:HG3	7	0.12
(1,2453)	1:A:116:LYS:HE3	1:A:119:LYS:HG2	7	0.12
(1,2453)	1:A:116:LYS:HE3	1:A:119:LYS:HG3	7	0.12
(1,2433)	1:A:30:LEU:HD11	1:A:31:SER:HA	7	0.12
(1,2433)	1:A:30:LEU:HD12	1:A:31:SER:HA	7	0.12
(1,2433)	1:A:30:LEU:HD13	1:A:31:SER:HA	7	0.12
(1,2433)	1:A:30:LEU:HD21	1:A:31:SER:HA	7	0.12
(1,2433)	1:A:30:LEU:HD22	1:A:31:SER:HA	7	0.12
(1,2433)	1:A:30:LEU:HD23	1:A:31:SER:HA	7	0.12
(1,2425)	1:A:20:MET:H	1:A:59:MET:HB2	14	0.12
(1,2408)	1:A:125:LEU:HD11	1:A:129:GLN:HG2	19	0.12
(1,2408)	1:A:125:LEU:HD11	1:A:129:GLN:HG3	19	0.12
(1,2408)	1:A:125:LEU:HD12	1:A:129:GLN:HG2	19	0.12
(1,2408)	1:A:125:LEU:HD12	1:A:129:GLN:HG3	19	0.12
(1,2408)	1:A:125:LEU:HD13	1:A:129:GLN:HG2	19	0.12
(1,2408)	1:A:125:LEU:HD13	1:A:129:GLN:HG3	19	0.12
(1,2408)	1:A:125:LEU:HD21	1:A:129:GLN:HG2	19	0.12
(1,2408)	1:A:125:LEU:HD21	1:A:129:GLN:HG3	19	0.12
(1,2408)	1:A:125:LEU:HD22	1:A:129:GLN:HG2	19	0.12
(1,2408)	1:A:125:LEU:HD22	1:A:129:GLN:HG3	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2408)	1:A:125:LEU:HD23	1:A:129:GLN:HG2	19	0.12
(1,2408)	1:A:125:LEU:HD23	1:A:129:GLN:HG3	19	0.12
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD11	11	0.12
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD12	11	0.12
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD13	11	0.12
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD21	11	0.12
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD22	11	0.12
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD23	11	0.12
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD11	11	0.12
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD12	11	0.12
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD13	11	0.12
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD21	11	0.12
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD22	11	0.12
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD23	11	0.12
(1,2188)	1:A:62:PRO:HA	1:A:63:LEU:HG	20	0.12
(1,1971)	1:A:66:ALA:HB1	1:A:76:LYS:HE2	20	0.12
(1,1971)	1:A:66:ALA:HB1	1:A:76:LYS:HE3	20	0.12
(1,1971)	1:A:66:ALA:HB2	1:A:76:LYS:HE2	20	0.12
(1,1971)	1:A:66:ALA:HB2	1:A:76:LYS:HE3	20	0.12
(1,1971)	1:A:66:ALA:HB3	1:A:76:LYS:HE2	20	0.12
(1,1971)	1:A:66:ALA:HB3	1:A:76:LYS:HE3	20	0.12
(1,1934)	1:A:20:MET:HG2	1:A:63:LEU:HD11	17	0.12
(1,1934)	1:A:20:MET:HG2	1:A:63:LEU:HD12	17	0.12
(1,1934)	1:A:20:MET:HG2	1:A:63:LEU:HD13	17	0.12
(1,1934)	1:A:20:MET:HG2	1:A:63:LEU:HD21	17	0.12
(1,1934)	1:A:20:MET:HG2	1:A:63:LEU:HD22	17	0.12
(1,1934)	1:A:20:MET:HG2	1:A:63:LEU:HD23	17	0.12
(1,1934)	1:A:20:MET:HG3	1:A:63:LEU:HD11	17	0.12
(1,1934)	1:A:20:MET:HG3	1:A:63:LEU:HD12	17	0.12
(1,1934)	1:A:20:MET:HG3	1:A:63:LEU:HD13	17	0.12
(1,1934)	1:A:20:MET:HG3	1:A:63:LEU:HD21	17	0.12
(1,1934)	1:A:20:MET:HG3	1:A:63:LEU:HD22	17	0.12
(1,1934)	1:A:20:MET:HG3	1:A:63:LEU:HD23	17	0.12
(1,1869)	1:A:10:ALA:HA	1:A:21:LEU:HD11	10	0.12
(1,1869)	1:A:10:ALA:HA	1:A:21:LEU:HD12	10	0.12
(1,1869)	1:A:10:ALA:HA	1:A:21:LEU:HD13	10	0.12
(1,1736)	1:A:5:LEU:HD11	1:A:48:ALA:HB1	7	0.12
(1,1736)	1:A:5:LEU:HD11	1:A:48:ALA:HB2	7	0.12
(1,1736)	1:A:5:LEU:HD11	1:A:48:ALA:HB3	7	0.12
(1,1736)	1:A:5:LEU:HD12	1:A:48:ALA:HB1	7	0.12
(1,1736)	1:A:5:LEU:HD12	1:A:48:ALA:HB2	7	0.12
(1,1736)	1:A:5:LEU:HD12	1:A:48:ALA:HB3	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1736)	1:A:5:LEU:HD13	1:A:48:ALA:HB1	7	0.12
(1,1736)	1:A:5:LEU:HD13	1:A:48:ALA:HB2	7	0.12
(1,1736)	1:A:5:LEU:HD13	1:A:48:ALA:HB3	7	0.12
(1,1736)	1:A:5:LEU:HD21	1:A:48:ALA:HB1	7	0.12
(1,1736)	1:A:5:LEU:HD21	1:A:48:ALA:HB2	7	0.12
(1,1736)	1:A:5:LEU:HD21	1:A:48:ALA:HB3	7	0.12
(1,1736)	1:A:5:LEU:HD22	1:A:48:ALA:HB1	7	0.12
(1,1736)	1:A:5:LEU:HD22	1:A:48:ALA:HB2	7	0.12
(1,1736)	1:A:5:LEU:HD22	1:A:48:ALA:HB3	7	0.12
(1,1736)	1:A:5:LEU:HD23	1:A:48:ALA:HB1	7	0.12
(1,1736)	1:A:5:LEU:HD23	1:A:48:ALA:HB2	7	0.12
(1,1736)	1:A:5:LEU:HD23	1:A:48:ALA:HB3	7	0.12
(1,1644)	1:A:167:VAL:HA	1:A:171:ILE:HD11	2	0.12
(1,1644)	1:A:167:VAL:HA	1:A:171:ILE:HD12	2	0.12
(1,1644)	1:A:167:VAL:HA	1:A:171:ILE:HD13	2	0.12
