Full wwPDB NMR Structure Validation Report (i)

Dec 24, 2024 – 06:33 PM EST

PDB ID	:	2LVV
BMRB ID	:	18011
Title	:	NMR structure of TB24
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Deposited on	:	2012-07-11

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:

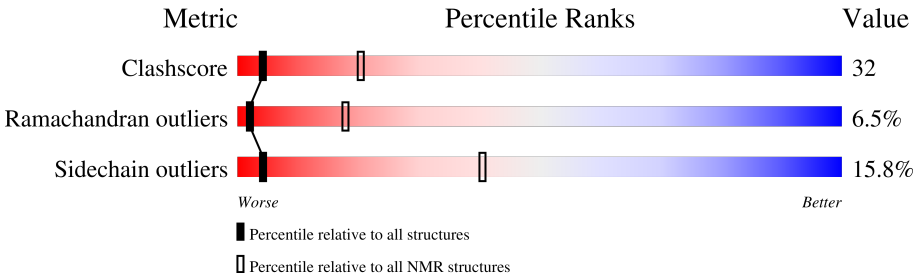
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 81%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	226	38% 33% 8% 18% ·

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:25-A:112, A:116-A:207 (180)	1.36	5

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

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

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

Cluster number	Models
1	2, 5, 9
2	4, 6
3	1, 8
Single-model clusters	3; 7; 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3391 atoms, of which 1675 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Flagellar calcium-binding protein TB-24.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	220	3391	1075	1675	285	346	10	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	ALA	conflict	UNP Q26680
A	219	LEU	-	expression tag	UNP Q26680
A	220	GLU	-	expression tag	UNP Q26680
A	221	HIS	-	expression tag	UNP Q26680
A	222	HIS	-	expression tag	UNP Q26680
A	223	HIS	-	expression tag	UNP Q26680
A	224	HIS	-	expression tag	UNP Q26680
A	225	HIS	-	expression tag	UNP Q26680
A	226	HIS	-	expression tag	UNP Q26680

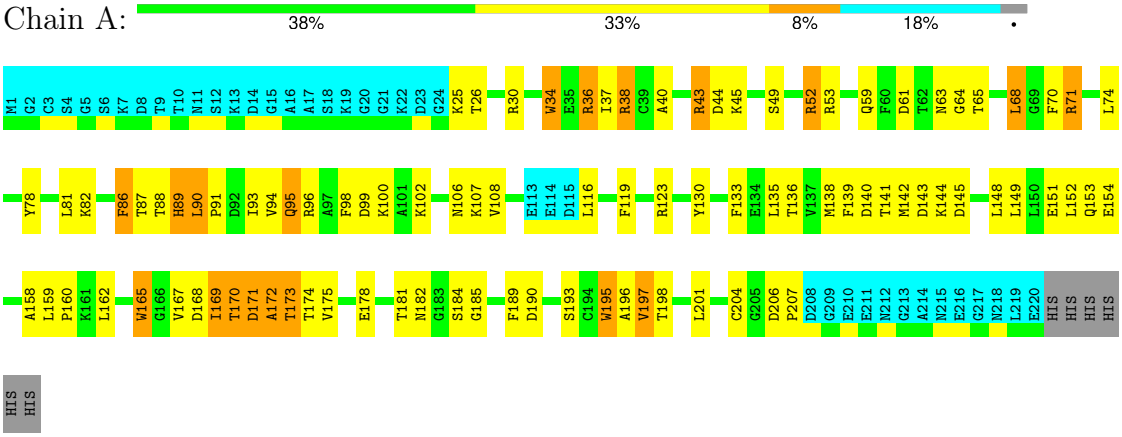
4 Residue-property plots (i)

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: Flagellar calcium-binding protein TB-24

Chain A:



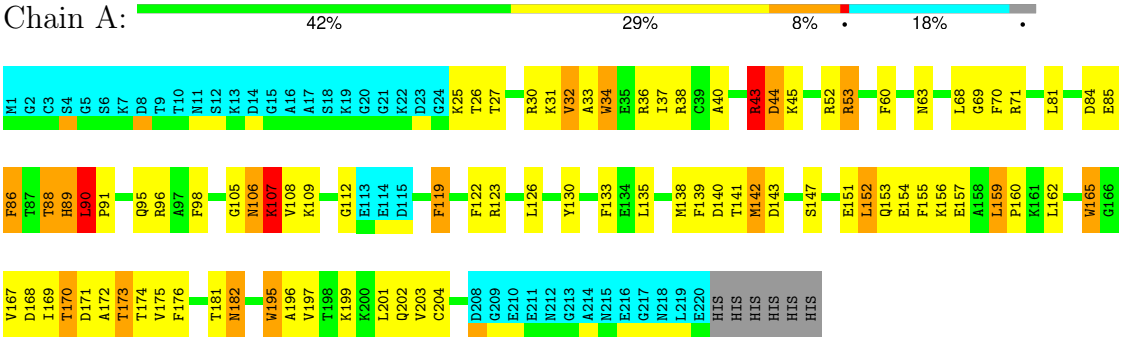
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Flagellar calcium-binding protein TB-24

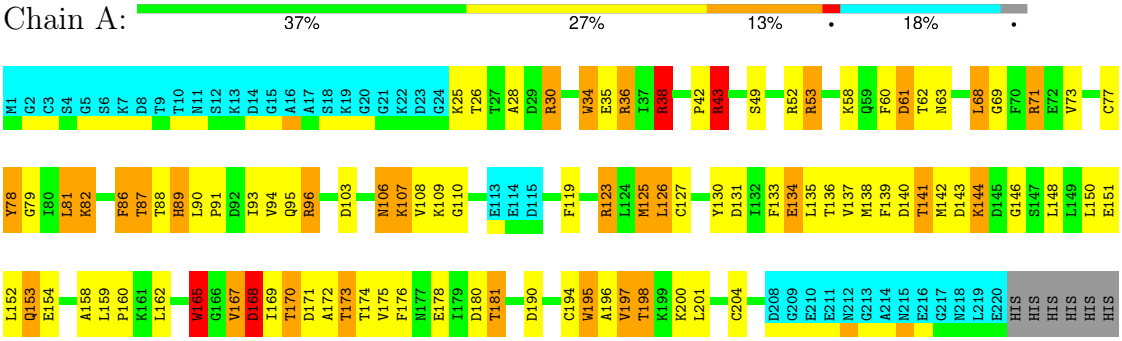
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Flagellar calcium-binding protein TB-24

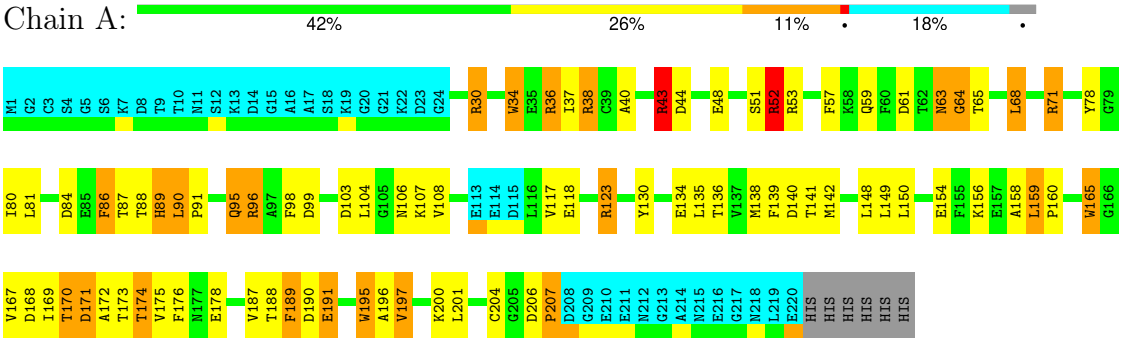
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Flagellar calcium-binding protein TB-24

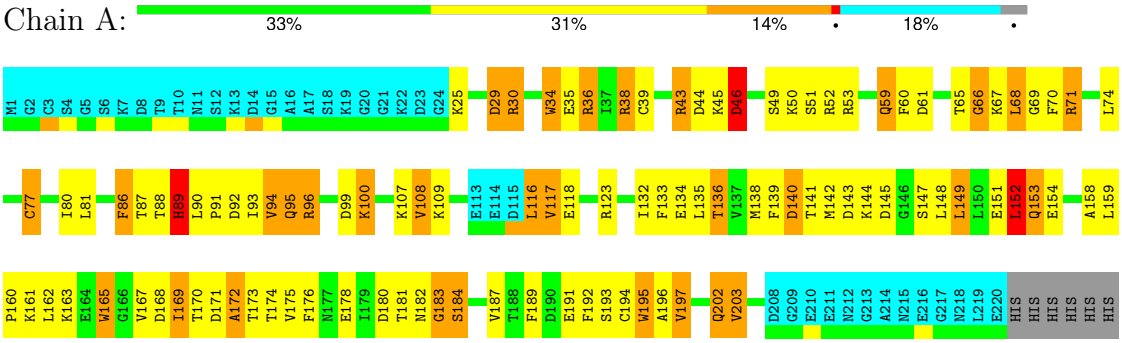
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Flagellar calcium-binding protein TB-24

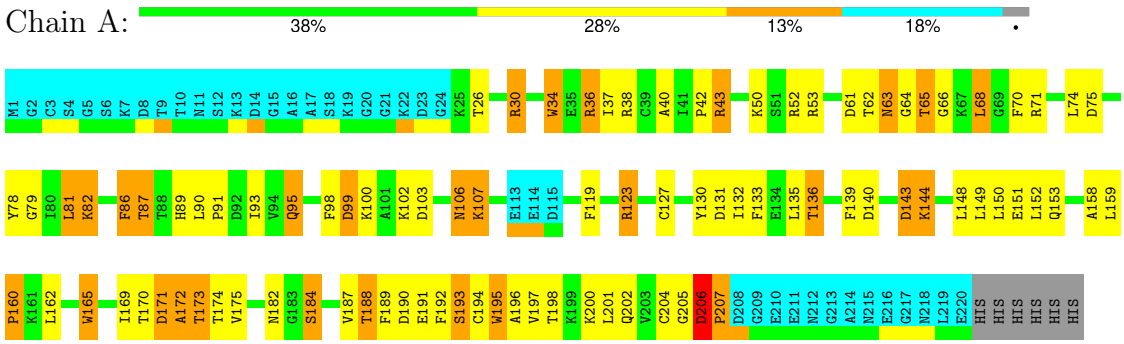
Chain A:



4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: Flagellar calcium-binding protein TB-24

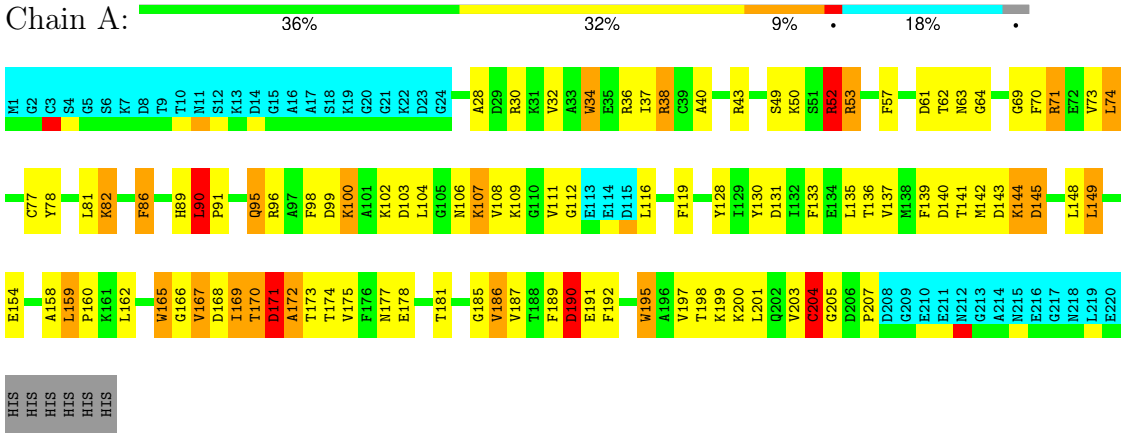
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Flagellar calcium-binding protein TB-24

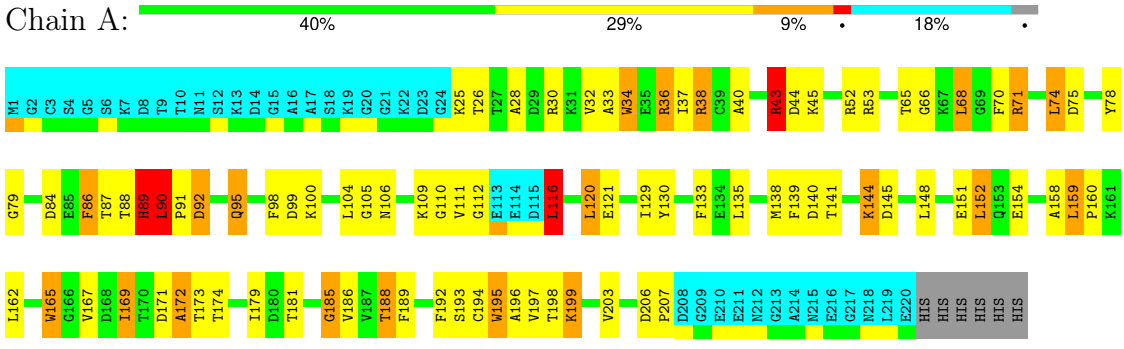
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Flagellar calcium-binding protein TB-24

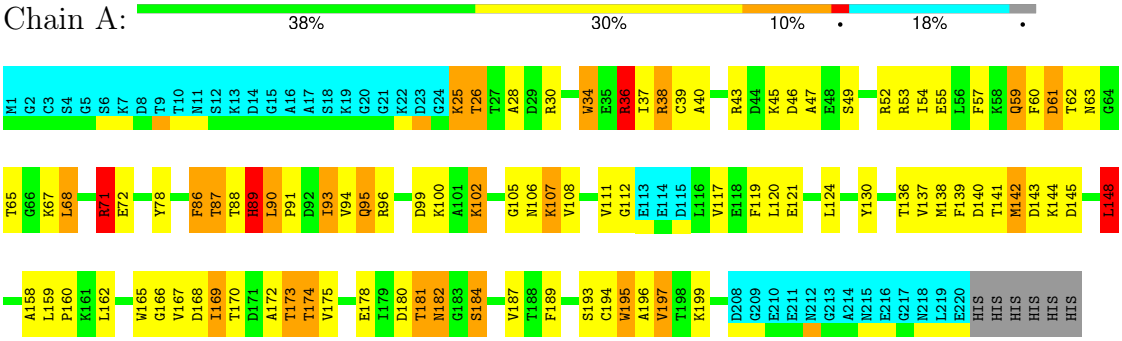
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Flagellar calcium-binding protein TB-24

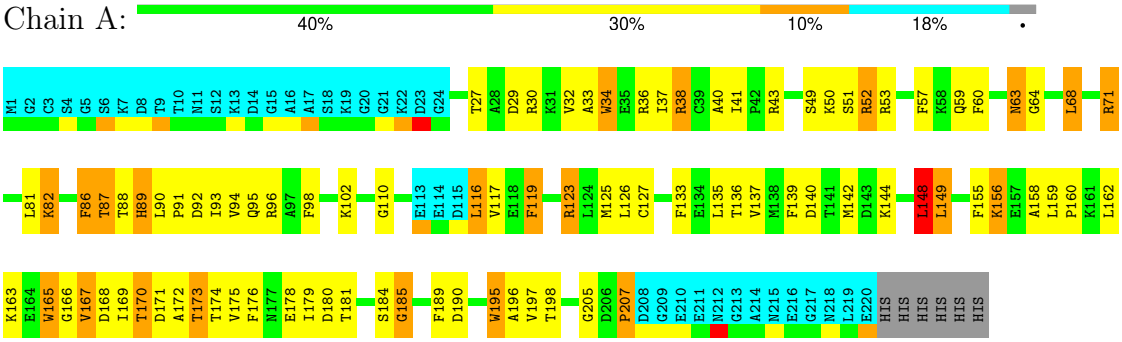
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Flagellar calcium-binding protein TB-24

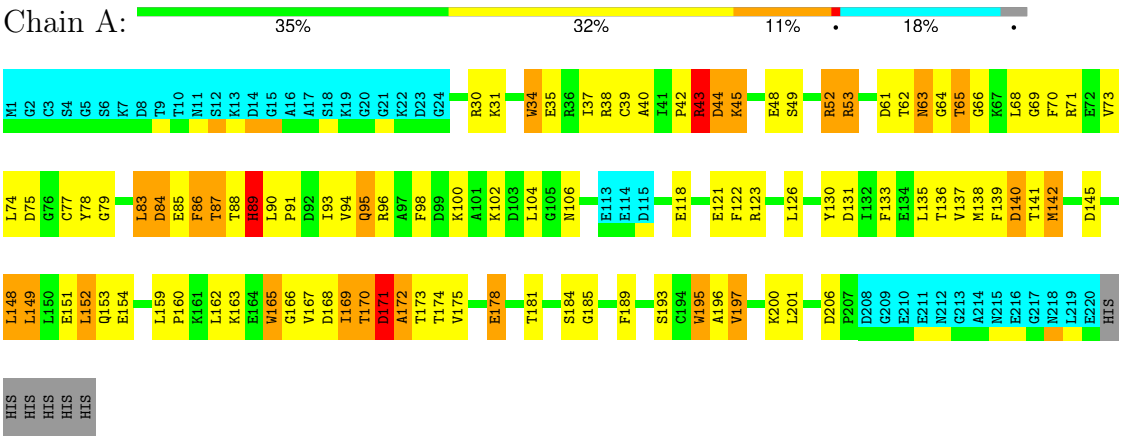
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Flagellar calcium-binding protein TB-24

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 10 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
XPLOR-NIH	refinement	

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	2286
Number of shifts mapped to atoms	2286
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.04±0.00	4±0/1470 (0.3± 0.0%)	1.29±0.00	17±1/1981 (0.9± 0.0%)
All	All	1.04	40/14700 (0.3%)	1.29	169/19810 (0.9%)

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	7.8±0.6
All	All	0	78

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	195	TRP	CG-CD2	-7.40	1.31	1.43	7	10
1	A	165	TRP	CG-CD2	-6.97	1.31	1.43	2	10
1	A	34	TRP	CG-CD2	-6.62	1.32	1.43	8	10
1	A	89	HIS	CG-ND1	-6.19	1.25	1.38	4	10

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	195	TRP	NE1-CE2-CZ2	9.25	140.57	130.40	9	10
1	A	165	TRP	NE1-CE2-CZ2	8.85	140.14	130.40	5	10
1	A	34	TRP	NE1-CE2-CZ2	8.58	139.84	130.40	8	10
1	A	195	TRP	NE1-CE2-CD2	-7.68	99.62	107.30	3	10
1	A	165	TRP	NE1-CE2-CD2	-7.37	99.94	107.30	5	10
1	A	34	TRP	NE1-CE2-CD2	-7.34	99.96	107.30	8	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	165	TRP	CG-CD1-NE1	-6.60	103.50	110.10	2	10
1	A	195	TRP	CG-CD1-NE1	-6.54	103.56	110.10	7	10
1	A	34	TRP	CG-CD1-NE1	-6.26	103.84	110.10	6	10
1	A	195	TRP	CD1-CG-CD2	6.10	111.18	106.30	1	10
1	A	34	TRP	CD1-NE1-CE2	6.06	114.46	109.00	9	10
1	A	165	TRP	CD1-CG-CD2	6.04	111.14	106.30	8	10
1	A	195	TRP	CG-CD2-CE3	-5.99	128.51	133.90	9	10
1	A	165	TRP	CD1-NE1-CE2	5.88	114.30	109.00	2	10
1	A	34	TRP	CD1-CG-CD2	5.88	111.01	106.30	4	10
1	A	195	TRP	CD1-NE1-CE2	5.80	114.22	109.00	2	10
1	A	195	TRP	CE2-CD2-CG	5.38	111.60	107.30	9	6
1	A	165	TRP	CG-CD2-CE3	-5.29	129.13	133.90	5	2
1	A	165	TRP	CE2-CD2-CG	5.11	111.39	107.30	5	1

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	38	ARG	Sidechain	10
1	A	71	ARG	Sidechain	10
1	A	36	ARG	Sidechain	9
1	A	52	ARG	Sidechain	9
1	A	30	ARG	Sidechain	9
1	A	43	ARG	Sidechain	8
1	A	53	ARG	Sidechain	8
1	A	96	ARG	Sidechain	8
1	A	123	ARG	Sidechain	7

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	1443	1443	1443	92±8
All	All	14430	14430	14430	919

