



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 9, 2025 – 08:08 PM EDT

PDB ID : 9MEM / pdb\_00009mem  
BMRB ID : 25290  
Title : Anabaena Sensory Rhodopsin Structure Determination from Paramagnetic Relaxation Enhancement and NMR Restraints  
Authors : Vaz, R.F.; Brown, L.; Ladizhansky, V.  
Deposited on : 2024-12-06

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
buster-report : 1.1.7 (2018)  
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) : 2.42

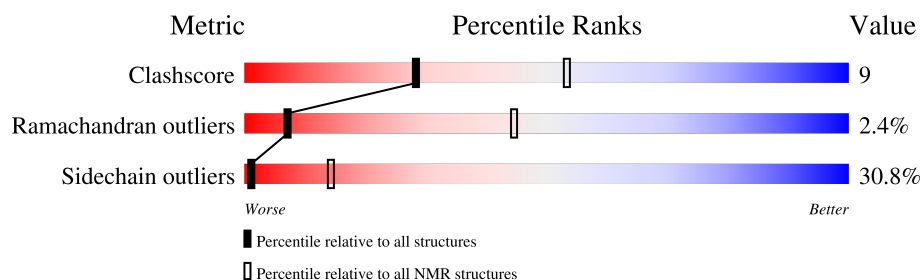
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLID-STATE NMR*


The overall completeness of chemical shifts assignment is 35%.

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	235	

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:6-A:91, A:103-A:222 (206)	1.42	1

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

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

The models can be grouped into 2 clusters and 3 single-model clusters were found.

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

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3788 atoms, of which 1900 are hydrogens and 0 are deuteriums.

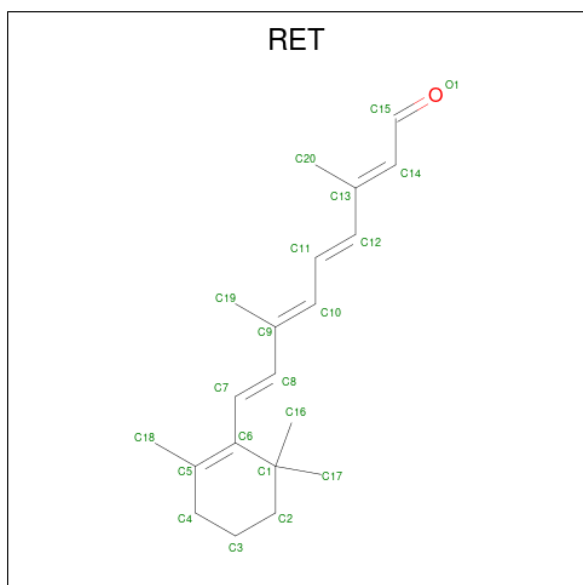
- Molecule 1 is a protein called Bacteriorhodopsin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	229	3740	1248	1872	298	311	11	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	HIS	-	expression tag	UNP Q8YSC4
A	231	HIS	-	expression tag	UNP Q8YSC4
A	232	HIS	-	expression tag	UNP Q8YSC4
A	233	HIS	-	expression tag	UNP Q8YSC4
A	234	HIS	-	expression tag	UNP Q8YSC4
A	235	HIS	-	expression tag	UNP Q8YSC4

- Molecule 2 is RETINAL (CCD ID: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



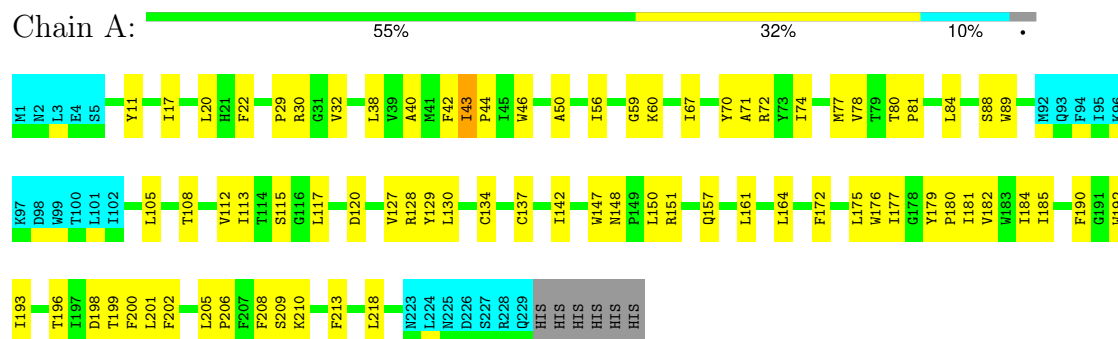
Mol	Chain	Residues	Atoms		
			Total	C	H
2	A	1	48	20	28