(1,1451)	1:A:17:GLU:HG2	1:A:19:ASP:H	11	0.12
(1,1451)	1:A:17:GLU:HG3	1:A:19:ASP:H	11	0.12
(1,1451)	1:A:17:GLU:HG2	1:A:19:ASP:H	12	0.12
(1,1451)	1:A:17:GLU:HG3	1:A:19:ASP:H	12	0.12
(1,1451)	1:A:17:GLU:HG2	1:A:19:ASP:H	17	0.12
(1,1451)	1:A:17:GLU:HG3	1:A:19:ASP:H	17	0.12
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD11	8	0.12
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD12	8	0.12
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD13	8	0.12
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD21	8	0.12
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD22	8	0.12
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD23	8	0.12
(1,1335)	1:A:162:VAL:HB	1:A:164:THR:H	5	0.12
(1,1335)	1:A:162:VAL:HB	1:A:164:THR:H	9	0.12
(1,1335)	1:A:162:VAL:HB	1:A:164:THR:H	19	0.12
(1,1176)	1:A:85:SER:H	1:A:85:SER:HB3	1	0.12
(1,1175)	1:A:85:SER:H	1:A:85:SER:HB2	18	0.12
(1,1162)	1:A:39:SER:H	1:A:39:SER:HB2	1	0.12
(1,1160)	1:A:75:ASN:H	1:A:78:THR:H	6	0.12
(1,1153)	1:A:32:ARG:HA	1:A:39:SER:H	18	0.12
(1,972)	1:A:83:LEU:HD21	1:A:87:GLU:H	2	0.11
(1,972)	1:A:83:LEU:HD22	1:A:87:GLU:H	2	0.11
(1,972)	1:A:83:LEU:HD23	1:A:87:GLU:H	2	0.11
(1,972)	1:A:83:LEU:HD21	1:A:87:GLU:H	8	0.11
(1,972)	1:A:83:LEU:HD22	1:A:87:GLU:H	8	0.11
(1,972)	1:A:83:LEU:HD23	1:A:87:GLU:H	8	0.11
(1,969)	1:A:83:LEU:HG	1:A:87:GLU:H	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,876)	1:A:181:LYS:H	1:A:182:ILE:HG21	13	0.11
(1,876)	1:A:181:LYS:H	1:A:182:ILE:HG22	13	0.11
(1,876)	1:A:181:LYS:H	1:A:182:ILE:HG23	13	0.11
(1,876)	1:A:181:LYS:H	1:A:182:ILE:HG21	18	0.11
(1,876)	1:A:181:LYS:H	1:A:182:ILE:HG22	18	0.11
(1,876)	1:A:181:LYS:H	1:A:182:ILE:HG23	18	0.11
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB1	2	0.11
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB2	2	0.11
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB3	2	0.11
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB1	12	0.11
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB2	12	0.11
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB3	12	0.11
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB1	19	0.11
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB2	19	0.11
(1,838)	1:A:8:ARG:H	1:A:10:ALA:HB3	19	0.11
(1,832)	1:A:4:GLU:HB2	1:A:8:ARG:H	4	0.11
(1,832)	1:A:4:GLU:HB3	1:A:8:ARG:H	4	0.11
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB2	9	0.11
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB3	9	0.11
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB2	12	0.11
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB3	12	0.11
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB2	14	0.11
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB3	14	0.11
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB2	15	0.11
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB3	15	0.11
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB2	19	0.11
(1,805)	1:A:178:GLN:H	1:A:181:LYS:HB3	19	0.11
(1,65)	1:A:155:LYS:H	1:A:155:LYS:HB2	3	0.11
(1,65)	1:A:155:LYS:H	1:A:155:LYS:HB3	3	0.11
(1,517)	1:A:61:CYS:H	1:A:61:CYS:HB3	20	0.11
(1,497)	1:A:155:LYS:HG3	1:A:156:VAL:H	10	0.11
(1,475)	1:A:99:ARG:H	1:A:99:ARG:HD2	8	0.11
(1,475)	1:A:99:ARG:H	1:A:99:ARG:HD3	8	0.11
(1,424)	1:A:4:GLU:HB2	1:A:5:LEU:H	13	0.11
(1,424)	1:A:4:GLU:HB3	1:A:5:LEU:H	13	0.11
(1,334)	1:A:114:ALA:H	1:A:148:ALA:H	7	0.11
(1,334)	1:A:114:ALA:H	1:A:148:ALA:H	13	0.11
(1,3298)	1:A:225:ASP:H	1:A:225:ASP:HB3	4	0.11
(1,3294)	1:A:225:ASP:HA	1:A:226:GLU:H	8	0.11
(1,3283)	1:A:222:PRO:HG2	1:A:223:GLN:H	16	0.11
(1,3283)	1:A:222:PRO:HG3	1:A:223:GLN:H	16	0.11
(1,3271)	1:A:217:GLU:HA	1:A:218:MET:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3230)	1:A:205:VAL:HA	1:A:206:GLU:H	1	0.11
(1,3205)	1:A:199:LYS:HA	1:A:200:ARG:H	12	0.11
(1,3156)	1:A:187:ASP:H	1:A:188:ARG:H	6	0.11
(1,3145)	1:A:185:GLN:HB2	1:A:186:VAL:H	9	0.11
(1,3145)	1:A:185:GLN:HB3	1:A:186:VAL:H	9	0.11
(1,3109)	1:A:175:LEU:HD11	1:A:179:LEU:HB2	5	0.11