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 32.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:VAL:HG22	1:A:168:ASP:H	0.97	1.18	9	2
1:A:90:LEU:H	1:A:90:LEU:HD13	0.96	1.16	6	2
1:A:90:LEU:HD13	1:A:90:LEU:N	0.96	1.75	7	2
1:A:90:LEU:HD23	1:A:90:LEU:H	0.94	1.18	8	1
1:A:170:THR:HG23	1:A:171:ASP:H	0.91	1.26	9	1
1:A:90:LEU:HD22	1:A:90:LEU:N	0.90	1.80	3	1
1:A:116:LEU:H	1:A:116:LEU:HD22	0.90	1.23	7	1
1:A:149:LEU:HD13	1:A:149:LEU:N	0.90	1.81	9	1
1:A:90:LEU:N	1:A:90:LEU:HD12	0.87	1.83	10	3
1:A:135:LEU:HD11	1:A:165:TRP:CH2	0.86	2.06	7	6
1:A:43:ARG:NH2	1:A:200:LYS:HZ1	0.83	1.71	2	1
1:A:167:VAL:HG12	1:A:168:ASP:H	0.82	1.32	8	4
1:A:197:VAL:HG13	1:A:198:THR:H	0.82	1.34	9	2
1:A:90:LEU:HD22	1:A:90:LEU:H	0.82	1.30	3	1
1:A:90:LEU:HD23	1:A:90:LEU:N	0.82	1.90	8	1
1:A:57:PHE:CZ	1:A:68:LEU:HD13	0.81	2.11	3	1
1:A:68:LEU:N	1:A:68:LEU:HD22	0.81	1.90	5	3
1:A:135:LEU:HD23	1:A:165:TRP:CH2	0.81	2.10	5	1
1:A:116:LEU:HD22	1:A:116:LEU:N	0.81	1.91	7	1
1:A:90:LEU:N	1:A:91:PRO:CD	0.80	2.45	6	10
1:A:148:LEU:HD12	1:A:148:LEU:N	0.78	1.93	7	4
1:A:68:LEU:HD12	1:A:68:LEU:N	0.78	1.93	7	3
1:A:135:LEU:HD12	1:A:135:LEU:C	0.78	1.99	5	1
1:A:197:VAL:HG13	1:A:198:THR:N	0.77	1.95	9	4
1:A:83:LEU:HD12	1:A:83:LEU:H	0.76	1.39	10	1
1:A:162:LEU:C	1:A:162:LEU:HD13	0.75	2.02	9	3
1:A:167:VAL:HG12	1:A:168:ASP:N	0.75	1.94	1	4
1:A:201:LEU:C	1:A:201:LEU:HD23	0.74	2.03	10	1
1:A:78:TYR:CD2	1:A:90:LEU:HD22	0.74	2.16	10	1
1:A:206:ASP:N	1:A:207:PRO:CD	0.74	2.50	3	1
1:A:90:LEU:HD13	1:A:90:LEU:H	0.72	1.44	7	1
1:A:90:LEU:N	1:A:90:LEU:CD1	0.72	2.49	7	6
1:A:176:PHE:CE1	1:A:187:VAL:HG23	0.72	2.19	4	1
1:A:106:ASN:N	1:A:106:ASN:HD22	0.72	1.82	2	2
1:A:93:ILE:HG23	1:A:94:VAL:N	0.71	1.99	9	5
1:A:155:PHE:CZ	1:A:172:ALA:HB1	0.71	2.20	1	2
1:A:106:ASN:HD22	1:A:107:LYS:N	0.71	1.82	5	1
1:A:162:LEU:HD11	1:A:167:VAL:CG1	0.71	2.16	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LEU:H	1:A:90:LEU:CD1	0.70	1.98	1	1
1:A:43:ARG:NH2	1:A:200:LYS:NZ	0.70	2.39	2	1
1:A:116:LEU:H	1:A:116:LEU:CD2	0.69	2.00	7	1
1:A:135:LEU:HD12	1:A:136:THR:N	0.69	2.02	5	1
1:A:168:ASP:O	1:A:169:ILE:HG22	0.69	1.88	8	1
1:A:162:LEU:HD11	1:A:192:PHE:CE2	0.68	2.23	6	1
1:A:135:LEU:HD21	1:A:165:TRP:CE2	0.68	2.24	10	1
1:A:126:LEU:C	1:A:126:LEU:HD13	0.68	2.09	9	1
1:A:167:VAL:HG22	1:A:168:ASP:N	0.68	1.98	9	1
1:A:165:TRP:CZ3	1:A:196:ALA:HB1	0.68	2.24	9	6
1:A:122:PHE:CZ	1:A:126:LEU:HD11	0.67	2.24	10	2
1:A:84:ASP:N	1:A:84:ASP:OD1	0.67	2.27	10	1
1:A:121:GLU:H	1:A:121:GLU:CD	0.67	1.93	8	3
1:A:141:THR:HG23	1:A:142:MET:N	0.67	2.04	1	4
1:A:99:ASP:CG	1:A:100:LYS:N	0.67	2.48	5	2
1:A:90:LEU:C	1:A:90:LEU:HD22	0.67	2.10	6	3
1:A:86:PHE:C	1:A:86:PHE:CD1	0.66	2.68	5	9
1:A:90:LEU:H	1:A:90:LEU:CD2	0.66	1.98	8	2
1:A:182:ASN:HD22	1:A:182:ASN:N	0.66	1.88	1	1
1:A:111:VAL:HG12	1:A:112:GLY:N	0.66	2.04	8	3
1:A:98:PHE:CZ	1:A:117:VAL:HG13	0.65	2.26	9	1
1:A:106:ASN:ND2	1:A:107:LYS:N	0.65	2.44	5	1
1:A:116:LEU:HD12	1:A:116:LEU:N	0.65	2.07	6	1
1:A:173:THR:CG2	1:A:174:THR:N	0.65	2.60	7	3
1:A:95:GLN:NE2	1:A:95:GLN:C	0.65	2.51	4	4
1:A:43:ARG:CZ	1:A:200:LYS:NZ	0.65	2.59	2	1
1:A:88:THR:C	1:A:89:HIS:CG	0.65	2.69	2	3
1:A:68:LEU:HD22	1:A:68:LEU:H	0.64	1.51	5	1
1:A:197:VAL:CG1	1:A:198:THR:N	0.64	2.60	6	4
1:A:131:ASP:OD2	1:A:165:TRP:CH2	0.64	2.51	5	1
1:A:106:ASN:N	1:A:106:ASN:ND2	0.64	2.44	2	1
1:A:89:HIS:O	1:A:89:HIS:CG	0.64	2.49	7	1
1:A:32:VAL:HG23	1:A:33:ALA:N	0.64	2.08	9	2
1:A:148:LEU:N	1:A:148:LEU:CD1	0.64	2.61	6	2
1:A:68:LEU:N	1:A:68:LEU:CD1	0.64	2.61	7	2
1:A:90:LEU:H	1:A:91:PRO:HD3	0.64	1.52	7	4
1:A:138:MET:CE	1:A:165:TRP:CD1	0.64	2.80	3	2
1:A:32:VAL:HG23	1:A:33:ALA:H	0.64	1.52	9	2
1:A:140:ASP:OD1	1:A:141:THR:N	0.64	2.31	4	1
1:A:167:VAL:CG2	1:A:168:ASP:H	0.63	2.02	9	1
1:A:90:LEU:HD12	1:A:90:LEU:H	0.63	1.50	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:174:THR:OG1	1:A:175:VAL:N	0.63	2.32	9	2
1:A:121:GLU:CD	1:A:121:GLU:N	0.63	2.52	8	2
1:A:170:THR:HG23	1:A:171:ASP:N	0.63	2.06	9	1
1:A:68:LEU:N	1:A:68:LEU:CD2	0.62	2.62	5	3
1:A:106:ASN:ND2	1:A:106:ASN:H	0.62	1.91	2	2
1:A:149:LEU:HD12	1:A:149:LEU:N	0.62	2.09	3	2
1:A:77:CYS:SG	1:A:78:TYR:N	0.62	2.73	2	2
1:A:116:LEU:N	1:A:116:LEU:CD1	0.62	2.63	6	1
1:A:93:ILE:CG2	1:A:94:VAL:N	0.62	2.63	9	2
1:A:182:ASN:N	1:A:182:ASN:ND2	0.62	2.46	1	1
1:A:197:VAL:CG1	1:A:198:THR:H	0.62	2.08	9	3
1:A:53:ARG:NH1	1:A:119:PHE:CD1	0.61	2.69	9	1
1:A:107:LYS:CB	1:A:107:LYS:NZ	0.61	2.63	2	1
1:A:90:LEU:N	1:A:91:PRO:HD2	0.61	2.10	2	10
1:A:130:TYR:C	1:A:130:TYR:CD1	0.61	2.73	5	6
1:A:92:ASP:OD1	1:A:93:ILE:N	0.61	2.32	4	2
1:A:60:PHE:CD1	1:A:60:PHE:N	0.60	2.67	9	2
1:A:194:CYS:SG	1:A:195:TRP:N	0.60	2.74	5	1
1:A:167:VAL:CG1	1:A:168:ASP:H	0.60	2.08	1	3
1:A:206:ASP:N	1:A:207:PRO:HD3	0.60	2.10	3	3
1:A:90:LEU:H	1:A:91:PRO:CD	0.60	2.09	7	1
1:A:90:LEU:N	1:A:91:PRO:HD3	0.60	2.12	1	4
1:A:135:LEU:HD21	1:A:165:TRP:CD2	0.60	2.30	10	1
1:A:142:MET:SD	1:A:143:ASP:OD1	0.60	2.59	1	1
1:A:143:ASP:CG	1:A:144:LYS:N	0.60	2.54	6	2
1:A:99:ASP:OD1	1:A:100:LYS:N	0.60	2.34	4	1
1:A:123:ARG:HH21	1:A:207:PRO:CD	0.60	2.10	5	1
1:A:170:THR:CG2	1:A:171:ASP:H	0.60	2.08	9	1
1:A:43:ARG:NE	1:A:130:TYR:OH	0.60	2.35	1	1
1:A:170:THR:HG22	1:A:171:ASP:OD1	0.60	1.97	3	1
1:A:38:ARG:NE	1:A:130:TYR:OH	0.60	2.35	3	1
1:A:32:VAL:CG1	1:A:33:ALA:N	0.59	2.64	1	1
1:A:69:GLY:O	1:A:73:VAL:HG23	0.59	1.97	6	3
1:A:171:ASP:OD1	1:A:171:ASP:N	0.59	2.32	3	3
1:A:29:ASP:OD1	1:A:29:ASP:N	0.59	2.34	4	1
1:A:61:ASP:OD1	1:A:62:THR:N	0.59	2.35	5	2
1:A:111:VAL:CG1	1:A:112:GLY:N	0.59	2.65	8	3
1:A:92:ASP:OD1	1:A:92:ASP:N	0.59	2.35	7	1
1:A:106:ASN:HD22	1:A:107:LYS:H	0.59	1.39	5	1
1:A:87:THR:HG23	1:A:89:HIS:NE2	0.58	2.13	8	1
1:A:141:THR:CG2	1:A:142:MET:N	0.58	2.66	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:182:ASN:HD22	1:A:182:ASN:H	0.58	1.41	1	1
1:A:135:LEU:C	1:A:135:LEU:CD1	0.58	2.71	5	1
1:A:36:ARG:NH2	1:A:39:CYS:CB	0.58	2.66	8	1
1:A:34:TRP:CZ3	1:A:133:PHE:CB	0.58	2.86	4	3
1:A:154:GLU:CD	1:A:154:GLU:N	0.58	2.56	1	3
1:A:87:THR:HG23	1:A:89:HIS:CE1	0.58	2.34	8	1
1:A:108:VAL:HG13	1:A:109:LYS:H	0.58	1.58	2	1
1:A:68:LEU:CD1	1:A:68:LEU:H	0.57	2.12	8	3
1:A:118:GLU:N	1:A:121:GLU:OE1	0.57	2.35	10	1
1:A:87:THR:OG1	1:A:133:PHE:CZ	0.57	2.52	2	1
1:A:151:GLU:N	1:A:151:GLU:CD	0.57	2.58	4	1
1:A:38:ARG:CG	1:A:39:CYS:N	0.57	2.67	4	1
1:A:83:LEU:H	1:A:83:LEU:CD1	0.57	2.08	10	1
1:A:108:VAL:HG13	1:A:109:LYS:N	0.57	2.15	2	2
1:A:63:ASN:ND2	1:A:65:THR:OG1	0.57	2.38	8	2
1:A:169:ILE:CG1	1:A:195:TRP:CH2	0.57	2.88	3	2
1:A:68:LEU:HD12	1:A:68:LEU:H	0.56	1.58	4	2
1:A:57:PHE:C	1:A:57:PHE:CD1	0.56	2.79	6	1
1:A:44:ASP:OD1	1:A:45:LYS:N	0.56	2.38	7	1
1:A:30:ARG:CG	1:A:86:PHE:CE1	0.56	2.88	2	1
1:A:135:LEU:CD1	1:A:165:TRP:CH2	0.56	2.85	7	3
1:A:77:CYS:SG	1:A:81:LEU:HD12	0.56	2.40	4	1
1:A:95:GLN:HE21	1:A:95:GLN:CA	0.56	2.13	10	1
1:A:26:THR:OG1	1:A:27:THR:N	0.56	2.38	1	1
1:A:138:MET:O	1:A:141:THR:HG22	0.56	2.01	8	1
1:A:27:THR:HG22	1:A:30:ARG:NH2	0.56	2.16	1	1
1:A:124:LEU:CD2	1:A:124:LEU:N	0.56	2.69	8	1
1:A:168:ASP:N	1:A:168:ASP:OD1	0.56	2.38	10	2
1:A:154:GLU:CD	1:A:154:GLU:H	0.56	2.02	1	3
1:A:167:VAL:CG1	1:A:168:ASP:N	0.56	2.69	10	3
1:A:41:ILE:CG2	1:A:126:LEU:HD11	0.56	2.30	9	1
1:A:88:THR:O	1:A:89:HIS:ND1	0.56	2.38	8	4
1:A:149:LEU:N	1:A:149:LEU:CD1	0.56	2.69	3	2
1:A:68:LEU:H	1:A:68:LEU:HD12	0.56	1.59	8	1
1:A:125:MET:C	1:A:125:MET:SD	0.55	2.84	2	1
1:A:159:LEU:HD11	1:A:172:ALA:HB2	0.55	1.77	4	2
1:A:53:ARG:NE	1:A:119:PHE:CE1	0.55	2.75	1	1
1:A:90:LEU:C	1:A:90:LEU:CD2	0.55	2.74	6	3
1:A:143:ASP:CG	1:A:144:LYS:H	0.55	2.04	6	2
1:A:88:THR:O	1:A:89:HIS:CG	0.55	2.60	2	3
1:A:94:VAL:HG13	1:A:95:GLN:N	0.55	2.16	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:MET:SD	1:A:126:LEU:HD22	0.55	2.41	2	1
1:A:145:ASP:N	1:A:145:ASP:OD1	0.55	2.40	6	2
1:A:139:PHE:CD1	1:A:139:PHE:N	0.55	2.73	5	6
1:A:180:ASP:OD1	1:A:181:THR:N	0.55	2.40	9	2
1:A:151:GLU:N	1:A:151:GLU:OE1	0.55	2.40	4	1
1:A:34:TRP:CH2	1:A:133:PHE:CB	0.55	2.89	7	3
1:A:180:ASP:OD2	1:A:184:SER:N	0.55	2.39	8	1
1:A:116:LEU:N	1:A:116:LEU:HD22	0.55	2.17	9	1
1:A:176:PHE:CZ	1:A:185:GLY:O	0.55	2.60	9	1
1:A:167:VAL:HG13	1:A:168:ASP:N	0.54	2.16	6	1
1:A:199:LYS:O	1:A:203:VAL:HG23	0.54	2.02	7	1
1:A:131:ASP:HB2	1:A:197:VAL:HG13	0.54	1.77	10	1
1:A:193:SER:O	1:A:197:VAL:HG23	0.54	2.03	10	1
1:A:188:THR:OG1	1:A:189:PHE:N	0.54	2.39	7	1
1:A:61:ASP:OD1	1:A:63:ASN:N	0.54	2.40	5	1
1:A:87:THR:HG23	1:A:89:HIS:CD2	0.54	2.37	8	1
1:A:61:ASP:CG	1:A:66:GLY:H	0.54	2.06	10	1
1:A:122:PHE:CE2	1:A:126:LEU:HD11	0.54	2.37	10	1
1:A:158:ALA:O	1:A:162:LEU:N	0.54	2.39	2	6
1:A:41:ILE:HG23	1:A:126:LEU:HD11	0.54	1.77	9	1
1:A:78:TYR:CD1	1:A:78:TYR:C	0.54	2.81	5	2
1:A:95:GLN:C	1:A:95:GLN:HE21	0.54	2.07	8	1
1:A:139:PHE:O	1:A:141:THR:N	0.53	2.41	8	6
1:A:169:ILE:O	1:A:169:ILE:HG23	0.53	2.03	5	3
1:A:171:ASP:OD2	1:A:174:THR:HG21	0.53	2.03	2	1
1:A:25:LYS:O	1:A:26:THR:HG23	0.53	2.03	8	1
1:A:102:LYS:O	1:A:106:ASN:ND2	0.53	2.41	8	1
1:A:151:GLU:O	1:A:153:GLN:N	0.53	2.42	1	4
1:A:70:PHE:CE2	1:A:74:LEU:HD12	0.53	2.37	6	1
1:A:162:LEU:HD13	1:A:163:LYS:N	0.53	2.19	9	1
1:A:90:LEU:N	1:A:90:LEU:CD2	0.53	2.63	8	2
1:A:89:HIS:O	1:A:89:HIS:CD2	0.53	2.61	7	1
1:A:70:PHE:CD2	1:A:95:GLN:NE2	0.53	2.76	1	1
1:A:84:ASP:CG	1:A:90:LEU:HD21	0.53	2.23	10	1
1:A:148:LEU:O	1:A:189:PHE:CD1	0.53	2.61	8	2
1:A:193:SER:O	1:A:196:ALA:N	0.53	2.42	5	1
1:A:162:LEU:O	1:A:165:TRP:N	0.53	2.42	9	5
1:A:78:TYR:CD1	1:A:78:TYR:O	0.53	2.62	7	3
1:A:139:PHE:C	1:A:141:THR:H	0.53	2.06	7	2
1:A:64:GLY:O	1:A:66:GLY:N	0.53	2.41	5	2
1:A:106:ASN:O	1:A:107:LYS:C	0.53	2.47	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:THR:OG1	1:A:171:ASP:N	0.53	2.41	4	2
1:A:175:VAL:O	1:A:178:GLU:N	0.53	2.42	9	5
1:A:95:GLN:NE2	1:A:95:GLN:O	0.53	2.42	6	5
1:A:59:GLN:N	1:A:59:GLN:OE1	0.53	2.42	8	1
1:A:60:PHE:O	1:A:62:THR:N	0.52	2.42	8	2
1:A:162:LEU:HD11	1:A:192:PHE:CZ	0.52	2.39	6	1
1:A:45:LYS:NZ	1:A:53:ARG:NH1	0.52	2.57	10	1
1:A:95:GLN:CA	1:A:95:GLN:NE2	0.52	2.72	10	1
1:A:103:ASP:O	1:A:106:ASN:ND2	0.52	2.43	2	3
1:A:104:LEU:C	1:A:106:ASN:H	0.52	2.08	10	2
1:A:195:TRP:CE3	1:A:195:TRP:C	0.52	2.83	5	3
1:A:203:VAL:HG23	1:A:204:CYS:N	0.52	2.20	1	1
1:A:53:ARG:CZ	1:A:53:ARG:CB	0.52	2.87	2	1
1:A:106:ASN:OD1	1:A:107:LYS:N	0.52	2.43	3	1
1:A:90:LEU:N	1:A:90:LEU:HD13	0.52	2.08	1	1
1:A:172:ALA:O	1:A:175:VAL:N	0.52	2.42	1	4
1:A:60:PHE:C	1:A:62:THR:H	0.52	2.07	8	1
1:A:154:GLU:O	1:A:158:ALA:N	0.52	2.42	7	3
1:A:34:TRP:HE1	1:A:38:ARG:HH21	0.52	1.48	6	1
1:A:139:PHE:O	1:A:142:MET:N	0.52	2.42	9	1
1:A:37:ILE:O	1:A:40:ALA:N	0.52	2.43	1	8
1:A:77:CYS:O	1:A:79:GLY:N	0.52	2.42	2	1
1:A:143:ASP:OD1	1:A:144:LYS:N	0.52	2.43	4	1
1:A:162:LEU:HD13	1:A:162:LEU:O	0.52	2.04	10	1
1:A:27:THR:O	1:A:31:LYS:N	0.51	2.43	1	1
1:A:131:ASP:OD2	1:A:165:TRP:CZ2	0.51	2.63	5	1
1:A:159:LEU:CB	1:A:160:PRO:CD	0.51	2.88	4	6
1:A:68:LEU:H	1:A:68:LEU:CD2	0.51	2.15	5	1
1:A:88:THR:O	1:A:89:HIS:CB	0.51	2.57	3	8
1:A:202:GLN:CD	1:A:202:GLN:C	0.51	2.69	4	1
1:A:134:GLU:O	1:A:138:MET:SD	0.51	2.69	3	1
1:A:90:LEU:HD22	1:A:90:LEU:O	0.51	2.05	1	1
1:A:176:PHE:CD1	1:A:176:PHE:C	0.51	2.84	1	2
1:A:106:ASN:C	1:A:108:VAL:H	0.51	2.07	6	1
1:A:126:LEU:HD13	1:A:126:LEU:O	0.51	2.04	9	1
1:A:138:MET:HE3	1:A:165:TRP:CD1	0.51	2.40	3	1
1:A:75:ASP:O	1:A:79:GLY:N	0.51	2.44	5	3
1:A:139:PHE:C	1:A:141:THR:N	0.51	2.63	8	5
1:A:182:ASN:O	1:A:183:GLY:C	0.51	2.48	4	1
1:A:95:GLN:HE21	1:A:95:GLN:C	0.51	2.09	10	1
1:A:143:ASP:C	1:A:145:ASP:H	0.51	2.09	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:PHE:CG	1:A:87:THR:N	0.51	2.79	9	6
1:A:188:THR:HG22	1:A:189:PHE:N	0.51	2.21	3	1
1:A:162:LEU:HD13	1:A:169:ILE:HD11	0.51	1.83	7	1
1:A:57:PHE:CD1	1:A:57:PHE:O	0.50	2.64	6	1
1:A:142:MET:SD	1:A:154:GLU:OE1	0.50	2.70	6	1
1:A:203:VAL:O	1:A:205:GLY:N	0.50	2.44	6	1
1:A:135:LEU:HD23	1:A:139:PHE:CE1	0.50	2.41	1	1
1:A:185:GLY:C	1:A:186:VAL:HG12	0.50	2.25	6	1
1:A:204:CYS:O	1:A:206:ASP:N	0.50	2.43	5	1
1:A:45:LYS:HZ1	1:A:53:ARG:NH1	0.50	2.03	10	1
1:A:105:GLY:O	1:A:109:LYS:NZ	0.50	2.42	1	1
1:A:90:LEU:HD22	1:A:91:PRO:N	0.50	2.22	6	2
1:A:135:LEU:CD2	1:A:165:TRP:CE2	0.50	2.93	10	1
1:A:123:ARG:NH2	1:A:207:PRO:CD	0.50	2.75	5	1
1:A:34:TRP:CD2	1:A:34:TRP:O	0.50	2.65	2	5
1:A:170:THR:O	1:A:172:ALA:N	0.50	2.45	6	1
1:A:57:PHE:C	1:A:59:GLN:N	0.50	2.64	8	2
1:A:123:ARG:NH2	1:A:204:CYS:O	0.50	2.45	3	1
1:A:173:THR:HG23	1:A:174:THR:N	0.50	2.21	7	1
1:A:87:THR:OG1	1:A:133:PHE:CE2	0.50	2.65	9	1
1:A:95:GLN:CG	1:A:96:ARG:N	0.50	2.74	3	1
1:A:99:ASP:N	1:A:99:ASP:OD1	0.50	2.42	7	2
1:A:28:ALA:O	1:A:32:VAL:HG23	0.50	2.06	6	1
1:A:98:PHE:CD1	1:A:98:PHE:C	0.49	2.85	1	4
1:A:64:GLY:C	1:A:66:GLY:N	0.49	2.64	10	2
1:A:144:LYS:C	1:A:145:ASP:CG	0.49	2.70	6	1
1:A:116:LEU:HD22	1:A:116:LEU:H	0.49	1.67	9	1
1:A:170:THR:C	1:A:171:ASP:CG	0.49	2.70	10	1
1:A:106:ASN:O	1:A:108:VAL:N	0.49	2.42	6	1
1:A:120:LEU:C	1:A:120:LEU:CD1	0.49	2.80	7	1
1:A:174:THR:HG22	1:A:175:VAL:N	0.49	2.22	8	1
1:A:43:ARG:NH1	1:A:43:ARG:O	0.49	2.45	3	1
1:A:34:TRP:CD1	1:A:137:VAL:HG21	0.49	2.43	8	5
1:A:98:PHE:CZ	1:A:117:VAL:HG23	0.49	2.42	3	1
1:A:51:SER:OG	1:A:52:ARG:N	0.49	2.46	3	1
1:A:131:ASP:OD1	1:A:200:LYS:CE	0.49	2.60	6	1
1:A:39:CYS:O	1:A:52:ARG:NH2	0.49	2.46	10	1