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Bacteriorhodopsin

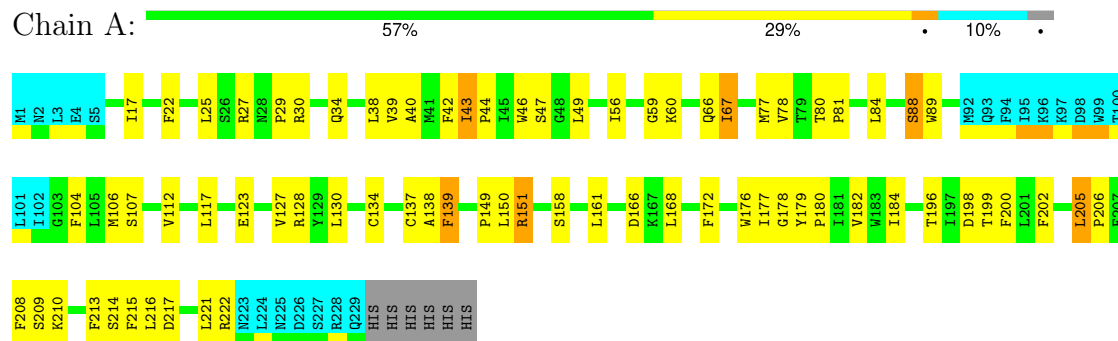


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

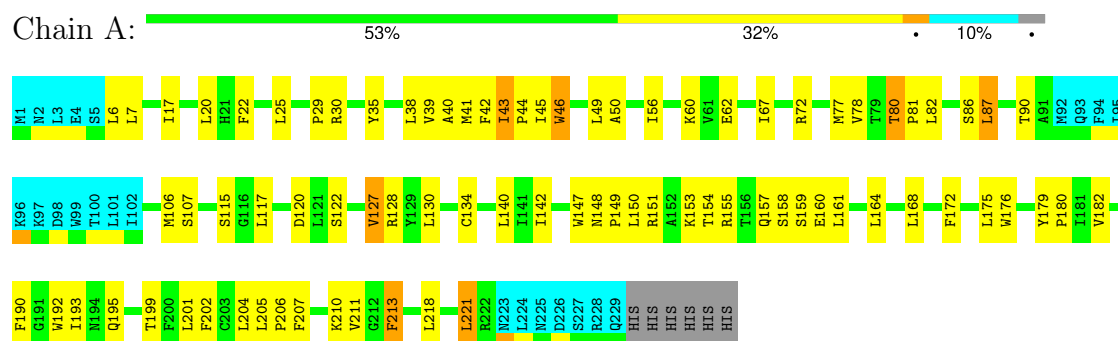
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Bacteriorhodopsin