(1,3109)	1:A:175:LEU:HD12	1:A:179:LEU:HB2	5	0.11
(1,3109)	1:A:175:LEU:HD13	1:A:179:LEU:HB2	5	0.11
(1,3109)	1:A:175:LEU:HD21	1:A:179:LEU:HB2	5	0.11
(1,3109)	1:A:175:LEU:HD22	1:A:179:LEU:HB2	5	0.11
(1,3109)	1:A:175:LEU:HD23	1:A:179:LEU:HB2	5	0.11
(1,3105)	1:A:175:LEU:HD11	1:A:178:GLN:HA	9	0.11
(1,3105)	1:A:175:LEU:HD12	1:A:178:GLN:HA	9	0.11
(1,3105)	1:A:175:LEU:HD13	1:A:178:GLN:HA	9	0.11
(1,3105)	1:A:175:LEU:HD21	1:A:178:GLN:HA	9	0.11
(1,3105)	1:A:175:LEU:HD22	1:A:178:GLN:HA	9	0.11
(1,3105)	1:A:175:LEU:HD23	1:A:178:GLN:HA	9	0.11
(1,2974)	1:A:131:VAL:HG11	1:A:132:ASP:HB2	18	0.11
(1,2974)	1:A:131:VAL:HG11	1:A:132:ASP:HB3	18	0.11
(1,2974)	1:A:131:VAL:HG12	1:A:132:ASP:HB2	18	0.11
(1,2974)	1:A:131:VAL:HG12	1:A:132:ASP:HB3	18	0.11
(1,2974)	1:A:131:VAL:HG13	1:A:132:ASP:HB2	18	0.11
(1,2974)	1:A:131:VAL:HG13	1:A:132:ASP:HB3	18	0.11
(1,2974)	1:A:131:VAL:HG21	1:A:132:ASP:HB2	18	0.11
(1,2974)	1:A:131:VAL:HG21	1:A:132:ASP:HB3	18	0.11
(1,2974)	1:A:131:VAL:HG22	1:A:132:ASP:HB2	18	0.11
(1,2974)	1:A:131:VAL:HG22	1:A:132:ASP:HB3	18	0.11
(1,2974)	1:A:131:VAL:HG23	1:A:132:ASP:HB2	18	0.11
(1,2974)	1:A:131:VAL:HG23	1:A:132:ASP:HB3	18	0.11
(1,2954)	1:A:123:SER:H	1:A:124:SER:HB2	13	0.11
(1,2954)	1:A:123:SER:H	1:A:124:SER:HB3	13	0.11
(1,2839)	1:A:90:LEU:HB2	1:A:92:LEU:H	19	0.11
(1,2839)	1:A:90:LEU:HB3	1:A:92:LEU:H	19	0.11
(1,2699)	1:A:48:ALA:H	1:A:50:MET:HB2	17	0.11
(1,2699)	1:A:48:ALA:H	1:A:50:MET:HB3	17	0.11
(1,2653)	1:A:29:ARG:HG2	1:A:31:SER:H	6	0.11
(1,2653)	1:A:29:ARG:HG3	1:A:31:SER:H	6	0.11
(1,2587)	1:A:10:ALA:HB1	1:A:20:MET:HB2	7	0.11
(1,2587)	1:A:10:ALA:HB1	1:A:20:MET:HB3	7	0.11
(1,2587)	1:A:10:ALA:HB2	1:A:20:MET:HB2	7	0.11
(1,2587)	1:A:10:ALA:HB2	1:A:20:MET:HB3	7	0.11
(1,2587)	1:A:10:ALA:HB3	1:A:20:MET:HB2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2587)	1:A:10:ALA:HB3	1:A:20:MET:HB3	7	0.11
(1,2581)	1:A:8:ARG:HB2	1:A:9:LEU:H	11	0.11
(1,2581)	1:A:8:ARG:HB3	1:A:9:LEU:H	11	0.11
(1,2581)	1:A:8:ARG:HB2	1:A:9:LEU:H	14	0.11
(1,2581)	1:A:8:ARG:HB3	1:A:9:LEU:H	14	0.11
(1,2581)	1:A:8:ARG:HB2	1:A:9:LEU:H	15	0.11
(1,2581)	1:A:8:ARG:HB3	1:A:9:LEU:H	15	0.11
(1,2581)	1:A:8:ARG:HB2	1:A:9:LEU:H	19	0.11
(1,2581)	1:A:8:ARG:HB3	1:A:9:LEU:H	19	0.11
(1,2548)	1:A:10:ALA:HA	1:A:49:VAL:HA	1	0.11
(1,2548)	1:A:10:ALA:HA	1:A:49:VAL:HA	14	0.11
(1,2548)	1:A:10:ALA:HA	1:A:49:VAL:HA	20	0.11
(1,2523)	1:A:132:ASP:HB2	1:A:133:LEU:HB2	4	0.11
(1,2523)	1:A:132:ASP:HB2	1:A:133:LEU:HB3	4	0.11
(1,2523)	1:A:132:ASP:HB2	1:A:133:LEU:HB2	15	0.11
(1,2523)	1:A:132:ASP:HB2	1:A:133:LEU:HB3	15	0.11
(1,2514)	1:A:132:ASP:HA	1:A:133:LEU:HD11	11	0.11
(1,2514)	1:A:132:ASP:HA	1:A:133:LEU:HD12	11	0.11
(1,2514)	1:A:132:ASP:HA	1:A:133:LEU:HD13	11	0.11
(1,2514)	1:A:132:ASP:HA	1:A:133:LEU:HD21	11	0.11
(1,2514)	1:A:132:ASP:HA	1:A:133:LEU:HD22	11	0.11
(1,2514)	1:A:132:ASP:HA	1:A:133:LEU:HD23	11	0.11
(1,2489)	1:A:95:ASN:HB2	1:A:96:ILE:HB	10	0.11
(1,2489)	1:A:95:ASN:HB3	1:A:96:ILE:HB	10	0.11
(1,2395)	1:A:108:ILE:HB	1:A:111:VAL:HG11	10	0.11
(1,2395)	1:A:108:ILE:HB	1:A:111:VAL:HG12	10	0.11
(1,2395)	1:A:108:ILE:HB	1:A:111:VAL:HG13	10	0.11
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD11	9	0.11
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD12	9	0.11
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD13	9	0.11
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD21	9	0.11
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD22	9	0.11
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD23	9	0.11
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD11	9	0.11
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD12	9	0.11
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD13	9	0.11
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD21	9	0.11
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD22	9	0.11
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD23	9	0.11
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD11	14	0.11