1:A:62:THR:O	1:A:63:ASN:CB	0.49	2.59	5	1
1:A:131:ASP:OD1	1:A:131:ASP:C	0.49	2.51	5	1
1:A:36:ARG:NH2	1:A:39:CYS:SG	0.49	2.85	8	1
1:A:87:THR:CG2	1:A:89:HIS:CD2	0.49	2.96	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:GLY:C	1:A:66:GLY:H	0.49	2.11	10	1
1:A:34:TRP:CH2	1:A:133:PHE:HB2	0.49	2.42	4	3
1:A:151:GLU:C	1:A:153:GLN:N	0.49	2.66	1	2
1:A:34:TRP:CH2	1:A:38:ARG:CB	0.49	2.96	4	1
1:A:93:ILE:CG2	1:A:94:VAL:H	0.49	2.20	9	1
1:A:169:ILE:HG12	1:A:195:TRP:CH2	0.48	2.43	3	3
1:A:61:ASP:C	1:A:61:ASP:OD1	0.48	2.50	6	1
1:A:127:CYS:SG	1:A:131:ASP:OD2	0.48	2.71	2	1
1:A:95:GLN:C	1:A:95:GLN:CD	0.48	2.72	3	1
1:A:149:LEU:HD22	1:A:149:LEU:H	0.48	1.68	9	1
1:A:178:GLU:CD	1:A:178:GLU:C	0.48	2.71	10	1
1:A:159:LEU:N	1:A:160:PRO:HD2	0.48	2.23	7	10
1:A:94:VAL:CG1	1:A:95:GLN:N	0.48	2.76	8	1
1:A:88:THR:C	1:A:89:HIS:ND1	0.48	2.66	8	2
1:A:190:ASP:O	1:A:194:CYS:SG	0.48	2.72	2	1
1:A:169:ILE:HG13	1:A:195:TRP:CH2	0.48	2.44	3	1
1:A:204:CYS:O	1:A:204:CYS:SG	0.48	2.72	3	1
1:A:84:ASP:OD1	1:A:84:ASP:C	0.48	2.52	7	1
1:A:199:LYS:O	1:A:203:VAL:CG2	0.48	2.62	7	1
1:A:57:PHE:O	1:A:59:GLN:N	0.48	2.47	8	2
1:A:95:GLN:CD	1:A:96:ARG:N	0.48	2.67	3	1
1:A:59:GLN:OE1	1:A:59:GLN:CA	0.48	2.62	8	1
1:A:107:LYS:CB	1:A:107:LYS:HZ3	0.48	2.21	2	1
1:A:169:ILE:HD11	1:A:175:VAL:HG11	0.48	1.84	2	1
1:A:201:LEU:O	1:A:204:CYS:N	0.48	2.47	5	1
1:A:30:ARG:HG2	1:A:86:PHE:CE1	0.48	2.44	2	1
1:A:35:GLU:CD	1:A:35:GLU:C	0.48	2.72	2	1
1:A:162:LEU:C	1:A:162:LEU:CD1	0.48	2.76	9	3
1:A:138:MET:O	1:A:161:LYS:NZ	0.48	2.47	4	1
1:A:40:ALA:O	1:A:52:ARG:NH1	0.48	2.47	6	1
1:A:171:ASP:OD1	1:A:174:THR:OG1	0.48	2.32	6	1
1:A:193:SER:OG	1:A:194:CYS:N	0.48	2.47	8	1
1:A:191:GLU:O	1:A:194:CYS:SG	0.48	2.67	5	1
1:A:126:LEU:C	1:A:126:LEU:CD1	0.48	2.82	9	1
1:A:142:MET:CG	1:A:142:MET:O	0.48	2.62	10	1
1:A:46:ASP:CG	1:A:47:ALA:H	0.47	2.12	8	1
1:A:200:LYS:O	1:A:204:CYS:SG	0.47	2.72	5	2
1:A:179:ILE:O	1:A:181:THR:N	0.47	2.46	7	1
1:A:169:ILE:O	1:A:169:ILE:CG2	0.47	2.63	9	3
1:A:48:GLU:OE1	1:A:48:GLU:N	0.47	2.47	3	1
1:A:159:LEU:N	1:A:160:PRO:CD	0.47	2.78	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:165:TRP:HZ3	1:A:196:ALA:HB1	0.47	1.69	5	2
1:A:144:LYS:CD	1:A:144:LYS:N	0.47	2.77	7	1
1:A:195:TRP:CE3	1:A:196:ALA:N	0.47	2.83	2	2
1:A:141:THR:HG23	1:A:141:THR:O	0.47	2.09	6	1
1:A:34:TRP:CZ3	1:A:133:PHE:HB3	0.47	2.45	4	7
1:A:201:LEU:HD23	1:A:201:LEU:O	0.47	2.10	1	2
1:A:134:GLU:CD	1:A:165:TRP:HE1	0.47	2.13	4	1
1:A:120:LEU:C	1:A:120:LEU:HD13	0.47	2.28	7	1
1:A:131:ASP:CB	1:A:197:VAL:HG13	0.47	2.40	10	1
1:A:26:THR:O	1:A:28:ALA:N	0.47	2.48	2	3
1:A:61:ASP:HA	1:A:68:LEU:HD11	0.47	1.86	2	1
1:A:144:LYS:C	1:A:146:GLY:N	0.47	2.67	2	1
1:A:26:THR:C	1:A:28:ALA:N	0.47	2.66	2	2
1:A:147:SER:HB3	1:A:149:LEU:HD11	0.46	1.87	4	1
1:A:135:LEU:HD23	1:A:138:MET:CE	0.46	2.40	7	2
1:A:46:ASP:CG	1:A:47:ALA:N	0.46	2.69	8	1
1:A:180:ASP:O	1:A:182:ASN:N	0.46	2.48	8	1
1:A:92:ASP:OD1	1:A:92:ASP:C	0.46	2.53	9	1
1:A:147:SER:CB	1:A:149:LEU:HD11	0.46	2.39	4	1
1:A:203:VAL:C	1:A:205:GLY:N	0.46	2.69	6	1
1:A:168:ASP:O	1:A:169:ILE:CG2	0.46	2.63	8	1
1:A:95:GLN:NE2	1:A:95:GLN:HA	0.46	2.26	10	2
1:A:69:GLY:C	1:A:98:PHE:CE2	0.46	2.89	1	1
1:A:95:GLN:HE22	1:A:99:ASP:CG	0.46	2.14	6	1
1:A:176:PHE:CE1	1:A:187:VAL:CG2	0.46	2.98	4	1
1:A:144:LYS:CB	1:A:144:LYS:NZ	0.46	2.78	5	1
1:A:142:MET:CE	1:A:158:ALA:HB2	0.46	2.41	9	1
1:A:70:PHE:CE2	1:A:95:GLN:NE2	0.46	2.84	1	1
1:A:63:ASN:OD1	1:A:63:ASN:N	0.46	2.48	3	2
1:A:78:TYR:N	1:A:78:TYR:CD1	0.46	2.81	3	1
1:A:171:ASP:O	1:A:175:VAL:CG2	0.46	2.63	3	1
1:A:187:VAL:HG13	1:A:187:VAL:O	0.46	2.11	3	1
1:A:206:ASP:H	1:A:207:PRO:HD3	0.46	1.71	3	1
1:A:70:PHE:CZ	1:A:74:LEU:HD13	0.46	2.45	5	3
1:A:104:LEU:C	1:A:106:ASN:N	0.46	2.69	10	2
1:A:32:VAL:CG2	1:A:33:ALA:N	0.46	2.77	9	1
1:A:86:PHE:O	1:A:86:PHE:CD1	0.46	2.69	6	1
1:A:36:ARG:HH22	1:A:39:CYS:CB	0.46	2.23	8	1
1:A:106:ASN:HD22	1:A:106:ASN:N	0.45	2.09	5	1
1:A:37:ILE:O	1:A:40:ALA:HB3	0.45	2.11	5	1
1:A:123:ARG:NH2	1:A:207:PRO:HD2	0.45	2.26	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ARG:CB	1:A:30:ARG:HH11	0.45	2.24	1	1
1:A:43:ARG:O	1:A:43:ARG:NE	0.45	2.49	3	1
1:A:81:LEU:CD1	1:A:81:LEU:N	0.45	2.79	3	1
1:A:69:GLY:O	1:A:73:VAL:CG2	0.45	2.64	6	2
1:A:191:GLU:OE1	1:A:191:GLU:CA	0.45	2.64	3	1
1:A:141:THR:CG2	1:A:142:MET:H	0.45	2.25	1	2
1:A:77:CYS:C	1:A:79:GLY:N	0.45	2.68	2	1
1:A:125:MET:CG	1:A:126:LEU:N	0.45	2.80	2	1
1:A:144:LYS:C	1:A:146:GLY:H	0.45	2.14	2	1
1:A:57:PHE:CE1	1:A:61:ASP:HB2	0.45	2.47	3	1
1:A:140:ASP:N	1:A:140:ASP:OD1	0.45	2.45	10	2
1:A:93:ILE:HG23	1:A:94:VAL:H	0.45	1.70	10	2
1:A:169:ILE:HD11	1:A:175:VAL:CG1	0.45	2.42	2	1
1:A:35:GLU:O	1:A:39:CYS:SG	0.45	2.74	4	1
1:A:64:GLY:C	1:A:65:THR:HG1	0.45	2.15	5	1
1:A:144:LYS:O	1:A:146:GLY:N	0.45	2.50	2	1
1:A:95:GLN:HE21	1:A:95:GLN:HA	0.45	1.72	10	1
1:A:196:ALA:O	1:A:197:VAL:C	0.45	2.55	4	8
1:A:49:SER:OG	1:A:50:LYS:N	0.45	2.50	6	1
1:A:139:PHE:HB2	1:A:189:PHE:CZ	0.45	2.47	6	1
1:A:177:ASN:OD1	1:A:177:ASN:N	0.45	2.50	6	1
1:A:98:PHE:CE2	1:A:117:VAL:CG2	0.44	3.00	3	1
1:A:148:LEU:C	1:A:149:LEU:HD13	0.44	2.28	9	1
1:A:134:GLU:O	1:A:137:VAL:HG22	0.44	2.12	2	1
1:A:173:THR:OG1	1:A:174:THR:N	0.44	2.50	3	1
1:A:189:PHE:O	1:A:190:ASP:C	0.44	2.55	6	4
1:A:135:LEU:O	1:A:138:MET:N	0.44	2.50	1	2
1:A:26:THR:C	1:A:28:ALA:H	0.44	2.15	2	1
1:A:68:LEU:CD1	1:A:68:LEU:N	0.44	2.81	8	1
1:A:70:PHE:CE2	1:A:95:GLN:CD	0.44	2.91	1	1
1:A:203:VAL:CG2	1:A:204:CYS:N	0.44	2.81	1	1
1:A:125:MET:HG3	1:A:126:LEU:N	0.44	2.27	2	1
1:A:135:LEU:CD1	1:A:196:ALA:HB3	0.44	2.43	10	1
1:A:131:ASP:CB	1:A:197:VAL:HG23	0.44	2.43	5	1
1:A:95:GLN:NE2	1:A:99:ASP:CG	0.44	2.71	6	1
1:A:189:PHE:O	1:A:191:GLU:N	0.44	2.51	6	1
1:A:65:THR:OG1	1:A:66:GLY:N	0.44	2.50	7	1
1:A:48:GLU:CD	1:A:49:SER:N	0.44	2.70	10	1
1:A:121:GLU:OE1	1:A:121:GLU:N	0.44	2.50	10	1
1:A:104:LEU:O	1:A:106:ASN:N	0.44	2.51	7	2
1:A:87:THR:HG21	1:A:133:PHE:CE1	0.44	2.47	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LYS:O	1:A:35:GLU:N	0.44	2.50	10	1
1:A:172:ALA:O	1:A:173:THR:C	0.44	2.56	4	10
1:A:81:LEU:O	1:A:82:LYS:C	0.44	2.56	9	3
1:A:193:SER:O	1:A:194:CYS:C	0.44	2.56	5	3
1:A:86:PHE:CD1	1:A:86:PHE:C	0.44	2.89	6	1
1:A:98:PHE:HE2	1:A:102:LYS:HZ2	0.44	1.56	10	1
1:A:70:PHE:CE2	1:A:95:GLN:OE1	0.44	2.70	1	1
1:A:38:ARG:HG3	1:A:130:TYR:CE2	0.44	2.48	8	4
1:A:30:ARG:HB2	1:A:86:PHE:CE1	0.44	2.48	3	1
1:A:188:THR:CG2	1:A:189:PHE:N	0.44	2.80	3	1
1:A:132:ILE:HG12	1:A:197:VAL:HG21	0.44	1.89	4	1
1:A:149:LEU:O	1:A:149:LEU:HD12	0.44	2.13	5	3
1:A:162:LEU:HD11	1:A:192:PHE:CE1	0.44	2.48	4	1
1:A:64:GLY:C	1:A:65:THR:HG23	0.44	2.33	10	1
1:A:165:TRP:CH2	1:A:200:LYS:HD3	0.44	2.47	10	1
1:A:151:GLU:CG	1:A:152:LEU:N	0.44	2.81	2	2
1:A:171:ASP:O	1:A:175:VAL:HG23	0.44	2.13	5	1
1:A:187:VAL:HG12	1:A:188:THR:N	0.44	2.28	5	1
1:A:124:LEU:N	1:A:124:LEU:HD22	0.44	2.27	8	1
1:A:201:LEU:C	1:A:201:LEU:CD2	0.44	2.76	10	1
1:A:103:ASP:C	1:A:106:ASN:HD21	0.43	2.15	2	1
1:A:141:THR:HG23	1:A:142:MET:H	0.43	1.73	1	1
1:A:159:LEU:CB	1:A:160:PRO:HD3	0.43	2.43	4	6
1:A:50:LYS:O	1:A:52:ARG:N	0.43	2.51	9	1
1:A:149:LEU:CD2	1:A:149:LEU:C	0.43	2.86	9	1
1:A:38:ARG:HG3	1:A:130:TYR:CZ	0.43	2.48	3	1
1:A:43:ARG:O	1:A:44:ASP:CB	0.43	2.64	4	1
1:A:90:LEU:O	1:A:94:VAL:CG2	0.43	2.67	4	1
1:A:154:GLU:N	1:A:154:GLU:OE1	0.43	2.51	7	1
1:A:105:GLY:C	1:A:106:ASN:HD22	0.43	2.16	8	1
1:A:61:ASP:OD2	1:A:64:GLY:N	0.43	2.51	3	1
1:A:171:ASP:CB	1:A:174:THR:OG1	0.43	2.67	4	2
1:A:53:ARG:CG	1:A:54:ILE:N	0.43	2.82	8	1
1:A:138:MET:HE1	1:A:165:TRP:CD1	0.43	2.48	10	1
1:A:139:PHE:O	1:A:140:ASP:C	0.43	2.57	4	4
1:A:61:ASP:C	1:A:63:ASN:H	0.43	2.17	2	1
1:A:146:GLY:C	1:A:148:LEU:N	0.43	2.71	2	1
1:A:175:VAL:O	1:A:176:PHE:C	0.43	2.57	3	1
1:A:151:GLU:HG2	1:A:152:LEU:N	0.43	2.29	5	1
1:A:135:LEU:CD2	1:A:139:PHE:CZ	0.43	3.02	1	1
1:A:30:ARG:NH1	1:A:140:ASP:HB2	0.43	2.29	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:162:LEU:O	1:A:165:TRP:CB	0.43	2.67	5	1
1:A:167:VAL:C	1:A:168:ASP:OD1	0.43	2.56	8	1
1:A:67:LYS:HB3	1:A:116:LEU:HD22	0.42	1.89	4	1
1:A:81:LEU:C	1:A:82:LYS:CG	0.42	2.87	9	2
1:A:142:MET:O	1:A:142:MET:SD	0.42	2.77	10	1
1:A:34:TRP:O	1:A:34:TRP:CG	0.42	2.72	2	1
1:A:111:VAL:CG1	1:A:112:GLY:H	0.42	2.26	8	1
1:A:144:LYS:O	1:A:144:LYS:CG	0.42	2.67	2	1
1:A:81:LEU:O	1:A:82:LYS:CB	0.42	2.65	5	1
1:A:100:LYS:NZ	1:A:100:LYS:HB2	0.42	2.29	6	1
1:A:127:CYS:SG	1:A:201:LEU:CD1	0.42	3.08	5	1
1:A:46:ASP:O	1:A:49:SER:N	0.42	2.52	4	1
1:A:162:LEU:O	1:A:163:LYS:C	0.42	2.58	9	3
1:A:143:ASP:OD1	1:A:143:ASP:N	0.42	2.52	5	1
1:A:106:ASN:C	1:A:108:VAL:N	0.42	2.72	6	1
1:A:60:PHE:C	1:A:62:THR:N	0.42	2.72	8	1
1:A:106:ASN:ND2	1:A:106:ASN:N	0.42	2.67	8	1
1:A:77:CYS:CB	1:A:83:LEU:HD11	0.42	2.45	10	1
1:A:199:LYS:C	1:A:201:LEU:N	0.42	2.73	1	1
1:A:34:TRP:CH2	1:A:133:PHE:HB3	0.42	2.49	9	2
1:A:180:ASP:OD1	1:A:180:ASP:C	0.42	2.57	9	1
1:A:90:LEU:CD1	1:A:90:LEU:H	0.42	2.20	10	1
1:A:38:ARG:HG2	1:A:39:CYS:N	0.42	2.30	4	1
1:A:92:ASP:CG	1:A:93:ILE:N	0.42	2.73	4	1
1:A:165:TRP:CZ3	1:A:200:LYS:HD2	0.42	2.50	3	1
1:A:180:ASP:CG	1:A:184:SER:H	0.42	2.16	8	1
1:A:169:ILE:CG2	1:A:170:THR:N	0.42	2.83	10	1
1:A:106:ASN:ND2	1:A:106:ASN:C	0.41	2.72	5	1
1:A:143:ASP:C	1:A:145:ASP:N	0.41	2.73	6	1
1:A:70:PHE:CZ	1:A:74:LEU:HD23	0.41	2.49	7	1
1:A:131:ASP:CG	1:A:197:VAL:HG23	0.41	2.35	5	1
1:A:201:LEU:O	1:A:205:GLY:N	0.41	2.52	5	1
1:A:50:LYS:O	1:A:51:SER:C	0.41	2.56	9	1
1:A:116:LEU:N	1:A:116:LEU:HD13	0.41	2.30	9	1
1:A:78:TYR:CE2	1:A:84:ASP:OD2	0.41	2.73	10	1
1:A:43:ARG:HB3	1:A:130:TYR:CE2	0.41	2.50	1	1
1:A:117:VAL:CG1	1:A:118:GLU:N	0.41	2.82	4	1
1:A:167:VAL:HG11	1:A:195:TRP:CH2	0.41	2.50	8	1
1:A:59:GLN:NE2	1:A:59:GLN:CA	0.41	2.82	9	1
1:A:151:GLU:O	1:A:152:LEU:C	0.41	2.59	4	4
1:A:197:VAL:O	1:A:201:LEU:N	0.41	2.53	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:PHE:O	1:A:71:ARG:C	0.41	2.59	6	1
1:A:125:MET:SD	1:A:126:LEU:N	0.41	2.93	9	1
1:A:44:ASP:O	1:A:45:LYS:C	0.41	2.58	1	1
1:A:84:ASP:O	1:A:85:GLU:C	0.41	2.59	1	1
1:A:88:THR:O	1:A:88:THR:HG22	0.41	2.16	1	1
1:A:169:ILE:O	1:A:170:THR:C	0.41	2.58	1	1
1:A:170:THR:HG22	1:A:171:ASP:N	0.41	2.31	1	1
1:A:57:PHE:O	1:A:57:PHE:CG	0.41	2.72	6	1
1:A:144:LYS:N	1:A:144:LYS:HD2	0.41	2.30	7	1
1:A:53:ARG:HG3	1:A:54:ILE:N	0.41	2.30	8	1
1:A:69:GLY:O	1:A:70:PHE:C	0.41	2.59	4	1
1:A:109:LYS:HG2	1:A:110:GLY:N	0.41	2.30	7	1
1:A:129:ILE:O	1:A:130:TYR:C	0.41	2.59	7	1
1:A:59:GLN:NE2	1:A:59:GLN:HA	0.41	2.31	9	1
1:A:61:ASP:C	1:A:63:ASN:N	0.41	2.74	10	1
1:A:32:VAL:HG13	1:A:33:ALA:N	0.41	2.29	1	1
1:A:70:PHE:CE1	1:A:95:GLN:HA	0.41	2.51	4	3
1:A:148:LEU:HD12	1:A:148:LEU:H	0.41	1.72	7	1
1:A:61:ASP:OD1	1:A:61:ASP:C	0.41	2.55	8	1
1:A:180:ASP:O	1:A:181:THR:C	0.41	2.58	8	1
1:A:135:LEU:HD11	1:A:196:ALA:HB3	0.41	1.91	9	1
1:A:136:THR:HG22	1:A:189:PHE:HD2	0.41	1.76	4	1
1:A:202:GLN:HG3	1:A:203:VAL:N	0.41	2.31	4	1
1:A:106:ASN:HD22	1:A:106:ASN:H	0.41	1.59	5	1
1:A:74:LEU:C	1:A:74:LEU:CD1	0.41	2.89	7	1
1:A:195:TRP:NE1	1:A:199:LYS:HE2	0.41	2.30	8	1
1:A:108:VAL:CG1	1:A:109:LYS:N	0.41	2.84	2	1
1:A:134:GLU:OE2	1:A:138:MET:SD	0.41	2.78	2	1
1:A:81:LEU:N	1:A:81:LEU:HD12	0.41	2.31	3	1
1:A:203:VAL:O	1:A:204:CYS:C	0.41	2.60	6	1
1:A:36:ARG:NH2	1:A:39:CYS:HB2	0.41	2.31	8	1
1:A:71:ARG:CG	1:A:72:GLU:N	0.41	2.84	8	1
1:A:171:ASP:N	1:A:171:ASP:OD1	0.41	2.51	9	1
1:A:136:THR:HG23	1:A:189:PHE:CD2	0.41	2.51	10	1
1:A:206:ASP:N	1:A:206:ASP:OD1	0.41	2.54	10	1
1:A:130:TYR:CD1	1:A:130:TYR:C	0.41	2.95	1	1
1:A:98:PHE:CE2	1:A:117:VAL:HG23	0.41	2.50	3	1
1:A:45:LYS:O	1:A:46:ASP:CB	0.41	2.68	4	1
1:A:135:LEU:HD21	1:A:193:SER:OG	0.41	2.16	5	1
1:A:149:LEU:O	1:A:150:LEU:HD12	0.41	2.16	5	1
1:A:156:LYS:O	1:A:160:PRO:CD	0.41	2.68	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:197:VAL:O	1:A:198:THR:C	0.40	2.59	2	1
1:A:93:ILE:HD13	1:A:132:ILE:HG21	0.40	1.93	5	1
1:A:104:LEU:N	1:A:104:LEU:CD2	0.40	2.83	6	1
1:A:128:TYR:CZ	1:A:197:VAL:HG11	0.40	2.51	6	1
1:A:170:THR:O	1:A:171:ASP:CB	0.40	2.67	10	1
1:A:34:TRP:CZ3	1:A:38:ARG:HB3	0.40	2.50	4	1
1:A:61:ASP:OD2	1:A:66:GLY:N	0.40	2.54	4	1
1:A:168:ASP:O	1:A:169:ILE:C	0.40	2.59	6	1
1:A:99:ASP:O	1:A:100:LYS:C	0.40	2.59	7	1
1:A:125:MET:SD	1:A:125:MET:C	0.40	3.00	9	1
1:A:30:ARG:CB	1:A:30:ARG:NH1	0.40	2.84	1	1
1:A:77:CYS:O	1:A:78:TYR:C	0.40	2.60	2	1
1:A:146:GLY:C	1:A:148:LEU:H	0.40	2.19	2	1
1:A:148:LEU:HD23	1:A:148:LEU:O	0.40	2.15	2	1
1:A:191:GLU:OE1	1:A:191:GLU:N	0.40	2.54	3	1
1:A:59:GLN:O	1:A:60:PHE:C	0.40	2.59	4	1
1:A:99:ASP:CG	1:A:100:LYS:H	0.40	2.17	5	1
1:A:182:ASN:OD1	1:A:182:ASN:N	0.40	2.54	5	1
1:A:37:ILE:O	1:A:38:ARG:C	0.40	2.60	9	1
1:A:84:ASP:C	1:A:84:ASP:OD1	0.40	2.59	1	1
1:A:107:LYS:O	1:A:108:VAL:C	0.40	2.60	3	2
1:A:136:THR:HG22	1:A:189:PHE:CD2	0.40	2.52	4	1
1:A:135:LEU:HD23	1:A:138:MET:HE1	0.40	1.92	7	1
1:A:43:ARG:HG3	1:A:130:TYR:CE1	0.40	2.51	10	1
1:A:30:ARG:NH2	1:A:140:ASP:CG	0.40	2.75	1	1
1:A:185:GLY:C	1:A:186:VAL:CG1	0.40	2.89	7	1
1:A:34:TRP:CZ2	1:A:38:ARG:HB2	0.40	2.52	8	1
1:A:53:ARG:NH1	1:A:119:PHE:CE1	0.40	2.90	9	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	180/226 (80%)	123±5 (68±3%)	45±7 (25±4%)	12±3 (6±2%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1800/2260 (80%)	1229 (68%)	454 (25%)	117 (6%)	2 18