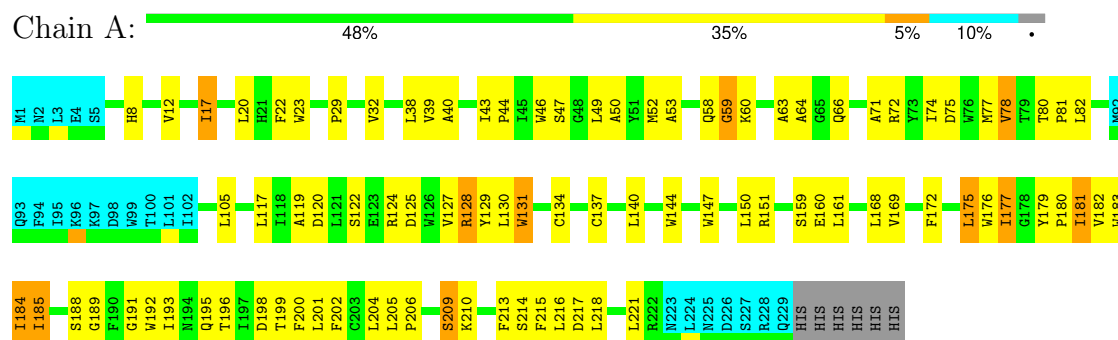
## 4.2.2 Score per residue for model 2

### • Molecule 1: Bacteriorhodopsin



## 4.2.3 Score per residue for model 3

### • Molecule 1: Bacteriorhodopsin



## 4.2.4 Score per residue for model 4

### • Molecule 1: Bacteriorhodopsin



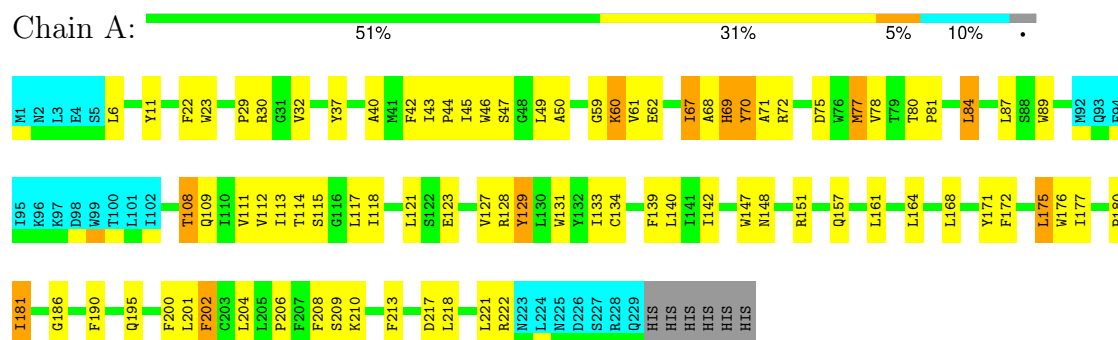
### 4.2.5 Score per residue for model 5

#### • Molecule 1: Bacteriorhodopsin



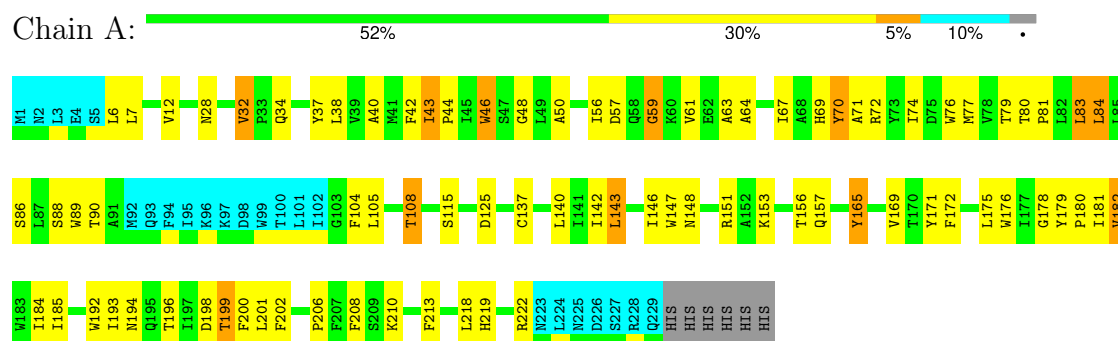
### 4.2.6 Score per residue for model 6

#### • Molecule 1: Bacteriorhodopsin



### 4.2.7 Score per residue for model 7

#### • Molecule 1: Bacteriorhodopsin



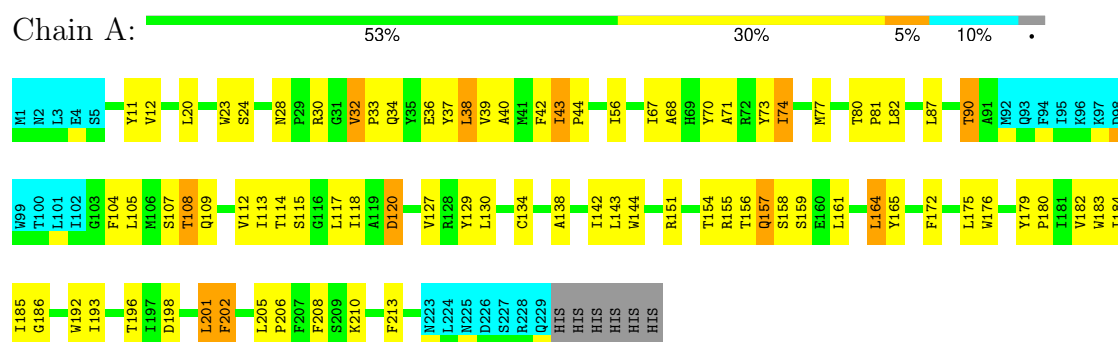
## 4.2.8 Score per residue for model 8

### • Molecule 1: Bacteriorhodopsin



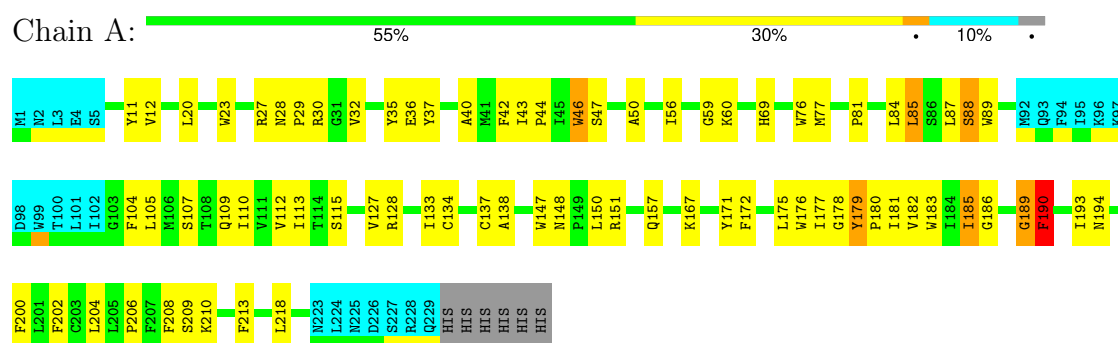
## 4.2.9 Score per residue for model 9

### • Molecule 1: Bacteriorhodopsin



## 4.2.10 Score per residue for model 10

### • Molecule 1: Bacteriorhodopsin





## 5 Refinement protocol and experimental data overview

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

Of the 100 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
X-PLOR NIH	structure calculation	
X-PLOR 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	2
Total number of shifts	1185
Number of shifts mapped to atoms	1185
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	35%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

## 6 Model quality

### 6.1 Standard geometry

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1672	1674	1674	29±5
2	A	20	28	27	2±0
All	All	16920	17020	17017	315