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD12	14	0.11
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD13	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD21	14	0.11
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD22	14	0.11
(1,2193)	1:A:123:SER:HB2	1:A:125:LEU:HD23	14	0.11
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD11	14	0.11
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD12	14	0.11
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD13	14	0.11
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD21	14	0.11
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD22	14	0.11
(1,2193)	1:A:123:SER:HB3	1:A:125:LEU:HD23	14	0.11
(1,2188)	1:A:62:PRO:HA	1:A:63:LEU:HG	17	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD11	8	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD12	8	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD13	8	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD21	8	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD22	8	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD23	8	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD11	9	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD12	9	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD13	9	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD21	9	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD22	9	0.11
(1,2047)	1:A:30:LEU:HA	1:A:30:LEU:HD23	9	0.11
(1,1973)	1:A:22:ARG:HD2	1:A:23:LYS:HD2	12	0.11
(1,1973)	1:A:22:ARG:HD2	1:A:23:LYS:HD3	12	0.11
(1,1973)	1:A:22:ARG:HD3	1:A:23:LYS:HD2	12	0.11
(1,1973)	1:A:22:ARG:HD3	1:A:23:LYS:HD3	12	0.11
(1,1949)	1:A:25:GLU:HA	1:A:25:GLU:HG2	6	0.11
(1,1923)	1:A:105:PHE:HD1	1:A:160:LYS:HB2	6	0.11
(1,1923)	1:A:105:PHE:HD1	1:A:160:LYS:HB3	6	0.11
(1,1923)	1:A:105:PHE:HD2	1:A:160:LYS:HB2	6	0.11
(1,1923)	1:A:105:PHE:HD2	1:A:160:LYS:HB3	6	0.11
(1,186)	1:A:6:ILE:HG21	1:A:26:GLU:H	10	0.11
(1,186)	1:A:6:ILE:HG22	1:A:26:GLU:H	10	0.11
(1,186)	1:A:6:ILE:HG23	1:A:26:GLU:H	10	0.11
(1,1842)	1:A:181:LYS:HA	1:A:181:LYS:HG3	7	0.11
(1,1765)	1:A:116:LYS:HB3	1:A:117:ILE:HD11	11	0.11
(1,1765)	1:A:116:LYS:HB3	1:A:117:ILE:HD12	11	0.11
(1,1765)	1:A:116:LYS:HB3	1:A:117:ILE:HD13	11	0.11
(1,1758)	1:A:10:ALA:HB1	1:A:16:ALA:HB1	11	0.11
(1,1758)	1:A:10:ALA:HB1	1:A:16:ALA:HB2	11	0.11
(1,1758)	1:A:10:ALA:HB1	1:A:16:ALA:HB3	11	0.11
(1,1758)	1:A:10:ALA:HB2	1:A:16:ALA:HB1	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1758)	1:A:10:ALA:HB2	1:A:16:ALA:HB2	11	0.11
(1,1758)	1:A:10:ALA:HB2	1:A:16:ALA:HB3	11	0.11
(1,1758)	1:A:10:ALA:HB3	1:A:16:ALA:HB1	11	0.11
(1,1758)	1:A:10:ALA:HB3	1:A:16:ALA:HB2	11	0.11
(1,1758)	1:A:10:ALA:HB3	1:A:16:ALA:HB3	11	0.11
(1,1736)	1:A:5:LEU:HD11	1:A:48:ALA:HB1	17	0.11
(1,1736)	1:A:5:LEU:HD11	1:A:48:ALA:HB2	17	0.11
(1,1736)	1:A:5:LEU:HD11	1:A:48:ALA:HB3	17	0.11
(1,1736)	1:A:5:LEU:HD12	1:A:48:ALA:HB1	17	0.11
(1,1736)	1:A:5:LEU:HD12	1:A:48:ALA:HB2	17	0.11
(1,1736)	1:A:5:LEU:HD12	1:A:48:ALA:HB3	17	0.11
(1,1736)	1:A:5:LEU:HD13	1:A:48:ALA:HB1	17	0.11
(1,1736)	1:A:5:LEU:HD13	1:A:48:ALA:HB2	17	0.11
(1,1736)	1:A:5:LEU:HD13	1:A:48:ALA:HB3	17	0.11
(1,1736)	1:A:5:LEU:HD21	1:A:48:ALA:HB1	17	0.11
(1,1736)	1:A:5:LEU:HD21	1:A:48:ALA:HB2	17	0.11
(1,1736)	1:A:5:LEU:HD21	1:A:48:ALA:HB3	17	0.11
(1,1736)	1:A:5:LEU:HD22	1:A:48:ALA:HB1	17	0.11
(1,1736)	1:A:5:LEU:HD22	1:A:48:ALA:HB2	17	0.11
(1,1736)	1:A:5:LEU:HD22	1:A:48:ALA:HB3	17	0.11
(1,1736)	1:A:5:LEU:HD23	1:A:48:ALA:HB1	17	0.11
(1,1736)	1:A:5:LEU:HD23	1:A:48:ALA:HB2	17	0.11
(1,1736)	1:A:5:LEU:HD23	1:A:48:ALA:HB3	17	0.11
(1,1693)	1:A:69:ILE:HG21	1:A:70:LYS:HG3	2	0.11
(1,1693)	1:A:69:ILE:HG22	1:A:70:LYS:HG3	2	0.11
(1,1693)	1:A:69:ILE:HG23	1:A:70:LYS:HG3	2	0.11
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD11	4	0.11
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD12	4	0.11
(1,1670)	1:A:95:ASN:HA	1:A:96:ILE:HD13	4	0.11
(1,1644)	1:A:167:VAL:HA	1:A:171:ILE:HD11	15	0.11
(1,1644)	1:A:167:VAL:HA	1:A:171:ILE:HD12	15	0.11