All 45 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	68	LEU	7
1	A	140	ASP	6
1	A	43	ARG	5
1	A	197	VAL	5
1	A	169	ILE	5
1	A	172	ALA	5
1	A	184	SER	5
1	A	170	THR	4
1	A	25	LYS	4
1	A	167	VAL	4
1	A	63	ASN	4
1	A	207	PRO	4
1	A	144	LYS	4
1	A	171	ASP	4
1	A	166	GLY	4
1	A	90	LEU	3
1	A	64	GLY	3
1	A	185	GLY	3
1	A	148	LEU	3
1	A	107	LYS	2
1	A	108	VAL	2
1	A	152	LEU	2
1	A	61	ASP	2
1	A	110	GLY	2
1	A	44	ASP	2
1	A	80	ILE	2
1	A	65	THR	2
1	A	181	THR	2
1	A	42	PRO	1
1	A	78	TYR	1
1	A	168	ASP	1
1	A	142	MET	1
1	A	189	PHE	1
1	A	46	ASP	1
1	A	59	GLN	1
1	A	66	GLY	1

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Mol	Chain	Res	Type	Models (Total)
1	A	145	ASP	1
1	A	183	GLY	1
1	A	206	ASP	1
1	A	190	ASP	1
1	A	204	CYS	1
1	A	105	GLY	1
1	A	116	LEU	1
1	A	89	HIS	1
1	A	205	GLY	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	158/192 (82%)	133±4 (84±3%)	25±4 (16±3%)	4 40
All	All	1580/1920 (82%)	1330 (84%)	250 (16%)	4 40

All 106 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	86	PHE	10
1	A	95	GLN	9
1	A	87	THR	7
1	A	136	THR	7
1	A	107	LYS	6
1	A	119	PHE	6
1	A	36	ARG	6
1	A	71	ARG	6
1	A	90	LEU	5
1	A	173	THR	5
1	A	43	ARG	5
1	A	159	LEU	4
1	A	174	THR	4
1	A	181	THR	4
1	A	82	LYS	4
1	A	100	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	149	LEU	4
1	A	102	LYS	4
1	A	170	THR	4
1	A	63	ASN	3
1	A	81	LEU	3
1	A	106	ASN	3
1	A	142	MET	3
1	A	156	LYS	3
1	A	202	GLN	3
1	A	49	SER	3
1	A	52	ARG	3
1	A	153	GLN	3
1	A	168	ASP	3
1	A	171	ASP	3
1	A	89	HIS	3
1	A	116	LEU	3
1	A	152	LEU	3
1	A	145	ASP	3
1	A	148	LEU	3
1	A	44	ASP	2
1	A	182	ASN	2
1	A	96	ARG	2
1	A	123	ARG	2
1	A	144	LYS	2
1	A	150	LEU	2
1	A	59	GLN	2
1	A	84	ASP	2
1	A	191	GLU	2
1	A	201	LEU	2
1	A	29	ASP	2
1	A	50	LYS	2
1	A	117	VAL	2
1	A	184	SER	2
1	A	26	THR	2
1	A	42	PRO	2
1	A	99	ASP	2
1	A	143	ASP	2
1	A	188	THR	2
1	A	192	PHE	2
1	A	74	LEU	2
1	A	167	VAL	2
1	A	178	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	187	VAL	2
1	A	199	LYS	2
1	A	120	LEU	2
1	A	45	LYS	2
1	A	25	LYS	1
1	A	32	VAL	1
1	A	88	THR	1
1	A	147	SER	1
1	A	157	GLU	1
1	A	162	LEU	1
1	A	38	ARG	1
1	A	58	LYS	1
1	A	125	MET	1
1	A	126	LEU	1
1	A	134	GLU	1
1	A	141	THR	1
1	A	165	TRP	1
1	A	198	THR	1
1	A	104	LEU	1
1	A	46	ASP	1
1	A	51	SER	1
1	A	65	THR	1
1	A	77	CYS	1
1	A	94	VAL	1
1	A	180	ASP	1
1	A	203	VAL	1
1	A	30	ARG	1
1	A	140	ASP	1
1	A	160	PRO	1
1	A	193	SER	1
1	A	206	ASP	1
1	A	53	ARG	1
1	A	103	ASP	1
1	A	109	LYS	1
1	A	186	VAL	1
1	A	190	ASP	1
1	A	204	CYS	1
1	A	92	ASP	1
1	A	55	GLU	1
1	A	67	LYS	1
1	A	68	LEU	1
1	A	93	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	27	THR	1
1	A	127	CYS	1
1	A	179	ILE	1
1	A	62	THR	1
1	A	83	LEU	1
1	A	85	GLU	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	2286
Number of shifts mapped to atoms	2286
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	211	-0.43 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	190	0.09 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	191	-0.18 ± 0.06	None needed (< 0.5 ppm)
^{15}N	191	0.41 ± 0.26	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 2019 atoms were assigned a chemical shift out of a possible 2496. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	855/905 (94%)	360/369 (98%)	335/360 (93%)	160/176 (91%)
Sidechain	1064/1391 (76%)	685/898 (76%)	373/441 (85%)	6/52 (12%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	100/200 (50%)	97/99 (98%)	0/97 (0%)	3/4 (75%)
Overall	2019/2496 (81%)	1142/1366 (84%)	708/898 (79%)	169/232 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 2283 atoms were assigned a chemical shift out of a possible 2909. 0 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1019/1114 (91%)	426/458 (93%)	402/440 (91%)	191/216 (88%)
Sidechain	1164/1595 (73%)	742/1023 (73%)	415/512 (81%)	7/60 (12%)
Aromatic	100/200 (50%)	97/99 (98%)	0/97 (0%)	3/4 (75%)
Overall	2283/2909 (78%)	1265/1580 (80%)	817/1049 (78%)	201/280 (72%)

7.1.4 Statistically unusual chemical shifts (i)

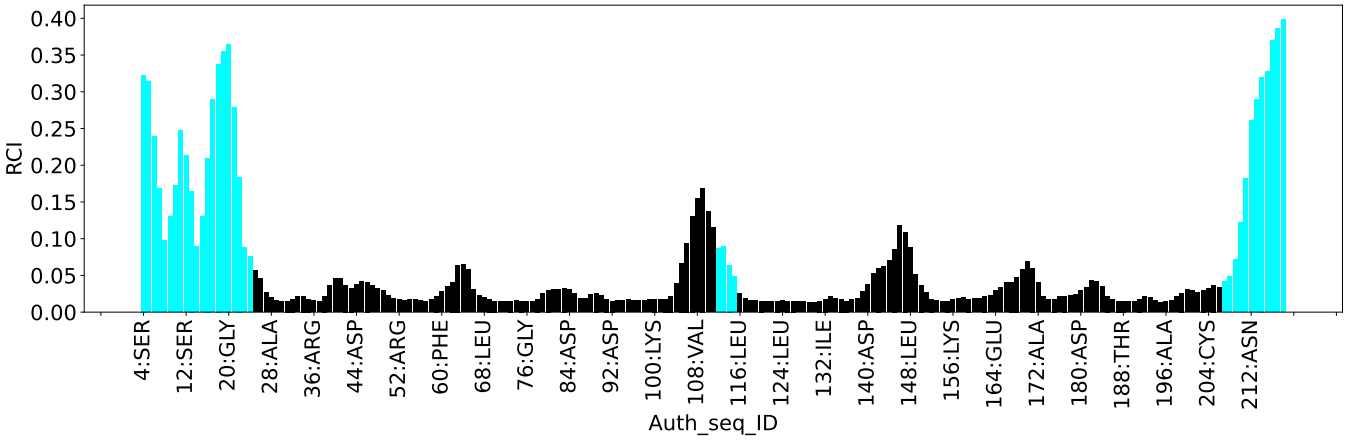
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	199	LYS	HD2	-0.44	0.58 – 2.64	-10.0
1	A	38	ARG	HB2	-0.57	0.52 – 3.08	-9.2
1	A	199	LYS	HD3	0.41	0.54 – 2.65	-5.6

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
4:SER
12:SER
20:GLY
28:ALA
36:ARG
44:ASP
52:ARG
60:PHE
68:LEU
76:GLY
84:ASP
92:ASP
100:LYS
108:VAL
116:LEU
124:LEU
132:ILE
140:ASP
148:LEU
156:LYS
164:GLU
172:ALA
180:ASP
188:THR
196:ALA
204:CYS
212:ASN
Auth_seq_ID

8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2687
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	489
Medium range (|i-j|>1 and |i-j|<5)	555
Long range (|i-j|≥5)	1487
Inter-chain	0
Hydrogen bond restraints	156
Disulfide bond restraints	0
Total dihedral-angle restraints	238
Number of unmapped restraints	0
Number of restraints per residue	12.9
Number of long range restraints per residue[1]	6.6

[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

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	14.6	0.2
0.2-0.5 (Medium)	12.1	0.5
>0.5 (Large)	33.9	10.37

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)	1.3	4.19
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

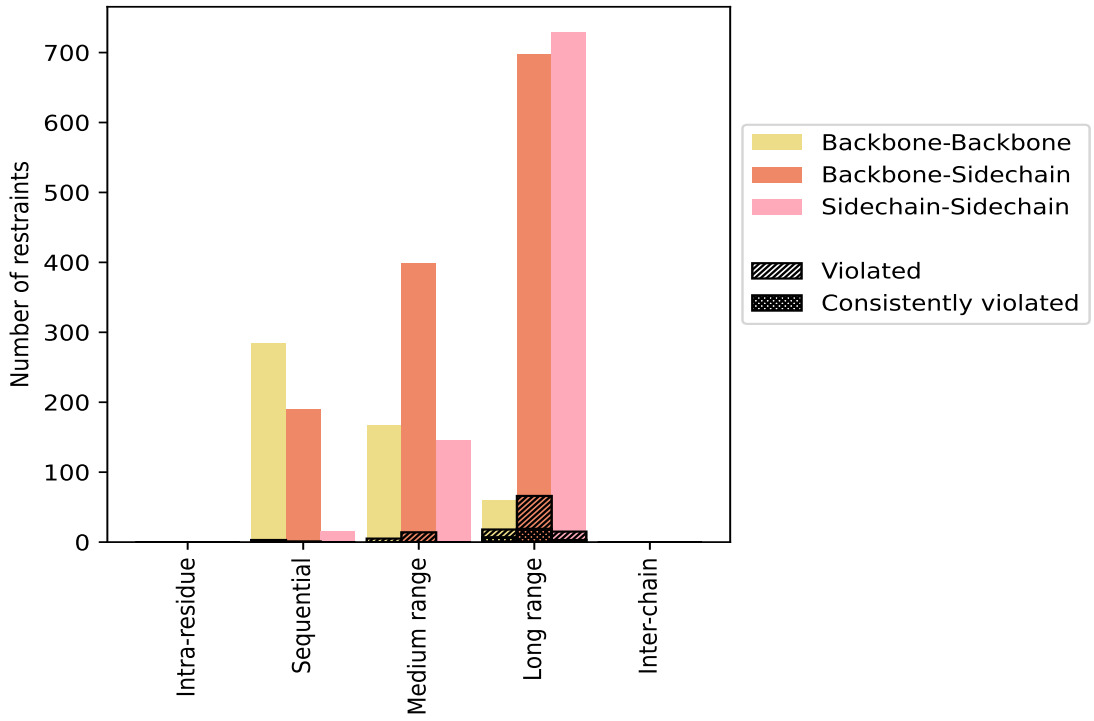
9.1 Summary of distance violations (i)

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)	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
Sequential (|i-j|=1)	489	18.2	4	0.8	0.1	0	0.0	0.0
Backbone-Backbone	284	10.6	3	1.1	0.1	0	0.0	0.0
Backbone-Sidechain	190	7.1	1	0.5	0.0	0	0.0	0.0
Sidechain-Sidechain	15	0.6	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	555	20.7	10	1.8	0.4	0	0.0	0.0
Backbone-Backbone	167	6.2	5	3.0	0.2	0	0.0	0.0
Backbone-Sidechain	242	9.0	5	2.1	0.2	0	0.0	0.0
Sidechain-Sidechain	146	5.4	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	1487	55.3	99	6.7	3.7	29	2.0	1.1
Backbone-Backbone	60	2.2	18	30.0	0.7	7	11.7	0.3
Backbone-Sidechain	698	26.0	66	9.5	2.5	19	2.7	0.7
Sidechain-Sidechain	729	27.1	15	2.1	0.6	3	0.4	0.1
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	156	5.8	9	5.8	0.3	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2687	100.0	122	4.5	4.5	29	1.1	1.1
Backbone-Backbone	511	19.0	26	5.1	1.0	7	1.4	0.3
Backbone-Sidechain	1286	47.9	81	6.3	3.0	19	1.5	0.7
Sidechain-Sidechain	890	33.1	15	1.7	0.6	3	0.3	0.1

[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



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

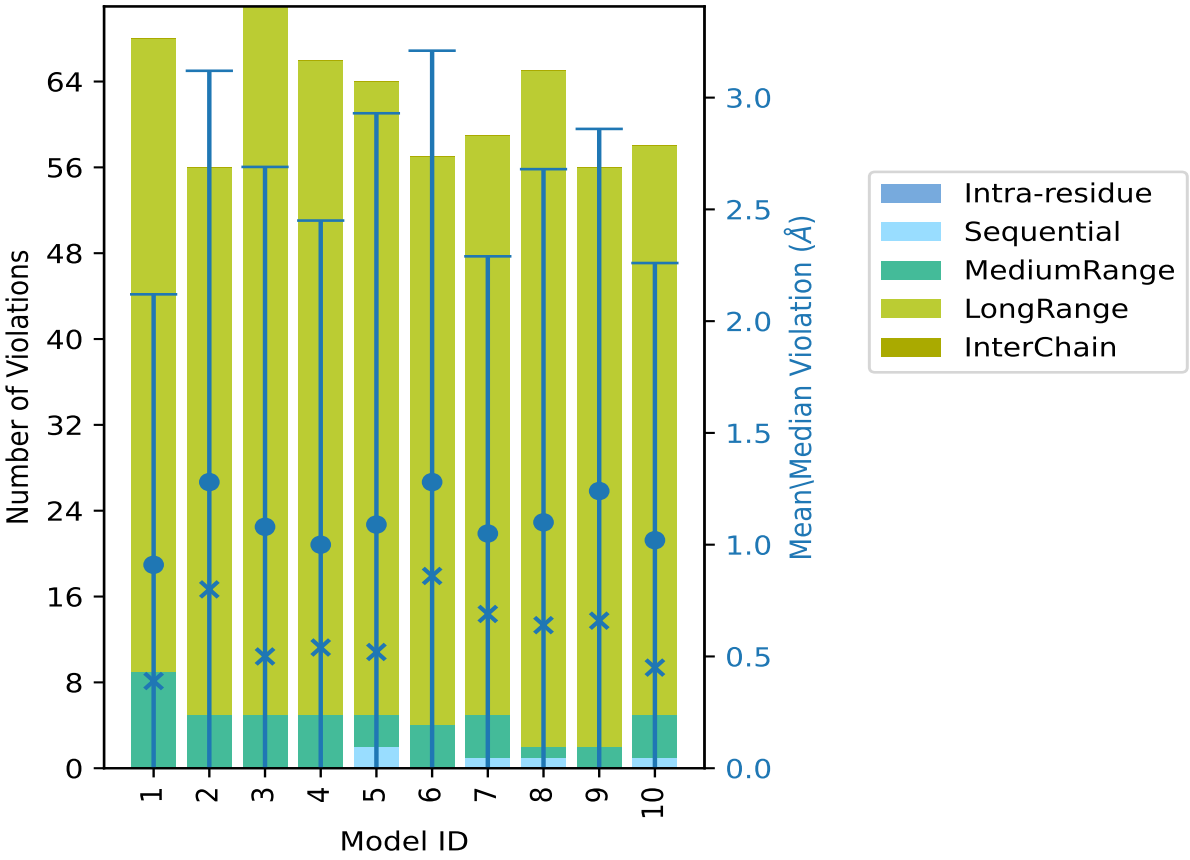
9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	9	59	0	68	0.91	5.95	1.21	0.39
2	0	0	5	51	0	56	1.28	9.34	1.84	0.8
3	0	0	5	66	0	71	1.08	7.82	1.61	0.5
4	0	0	5	61	0	66	1.0	7.81	1.45	0.54
5	0	2	3	59	0	64	1.09	10.37	1.84	0.52
6	0	0	4	53	0	57	1.28	10.06	1.93	0.86
7	0	1	4	54	0	59	1.05	6.52	1.24	0.69
8	0	1	1	63	0	65	1.1	9.09	1.58	0.64
9	0	0	2	54	0	56	1.24	8.19	1.62	0.66
10	0	1	4	53	0	58	1.02	5.84	1.24	0.45

[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



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

9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2418(IR:0, SQ:485, MR:545, LR:1388, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	3	4	19	0	26	1	10.0
0	1	3	11	0	15	2	20.0
0	0	2	6	0	8	3	30.0

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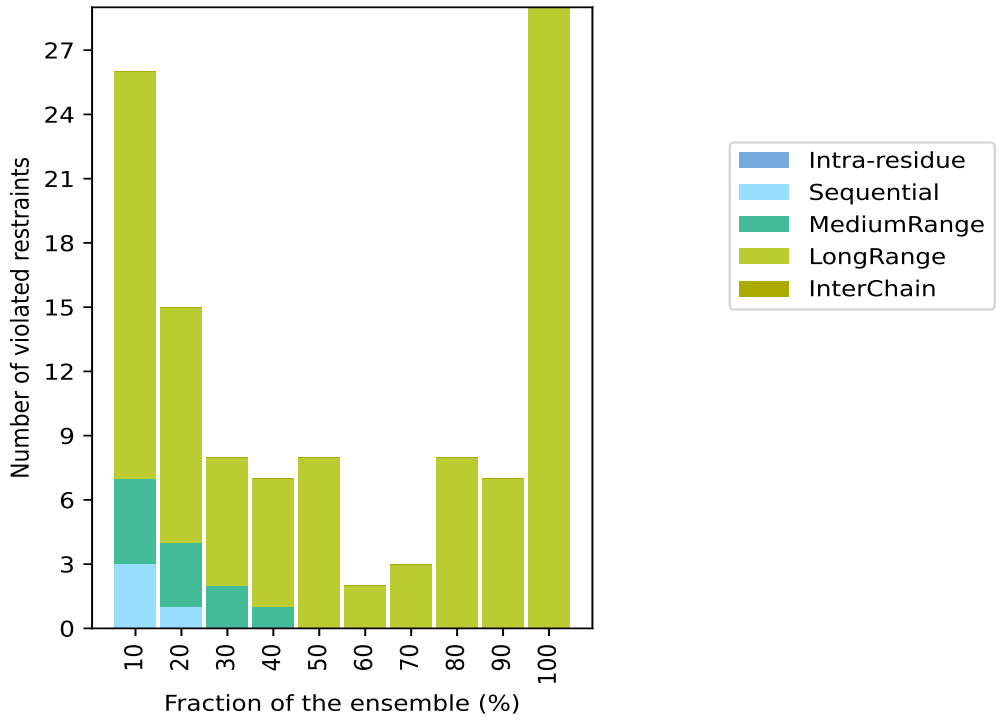
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	1	6	0	7	4	40.0
0	0	0	8	0	8	5	50.0
0	0	0	2	0	2	6	60.0
0	0	0	3	0	3	7	70.0
0	0	0	8	0	8	8	80.0
0	0	0	7	0	7	9	90.0
0	0	0	29	0	29	10	100.0

[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

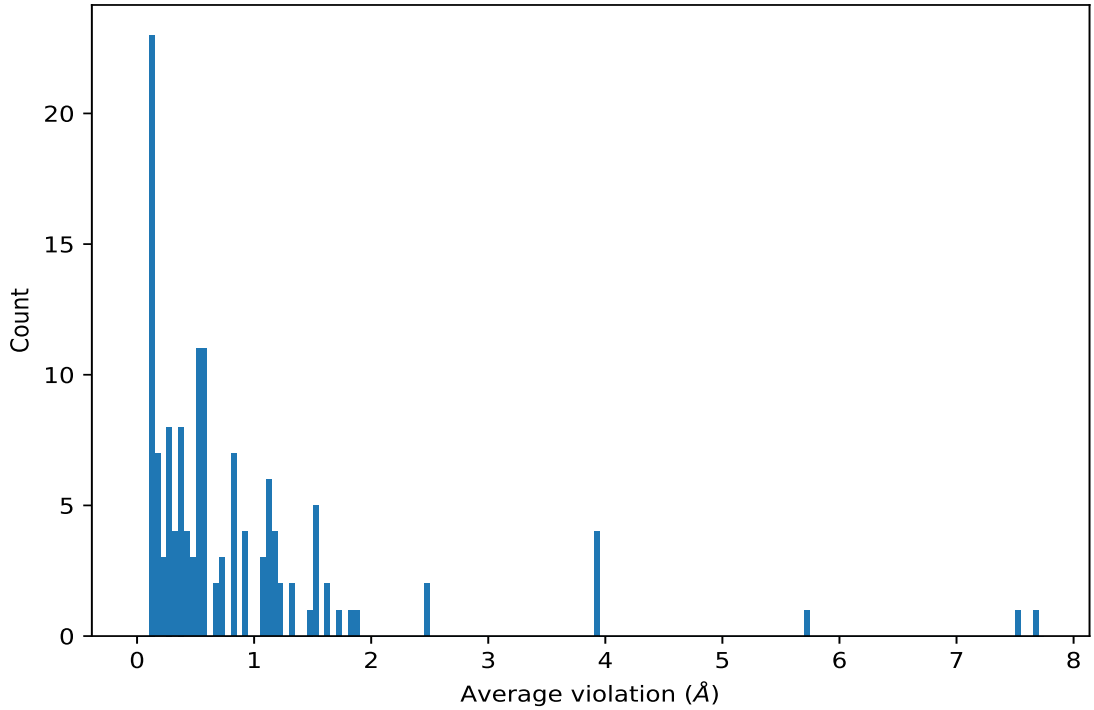


9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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

in the ensemble



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of theviolation 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)
(3,644)	1:24:A:GLY:H	1:88:A:THR:HA	10	7.68	1.66	8.0
(1,143)	1:24:A:GLY:H	1:88:A:THR:HB	10	7.5	1.91	7.82
(3,645)	1:25:A:LYS:H	1:87:A:THR:HA	10	5.71	1.04	5.9
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE2	10	3.92	0.84	4.3
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE3	10	3.92	0.84	4.3
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE2	10	3.92	0.84	4.3
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE3	10	3.92	0.84	4.3
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB2	10	2.45	0.76	2.48
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB3	10	2.45	0.76	2.48
(3,653)	1:67:A:LYS:H	1:117:A:VAL:H	10	1.9	0.78	1.62
(3,659)	1:78:A:TYR:H	1:84:A:ASP:H	10	1.81	0.27	1.81
(3,96)	1:83:A:LEU:HG	1:133:A:PHE:HZ	10	1.73	0.07	1.74
(2,1589)	1:99:A:ASP:H	1:125:A:MET:HE1	10	1.64	0.34	1.69
(3,703)	1:186:A:VAL:H	1:180:A:ASP:HA	10	1.61	0.75	1.7
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD2	10	1.51	0.44	1.54