(1,1644)	1:A:167:VAL:HA	1:A:171:ILE:HD13	15	0.11
(1,1551)	1:A:16:ALA:H	1:A:21:LEU:HD11	11	0.11
(1,1551)	1:A:16:ALA:H	1:A:21:LEU:HD12	11	0.11
(1,1551)	1:A:16:ALA:H	1:A:21:LEU:HD13	11	0.11
(1,1549)	1:A:147:SER:H	1:A:151:ILE:HD11	7	0.11
(1,1549)	1:A:147:SER:H	1:A:151:ILE:HD12	7	0.11
(1,1549)	1:A:147:SER:H	1:A:151:ILE:HD13	7	0.11
(1,1537)	1:A:118:LEU:HD11	1:A:123:SER:H	6	0.11
(1,1537)	1:A:118:LEU:HD12	1:A:123:SER:H	6	0.11
(1,1537)	1:A:118:LEU:HD13	1:A:123:SER:H	6	0.11
(1,1537)	1:A:118:LEU:HD21	1:A:123:SER:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1537)	1:A:118:LEU:HD22	1:A:123:SER:H	6	0.11
(1,1537)	1:A:118:LEU:HD23	1:A:123:SER:H	6	0.11
(1,1481)	1:A:29:ARG:HD2	1:A:30:LEU:H	4	0.11
(1,1481)	1:A:29:ARG:HD3	1:A:30:LEU:H	4	0.11
(1,1473)	1:A:28:LEU:HD21	1:A:29:ARG:H	14	0.11
(1,1473)	1:A:28:LEU:HD22	1:A:29:ARG:H	14	0.11
(1,1473)	1:A:28:LEU:HD23	1:A:29:ARG:H	14	0.11
(1,1451)	1:A:17:GLU:HG2	1:A:19:ASP:H	13	0.11
(1,1451)	1:A:17:GLU:HG3	1:A:19:ASP:H	13	0.11
(1,1451)	1:A:17:GLU:HG2	1:A:19:ASP:H	18	0.11
(1,1451)	1:A:17:GLU:HG3	1:A:19:ASP:H	18	0.11
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD11	3	0.11
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD12	3	0.11
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD13	3	0.11
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD21	3	0.11
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD22	3	0.11
(1,1393)	1:A:14:GLY:H	1:A:15:LEU:HD23	3	0.11
(1,1293)	1:A:43:THR:HG21	1:A:45:THR:H	14	0.11
(1,1293)	1:A:43:THR:HG22	1:A:45:THR:H	14	0.11
(1,1293)	1:A:43:THR:HG23	1:A:45:THR:H	14	0.11
(1,1270)	1:A:33:VAL:H	1:A:34:LYS:HG2	6	0.11
(1,1270)	1:A:33:VAL:H	1:A:34:LYS:HG3	6	0.11
(1,1252)	1:A:52:LEU:HD11	1:A:57:SER:H	4	0.11
(1,1252)	1:A:52:LEU:HD12	1:A:57:SER:H	4	0.11
(1,1252)	1:A:52:LEU:HD13	1:A:57:SER:H	4	0.11
(1,1252)	1:A:52:LEU:HD21	1:A:57:SER:H	4	0.11
(1,1252)	1:A:52:LEU:HD22	1:A:57:SER:H	4	0.11
(1,1252)	1:A:52:LEU:HD23	1:A:57:SER:H	4	0.11
(1,1252)	1:A:52:LEU:HD11	1:A:57:SER:H	14	0.11
(1,1252)	1:A:52:LEU:HD12	1:A:57:SER:H	14	0.11
(1,1252)	1:A:52:LEU:HD13	1:A:57:SER:H	14	0.11
(1,1252)	1:A:52:LEU:HD21	1:A:57:SER:H	14	0.11
(1,1252)	1:A:52:LEU:HD22	1:A:57:SER:H	14	0.11
(1,1252)	1:A:52:LEU:HD23	1:A:57:SER:H	14	0.11
(1,1198)	1:A:59:MET:H	1:A:59:MET:HB3	18	0.11
(1,1176)	1:A:85:SER:H	1:A:85:SER:HB3	14	0.11
(1,1176)	1:A:85:SER:H	1:A:85:SER:HB3	20	0.11
(1,1150)	1:A:36:VAL:H	1:A:39:SER:H	14	0.11
(1,1086)	1:A:3:SER:H	1:A:4:GLU:HB2	8	0.11
(1,1086)	1:A:3:SER:H	1:A:4:GLU:HB3	8	0.11
(1,1066)	1:A:49:VAL:HB	1:A:51:CYS:H	5	0.11

10 Dihedral-angle violation analysis (i)

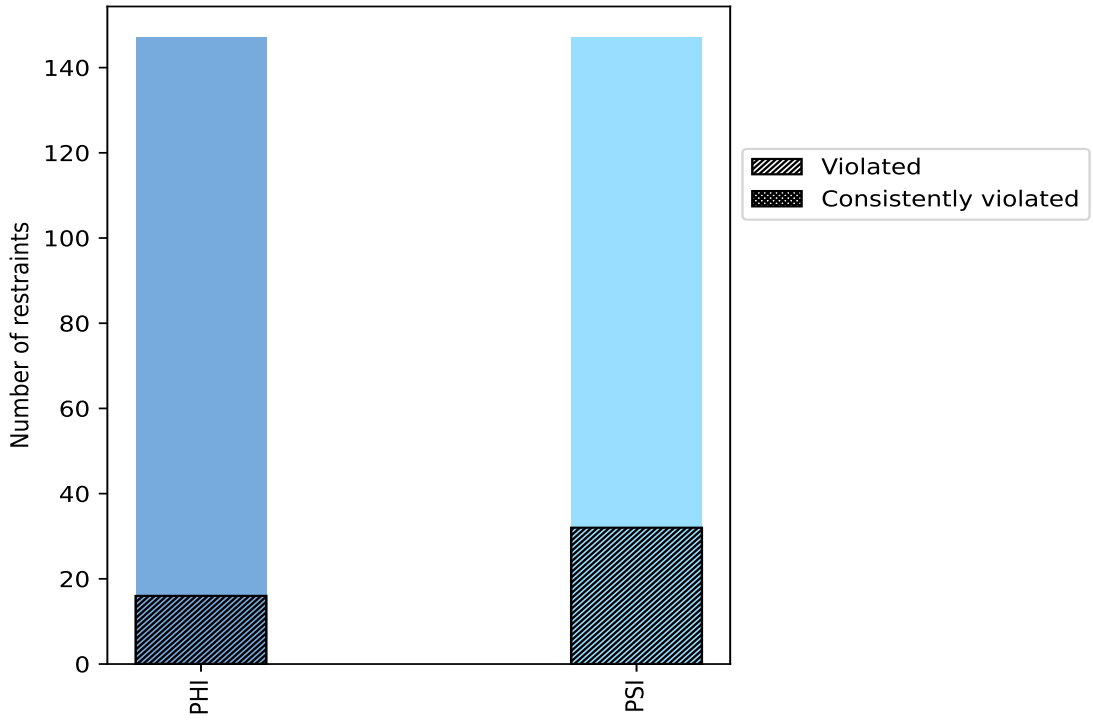
10.1 Summary of dihedral-angle violations (i)

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]
PHI	147	50.0	16	10.9	5.4	0	0.0	0.0
PSI	147	50.0	32	21.8	10.9	0	0.0	0.0
Total	294	100.0	48	16.3	16.3	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)



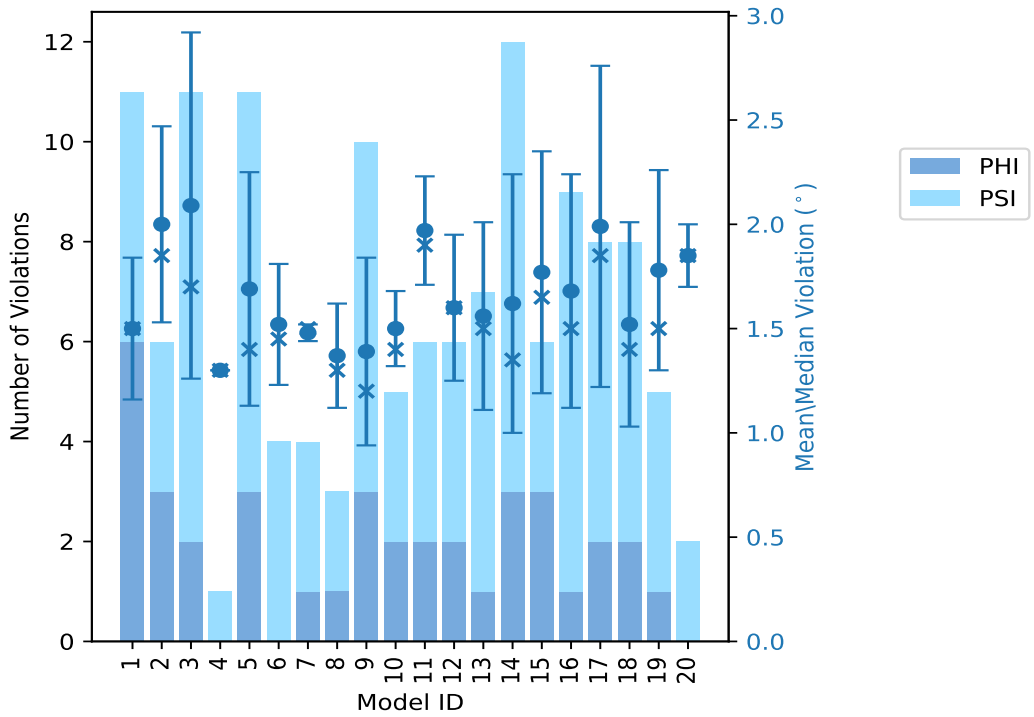
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PHI	PSI	Total				
1	6	5	11	1.5	2.1	0.34	1.5
2	3	3	6	2.0	2.7	0.47	1.85
3	2	9	11	2.09	3.9	0.83	1.7
4	0	1	1	1.3	1.3	0.0	1.3
5	3	8	11	1.69	2.8	0.56	1.4
6	0	4	4	1.52	2.0	0.29	1.45
7	1	3	4	1.48	1.5	0.04	1.5
8	1	2	3	1.37	1.7	0.25	1.3
9	3	7	10	1.39	2.7	0.45	1.2
10	2	3	5	1.5	1.8	0.18	1.4
11	2	4	6	1.97	2.4	0.26	1.9
12	2	4	6	1.6	2.2	0.35	1.6
13	1	6	7	1.56	2.5	0.45	1.5
14	3	9	12	1.62	3.4	0.62	1.35
15	3	3	6	1.77	2.9	0.58	1.65
16	1	8	9	1.68	3.0	0.56	1.5
17	2	6	8	1.99	3.4	0.77	1.85
18	2	6	8	1.52	2.7	0.49	1.4
19	1	4	5	1.78	2.5	0.48	1.5
20	0	2	2	1.85	2.0	0.15	1.85

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
9	17	26	1	5.0
3	1	4	2	10.0
1	5	6	3	15.0
0	0	0	4	20.0
2	3	5	5	25.0
0	2	2	6	30.0
0	2	2	7	35.0
0	0	0	8	40.0
0	1	1	9	45.0
1	0	1	10	50.0
0	0	0	11	55.0

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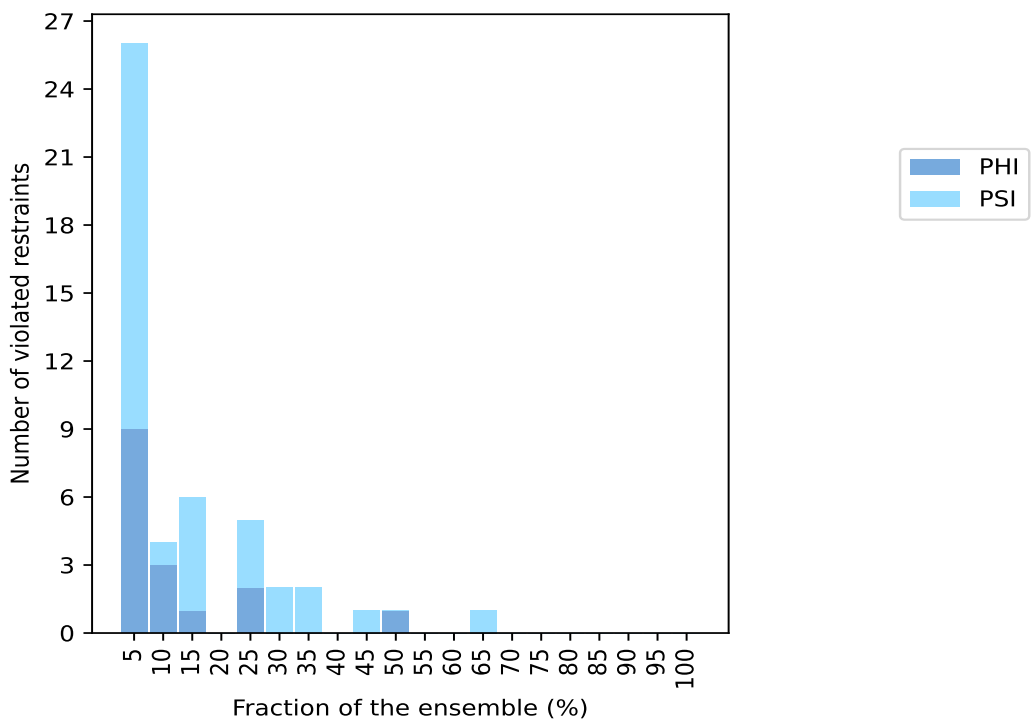
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	1	1	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

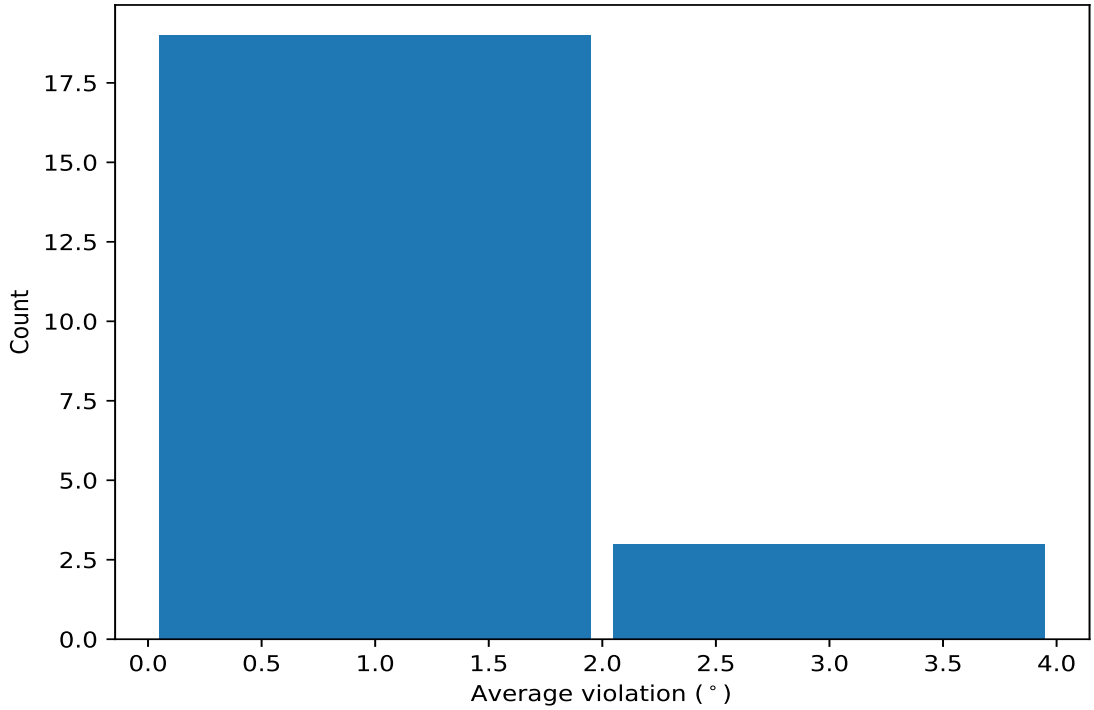


10.4 Most violated dihedral-angle restraints in the ensemble (i)

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
(1,56)	1:A:43:THR:N	1:A:43:THR:CA	1:A:43:THR:C	1:A:44:GLU:N	13	1.62	0.55	1.4
(1,219)	1:A:157:ASP:C	1:A:158:LYS:N	1:A:158:LYS:CA	1:A:158:LYS:C	10	2.07	0.46	2.05
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ARG:N	9	1.51	0.25	1.5
(1,232)	1:A:164:THR:N	1:A:164:THR:CA	1:A:164:THR:C	1:A:165:SER:N	7	1.91	0.61	1.9
(1,214)	1:A:152:LEU:N	1:A:152:LEU:CA	1:A:152:LEU:C	1:A:153:LYS:N	7	1.77	0.71	1.4
(1,196)	1:A:143:ALA:N	1:A:143:ALA:CA	1:A:143:ALA:C	1:A:144:ALA:N	6	2.2	0.74	2.2
(1,48)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:VAL:N	6	1.68	0.58	1.5
(1,2)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	1:A:5:LEU:N	5	1.76	0.14	1.7
(1,210)	1:A:150:LYS:N	1:A:150:LYS:CA	1:A:150:LYS:C	1:A:151:ILE:N	5	1.68	0.43	1.4
(1,54)	1:A:42:THR:N	1:A:42:THR:CA	1:A:42:THR:C	1:A:43:THR:N	5	1.48	0.27	1.3
(1,133)	1:A:86:PHE:C	1:A:87:GLU:N	1:A:87:GLU:CA	1:A:87:GLU:C	5	1.44	0.17	1.5
(1,215)	1:A:155:LYS:C	1:A:156:VAL:N	1:A:156:VAL:CA	1:A:156:VAL:C	5	1.36	0.26	1.2
(1,92)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	3	1.83	0.17	1.9
(1,58)	1:A:44:GLU:N	1:A:44:GLU:CA	1:A:44:GLU:C	1:A:45:THR:N	3	1.7	0.71	1.3
(1,154)	1:A:104:GLN:N	1:A:104:GLN:CA	1:A:104:GLN:C	1:A:105:PHE:N	3	1.5	0.22	1.4
(1,93)	1:A:64:ASP:C	1:A:65:ARG:N	1:A:65:ARG:CA	1:A:65:ARG:C	3	1.33	0.12	1.3
(1,178)	1:A:118:LEU:N	1:A:118:LEU:CA	1:A:118:LEU:C	1:A:119:LYS:N	3	1.33	0.09	1.4
(1,256)	1:A:179:LEU:N	1:A:179:LEU:CA	1:A:179:LEU:C	1:A:180:GLU:N	3	1.17	0.09	1.1
(1,53)	1:A:41:ARG:C	1:A:42:THR:N	1:A:42:THR:CA	1:A:42:THR:C	2	3.65	0.25	3.65
(1,222)	1:A:159:ASN:N	1:A:159:ASN:CA	1:A:159:ASN:C	1:A:160:LYS:N	2	1.9	0.3	1.9

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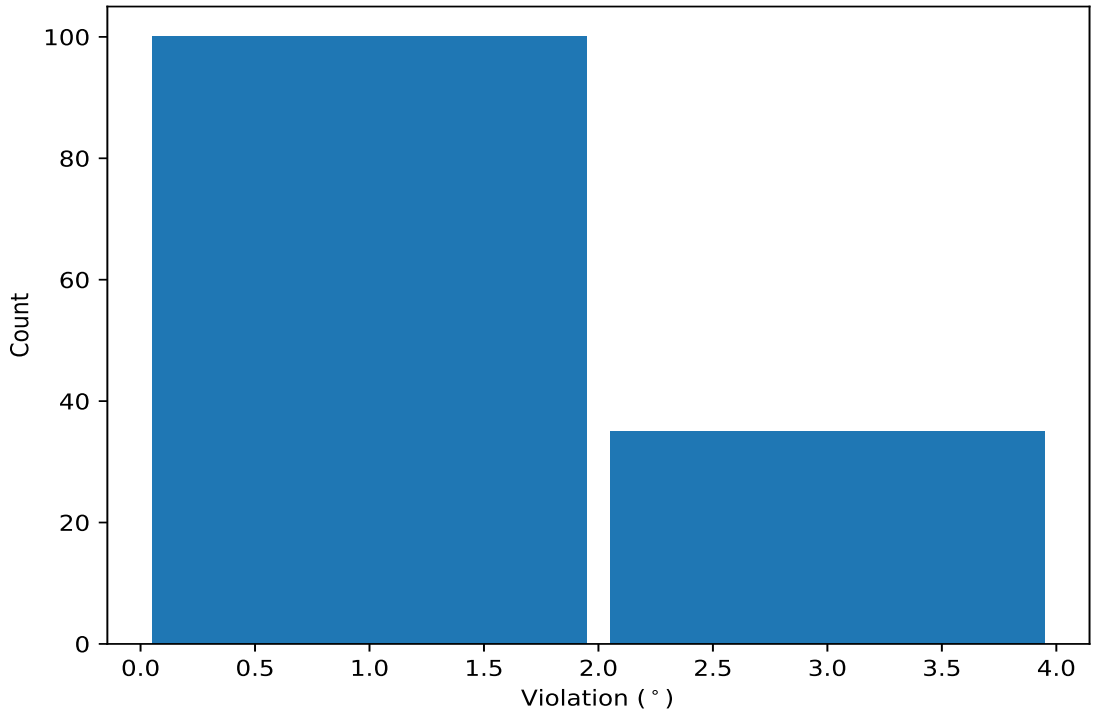
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,273)	1:A:231:ASP:C	1:A:232:TYR:N	1:A:232:TYR:CA	1:A:232:TYR:C	2	1.45	0.35	1.45
(1,141)	1:A:97:GLY:C	1:A:98:ILE:N	1:A:98:ILE:CA	1:A:98:ILE:C	2	1.4	0.3	1.4

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,53)	1:A:41:ARG:C	1:A:42:THR:N	1:A:42:THR:CA	1:A:42:THR:C	3	3.9
(1,53)	1:A:41:ARG:C	1:A:42:THR:N	1:A:42:THR:CA	1:A:42:THR:C	14	3.4
(1,196)	1:A:143:ALA:N	1:A:143:ALA:CA	1:A:143:ALA:C	1:A:144:ALA:N	17	3.4
(1,56)	1:A:43:THR:N	1:A:43:THR:CA	1:A:43:THR:C	1:A:44:GLU:N	3	3.1
(1,214)	1:A:152:LEU:N	1:A:152:LEU:CA	1:A:152:LEU:C	1:A:153:LYS:N	16	3.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,219)	1:A:157:ASP:C	1:A:158:LYS:N	1:A:158:LYS:CA	1:A:158:LYS:C	15	2.9
(1,48)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:VAL:N	17	2.8
(1,190)	1:A:129:GLN:N	1:A:129:GLN:CA	1:A:129:GLN:C	1:A:130:GLN:N	5	2.8
(1,58)	1:A:44:GLU:N	1:A:44:GLU:CA	1:A:44:GLU:C	1:A:45:THR:N	18	2.7
(1,232)	1:A:164:THR:N	1:A:164:THR:CA	1:A:164:THR:C	1:A:165:SER:N	3	2.7
(1,219)	1:A:157:ASP:C	1:A:158:LYS:N	1:A:158:LYS:CA	1:A:158:LYS:C	2	2.7
(1,196)	1:A:143:ALA:N	1:A:143:ALA:CA	1:A:143:ALA:C	1:A:144:ALA:N	9	2.7
(1,46)	1:A:31:SER:N	1:A:31:SER:CA	1:A:31:SER:C	1:A:32:ARG:N	3	2.5
(1,232)	1:A:164:THR:N	1:A:164:THR:CA	1:A:164:THR:C	1:A:165:SER:N	13	2.5
(1,232)	1:A:164:THR:N	1:A:164:THR:CA	1:A:164:THR:C	1:A:165:SER:N	19	2.5
(1,214)	1:A:152:LEU:N	1:A:152:LEU:CA	1:A:152:LEU:C	1:A:153:LYS:N	2	2.5
(1,56)	1:A:43:THR:N	1:A:43:THR:CA	1:A:43:THR:C	1:A:44:GLU:N	17	2.4
(1,219)	1:A:157:ASP:C	1:A:158:LYS:N	1:A:158:LYS:CA	1:A:158:LYS:C	11	2.4
(1,196)	1:A:143:ALA:N	1:A:143:ALA:CA	1:A:143:ALA:C	1:A:144:ALA:N	5	2.4
(1,222)	1:A:159:ASN:N	1:A:159:ASN:CA	1:A:159:ASN:C	1:A:160:LYS:N	3	2.2
(1,219)	1:A:157:ASP:C	1:A:158:LYS:N	1:A:158:LYS:CA	1:A:158:LYS:C	12	2.2
(1,210)	1:A:150:LYS:N	1:A:150:LYS:CA	1:A:150:LYS:C	1:A:151:ILE:N	11	2.2
(1,210)	1:A:150:LYS:N	1:A:150:LYS:CA	1:A:150:LYS:C	1:A:151:ILE:N	14	2.2
(1,188)	1:A:128:THR:N	1:A:128:THR:CA	1:A:128:THR:C	1:A:129:GLN:N	19	2.2
(1,219)	1:A:157:ASP:C	1:A:158:LYS:N	1:A:158:LYS:CA	1:A:158:LYS:C	5	2.1