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD3	10	1.51	0.44	1.54
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD2	10	1.51	0.44	1.54
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD3	10	1.51	0.44	1.54
(3,702)	1:185:A:GLY:H	1:180:A:ASP:HA	10	1.5	0.54	1.42
(3,661)	1:78:A:TYR:H	1:90:A:LEU:HG	10	1.46	0.45	1.5
(3,664)	1:86:A:PHE:H	1:133:A:PHE:HZ	10	1.33	0.25	1.35
(3,125)	1:150:A:LEU:HA	1:187:A:VAL:HB	10	1.31	0.91	0.9
(3,674)	1:135:A:LEU:H	1:165:A:TRP:HD1	10	1.21	0.25	1.25
(3,115)	1:133:A:PHE:HA	1:86:A:PHE:HZ	10	1.15	0.39	1.06
(3,670)	1:134:A:GLU:H	1:34:A:TRP:HE3	10	1.13	0.16	1.12
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD1	10	1.1	0.29	1.1
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD2	10	1.1	0.29	1.1
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE1	10	1.1	0.39	1.16
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE2	10	1.1	0.39	1.16
(3,678)	1:148:A:LEU:H	1:189:A:PHE:H	10	1.08	0.19	1.04
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG12	10	0.95	0.38	0.91
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG13	10	0.95	0.38	0.91
(3,700)	1:175:A:VAL:H	1:155:A:PHE:HZ	10	0.84	0.36	0.8
(3,91)	1:68:A:LEU:HG	1:73:A:VAL:HA	10	0.84	0.43	0.8
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD1	10	0.81	0.27	0.82
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD2	10	0.81	0.27	0.82
(3,100)	1:94:A:VAL:HA	1:70:A:PHE:HZ	10	0.73	0.24	0.7
(2,1015)	1:162:A:LEU:HB2	1:195:A:TRP:HE3	10	0.38	0.27	0.28
(2,1015)	1:162:A:LEU:HB3	1:195:A:TRP:HE3	10	0.38	0.27	0.28
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG21	10	0.3	0.11	0.3
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG22	10	0.3	0.11	0.3
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG23	10	0.3	0.11	0.3
(3,601)	1:133:A:PHE:H	1:34:A:TRP:HZ2	10	0.13	0.02	0.13
(3,124)	1:137:A:VAL:HB	1:34:A:TRP:HZ2	9	1.21	0.75	0.94
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG2	9	1.17	0.29	1.19
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG3	9	1.17	0.29	1.19
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG2	9	1.17	0.29	1.19
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG3	9	1.17	0.29	1.19
(3,94)	1:73:A:VAL:HA	1:60:A:PHE:HZ	9	0.54	0.22	0.59
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD1	9	0.37	0.16	0.34
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD2	9	0.37	0.16	0.34
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD1	9	0.36	0.13	0.41
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD2	9	0.36	0.13	0.41
(3,642)	1:197:A:VAL:H	1:165:A:TRP:HZ2	9	0.18	0.03	0.18
(3,708)	1:197:A:VAL:H	1:165:A:TRP:HZ2	9	0.18	0.03	0.18
(3,649)	1:44:A:ASP:H	1:49:A:SER:HA	8	0.82	0.4	0.8
(3,654)	1:68:A:LEU:H	1:117:A:VAL:H	8	0.74	0.37	0.78

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE1	8	0.58	0.31	0.54
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE2	8	0.58	0.31	0.54
(3,104)	1:115:A:ASP:HA	1:98:A:PHE:HZ	8	0.57	0.26	0.57
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB2	8	0.5	0.19	0.48
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB3	8	0.5	0.19	0.48
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE1	8	0.46	0.2	0.4
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE2	8	0.46	0.2	0.4
(3,111)	1:131:A:ASP:HA	1:197:A:VAL:HA	8	0.42	0.23	0.36
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD1	8	0.38	0.25	0.32
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD2	8	0.38	0.25	0.32
(5,118)	1:157:A:GLU:O	1:161:A:LYS:H	8	0.11	0.01	0.12
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD1	7	0.6	0.29	0.72
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD2	7	0.6	0.29	0.72
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE1	7	0.4	0.13	0.38
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE2	7	0.4	0.13	0.38
(3,99)	1:93:A:ILE:HB	1:133:A:PHE:HZ	7	0.3	0.19	0.29
(2,801)	1:77:A:CYS:HA	1:83:A:LEU:HB2	6	0.54	0.19	0.46
(2,801)	1:77:A:CYS:HA	1:83:A:LEU:HB3	6	0.54	0.19	0.46
(2,840)	1:91:A:PRO:HD2	1:74:A:LEU:HB2	6	0.5	0.34	0.42
(2,840)	1:91:A:PRO:HD2	1:74:A:LEU:HB3	6	0.5	0.34	0.42
(2,840)	1:91:A:PRO:HD3	1:74:A:LEU:HB2	6	0.5	0.34	0.42
(2,840)	1:91:A:PRO:HD3	1:74:A:LEU:HB3	6	0.5	0.34	0.42
(2,1565)	1:78:A:TYR:H	1:90:A:LEU:HB2	5	1.05	0.55	1.24
(2,1565)	1:78:A:TYR:H	1:90:A:LEU:HB3	5	1.05	0.55	1.24
(2,1595)	1:114:A:GLU:H	1:102:A:LYS:HB2	5	0.93	0.29	0.96
(2,1595)	1:114:A:GLU:H	1:102:A:LYS:HB3	5	0.93	0.29	0.96
(2,779)	1:68:A:LEU:HD11	1:62:A:THR:HB	5	0.56	0.31	0.42
(2,779)	1:68:A:LEU:HD12	1:62:A:THR:HB	5	0.56	0.31	0.42
(2,779)	1:68:A:LEU:HD13	1:62:A:THR:HB	5	0.56	0.31	0.42
(2,779)	1:68:A:LEU:HD21	1:62:A:THR:HB	5	0.56	0.31	0.42
(2,779)	1:68:A:LEU:HD22	1:62:A:THR:HB	5	0.56	0.31	0.42
(2,779)	1:68:A:LEU:HD23	1:62:A:THR:HB	5	0.56	0.31	0.42
(3,647)	1:43:A:ARG:H	1:49:A:SER:HA	5	0.46	0.22	0.37
(2,975)	1:143:A:ASP:HB2	1:189:A:PHE:HD1	5	0.32	0.22	0.18
(2,975)	1:143:A:ASP:HB2	1:189:A:PHE:HD2	5	0.32	0.22	0.18
(2,975)	1:143:A:ASP:HB3	1:189:A:PHE:HD1	5	0.32	0.22	0.18
(2,975)	1:143:A:ASP:HB3	1:189:A:PHE:HD2	5	0.32	0.22	0.18
(3,666)	1:94:A:VAL:H	1:70:A:PHE:HZ	5	0.26	0.07	0.24
(3,607)	1:135:A:LEU:H	1:165:A:TRP:HH2	5	0.15	0.02	0.15
(3,675)	1:135:A:LEU:H	1:165:A:TRP:HH2	5	0.15	0.02	0.15
(5,52)	1:91:A:PRO:O	1:95:A:GLN:H	5	0.13	0.03	0.11
(2,883)	1:106:A:ASN:HA	1:112:A:GLY:HA2	4	0.85	0.45	0.93