(1,214)	1:A:152:LEU:N	1:A:152:LEU:CA	1:A:152:LEU:C	1:A:153:LYS:N	1	2.1
(1,191)	1:A:139:LEU:C	1:A:140:PHE:N	1:A:140:PHE:CA	1:A:140:PHE:C	2	2.1
(1,92)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	15	2.0
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ARG:N	5	2.0
(1,56)	1:A:43:THR:N	1:A:43:THR:CA	1:A:43:THR:C	1:A:44:GLU:N	20	2.0
(1,48)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:VAL:N	6	2.0
(1,219)	1:A:157:ASP:C	1:A:158:LYS:N	1:A:158:LYS:CA	1:A:158:LYS:C	1	2.0
(1,200)	1:A:145:LEU:N	1:A:145:LEU:CA	1:A:145:LEU:C	1:A:146:LEU:N	5	2.0
(1,2)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	1:A:5:LEU:N	16	2.0
(1,196)	1:A:143:ALA:N	1:A:143:ALA:CA	1:A:143:ALA:C	1:A:144:ALA:N	16	2.0
(1,92)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	11	1.9
(1,59)	1:A:44:GLU:C	1:A:45:THR:N	1:A:45:THR:CA	1:A:45:THR:C	14	1.9
(1,54)	1:A:42:THR:N	1:A:42:THR:CA	1:A:42:THR:C	1:A:43:THR:N	11	1.9
(1,232)	1:A:164:THR:N	1:A:164:THR:CA	1:A:164:THR:C	1:A:165:SER:N	17	1.9
(1,273)	1:A:231:ASP:C	1:A:232:TYR:N	1:A:232:TYR:CA	1:A:232:TYR:C	12	1.8
(1,215)	1:A:155:LYS:C	1:A:156:VAL:N	1:A:156:VAL:CA	1:A:156:VAL:C	10	1.8
(1,2)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	1:A:5:LEU:N	1	1.8
(1,194)	1:A:142:SER:N	1:A:142:SER:CA	1:A:142:SER:C	1:A:143:ALA:N	17	1.8
(1,154)	1:A:104:GLN:N	1:A:104:GLN:CA	1:A:104:GLN:C	1:A:105:PHE:N	13	1.8
(1,9)	1:A:7:GLY:C	1:A:8:ARG:N	1:A:8:ARG:CA	1:A:8:ARG:C	11	1.7
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ARG:N	1	1.7
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ARG:N	11	1.7
(1,54)	1:A:42:THR:N	1:A:42:THR:CA	1:A:42:THR:C	1:A:43:THR:N	14	1.7
(1,269)	1:A:220:HIS:C	1:A:221:LYS:N	1:A:221:LYS:CA	1:A:221:LYS:C	3	1.7
(1,219)	1:A:157:ASP:C	1:A:158:LYS:N	1:A:158:LYS:CA	1:A:158:LYS:C	8	1.7
(1,2)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	1:A:5:LEU:N	12	1.7
(1,2)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	1:A:5:LEU:N	20	1.7
(1,141)	1:A:97:GLY:C	1:A:98:ILE:N	1:A:98:ILE:CA	1:A:98:ILE:C	18	1.7
(1,133)	1:A:86:PHE:C	1:A:87:GLU:N	1:A:87:GLU:CA	1:A:87:GLU:C	15	1.7
(1,92)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	16	1.6
(1,56)	1:A:43:THR:N	1:A:43:THR:CA	1:A:43:THR:C	1:A:44:GLU:N	2	1.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,56)	1:A:43:THR:N	1:A:43:THR:CA	1:A:43:THR:C	1:A:44:GLU:N	13	1.6
(1,48)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:VAL:N	2	1.6
(1,222)	1:A:159:ASN:N	1:A:159:ASN:CA	1:A:159:ASN:C	1:A:160:LYS:N	18	1.6
(1,219)	1:A:157:ASP:C	1:A:158:LYS:N	1:A:158:LYS:CA	1:A:158:LYS:C	9	1.6
(1,219)	1:A:157:ASP:C	1:A:158:LYS:N	1:A:158:LYS:CA	1:A:158:LYS:C	10	1.6
(1,2)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	1:A:5:LEU:N	15	1.6
(1,93)	1:A:64:ASP:C	1:A:65:ARG:N	1:A:65:ARG:CA	1:A:65:ARG:C	1	1.5
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ARG:N	6	1.5
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ARG:N	12	1.5
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ARG:N	14	1.5
(1,78)	1:A:54:LEU:N	1:A:54:LEU:CA	1:A:54:LEU:C	1:A:55:ALA:N	19	1.5
(1,56)	1:A:43:THR:N	1:A:43:THR:CA	1:A:43:THR:C	1:A:44:GLU:N	7	1.5
(1,34)	1:A:25:GLU:N	1:A:25:GLU:CA	1:A:25:GLU:C	1:A:26:GLU:N	7	1.5
(1,291)	1:A:240:LEU:C	1:A:241:GLU:N	1:A:241:GLU:CA	1:A:241:GLU:C	1	1.5
(1,219)	1:A:157:ASP:C	1:A:158:LYS:N	1:A:158:LYS:CA	1:A:158:LYS:C	16	1.5
(1,215)	1:A:155:LYS:C	1:A:156:VAL:N	1:A:156:VAL:CA	1:A:156:VAL:C	2	1.5
(1,196)	1:A:143:ALA:N	1:A:143:ALA:CA	1:A:143:ALA:C	1:A:144:ALA:N	13	1.5
(1,133)	1:A:86:PHE:C	1:A:87:GLU:N	1:A:87:GLU:CA	1:A:87:GLU:C	7	1.5
(1,133)	1:A:86:PHE:C	1:A:87:GLU:N	1:A:87:GLU:CA	1:A:87:GLU:C	18	1.5
(1,56)	1:A:43:THR:N	1:A:43:THR:CA	1:A:43:THR:C	1:A:44:GLU:N	6	1.4
(1,56)	1:A:43:THR:N	1:A:43:THR:CA	1:A:43:THR:C	1:A:44:GLU:N	19	1.4
(1,48)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:VAL:N	10	1.4
(1,272)	1:A:228:LEU:N	1:A:228:LEU:CA	1:A:228:LEU:C	1:A:229:THR:N	17	1.4
(1,232)	1:A:164:THR:N	1:A:164:THR:CA	1:A:164:THR:C	1:A:165:SER:N	5	1.4