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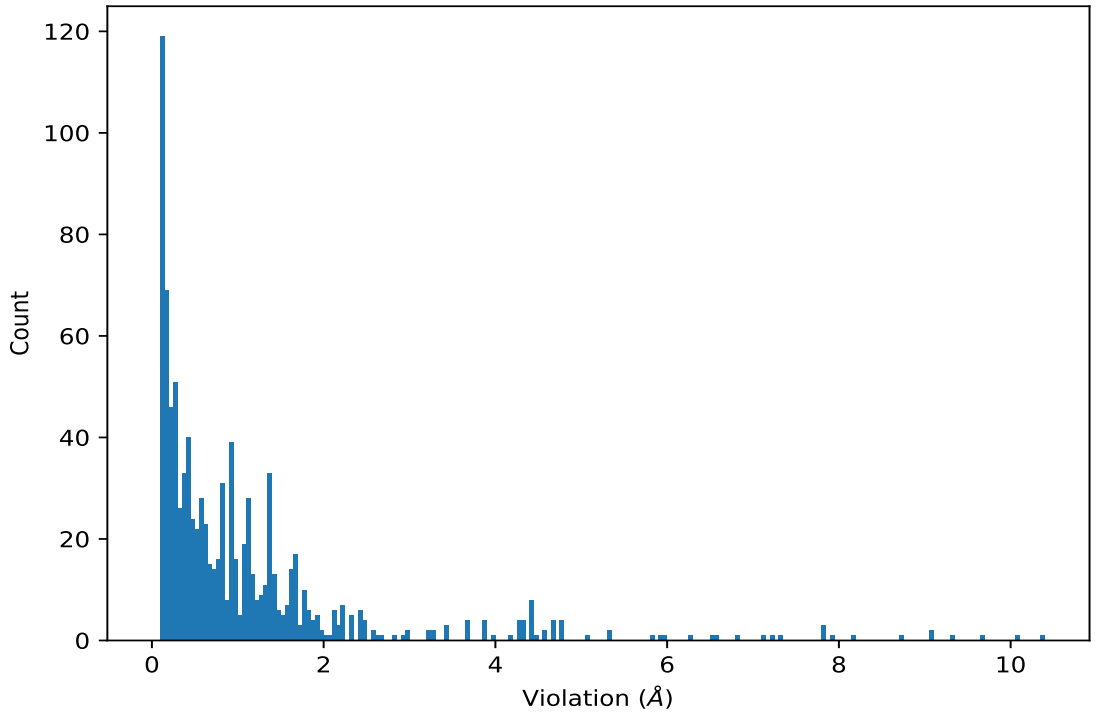
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,883)	1:106:A:ASN:HA	1:112:A:GLY:HA3	4	0.85	0.45	0.93
(2,1005)	1:158:A:ALA:HA	1:142:A:MET:HB2	4	0.65	0.06	0.66
(2,1005)	1:158:A:ALA:HA	1:142:A:MET:HB3	4	0.65	0.06	0.66
(3,112)	1:131:A:ASP:HA	1:34:A:TRP:HH2	4	0.22	0.1	0.2
(3,669)	1:134:A:GLU:H	1:34:A:TRP:HE1	4	0.19	0.06	0.2
(3,603)	1:134:A:GLU:H	1:165:A:TRP:HE1	4	0.16	0.03	0.15
(3,671)	1:134:A:GLU:H	1:165:A:TRP:HE1	4	0.16	0.03	0.15
(3,189)	1:38:A:ARG:H	1:34:A:TRP:HZ3	4	0.12	0.01	0.12
(3,696)	1:169:A:ILE:H	1:163:A:LYS:HA	3	0.74	0.19	0.67
(3,679)	1:149:A:LEU:H	1:189:A:PHE:HZ	3	0.4	0.36	0.19
(3,321)	1:92:A:ASP:H	1:89:A:HIS:HA	3	0.27	0.04	0.29
(3,710)	1:197:A:VAL:H	1:165:A:TRP:HZ3	3	0.22	0.09	0.19
(2,1608)	1:149:A:LEU:H	1:189:A:PHE:HB2	3	0.16	0.04	0.14
(2,1608)	1:149:A:LEU:H	1:189:A:PHE:HB3	3	0.16	0.04	0.14
(3,315)	1:89:A:HIS:H	1:87:A:THR:HB	3	0.13	0.04	0.11
(3,602)	1:134:A:GLU:H	1:34:A:TRP:HH2	3	0.13	0.02	0.12
(3,668)	1:134:A:GLU:H	1:34:A:TRP:HH2	3	0.13	0.02	0.12
(2,1534)	1:40:A:ALA:H	1:130:A:TYR:HE1	2	0.54	0.28	0.54
(2,1534)	1:40:A:ALA:H	1:130:A:TYR:HE2	2	0.54	0.28	0.54
(3,14)	1:79:A:GLY:HA2	1:82:A:LYS:HA	2	0.26	0.09	0.26
(3,14)	1:79:A:GLY:HA3	1:82:A:LYS:HA	2	0.26	0.09	0.26
(3,487)	1:173:A:THR:H	1:171:A:ASP:HA	2	0.21	0.05	0.21
(3,80)	1:186:A:VAL:HB	1:150:A:LEU:HA	2	0.15	0.03	0.15
(3,128)	1:186:A:VAL:HB	1:150:A:LEU:HA	2	0.15	0.03	0.15
(3,563)	1:198:A:THR:H	1:197:A:VAL:HB	2	0.13	0.01	0.13
(3,599)	1:130:A:TYR:H	1:34:A:TRP:HH2	2	0.13	0.01	0.13
(3,610)	1:149:A:LEU:H	1:189:A:PHE:H	2	0.13	0.01	0.13
(3,667)	1:130:A:TYR:H	1:34:A:TRP:HH2	2	0.13	0.01	0.13
(3,681)	1:149:A:LEU:H	1:189:A:PHE:H	2	0.13	0.01	0.13
(5,124)	1:160:A:PRO:O	1:164:A:GLU:H	2	0.13	0.01	0.13
(3,10)	1:74:A:LEU:HA	1:70:A:PHE:HZ	2	0.12	0.02	0.12
(3,631)	1:174:A:THR:H	1:155:A:PHE:HZ	2	0.12	0.02	0.12
(3,699)	1:174:A:THR:H	1:155:A:PHE:HZ	2	0.12	0.02	0.12
(5,140)	1:192:A:PHE:O	1:196:A:ALA:H	2	0.11	0.01	0.11
(3,595)	1:78:A:TYR:H	1:83:A:LEU:H	2	0.11	0.0	0.11
(3,660)	1:78:A:TYR:H	1:83:A:LEU:H	2	0.11	0.0	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:24:A:GLY:H	1:88:A:THR:HB	5	10.37
(1,143)	1:24:A:GLY:H	1:88:A:THR:HB	6	10.06
(3,644)	1:24:A:GLY:H	1:88:A:THR:HA	6	9.66
(3,644)	1:24:A:GLY:H	1:88:A:THR:HA	2	9.34
(3,644)	1:24:A:GLY:H	1:88:A:THR:HA	8	9.09
(3,644)	1:24:A:GLY:H	1:88:A:THR:HA	5	9.05
(1,143)	1:24:A:GLY:H	1:88:A:THR:HB	2	8.72
(3,644)	1:24:A:GLY:H	1:88:A:THR:HA	9	8.19
(1,143)	1:24:A:GLY:H	1:88:A:THR:HB	8	7.93
(3,644)	1:24:A:GLY:H	1:88:A:THR:HA	3	7.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:24:A:GLY:H	1:88:A:THR:HB	3	7.82
(1,143)	1:24:A:GLY:H	1:88:A:THR:HB	4	7.81
(3,645)	1:25:A:LYS:H	1:87:A:THR:HA	3	7.31
(3,644)	1:24:A:GLY:H	1:88:A:THR:HA	4	7.2
(1,143)	1:24:A:GLY:H	1:88:A:THR:HB	9	7.14
(3,645)	1:25:A:LYS:H	1:87:A:THR:HA	6	6.81
(3,645)	1:25:A:LYS:H	1:87:A:THR:HA	5	6.56
(3,644)	1:24:A:GLY:H	1:88:A:THR:HA	7	6.52
(3,645)	1:25:A:LYS:H	1:87:A:THR:HA	2	6.27
(3,645)	1:25:A:LYS:H	1:87:A:THR:HA	1	5.95
(1,143)	1:24:A:GLY:H	1:88:A:THR:HB	7	5.91
(3,645)	1:25:A:LYS:H	1:87:A:THR:HA	10	5.84
(3,645)	1:25:A:LYS:H	1:87:A:THR:HA	9	5.35
(3,644)	1:24:A:GLY:H	1:88:A:THR:HA	1	5.33
(1,143)	1:24:A:GLY:H	1:88:A:THR:HB	1	5.06
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE2	2	4.79
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE3	2	4.79
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE2	2	4.79
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE3	2	4.79
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE2	9	4.69
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE3	9	4.69
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE2	9	4.69
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE3	9	4.69
(3,645)	1:25:A:LYS:H	1:87:A:THR:HA	7	4.58
(3,644)	1:24:A:GLY:H	1:88:A:THR:HA	10	4.56
(3,645)	1:25:A:LYS:H	1:87:A:THR:HA	4	4.46
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE2	3	4.44
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE3	3	4.44
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE2	3	4.44
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE3	3	4.44
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE2	10	4.41
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE3	10	4.41
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE2	10	4.41
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE3	10	4.41
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE2	8	4.33
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE3	8	4.33
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE2	8	4.33
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE3	8	4.33
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE2	1	4.28
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE3	1	4.28
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE2	1	4.28
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE3	1	4.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:24:A:GLY:H	1:88:A:THR:HB	10	4.17
(3,645)	1:25:A:LYS:H	1:87:A:THR:HA	8	3.99
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE2	4	3.89
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE3	4	3.89
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE2	4	3.89
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE3	4	3.89
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE2	5	3.69
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE3	5	3.69
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE2	5	3.69
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE3	5	3.69
(3,653)	1:67:A:LYS:H	1:117:A:VAL:H	3	3.42
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB2	6	3.41
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB3	6	3.41
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB2	4	3.25
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB3	4	3.25
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB2	3	3.23
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB3	3	3.23
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB2	8	2.97
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB3	8	2.97
(3,703)	1:186:A:VAL:H	1:180:A:ASP:HA	10	2.93
(3,653)	1:67:A:LYS:H	1:117:A:VAL:H	4	2.82
(3,653)	1:67:A:LYS:H	1:117:A:VAL:H	9	2.66
(3,702)	1:185:A:GLY:H	1:180:A:ASP:HA	10	2.64
(3,125)	1:150:A:LEU:HA	1:187:A:VAL:HB	6	2.56
(3,125)	1:150:A:LEU:HA	1:187:A:VAL:HB	9	2.56
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB2	5	2.48
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB3	5	2.48
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB2	10	2.47
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB3	10	2.47
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE2	6	2.42
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE3	6	2.42
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE2	6	2.42
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE3	6	2.42
(3,703)	1:186:A:VAL:H	1:180:A:ASP:HA	9	2.41
(3,661)	1:78:A:TYR:H	1:90:A:LEU:HG	7	2.41
(2,1589)	1:99:A:ASP:H	1:125:A:MET:HE1	9	2.31
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE2	7	2.31
(1,104)	1:166:A:GLY:HA2	1:199:A:LYS:HE3	7	2.31
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE2	7	2.31
(1,104)	1:166:A:GLY:HA3	1:199:A:LYS:HE3	7	2.31
(3,659)	1:78:A:TYR:H	1:84:A:ASP:H	9	2.24
(3,125)	1:150:A:LEU:HA	1:187:A:VAL:HB	3	2.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD2	3	2.22
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD3	3	2.22
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD2	3	2.22
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD3	3	2.22
(3,124)	1:137:A:VAL:HB	1:34:A:TRP:HZ2	2	2.21
(3,125)	1:150:A:LEU:HA	1:187:A:VAL:HB	2	2.19
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB2	2	2.16
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB3	2	2.16
(3,659)	1:78:A:TYR:H	1:84:A:ASP:H	6	2.13
(3,124)	1:137:A:VAL:HB	1:34:A:TRP:HZ2	8	2.13
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD2	2	2.12
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD3	2	2.12
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD2	2	2.12
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD3	2	2.12
(3,653)	1:67:A:LYS:H	1:117:A:VAL:H	8	2.06
(3,703)	1:186:A:VAL:H	1:180:A:ASP:HA	5	2.05
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB2	7	1.99
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB3	7	1.99
(3,702)	1:185:A:GLY:H	1:180:A:ASP:HA	3	1.94
(3,703)	1:186:A:VAL:H	1:180:A:ASP:HA	3	1.92
(3,124)	1:137:A:VAL:HB	1:34:A:TRP:HZ2	10	1.92
(3,659)	1:78:A:TYR:H	1:84:A:ASP:H	5	1.91
(3,659)	1:78:A:TYR:H	1:84:A:ASP:H	8	1.91
(3,96)	1:83:A:LEU:HG	1:133:A:PHE:HZ	5	1.88
(3,702)	1:185:A:GLY:H	1:180:A:ASP:HA	4	1.87
(3,703)	1:186:A:VAL:H	1:180:A:ASP:HA	4	1.86
(2,1589)	1:99:A:ASP:H	1:125:A:MET:HE1	2	1.85
(3,664)	1:86:A:PHE:H	1:133:A:PHE:HZ	1	1.82
(3,659)	1:78:A:TYR:H	1:84:A:ASP:H	1	1.81
(3,659)	1:78:A:TYR:H	1:84:A:ASP:H	2	1.81
(3,659)	1:78:A:TYR:H	1:84:A:ASP:H	7	1.8
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE1	2	1.8
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE2	2	1.8
(3,661)	1:78:A:TYR:H	1:90:A:LEU:HG	1	1.79
(3,124)	1:137:A:VAL:HB	1:34:A:TRP:HZ2	3	1.79
(2,1565)	1:78:A:TYR:H	1:90:A:LEU:HB2	7	1.79
(2,1565)	1:78:A:TYR:H	1:90:A:LEU:HB3	7	1.79
(3,659)	1:78:A:TYR:H	1:84:A:ASP:H	10	1.77
(3,115)	1:133:A:PHE:HA	1:86:A:PHE:HZ	7	1.77
(3,96)	1:83:A:LEU:HG	1:133:A:PHE:HZ	3	1.77
(3,96)	1:83:A:LEU:HG	1:133:A:PHE:HZ	4	1.77
(3,96)	1:83:A:LEU:HG	1:133:A:PHE:HZ	6	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1589)	1:99:A:ASP:H	1:125:A:MET:HE1	1	1.76
(3,96)	1:83:A:LEU:HG	1:133:A:PHE:HZ	8	1.74
(3,702)	1:185:A:GLY:H	1:180:A:ASP:HA	5	1.73
(3,96)	1:83:A:LEU:HG	1:133:A:PHE:HZ	2	1.73
(2,1589)	1:99:A:ASP:H	1:125:A:MET:HE1	8	1.7
(2,1589)	1:99:A:ASP:H	1:125:A:MET:HE1	10	1.7
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG2	9	1.7
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG3	9	1.7
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG2	9	1.7
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG3	9	1.7
(3,96)	1:83:A:LEU:HG	1:133:A:PHE:HZ	1	1.69
(3,96)	1:83:A:LEU:HG	1:133:A:PHE:HZ	9	1.69
(2,1589)	1:99:A:ASP:H	1:125:A:MET:HE1	5	1.69
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD2	10	1.67
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD3	10	1.67
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD2	10	1.67
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD3	10	1.67
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD2	9	1.66
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD3	9	1.66
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD2	9	1.66
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD3	9	1.66
(3,674)	1:135:A:LEU:H	1:165:A:TRP:HD1	1	1.65
(3,661)	1:78:A:TYR:H	1:90:A:LEU:HG	6	1.65
(3,115)	1:133:A:PHE:HA	1:86:A:PHE:HZ	4	1.65
(3,664)	1:86:A:PHE:H	1:133:A:PHE:HZ	8	1.64
(3,96)	1:83:A:LEU:HG	1:133:A:PHE:HZ	7	1.64
(2,1589)	1:99:A:ASP:H	1:125:A:MET:HE1	7	1.64
(3,661)	1:78:A:TYR:H	1:90:A:LEU:HG	9	1.63
(3,653)	1:67:A:LYS:H	1:117:A:VAL:H	5	1.63
(3,649)	1:44:A:ASP:H	1:49:A:SER:HA	8	1.62
(3,115)	1:133:A:PHE:HA	1:86:A:PHE:HZ	8	1.62
(3,96)	1:83:A:LEU:HG	1:133:A:PHE:HZ	10	1.61
(2,1589)	1:99:A:ASP:H	1:125:A:MET:HE1	3	1.61
(3,661)	1:78:A:TYR:H	1:90:A:LEU:HG	10	1.6
(3,653)	1:67:A:LYS:H	1:117:A:VAL:H	10	1.6
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD2	6	1.59
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD3	6	1.59
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD2	6	1.59
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD3	6	1.59
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB2	1	1.56
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB3	1	1.56
(3,703)	1:186:A:VAL:H	1:180:A:ASP:HA	8	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,702)	1:185:A:GLY:H	1:180:A:ASP:HA	1	1.53
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD2	7	1.5
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD3	7	1.5
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD2	7	1.5
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD3	7	1.5
(3,91)	1:68:A:LEU:HG	1:73:A:VAL:HA	10	1.48
(3,700)	1:175:A:VAL:H	1:155:A:PHE:HZ	9	1.47
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD2	8	1.46
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD3	8	1.46
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD2	8	1.46
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD3	8	1.46
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD1	9	1.45
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD2	9	1.45
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG2	6	1.45
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG3	6	1.45
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG2	6	1.45
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG3	6	1.45
(3,664)	1:86:A:PHE:H	1:133:A:PHE:HZ	5	1.44
(3,653)	1:67:A:LYS:H	1:117:A:VAL:H	1	1.44
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG12	2	1.43
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG13	2	1.43
(3,678)	1:148:A:LEU:H	1:189:A:PHE:H	4	1.42
(3,674)	1:135:A:LEU:H	1:165:A:TRP:HD1	3	1.41
(3,659)	1:78:A:TYR:H	1:84:A:ASP:H	3	1.41
(2,1595)	1:114:A:GLU:H	1:102:A:LYS:HB2	2	1.4
(2,1595)	1:114:A:GLU:H	1:102:A:LYS:HB3	2	1.4
(3,703)	1:186:A:VAL:H	1:180:A:ASP:HA	1	1.39
(3,674)	1:135:A:LEU:H	1:165:A:TRP:HD1	4	1.39
(3,664)	1:86:A:PHE:H	1:133:A:PHE:HZ	10	1.39
(3,661)	1:78:A:TYR:H	1:90:A:LEU:HG	8	1.39
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG12	6	1.39
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG13	6	1.39
(2,1565)	1:78:A:TYR:H	1:90:A:LEU:HB2	1	1.39
(2,1565)	1:78:A:TYR:H	1:90:A:LEU:HB3	1	1.39
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE1	10	1.39
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE2	10	1.39
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG2	1	1.39
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG3	1	1.39
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG2	1	1.39
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG3	1	1.39
(2,883)	1:106:A:ASN:HA	1:112:A:GLY:HA2	7	1.38
(2,883)	1:106:A:ASN:HA	1:112:A:GLY:HA3	7	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,674)	1:135:A:LEU:H	1:165:A:TRP:HD1	9	1.37
(3,670)	1:134:A:GLU:H	1:34:A:TRP:HE3	9	1.36
(3,664)	1:86:A:PHE:H	1:133:A:PHE:HZ	3	1.36
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD1	2	1.36
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD2	2	1.36
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD1	6	1.36
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD2	6	1.36
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD1	7	1.36
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD2	7	1.36
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD1	2	1.36
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD2	2	1.36
(3,678)	1:148:A:LEU:H	1:189:A:PHE:H	7	1.35
(3,674)	1:135:A:LEU:H	1:165:A:TRP:HD1	10	1.35
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG12	7	1.35
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG13	7	1.35
(3,664)	1:86:A:PHE:H	1:133:A:PHE:HZ	4	1.33
(3,661)	1:78:A:TYR:H	1:90:A:LEU:HG	4	1.33
(3,100)	1:94:A:VAL:HA	1:70:A:PHE:HZ	1	1.33
(3,702)	1:185:A:GLY:H	1:180:A:ASP:HA	8	1.32
(3,91)	1:68:A:LEU:HG	1:73:A:VAL:HA	6	1.32
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG2	2	1.32
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG3	2	1.32
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG2	2	1.32
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG3	2	1.32
(3,659)	1:78:A:TYR:H	1:84:A:ASP:H	4	1.31
(3,91)	1:68:A:LEU:HG	1:73:A:VAL:HA	8	1.31
(3,670)	1:134:A:GLU:H	1:34:A:TRP:HE3	5	1.29
(3,670)	1:134:A:GLU:H	1:34:A:TRP:HE3	10	1.29
(3,653)	1:67:A:LYS:H	1:117:A:VAL:H	6	1.27
(3,653)	1:67:A:LYS:H	1:117:A:VAL:H	7	1.27
(3,654)	1:68:A:LEU:H	1:117:A:VAL:H	9	1.26
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG12	9	1.26
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG13	9	1.26
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE1	3	1.25
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE2	3	1.25
(2,1565)	1:78:A:TYR:H	1:90:A:LEU:HB2	6	1.24
(2,1565)	1:78:A:TYR:H	1:90:A:LEU:HB3	6	1.24
(3,670)	1:134:A:GLU:H	1:34:A:TRP:HE3	1	1.23
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE1	1	1.22
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE2	1	1.22
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE1	4	1.22
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE2	4	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,678)	1:148:A:LEU:H	1:189:A:PHE:H	9	1.21
(3,664)	1:86:A:PHE:H	1:133:A:PHE:HZ	9	1.2
(3,115)	1:133:A:PHE:HA	1:86:A:PHE:HZ	6	1.2
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG12	1	1.2
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG13	1	1.2
(2,1589)	1:99:A:ASP:H	1:125:A:MET:HE1	4	1.2
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG2	8	1.19
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG3	8	1.19
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG2	8	1.19
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG3	8	1.19
(3,702)	1:185:A:GLY:H	1:180:A:ASP:HA	2	1.18
(3,654)	1:68:A:LEU:H	1:117:A:VAL:H	3	1.18
(3,700)	1:175:A:VAL:H	1:155:A:PHE:HZ	2	1.17
(3,670)	1:134:A:GLU:H	1:34:A:TRP:HE3	4	1.17
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE1	6	1.15
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE2	6	1.15
(2,779)	1:68:A:LEU:HD11	1:62:A:THR:HB	7	1.15
(2,779)	1:68:A:LEU:HD12	1:62:A:THR:HB	7	1.15
(2,779)	1:68:A:LEU:HD13	1:62:A:THR:HB	7	1.15
(2,779)	1:68:A:LEU:HD21	1:62:A:THR:HB	7	1.15
(2,779)	1:68:A:LEU:HD22	1:62:A:THR:HB	7	1.15
(2,779)	1:68:A:LEU:HD23	1:62:A:THR:HB	7	1.15
(3,702)	1:185:A:GLY:H	1:180:A:ASP:HA	6	1.14
(3,702)	1:185:A:GLY:H	1:180:A:ASP:HA	7	1.14
(3,674)	1:135:A:LEU:H	1:165:A:TRP:HD1	2	1.14
(3,664)	1:86:A:PHE:H	1:133:A:PHE:HZ	2	1.14
(3,700)	1:175:A:VAL:H	1:155:A:PHE:HZ	6	1.13
(3,664)	1:86:A:PHE:H	1:133:A:PHE:HZ	7	1.13
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD1	1	1.13
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD2	1	1.13
(3,678)	1:148:A:LEU:H	1:189:A:PHE:H	5	1.11
(3,661)	1:78:A:TYR:H	1:90:A:LEU:HG	3	1.1
(3,125)	1:150:A:LEU:HA	1:187:A:VAL:HB	8	1.1
(3,104)	1:115:A:ASP:HA	1:98:A:PHE:HZ	3	1.1
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE1	5	1.1
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE2	5	1.1
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE1	9	1.1
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE2	9	1.1
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD2	1	1.1
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD3	1	1.1
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD2	1	1.1
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD3	1	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,674)	1:135:A:LEU:H	1:165:A:TRP:HD1	8	1.08
(3,670)	1:134:A:GLU:H	1:34:A:TRP:HE3	7	1.08
(3,91)	1:68:A:LEU:HG	1:73:A:VAL:HA	4	1.08
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD1	4	1.08
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD2	4	1.08
(3,700)	1:175:A:VAL:H	1:155:A:PHE:HZ	7	1.07
(3,115)	1:133:A:PHE:HA	1:86:A:PHE:HZ	1	1.07
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD1	5	1.07
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD2	5	1.07
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD1	1	1.07
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD2	1	1.07
(2,1015)	1:162:A:LEU:HB2	1:195:A:TRP:HE3	5	1.07
(2,1015)	1:162:A:LEU:HB3	1:195:A:TRP:HE3	5	1.07
(3,115)	1:133:A:PHE:HA	1:86:A:PHE:HZ	3	1.06
(2,883)	1:106:A:ASN:HA	1:112:A:GLY:HA2	6	1.06
(2,883)	1:106:A:ASN:HA	1:112:A:GLY:HA3	6	1.06
(3,670)	1:134:A:GLU:H	1:34:A:TRP:HE3	3	1.05
(3,661)	1:78:A:TYR:H	1:90:A:LEU:HG	2	1.05
(3,649)	1:44:A:ASP:H	1:49:A:SER:HA	2	1.05
(3,678)	1:148:A:LEU:H	1:189:A:PHE:H	10	1.04
(3,678)	1:148:A:LEU:H	1:189:A:PHE:H	2	1.03
(3,678)	1:148:A:LEU:H	1:189:A:PHE:H	6	1.03
(3,670)	1:134:A:GLU:H	1:34:A:TRP:HE3	2	1.03
(3,696)	1:169:A:ILE:H	1:163:A:LYS:HA	8	1.0
(3,115)	1:133:A:PHE:HA	1:86:A:PHE:HZ	5	0.99
(3,703)	1:186:A:VAL:H	1:180:A:ASP:HA	6	0.98
(3,674)	1:135:A:LEU:H	1:165:A:TRP:HD1	6	0.98
(3,654)	1:68:A:LEU:H	1:117:A:VAL:H	8	0.98
(3,91)	1:68:A:LEU:HG	1:73:A:VAL:HA	2	0.98
(2,1589)	1:99:A:ASP:H	1:125:A:MET:HE1	6	0.98
(2,1595)	1:114:A:GLU:H	1:102:A:LYS:HB2	4	0.97
(2,1595)	1:114:A:GLU:H	1:102:A:LYS:HB3	4	0.97
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB2	9	0.97
(2,832)	1:88:A:THR:HA	1:25:A:LYS:HB3	9	0.97
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD1	7	0.96
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD2	7	0.96
(2,1595)	1:114:A:GLU:H	1:102:A:LYS:HB2	5	0.96
(2,1595)	1:114:A:GLU:H	1:102:A:LYS:HB3	5	0.96
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD1	6	0.96
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD2	6	0.96
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD1	8	0.95
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD2	8	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD1	3	0.95
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD2	3	0.95
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD2	5	0.95
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD3	5	0.95
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD2	5	0.95
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD3	5	0.95
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE1	3	0.95
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE2	3	0.95
(2,840)	1:91:A:PRO:HD2	1:74:A:LEU:HB2	7	0.95
(2,840)	1:91:A:PRO:HD2	1:74:A:LEU:HB3	7	0.95
(2,840)	1:91:A:PRO:HD3	1:74:A:LEU:HB2	7	0.95
(2,840)	1:91:A:PRO:HD3	1:74:A:LEU:HB3	7	0.95
(3,678)	1:148:A:LEU:H	1:189:A:PHE:H	8	0.94
(3,674)	1:135:A:LEU:H	1:165:A:TRP:HD1	7	0.94
(3,670)	1:134:A:GLU:H	1:34:A:TRP:HE3	8	0.94
(3,124)	1:137:A:VAL:HB	1:34:A:TRP:HZ2	4	0.94
(3,111)	1:131:A:ASP:HA	1:197:A:VAL:HA	7	0.94
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD1	9	0.94
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD2	9	0.94
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD1	4	0.94
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD2	4	0.94
(3,654)	1:68:A:LEU:H	1:117:A:VAL:H	4	0.93
(3,649)	1:44:A:ASP:H	1:49:A:SER:HA	1	0.92
(3,94)	1:73:A:VAL:HA	1:60:A:PHE:HZ	5	0.92
(3,679)	1:149:A:LEU:H	1:189:A:PHE:HZ	3	0.91
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG2	3	0.91
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG3	3	0.91
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG2	3	0.91
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG3	3	0.91
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG2	4	0.9
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG3	4	0.9
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG2	4	0.9
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG3	4	0.9
(2,840)	1:91:A:PRO:HD2	1:74:A:LEU:HB2	6	0.9
(2,840)	1:91:A:PRO:HD2	1:74:A:LEU:HB3	6	0.9
(2,840)	1:91:A:PRO:HD3	1:74:A:LEU:HB2	6	0.9
(2,840)	1:91:A:PRO:HD3	1:74:A:LEU:HB3	6	0.9
(3,664)	1:86:A:PHE:H	1:133:A:PHE:HZ	6	0.89
(3,678)	1:148:A:LEU:H	1:189:A:PHE:H	3	0.87
(3,647)	1:43:A:ARG:H	1:49:A:SER:HA	8	0.87
(3,670)	1:134:A:GLU:H	1:34:A:TRP:HE3	6	0.86
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG2	7	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG3	7	0.86
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG2	7	0.86
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG3	7	0.86
(3,653)	1:67:A:LYS:H	1:117:A:VAL:H	2	0.85
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE1	10	0.85
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE2	10	0.85
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG2	10	0.85
(2,1025)	1:166:A:GLY:HA2	1:199:A:LYS:HG3	10	0.85
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG2	10	0.85
(2,1025)	1:166:A:GLY:HA3	1:199:A:LYS:HG3	10	0.85
(3,649)	1:44:A:ASP:H	1:49:A:SER:HA	9	0.84
(2,1595)	1:114:A:GLU:H	1:102:A:LYS:HB2	3	0.84
(2,1595)	1:114:A:GLU:H	1:102:A:LYS:HB3	3	0.84
(3,700)	1:175:A:VAL:H	1:155:A:PHE:HZ	1	0.83
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD1	5	0.83
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD2	5	0.83
(3,678)	1:148:A:LEU:H	1:189:A:PHE:H	1	0.82
(2,1534)	1:40:A:ALA:H	1:130:A:TYR:HE1	5	0.82
(2,1534)	1:40:A:ALA:H	1:130:A:TYR:HE2	5	0.82
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE1	8	0.82
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE2	8	0.82
(3,100)	1:94:A:VAL:HA	1:70:A:PHE:HZ	2	0.81
(3,100)	1:94:A:VAL:HA	1:70:A:PHE:HZ	3	0.81
(3,115)	1:133:A:PHE:HA	1:86:A:PHE:HZ	2	0.8
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD1	10	0.8
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD2	10	0.8
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD2	4	0.8
(2,1024)	1:166:A:GLY:HA2	1:199:A:LYS:HD3	4	0.8
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD2	4	0.8
(2,1024)	1:166:A:GLY:HA3	1:199:A:LYS:HD3	4	0.8
(2,883)	1:106:A:ASN:HA	1:112:A:GLY:HA2	8	0.8
(2,883)	1:106:A:ASN:HA	1:112:A:GLY:HA3	8	0.8
(2,801)	1:77:A:CYS:HA	1:83:A:LEU:HB2	6	0.8
(2,801)	1:77:A:CYS:HA	1:83:A:LEU:HB3	6	0.8
(3,674)	1:135:A:LEU:H	1:165:A:TRP:HD1	5	0.79
(3,100)	1:94:A:VAL:HA	1:70:A:PHE:HZ	9	0.79
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE1	6	0.79
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE2	6	0.79
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB2	6	0.79
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB3	6	0.79
(3,700)	1:175:A:VAL:H	1:155:A:PHE:HZ	4	0.78
(2,801)	1:77:A:CYS:HA	1:83:A:LEU:HB2	2	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,801)	1:77:A:CYS:HA	1:83:A:LEU:HB3	2	0.78
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB2	5	0.78
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB3	5	0.78
(3,115)	1:133:A:PHE:HA	1:86:A:PHE:HZ	10	0.77
(3,649)	1:44:A:ASP:H	1:49:A:SER:HA	3	0.76
(3,104)	1:115:A:ASP:HA	1:98:A:PHE:HZ	8	0.76
(3,703)	1:186:A:VAL:H	1:180:A:ASP:HA	2	0.75
(3,94)	1:73:A:VAL:HA	1:60:A:PHE:HZ	1	0.75
(3,649)	1:44:A:ASP:H	1:49:A:SER:HA	7	0.74
(2,975)	1:143:A:ASP:HB2	1:189:A:PHE:HD1	9	0.74
(2,975)	1:143:A:ASP:HB2	1:189:A:PHE:HD2	9	0.74
(2,975)	1:143:A:ASP:HB3	1:189:A:PHE:HD1	9	0.74
(2,975)	1:143:A:ASP:HB3	1:189:A:PHE:HD2	9	0.74
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD1	3	0.73
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD2	3	0.73
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD1	4	0.73
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD2	4	0.73
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD1	1	0.72
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD2	1	0.72
(3,100)	1:94:A:VAL:HA	1:70:A:PHE:HZ	6	0.71
(2,1005)	1:158:A:ALA:HA	1:142:A:MET:HB2	9	0.71
(2,1005)	1:158:A:ALA:HA	1:142:A:MET:HB3	9	0.71
(3,100)	1:94:A:VAL:HA	1:70:A:PHE:HZ	7	0.7
(3,125)	1:150:A:LEU:HA	1:187:A:VAL:HB	7	0.69
(3,100)	1:94:A:VAL:HA	1:70:A:PHE:HZ	8	0.68
(2,1005)	1:158:A:ALA:HA	1:142:A:MET:HB2	3	0.68
(2,1005)	1:158:A:ALA:HA	1:142:A:MET:HB3	3	0.68
(3,696)	1:169:A:ILE:H	1:163:A:LYS:HA	4	0.67
(3,661)	1:78:A:TYR:H	1:90:A:LEU:HG	5	0.67
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE1	2	0.67
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE2	2	0.67
(3,700)	1:175:A:VAL:H	1:155:A:PHE:HZ	5	0.66
(3,94)	1:73:A:VAL:HA	1:60:A:PHE:HZ	8	0.66
(2,1005)	1:158:A:ALA:HA	1:142:A:MET:HB2	6	0.65
(2,1005)	1:158:A:ALA:HA	1:142:A:MET:HB3	6	0.65
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE1	7	0.65
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE2	7	0.65
(3,654)	1:68:A:LEU:H	1:117:A:VAL:H	5	0.64
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD1	8	0.64
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD2	8	0.64
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE1	6	0.64
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE2	6	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,700)	1:175:A:VAL:H	1:155:A:PHE:HZ	8	0.63
(2,840)	1:91:A:PRO:HD2	1:74:A:LEU:HB2	8	0.63
(2,840)	1:91:A:PRO:HD2	1:74:A:LEU:HB3	8	0.63
(2,840)	1:91:A:PRO:HD3	1:74:A:LEU:HB2	8	0.63
(2,840)	1:91:A:PRO:HD3	1:74:A:LEU:HB3	8	0.63
(3,124)	1:137:A:VAL:HB	1:34:A:TRP:HZ2	5	0.62
(3,104)	1:115:A:ASP:HA	1:98:A:PHE:HZ	4	0.62
(3,100)	1:94:A:VAL:HA	1:70:A:PHE:HZ	10	0.62
(3,99)	1:93:A:ILE:HB	1:133:A:PHE:HZ	8	0.62
(3,94)	1:73:A:VAL:HA	1:60:A:PHE:HZ	10	0.62
(3,91)	1:68:A:LEU:HG	1:73:A:VAL:HA	5	0.62
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG12	4	0.62
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG13	4	0.62
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE1	1	0.62
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE2	1	0.62
(3,104)	1:115:A:ASP:HA	1:98:A:PHE:HZ	9	0.61
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD1	3	0.61
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD2	3	0.61
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD1	10	0.6
(2,1625)	1:175:A:VAL:H	1:155:A:PHE:HD2	10	0.6
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG12	10	0.6
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG13	10	0.6
(3,94)	1:73:A:VAL:HA	1:60:A:PHE:HZ	7	0.59
(2,1015)	1:162:A:LEU:HB2	1:195:A:TRP:HE3	6	0.58
(2,1015)	1:162:A:LEU:HB3	1:195:A:TRP:HE3	6	0.58
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB2	1	0.58
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB3	1	0.58
(3,115)	1:133:A:PHE:HA	1:86:A:PHE:HZ	9	0.57
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG12	8	0.57
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG13	8	0.57
(2,1565)	1:78:A:TYR:H	1:90:A:LEU:HB2	4	0.57
(2,1565)	1:78:A:TYR:H	1:90:A:LEU:HB3	4	0.57
(3,702)	1:185:A:GLY:H	1:180:A:ASP:HA	9	0.56
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE1	9	0.56
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE2	9	0.56
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD1	9	0.56
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD2	9	0.56
(2,1005)	1:158:A:ALA:HA	1:142:A:MET:HB2	5	0.56
(2,1005)	1:158:A:ALA:HA	1:142:A:MET:HB3	5	0.56
(2,779)	1:68:A:LEU:HD11	1:62:A:THR:HB	3	0.56
(2,779)	1:68:A:LEU:HD12	1:62:A:THR:HB	3	0.56
(2,779)	1:68:A:LEU:HD13	1:62:A:THR:HB	3	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,779)	1:68:A:LEU:HD21	1:62:A:THR:HB	3	0.56
(2,779)	1:68:A:LEU:HD22	1:62:A:THR:HB	3	0.56
(2,779)	1:68:A:LEU:HD23	1:62:A:THR:HB	3	0.56
(3,125)	1:150:A:LEU:HA	1:187:A:VAL:HB	4	0.55
(3,696)	1:169:A:ILE:H	1:163:A:LYS:HA	7	0.54
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG12	3	0.54
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG13	3	0.54
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB2	7	0.54
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB3	7	0.54
(3,124)	1:137:A:VAL:HB	1:34:A:TRP:HZ2	7	0.53
(3,104)	1:115:A:ASP:HA	1:98:A:PHE:HZ	7	0.53
(3,100)	1:94:A:VAL:HA	1:70:A:PHE:HZ	5	0.53
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD1	4	0.53
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD2	4	0.53
(3,111)	1:131:A:ASP:HA	1:197:A:VAL:HA	6	0.52
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG12	5	0.52
(2,1603)	1:129:A:ILE:H	1:41:A:ILE:HG13	5	0.52
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD1	9	0.52
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD2	9	0.52
(3,99)	1:93:A:ILE:HB	1:133:A:PHE:HZ	2	0.51
(3,91)	1:68:A:LEU:HG	1:73:A:VAL:HA	7	0.51
(3,647)	1:43:A:ARG:H	1:49:A:SER:HA	5	0.5
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD1	3	0.5
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD2	3	0.5
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD1	6	0.5
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD2	6	0.5
(2,1595)	1:114:A:GLU:H	1:102:A:LYS:HB2	7	0.49
(2,1595)	1:114:A:GLU:H	1:102:A:LYS:HB3	7	0.49
(2,1532)	1:38:A:ARG:H	1:130:A:TYR:HE1	5	0.49
(2,1532)	1:38:A:ARG:H	1:130:A:TYR:HE2	5	0.49
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE1	5	0.48
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE2	5	0.48
(2,801)	1:77:A:CYS:HA	1:83:A:LEU:HB2	3	0.48
(2,801)	1:77:A:CYS:HA	1:83:A:LEU:HB3	3	0.48
(3,700)	1:175:A:VAL:H	1:155:A:PHE:HZ	3	0.47
(3,125)	1:150:A:LEU:HA	1:187:A:VAL:HB	1	0.47
(3,111)	1:131:A:ASP:HA	1:197:A:VAL:HA	5	0.47
(3,104)	1:115:A:ASP:HA	1:98:A:PHE:HZ	10	0.47
(2,1015)	1:162:A:LEU:HB2	1:195:A:TRP:HE3	7	0.47
(2,1015)	1:162:A:LEU:HB3	1:195:A:TRP:HE3	7	0.47
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE1	9	0.47
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE2	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,125)	1:150:A:LEU:HA	1:187:A:VAL:HB	5	0.46
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD1	5	0.46
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD2	5	0.46
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG21	2	0.46
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG22	2	0.46
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG23	2	0.46
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD1	1	0.45
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD2	1	0.45
(3,94)	1:73:A:VAL:HA	1:60:A:PHE:HZ	6	0.44
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD1	9	0.44
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD2	9	0.44
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE1	3	0.44
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE2	3	0.44
(2,801)	1:77:A:CYS:HA	1:83:A:LEU:HB2	10	0.44
(2,801)	1:77:A:CYS:HA	1:83:A:LEU:HB3	10	0.44
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG21	8	0.44
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG22	8	0.44
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG23	8	0.44
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE1	3	0.42
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE2	3	0.42
(2,779)	1:68:A:LEU:HD11	1:62:A:THR:HB	4	0.42
(2,779)	1:68:A:LEU:HD12	1:62:A:THR:HB	4	0.42
(2,779)	1:68:A:LEU:HD13	1:62:A:THR:HB	4	0.42
(2,779)	1:68:A:LEU:HD21	1:62:A:THR:HB	4	0.42
(2,779)	1:68:A:LEU:HD22	1:62:A:THR:HB	4	0.42
(2,779)	1:68:A:LEU:HD23	1:62:A:THR:HB	4	0.42
(3,654)	1:68:A:LEU:H	1:117:A:VAL:H	2	0.41
(3,124)	1:137:A:VAL:HB	1:34:A:TRP:HZ2	6	0.41
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD1	8	0.41
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD2	8	0.41
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD1	2	0.41
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD2	2	0.41
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD1	7	0.41
(2,1525)	1:32:A:VAL:H	1:86:A:PHE:HD2	7	0.41
(2,801)	1:77:A:CYS:HA	1:83:A:LEU:HB2	7	0.41
(2,801)	1:77:A:CYS:HA	1:83:A:LEU:HB3	7	0.41
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB2	3	0.41
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB3	3	0.41
(3,111)	1:131:A:ASP:HA	1:197:A:VAL:HA	2	0.4
(3,91)	1:68:A:LEU:HG	1:73:A:VAL:HA	1	0.4
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD1	8	0.4
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD2	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,779)	1:68:A:LEU:HD11	1:62:A:THR:HB	5	0.4
(2,779)	1:68:A:LEU:HD12	1:62:A:THR:HB	5	0.4
(2,779)	1:68:A:LEU:HD13	1:62:A:THR:HB	5	0.4
(2,779)	1:68:A:LEU:HD21	1:62:A:THR:HB	5	0.4
(2,779)	1:68:A:LEU:HD22	1:62:A:THR:HB	5	0.4
(2,779)	1:68:A:LEU:HD23	1:62:A:THR:HB	5	0.4
(3,91)	1:68:A:LEU:HG	1:73:A:VAL:HA	3	0.39
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD1	4	0.39
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD2	4	0.39
(2,1042)	1:169:A:ILE:HG21	1:195:A:TRP:HE3	8	0.39
(2,1042)	1:169:A:ILE:HG22	1:195:A:TRP:HE3	8	0.39
(2,1042)	1:169:A:ILE:HG23	1:195:A:TRP:HE3	8	0.39
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG21	9	0.39
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG22	9	0.39
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG23	9	0.39
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG21	10	0.39
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG22	10	0.39
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG23	10	0.39
(3,666)	1:94:A:VAL:H	1:70:A:PHE:HZ	1	0.38
(3,112)	1:131:A:ASP:HA	1:34:A:TRP:HH2	9	0.38
(3,94)	1:73:A:VAL:HA	1:60:A:PHE:HZ	2	0.38
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD1	8	0.38
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD2	8	0.38
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE1	5	0.38
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE2	5	0.38
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE1	2	0.38
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE2	2	0.38
(3,647)	1:43:A:ARG:H	1:49:A:SER:HA	1	0.37
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD1	10	0.37
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD2	10	0.37
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD1	5	0.37
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD2	5	0.37
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE1	9	0.37
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE2	9	0.37
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG21	6	0.37
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG22	6	0.37
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG23	6	0.37
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE1	8	0.36
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE2	8	0.36
(3,649)	1:44:A:ASP:H	1:49:A:SER:HA	10	0.35
(3,100)	1:94:A:VAL:HA	1:70:A:PHE:HZ	4	0.35
(3,14)	1:79:A:GLY:HA2	1:82:A:LYS:HA	4	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,14)	1:79:A:GLY:HA3	1:82:A:LYS:HA	4	0.35
(3,710)	1:197:A:VAL:H	1:165:A:TRP:HZ3	6	0.34
(3,99)	1:93:A:ILE:HB	1:133:A:PHE:HZ	7	0.34
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD1	5	0.34
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD2	5	0.34
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB2	4	0.34
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB3	4	0.34
(3,111)	1:131:A:ASP:HA	1:197:A:VAL:HA	1	0.33
(3,104)	1:115:A:ASP:HA	1:98:A:PHE:HZ	5	0.33
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD1	9	0.33
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD2	9	0.33
(2,1015)	1:162:A:LEU:HB2	1:195:A:TRP:HE3	3	0.33
(2,1015)	1:162:A:LEU:HB3	1:195:A:TRP:HE3	3	0.33
(2,975)	1:143:A:ASP:HB2	1:189:A:PHE:HD1	7	0.33
(2,975)	1:143:A:ASP:HB2	1:189:A:PHE:HD2	7	0.33
(2,975)	1:143:A:ASP:HB3	1:189:A:PHE:HD1	7	0.33
(2,975)	1:143:A:ASP:HB3	1:189:A:PHE:HD2	7	0.33
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE1	4	0.33
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE2	4	0.33
(1,80)	1:54:A:ILE:HG12	1:119:A:PHE:HZ	9	0.32
(1,80)	1:54:A:ILE:HG13	1:119:A:PHE:HZ	9	0.32
(2,801)	1:77:A:CYS:HA	1:83:A:LEU:HB2	8	0.31
(2,801)	1:77:A:CYS:HA	1:83:A:LEU:HB3	8	0.31
(3,654)	1:68:A:LEU:H	1:117:A:VAL:H	10	0.3
(3,321)	1:92:A:ASP:H	1:89:A:HIS:HA	7	0.3
(3,124)	1:137:A:VAL:HB	1:34:A:TRP:HZ2	1	0.3
(3,111)	1:131:A:ASP:HA	1:197:A:VAL:HA	4	0.3
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD1	10	0.3
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD2	10	0.3
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE1	4	0.3
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE2	4	0.3
(3,703)	1:186:A:VAL:H	1:180:A:ASP:HA	7	0.29
(3,647)	1:43:A:ARG:H	1:49:A:SER:HA	3	0.29
(3,321)	1:92:A:ASP:H	1:89:A:HIS:HA	1	0.29
(3,99)	1:93:A:ILE:HB	1:133:A:PHE:HZ	9	0.29
(3,94)	1:73:A:VAL:HA	1:60:A:PHE:HZ	9	0.29
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB2	8	0.29
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB3	8	0.29
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB2	10	0.29
(1,147)	1:113:A:GLU:H	1:106:A:ASN:HB3	10	0.29
(3,647)	1:43:A:ARG:H	1:49:A:SER:HA	4	0.28
(2,1015)	1:162:A:LEU:HB2	1:195:A:TRP:HE3	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1015)	1:162:A:LEU:HB3	1:195:A:TRP:HE3	1	0.28
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE1	2	0.28
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE2	2	0.28
(3,669)	1:134:A:GLU:H	1:34:A:TRP:HE1	10	0.27
(3,666)	1:94:A:VAL:H	1:70:A:PHE:HZ	3	0.27
(3,91)	1:68:A:LEU:HG	1:73:A:VAL:HA	9	0.27
(2,1565)	1:78:A:TYR:H	1:90:A:LEU:HB2	5	0.27
(2,1565)	1:78:A:TYR:H	1:90:A:LEU:HB3	5	0.27
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD1	10	0.27
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD2	10	0.27
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE1	7	0.27
(2,1526)	1:32:A:VAL:H	1:86:A:PHE:HE2	7	0.27
(2,1015)	1:162:A:LEU:HB2	1:195:A:TRP:HE3	9	0.27
(2,1015)	1:162:A:LEU:HB3	1:195:A:TRP:HE3	9	0.27
(2,779)	1:68:A:LEU:HD11	1:62:A:THR:HB	10	0.27
(2,779)	1:68:A:LEU:HD12	1:62:A:THR:HB	10	0.27
(2,779)	1:68:A:LEU:HD13	1:62:A:THR:HB	10	0.27
(2,779)	1:68:A:LEU:HD21	1:62:A:THR:HB	10	0.27
(2,779)	1:68:A:LEU:HD22	1:62:A:THR:HB	10	0.27
(2,779)	1:68:A:LEU:HD23	1:62:A:THR:HB	10	0.27
(3,487)	1:173:A:THR:H	1:171:A:ASP:HA	3	0.26
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD1	4	0.26
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD2	4	0.26
(2,1534)	1:40:A:ALA:H	1:130:A:TYR:HE1	1	0.26
(2,1534)	1:40:A:ALA:H	1:130:A:TYR:HE2	1	0.26
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE1	1	0.26
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE2	1	0.26
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE1	8	0.26
(2,1528)	1:33:A:ALA:H	1:86:A:PHE:HE2	8	0.26
(3,649)	1:44:A:ASP:H	1:49:A:SER:HA	5	0.25
(2,1666)	1:198:A:THR:H	1:132:A:ILE:HG12	8	0.25
(2,1666)	1:198:A:THR:H	1:132:A:ILE:HG13	8	0.25
(3,708)	1:197:A:VAL:H	1:165:A:TRP:HZ2	3	0.24
(3,666)	1:94:A:VAL:H	1:70:A:PHE:HZ	8	0.24
(3,666)	1:94:A:VAL:H	1:70:A:PHE:HZ	9	0.24
(3,654)	1:68:A:LEU:H	1:117:A:VAL:H	6	0.24
(3,642)	1:197:A:VAL:H	1:165:A:TRP:HZ2	3	0.24
(3,111)	1:131:A:ASP:HA	1:197:A:VAL:HA	8	0.24
(2,1015)	1:162:A:LEU:HB2	1:195:A:TRP:HE3	2	0.24
(2,1015)	1:162:A:LEU:HB3	1:195:A:TRP:HE3	2	0.24
(2,1015)	1:162:A:LEU:HB2	1:195:A:TRP:HE3	8	0.24
(2,1015)	1:162:A:LEU:HB3	1:195:A:TRP:HE3	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,708)	1:197:A:VAL:H	1:165:A:TRP:HZ2	10	0.23
(3,642)	1:197:A:VAL:H	1:165:A:TRP:HZ2	10	0.23
(3,125)	1:150:A:LEU:HA	1:187:A:VAL:HB	10	0.23
(3,112)	1:131:A:ASP:HA	1:34:A:TRP:HH2	7	0.23
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD1	2	0.23
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD2	2	0.23
(3,669)	1:134:A:GLU:H	1:34:A:TRP:HE1	4	0.22
(3,648)	1:43:A:ARG:H	1:49:A:SER:HB2	5	0.22
(3,648)	1:43:A:ARG:H	1:49:A:SER:HB3	5	0.22
(3,321)	1:92:A:ASP:H	1:89:A:HIS:HA	6	0.22
(2,1608)	1:149:A:LEU:H	1:189:A:PHE:HB2	3	0.22
(2,1608)	1:149:A:LEU:H	1:189:A:PHE:HB3	3	0.22
(2,994)	1:151:A:GLU:HA	1:176:A:PHE:HD1	4	0.22
(2,994)	1:151:A:GLU:HA	1:176:A:PHE:HD2	4	0.22
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG21	7	0.22
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG22	7	0.22
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG23	7	0.22
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD1	3	0.21
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD2	3	0.21
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD1	7	0.21
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD2	7	0.21
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD1	1	0.21
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD2	1	0.21
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG21	1	0.21
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG22	1	0.21
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG23	1	0.21
(3,708)	1:197:A:VAL:H	1:165:A:TRP:HZ2	6	0.2
(3,642)	1:197:A:VAL:H	1:165:A:TRP:HZ2	6	0.2
(3,94)	1:73:A:VAL:HA	1:60:A:PHE:HZ	4	0.2
(2,840)	1:91:A:PRO:HD2	1:74:A:LEU:HB2	5	0.2
(2,840)	1:91:A:PRO:HD2	1:74:A:LEU:HB3	5	0.2
(2,840)	1:91:A:PRO:HD3	1:74:A:LEU:HB2	5	0.2
(2,840)	1:91:A:PRO:HD3	1:74:A:LEU:HB3	5	0.2
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG21	4	0.2
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG22	4	0.2
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG23	4	0.2
(5,52)	1:91:A:PRO:O	1:95:A:GLN:H	1	0.19
(3,710)	1:197:A:VAL:H	1:165:A:TRP:HZ3	3	0.19
(3,700)	1:175:A:VAL:H	1:155:A:PHE:HZ	10	0.19
(3,679)	1:149:A:LEU:H	1:189:A:PHE:HZ	1	0.19
(3,671)	1:134:A:GLU:H	1:165:A:TRP:HE1	1	0.19
(3,603)	1:134:A:GLU:H	1:165:A:TRP:HE1	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,601)	1:133:A:PHE:H	1:34:A:TRP:HZ2	9	0.19
(3,315)	1:89:A:HIS:H	1:87:A:THR:HB	5	0.19
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD1	2	0.19
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD2	2	0.19
(2,840)	1:91:A:PRO:HD2	1:74:A:LEU:HB2	3	0.19
(2,840)	1:91:A:PRO:HD2	1:74:A:LEU:HB3	3	0.19
(2,840)	1:91:A:PRO:HD3	1:74:A:LEU:HB2	3	0.19
(2,840)	1:91:A:PRO:HD3	1:74:A:LEU:HB3	3	0.19
(3,708)	1:197:A:VAL:H	1:165:A:TRP:HZ2	5	0.18
(3,708)	1:197:A:VAL:H	1:165:A:TRP:HZ2	8	0.18
(3,675)	1:135:A:LEU:H	1:165:A:TRP:HH2	4	0.18
(3,666)	1:94:A:VAL:H	1:70:A:PHE:HZ	5	0.18
(3,642)	1:197:A:VAL:H	1:165:A:TRP:HZ2	5	0.18
(3,642)	1:197:A:VAL:H	1:165:A:TRP:HZ2	8	0.18
(3,607)	1:135:A:LEU:H	1:165:A:TRP:HH2	4	0.18
(3,44)	1:83:A:LEU:HG	1:133:A:PHE:HZ	5	0.18
(2,975)	1:143:A:ASP:HB2	1:189:A:PHE:HD1	3	0.18
(2,975)	1:143:A:ASP:HB2	1:189:A:PHE:HD2	3	0.18
(2,975)	1:143:A:ASP:HB3	1:189:A:PHE:HD1	3	0.18
(2,975)	1:143:A:ASP:HB3	1:189:A:PHE:HD2	3	0.18
(2,975)	1:143:A:ASP:HB2	1:189:A:PHE:HD1	6	0.18
(2,975)	1:143:A:ASP:HB2	1:189:A:PHE:HD2	6	0.18
(2,975)	1:143:A:ASP:HB3	1:189:A:PHE:HD1	6	0.18
(2,975)	1:143:A:ASP:HB3	1:189:A:PHE:HD2	6	0.18
(3,708)	1:197:A:VAL:H	1:165:A:TRP:HZ2	2	0.17
(3,708)	1:197:A:VAL:H	1:165:A:TRP:HZ2	7	0.17
(3,671)	1:134:A:GLU:H	1:165:A:TRP:HE1	3	0.17
(3,669)	1:134:A:GLU:H	1:34:A:TRP:HE1	5	0.17
(3,642)	1:197:A:VAL:H	1:165:A:TRP:HZ2	2	0.17
(3,642)	1:197:A:VAL:H	1:165:A:TRP:HZ2	7	0.17
(3,603)	1:134:A:GLU:H	1:165:A:TRP:HE1	3	0.17
(3,128)	1:186:A:VAL:HB	1:150:A:LEU:HA	10	0.17
(3,112)	1:131:A:ASP:HA	1:34:A:TRP:HH2	10	0.17
(3,104)	1:115:A:ASP:HA	1:98:A:PHE:HZ	6	0.17
(3,80)	1:186:A:VAL:HB	1:150:A:LEU:HA	10	0.17
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD1	1	0.17
(2,1548)	1:66:A:GLY:H	1:57:A:PHE:HD2	1	0.17
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE1	8	0.17
(2,857)	1:94:A:VAL:HA	1:128:A:TYR:HE2	8	0.17
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE1	10	0.17
(2,843)	1:93:A:ILE:HB	1:128:A:TYR:HE2	10	0.17
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG21	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG22	3	0.17
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG23	3	0.17
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG21	5	0.17
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG22	5	0.17
(1,85)	1:83:A:LEU:HG	1:129:A:ILE:HG23	5	0.17
(3,668)	1:134:A:GLU:H	1:34:A:TRP:HH2	4	0.16
(3,602)	1:134:A:GLU:H	1:34:A:TRP:HH2	4	0.16
(3,487)	1:173:A:THR:H	1:171:A:ASP:HA	2	0.16
(3,120)	1:135:A:LEU:HG	1:165:A:TRP:HZ3	5	0.16
(3,111)	1:131:A:ASP:HA	1:197:A:VAL:HA	9	0.16
(3,66)	1:135:A:LEU:HG	1:165:A:TRP:HZ3	5	0.16
(3,14)	1:79:A:GLY:HA2	1:82:A:LYS:HA	3	0.16
(3,14)	1:79:A:GLY:HA3	1:82:A:LYS:HA	3	0.16
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD1	2	0.16
(2,1635)	1:185:A:GLY:H	1:176:A:PHE:HD2	2	0.16
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD1	3	0.16
(2,1540)	1:54:A:ILE:H	1:119:A:PHE:HD2	3	0.16
(2,975)	1:143:A:ASP:HB2	1:189:A:PHE:HD1	8	0.16
(2,975)	1:143:A:ASP:HB2	1:189:A:PHE:HD2	8	0.16
(2,975)	1:143:A:ASP:HB3	1:189:A:PHE:HD1	8	0.16
(2,975)	1:143:A:ASP:HB3	1:189:A:PHE:HD2	8	0.16
(3,708)	1:197:A:VAL:H	1:165:A:TRP:HZ2	1	0.15
(3,675)	1:135:A:LEU:H	1:165:A:TRP:HH2	3	0.15
(3,675)	1:135:A:LEU:H	1:165:A:TRP:HH2	6	0.15
(3,642)	1:197:A:VAL:H	1:165:A:TRP:HZ2	1	0.15
(3,607)	1:135:A:LEU:H	1:165:A:TRP:HH2	3	0.15
(3,607)	1:135:A:LEU:H	1:165:A:TRP:HH2	6	0.15
(3,601)	1:133:A:PHE:H	1:34:A:TRP:HZ2	4	0.15
(2,1015)	1:162:A:LEU:HB2	1:195:A:TRP:HE3	10	0.15
(2,1015)	1:162:A:LEU:HB3	1:195:A:TRP:HE3	10	0.15
(2,883)	1:106:A:ASN:HA	1:112:A:GLY:HA2	1	0.15
(2,883)	1:106:A:ASN:HA	1:112:A:GLY:HA3	1	0.15
(5,124)	1:160:A:PRO:O	1:164:A:GLU:H	1	0.14
(3,699)	1:174:A:THR:H	1:155:A:PHE:HZ	3	0.14
(3,681)	1:149:A:LEU:H	1:189:A:PHE:H	3	0.14
(3,667)	1:130:A:TYR:H	1:34:A:TRP:HH2	1	0.14
(3,631)	1:174:A:THR:H	1:155:A:PHE:HZ	3	0.14
(3,610)	1:149:A:LEU:H	1:189:A:PHE:H	3	0.14
(3,601)	1:133:A:PHE:H	1:34:A:TRP:HZ2	6	0.14
(3,599)	1:130:A:TYR:H	1:34:A:TRP:HH2	1	0.14
(3,563)	1:198:A:THR:H	1:197:A:VAL:HB	5	0.14
(3,45)	1:83:A:LEU:HG	1:77:A:CYS:HA	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,10)	1:74:A:LEU:HA	1:70:A:PHE:HZ	10	0.14
(2,1638)	1:187:A:VAL:H	1:176:A:PHE:HD1	8	0.14
(2,1638)	1:187:A:VAL:H	1:176:A:PHE:HD2	8	0.14
(2,1608)	1:149:A:LEU:H	1:189:A:PHE:HB2	9	0.14
(2,1608)	1:149:A:LEU:H	1:189:A:PHE:HB3	9	0.14
(5,128)	1:173:A:THR:O	1:177:A:ASN:H	1	0.13
(5,118)	1:157:A:GLU:O	1:161:A:LYS:H	3	0.13
(3,708)	1:197:A:VAL:H	1:165:A:TRP:HZ2	4	0.13
(3,675)	1:135:A:LEU:H	1:165:A:TRP:HH2	1	0.13
(3,675)	1:135:A:LEU:H	1:165:A:TRP:HH2	2	0.13
(3,671)	1:134:A:GLU:H	1:165:A:TRP:HE1	4	0.13
(3,671)	1:134:A:GLU:H	1:165:A:TRP:HE1	10	0.13
(3,642)	1:197:A:VAL:H	1:165:A:TRP:HZ2	4	0.13
(3,607)	1:135:A:LEU:H	1:165:A:TRP:HH2	1	0.13
(3,607)	1:135:A:LEU:H	1:165:A:TRP:HH2	2	0.13
(3,603)	1:134:A:GLU:H	1:165:A:TRP:HE1	4	0.13
(3,603)	1:134:A:GLU:H	1:165:A:TRP:HE1	10	0.13
(3,601)	1:133:A:PHE:H	1:34:A:TRP:HZ2	1	0.13
(3,601)	1:133:A:PHE:H	1:34:A:TRP:HZ2	5	0.13
(3,601)	1:133:A:PHE:H	1:34:A:TRP:HZ2	7	0.13
(3,601)	1:133:A:PHE:H	1:34:A:TRP:HZ2	10	0.13
(3,189)	1:38:A:ARG:H	1:34:A:TRP:HZ3	1	0.13
(3,99)	1:93:A:ILE:HB	1:133:A:PHE:HZ	5	0.13
(3,99)	1:93:A:ILE:HB	1:133:A:PHE:HZ	6	0.13
(2,1608)	1:149:A:LEU:H	1:189:A:PHE:HB2	8	0.13
(2,1608)	1:149:A:LEU:H	1:189:A:PHE:HB3	8	0.13
(2,1015)	1:162:A:LEU:HB2	1:195:A:TRP:HE3	4	0.13
(2,1015)	1:162:A:LEU:HB3	1:195:A:TRP:HE3	4	0.13
(2,840)	1:91:A:PRO:HD2	1:74:A:LEU:HB2	1	0.13
(2,840)	1:91:A:PRO:HD2	1:74:A:LEU:HB3	1	0.13
(2,840)	1:91:A:PRO:HD3	1:74:A:LEU:HB2	1	0.13
(2,840)	1:91:A:PRO:HD3	1:74:A:LEU:HB3	1	0.13
(5,140)	1:192:A:PHE:O	1:196:A:ALA:H	1	0.12
(5,124)	1:160:A:PRO:O	1:164:A:GLU:H	3	0.12
(5,118)	1:157:A:GLU:O	1:161:A:LYS:H	1	0.12
(5,118)	1:157:A:GLU:O	1:161:A:LYS:H	9	0.12
(5,118)	1:157:A:GLU:O	1:161:A:LYS:H	10	0.12
(5,104)	1:134:A:GLU:O	1:138:A:MET:H	4	0.12
(5,62)	1:96:A:ARG:O	1:100:A:LYS:H	2	0.12
(5,52)	1:91:A:PRO:O	1:95:A:GLN:H	4	0.12
(3,710)	1:197:A:VAL:H	1:165:A:TRP:HZ3	8	0.12
(3,687)	1:165:A:TRP:HE1	1:134:A:GLU:HA	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,681)	1:149:A:LEU:H	1:189:A:PHE:H	8	0.12
(3,668)	1:134:A:GLU:H	1:34:A:TRP:HH2	3	0.12
(3,667)	1:130:A:TYR:H	1:34:A:TRP:HH2	4	0.12
(3,619)	1:165:A:TRP:HE1	1:134:A:GLU:HA	9	0.12
(3,610)	1:149:A:LEU:H	1:189:A:PHE:H	8	0.12
(3,602)	1:134:A:GLU:H	1:34:A:TRP:HH2	3	0.12
(3,601)	1:133:A:PHE:H	1:34:A:TRP:HZ2	3	0.12
(3,599)	1:130:A:TYR:H	1:34:A:TRP:HH2	4	0.12
(3,567)	1:203:A:VAL:H	1:204:A:CYS:HA	5	0.12
(3,563)	1:198:A:THR:H	1:197:A:VAL:HB	7	0.12
(3,472)	1:167:A:VAL:H	1:165:A:TRP:HA	9	0.12
(3,189)	1:38:A:ARG:H	1:34:A:TRP:HZ3	6	0.12
(3,128)	1:186:A:VAL:HB	1:150:A:LEU:HA	1	0.12
(3,112)	1:131:A:ASP:HA	1:34:A:TRP:HH2	6	0.12
(3,97)	1:84:A:ASP:HA	1:90:A:LEU:HG	4	0.12
(3,80)	1:186:A:VAL:HB	1:150:A:LEU:HA	1	0.12
(3,46)	1:84:A:ASP:HA	1:90:A:LEU:HG	4	0.12
(3,21)	1:129:A:ILE:HA	1:132:A:ILE:HB	10	0.12
(5,118)	1:157:A:GLU:O	1:161:A:LYS:H	6	0.11
(5,118)	1:157:A:GLU:O	1:161:A:LYS:H	7	0.11
(5,52)	1:91:A:PRO:O	1:95:A:GLN:H	5	0.11
(5,52)	1:91:A:PRO:O	1:95:A:GLN:H	6	0.11
(5,52)	1:91:A:PRO:O	1:95:A:GLN:H	8	0.11
(5,4)	1:28:A:ALA:O	1:32:A:VAL:H	2	0.11
(3,692)	1:168:A:ASP:H	1:195:A:TRP:HZ2	8	0.11
(3,680)	1:149:A:LEU:H	1:188:A:THR:HA	9	0.11
(3,679)	1:149:A:LEU:H	1:189:A:PHE:HZ	8	0.11
(3,669)	1:134:A:GLU:H	1:34:A:TRP:HE1	1	0.11
(3,668)	1:134:A:GLU:H	1:34:A:TRP:HH2	7	0.11
(3,660)	1:78:A:TYR:H	1:83:A:LEU:H	2	0.11
(3,625)	1:168:A:ASP:H	1:195:A:TRP:HZ2	8	0.11
(3,602)	1:134:A:GLU:H	1:34:A:TRP:HH2	7	0.11
(3,601)	1:133:A:PHE:H	1:34:A:TRP:HZ2	2	0.11
(3,595)	1:78:A:TYR:H	1:83:A:LEU:H	2	0.11
(3,577)	1:209:A:GLY:H	1:207:A:PRO:HA	1	0.11
(3,315)	1:89:A:HIS:H	1:87:A:THR:HB	2	0.11
(3,189)	1:38:A:ARG:H	1:34:A:TRP:HZ3	3	0.11
(3,189)	1:38:A:ARG:H	1:34:A:TRP:HZ3	7	0.11
(3,77)	1:169:A:ILE:HB	1:195:A:TRP:HZ3	6	0.11
(3,10)	1:74:A:LEU:HA	1:70:A:PHE:HZ	7	0.11
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD1	7	0.11
(2,1637)	1:186:A:VAL:H	1:176:A:PHE:HD2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,140)	1:192:A:PHE:O	1:196:A:ALA:H	4	0.1
(5,118)	1:157:A:GLU:O	1:161:A:LYS:H	4	0.1
(5,118)	1:157:A:GLU:O	1:161:A:LYS:H	5	0.1
(5,18)	1:35:A:GLU:O	1:39:A:CYS:H	1	0.1
(3,699)	1:174:A:THR:H	1:155:A:PHE:HZ	10	0.1
(3,660)	1:78:A:TYR:H	1:83:A:LEU:H	9	0.1
(3,631)	1:174:A:THR:H	1:155:A:PHE:HZ	10	0.1
(3,601)	1:133:A:PHE:H	1:34:A:TRP:HZ2	8	0.1
(3,595)	1:78:A:TYR:H	1:83:A:LEU:H	9	0.1
(3,315)	1:89:A:HIS:H	1:87:A:THR:HB	10	0.1
(3,209)	1:45:A:LYS:H	1:44:A:ASP:HA	10	0.1
(3,178)	1:36:A:ARG:H	1:37:A:ILE:HA	8	0.1
(3,99)	1:93:A:ILE:HB	1:133:A:PHE:HZ	3	0.1
(3,19)	1:126:A:LEU:HA	1:129:A:ILE:HB	2	0.1