(1,228)	1:A:162:VAL:N	1:A:162:VAL:CA	1:A:162:VAL:C	1:A:163:ALA:N	3	1.4
(1,214)	1:A:152:LEU:N	1:A:152:LEU:CA	1:A:152:LEU:C	1:A:153:LYS:N	14	1.4
(1,210)	1:A:150:LYS:N	1:A:150:LYS:CA	1:A:150:LYS:C	1:A:151:ILE:N	3	1.4
(1,210)	1:A:150:LYS:N	1:A:150:LYS:CA	1:A:150:LYS:C	1:A:151:ILE:N	16	1.4
(1,178)	1:A:118:LEU:N	1:A:118:LEU:CA	1:A:118:LEU:C	1:A:119:LYS:N	3	1.4
(1,178)	1:A:118:LEU:N	1:A:118:LEU:CA	1:A:118:LEU:C	1:A:119:LYS:N	10	1.4
(1,154)	1:A:104:GLN:N	1:A:104:GLN:CA	1:A:104:GLN:C	1:A:105:PHE:N	7	1.4
(1,12)	1:A:9:LEU:N	1:A:9:LEU:CA	1:A:9:LEU:C	1:A:10:ALA:N	3	1.4
(1,93)	1:A:64:ASP:C	1:A:65:ARG:N	1:A:65:ARG:CA	1:A:65:ARG:C	15	1.3
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ARG:N	8	1.3
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ARG:N	10	1.3
(1,58)	1:A:44:GLU:N	1:A:44:GLU:CA	1:A:44:GLU:C	1:A:45:THR:N	14	1.3
(1,56)	1:A:43:THR:N	1:A:43:THR:CA	1:A:43:THR:C	1:A:44:GLU:N	4	1.3
(1,54)	1:A:42:THR:N	1:A:42:THR:CA	1:A:42:THR:C	1:A:43:THR:N	5	1.3
(1,54)	1:A:42:THR:N	1:A:42:THR:CA	1:A:42:THR:C	1:A:43:THR:N	18	1.3
(1,294)	1:A:242:ASN:N	1:A:242:ASN:CA	1:A:242:ASN:C	1:A:243:ALA:N	14	1.3
(1,263)	1:A:188:ARG:C	1:A:189:GLU:N	1:A:189:GLU:CA	1:A:189:GLU:C	19	1.3
(1,256)	1:A:179:LEU:N	1:A:179:LEU:CA	1:A:179:LEU:C	1:A:180:GLU:N	9	1.3
(1,184)	1:A:121:TYR:N	1:A:121:TYR:CA	1:A:121:TYR:C	1:A:122:GLU:N	16	1.3
(1,154)	1:A:104:GLN:N	1:A:104:GLN:CA	1:A:104:GLN:C	1:A:105:PHE:N	3	1.3
(1,133)	1:A:86:PHE:C	1:A:87:GLU:N	1:A:87:GLU:CA	1:A:87:GLU:C	1	1.3
(1,93)	1:A:64:ASP:C	1:A:65:ARG:N	1:A:65:ARG:CA	1:A:65:ARG:C	9	1.2
(1,70)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:CYS:N	16	1.2
(1,56)	1:A:43:THR:N	1:A:43:THR:CA	1:A:43:THR:C	1:A:44:GLU:N	9	1.2
(1,56)	1:A:43:THR:N	1:A:43:THR:CA	1:A:43:THR:C	1:A:44:GLU:N	12	1.2
(1,56)	1:A:43:THR:N	1:A:43:THR:CA	1:A:43:THR:C	1:A:44:GLU:N	14	1.2
(1,54)	1:A:42:THR:N	1:A:42:THR:CA	1:A:42:THR:C	1:A:43:THR:N	9	1.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,48)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:VAL:N	13	1.2
(1,246)	1:A:174:ARG:N	1:A:174:ARG:CA	1:A:174:ARG:C	1:A:175:LEU:N	14	1.2
(1,232)	1:A:164:THR:N	1:A:164:THR:CA	1:A:164:THR:C	1:A:165:SER:N	6	1.2
(1,232)	1:A:164:THR:N	1:A:164:THR:CA	1:A:164:THR:C	1:A:165:SER:N	9	1.2
(1,215)	1:A:155:LYS:C	1:A:156:VAL:N	1:A:156:VAL:CA	1:A:156:VAL:C	5	1.2
(1,215)	1:A:155:LYS:C	1:A:156:VAL:N	1:A:156:VAL:CA	1:A:156:VAL:C	14	1.2
(1,214)	1:A:152:LEU:N	1:A:152:LEU:CA	1:A:152:LEU:C	1:A:153:LYS:N	18	1.2
(1,210)	1:A:150:LYS:N	1:A:150:LYS:CA	1:A:150:LYS:C	1:A:151:ILE:N	9	1.2
(1,202)	1:A:146:LEU:N	1:A:146:LEU:CA	1:A:146:LEU:C	1:A:147:SER:N	5	1.2
(1,196)	1:A:143:ALA:N	1:A:143:ALA:CA	1:A:143:ALA:C	1:A:144:ALA:N	12	1.2
(1,178)	1:A:118:LEU:N	1:A:118:LEU:CA	1:A:118:LEU:C	1:A:119:LYS:N	1	1.2
(1,133)	1:A:86:PHE:C	1:A:87:GLU:N	1:A:87:GLU:CA	1:A:87:GLU:C	13	1.2
(1,105)	1:A:70:LYS:C	1:A:71:LEU:N	1:A:71:LEU:CA	1:A:71:LEU:C	9	1.2
(1,1)	1:A:3:SER:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	1	1.2
(1,8)	1:A:7:GLY:N	1:A:7:GLY:CA	1:A:7:GLY:C	1:A:8:ARG:N	16	1.1
(1,60)	1:A:45:THR:N	1:A:45:THR:CA	1:A:45:THR:C	1:A:46:SER:N	9	1.1
(1,58)	1:A:44:GLU:N	1:A:44:GLU:CA	1:A:44:GLU:C	1:A:45:THR:N	8	1.1
(1,56)	1:A:43:THR:N	1:A:43:THR:CA	1:A:43:THR:C	1:A:44:GLU:N	1	1.1
(1,48)	1:A:32:ARG:N	1:A:32:ARG:CA	1:A:32:ARG:C	1:A:33:VAL:N	18	1.1
(1,273)	1:A:231:ASP:C	1:A:232:TYR:N	1:A:232:TYR:CA	1:A:232:TYR:C	1	1.1
(1,256)	1:A:179:LEU:N	1:A:179:LEU:CA	1:A:179:LEU:C	1:A:180:GLU:N	14	1.1
(1,256)	1:A:179:LEU:N	1:A:179:LEU:CA	1:A:179:LEU:C	1:A:180:GLU:N	18	1.1
(1,236)	1:A:169:LYS:N	1:A:169:LYS:CA	1:A:169:LYS:C	1:A:170:ALA:N	15	1.1
(1,215)	1:A:155:LYS:C	1:A:156:VAL:N	1:A:156:VAL:CA	1:A:156:VAL:C	17	1.1
(1,214)	1:A:152:LEU:N	1:A:152:LEU:CA	1:A:152:LEU:C	1:A:153:LYS:N	5	1.1
(1,214)	1:A:152:LEU:N	1:A:152:LEU:CA	1:A:152:LEU:C	1:A:153:LYS:N	13	1.1
(1,201)	1:A:145:LEU:C	1:A:146:LEU:N	1:A:146:LEU:CA	1:A:146:LEU:C	5	1.1
(1,141)	1:A:97:GLY:C	1:A:98:ILE:N	1:A:98:ILE:CA	1:A:98:ILE:C	17	1.1