10 Dihedral-angle violation analysis

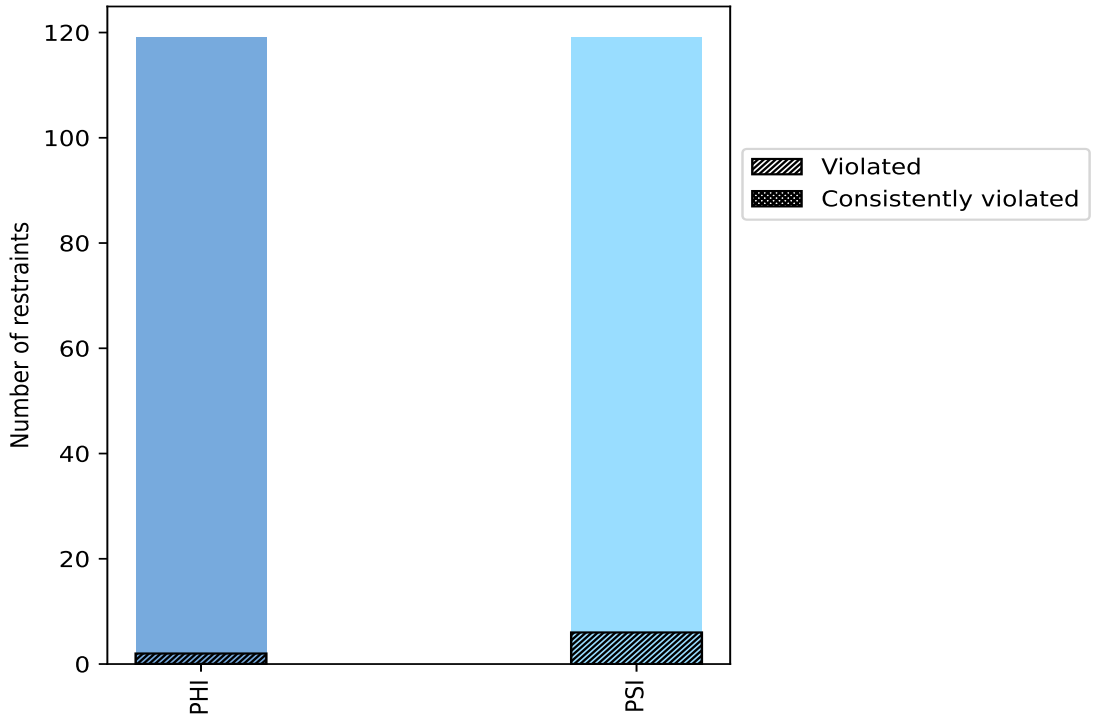
10.1 Summary of dihedral-angle violations

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	119	50.0	2	1.7	0.8	0	0.0	0.0
PSI	119	50.0	6	5.0	2.5	0	0.0	0.0
Total	238	100.0	8	3.4	3.4	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



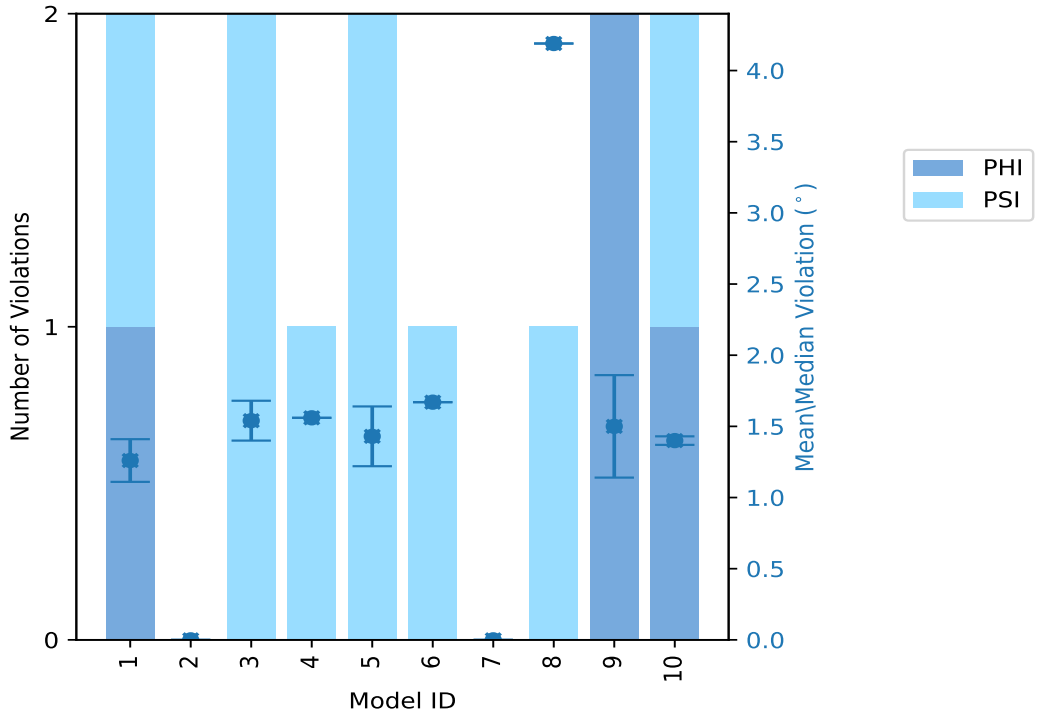
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	1	1	2	1.26	1.41	0.15	1.26
2	0	0	0	0.0	0.0	0.0	0.0
3	0	2	2	1.54	1.67	0.14	1.54
4	0	1	1	1.56	1.56	0.0	1.56
5	0	2	2	1.43	1.64	0.21	1.43
6	0	1	1	1.67	1.67	0.0	1.67
7	0	0	0	0.0	0.0	0.0	0.0
8	0	1	1	4.19	4.19	0.0	4.19
9	2	0	2	1.5	1.86	0.36	1.5
10	1	1	2	1.4	1.43	0.03	1.4

10.2.1 Bar graph : Dihedral violation statistics for each model



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

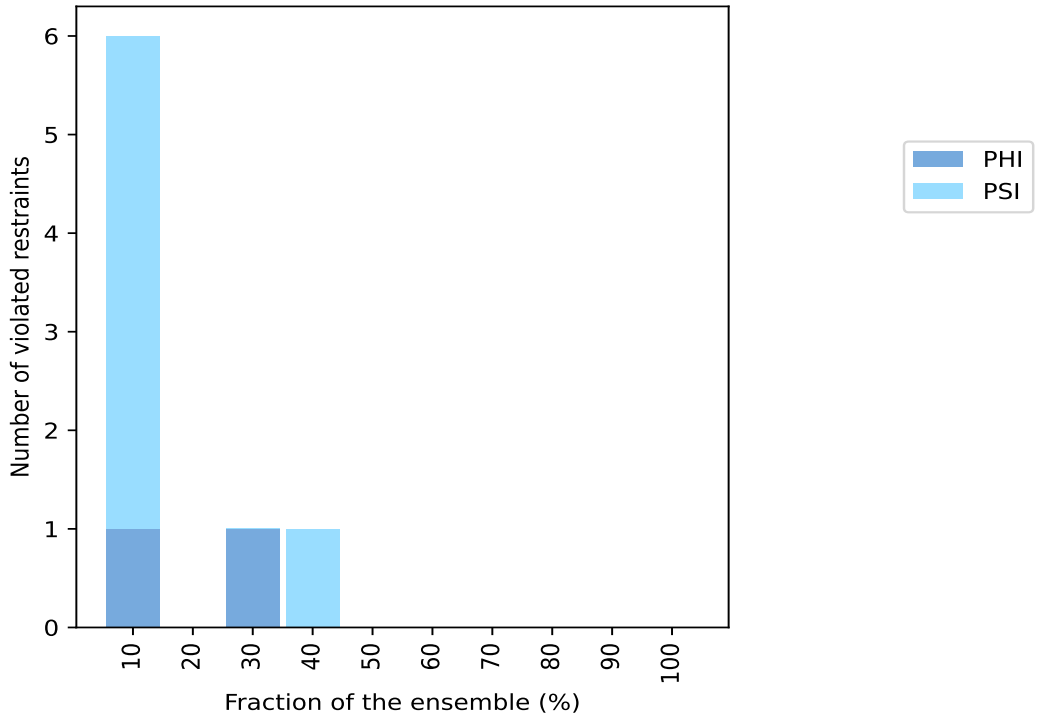
10.3 Dihedral-angle violation statistics for the ensemble

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]	%
1	5	6	1	10.0
0	0	0	2	20.0
1	0	1	3	30.0
0	1	1	4	40.0
0	0	0	5	50.0
0	0	0	6	60.0
0	0	0	7	70.0
0	0	0	8	80.0
0	0	0	9	90.0
0	0	0	10	100.0

[1] Number of models with violations

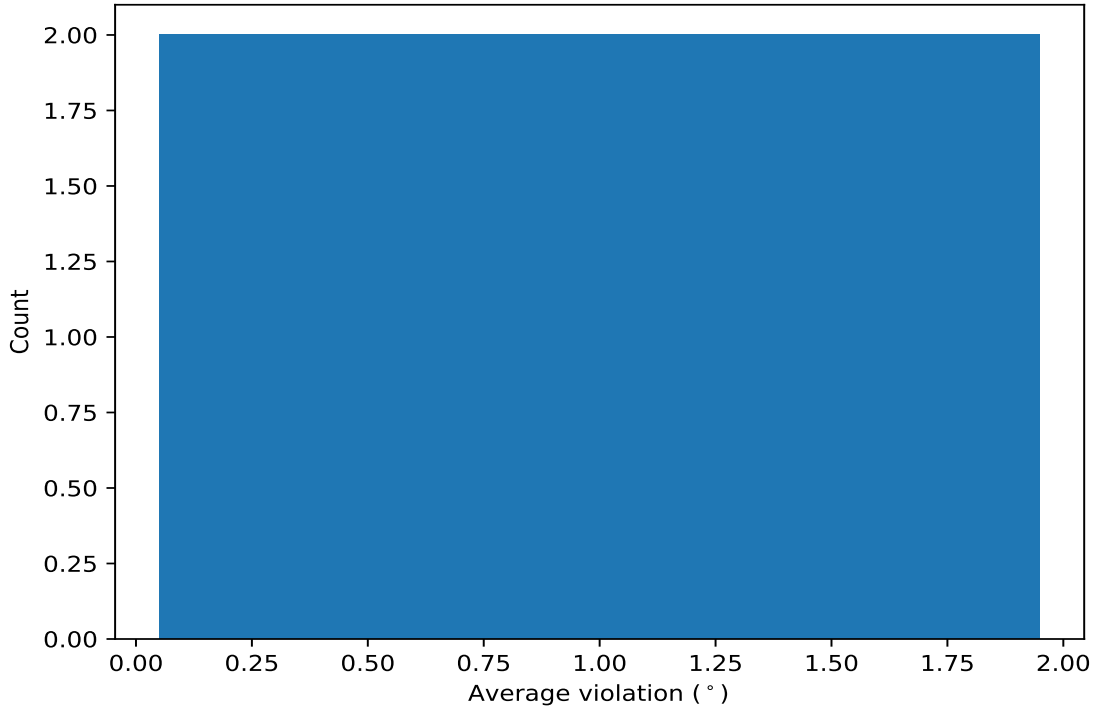
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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



10.4.2 Table: Most violated dihedral-angle restraints

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.

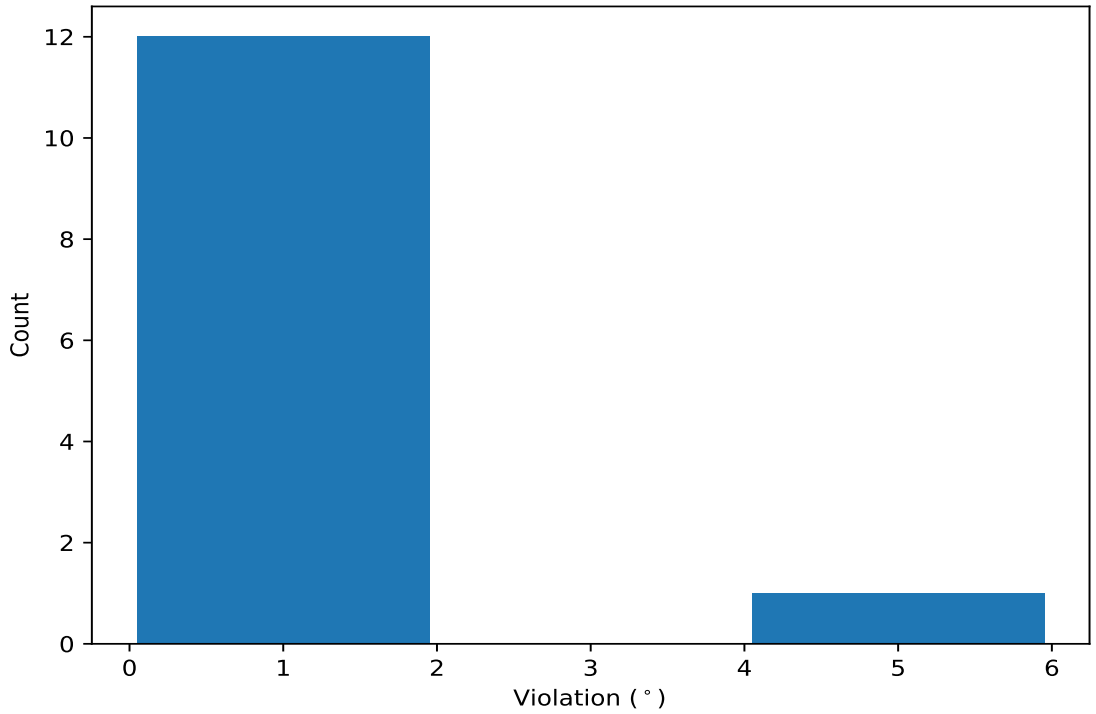
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,230)	1:196:A:ALA:N	1:196:A:ALA:CA	1:196:A:ALA:C	1:197:A:VAL:N	4	1.45	0.23	1.5
(1,75)	1:138:A:MET:C	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	3	1.57	0.21	1.43

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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 (°)
(1,158)	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	1:89:A:HIS:N	8	4.19
(1,75)	1:138:A:MET:C	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	9	1.86
(1,230)	1:196:A:ALA:N	1:196:A:ALA:CA	1:196:A:ALA:C	1:197:A:VAL:N	6	1.67
(1,212)	1:172:A:ALA:N	1:172:A:ALA:CA	1:172:A:ALA:C	1:173:A:THR:N	3	1.67
(1,230)	1:196:A:ALA:N	1:196:A:ALA:CA	1:196:A:ALA:C	1:197:A:VAL:N	5	1.64
(1,156)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:ILE:N	4	1.56
(1,75)	1:138:A:MET:C	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	10	1.43
(1,75)	1:138:A:MET:C	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1	1.41
(1,173)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:ASN:N	3	1.4
(1,230)	1:196:A:ALA:N	1:196:A:ALA:CA	1:196:A:ALA:C	1:197:A:VAL:N	10	1.37
(1,172)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLY:N	5	1.22
(1,101)	1:185:A:GLY:C	1:186:A:VAL:N	1:186:A:VAL:CA	1:186:A:VAL:C	9	1.14
(1,230)	1:196:A:ALA:N	1:196:A:ALA:CA	1:196:A:ALA:C	1:197:A:VAL:N	1	1.11