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:ALA:O	1:A:44:PRO:CD	0.89	2.20	5	10
1:A:176:TRP:O	1:A:180:PRO:CD	0.88	2.21	5	10
1:A:202:PHE:O	1:A:206:PRO:CD	0.88	2.22	2	10
1:A:77:MET:O	1:A:81:PRO:CD	0.84	2.26	7	10
1:A:77:MET:O	1:A:81:PRO:HD2	0.81	1.75	7	10
1:A:40:ALA:O	1:A:44:PRO:HD2	0.80	1.77	6	10
1:A:202:PHE:O	1:A:206:PRO:HD2	0.79	1.78	9	10
1:A:176:TRP:O	1:A:180:PRO:HD2	0.76	1.80	7	10
1:A:122:SER:HB2	1:A:127:VAL:HG11	0.76	1.55	3	1
1:A:193:ILE:HD12	1:A:194:ASN:O	0.70	1.86	8	2
1:A:43:ILE:HG23	1:A:44:PRO:CD	0.67	2.19	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:202:PHE:O	1:A:205:LEU:N	0.67	2.27	2	3
1:A:182:VAL:HG23	1:A:183:TRP:CD2	0.67	2.24	9	3
1:A:179:TYR:CE1	1:A:205:LEU:HD12	0.66	2.25	9	1
1:A:50:ALA:HB3	1:A:75:ASP:OD2	0.65	1.91	3	2
1:A:158:SER:OG	1:A:161:LEU:HB2	0.64	1.92	9	3
1:A:60:LYS:CB	1:A:68:ALA:HB1	0.64	2.22	6	1
1:A:112:VAL:HG22	1:A:138:ALA:CB	0.64	2.22	9	1
1:A:176:TRP:O	1:A:179:TYR:N	0.64	2.30	7	3
2:A:301:RET:H8	2:A:301:RET:H161	0.63	1.71	5	10
1:A:40:ALA:O	1:A:43:ILE:N	0.63	2.31	10	7
1:A:176:TRP:O	1:A:180:PRO:HD3	0.63	1.91	5	1
1:A:112:VAL:HG22	1:A:138:ALA:HB1	0.63	1.71	9	1
1:A:108:THR:O	1:A:112:VAL:HG23	0.62	1.94	9	4
1:A:67:ILE:O	1:A:67:ILE:HG23	0.62	1.94	6	1
1:A:185:ILE:HD12	1:A:185:ILE:O	0.62	1.94	9	1
1:A:43:ILE:HD11	1:A:82:LEU:HB2	0.61	1.70	3	2
1:A:201:LEU:O	1:A:205:LEU:HD23	0.61	1.94	9	1
1:A:178:GLY:O	1:A:182:VAL:HG13	0.61	1.95	4	5
1:A:86:SER:O	1:A:90:THR:HG23	0.61	1.95	2	1
1:A:109:GLN:O	1:A:113:ILE:HD12	0.61	1.95	6	1
1:A:8:HIS:CE1	1:A:199:THR:HG21	0.61	2.30	3	1
1:A:17:ILE:O	1:A:17:ILE:HD12	0.61	1.95	5	2
1:A:40:ALA:O	1:A:44:PRO:HD3	0.61	1.95	5	5
1:A:60:LYS:HB2	1:A:68:ALA:HB1	0.60	1.72	6	1
1:A:177:ILE:O	1:A:181:ILE:HD13	0.60	1.96	6	2
1:A:80:THR:HG23	1:A:176:TRP:HZ2	0.60	1.56	6	1
1:A:164:LEU:HD13	1:A:165:TYR:N	0.59	2.11	9	1
1:A:113:ILE:HD13	2:A:301:RET:C17	0.59	2.27	8	1
1:A:62:GLU:HB2	1:A:68:ALA:HB2	0.59	1.73	6	1
1:A:43:ILE:HG23	1:A:44:PRO:HD3	0.58	1.75	1	3
1:A:190:PHE:CB	1:A:193:ILE:HD11	0.58	2.28	10	1
1:A:202:PHE:O	1:A:206:PRO:HD3	0.58	1.99	2	2
1:A:68:ALA:HB1	1:A:120:ASP:HB2	0.57	1.75	9	1
1:A:129:TYR:O	1:A:133:ILE:HD13	0.56	1.98	6	1
1:A:80:THR:O	1:A:84:LEU:HD22	0.56	2.01	6	1
1:A:168:LEU:HD13	1:A:217:ASP:OD2	0.56	1.99	6	1
1:A:77:MET:O	1:A:80:THR:N	0.56	2.38	7	1
1:A:59:GLY:O	1:A:71:ALA:HB3	0.56	2.00	6	1
1:A:179:TYR:HE1	1:A:205:LEU:HD12	0.55	1.59	9	1
1:A:43:ILE:HD11	1:A:82:LEU:HB3	0.54	1.79	5	1
1:A:9:TRP:O	1:A:12:VAL:HG12	0.54	2.02	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:MET:SD	1:A:117:LEU:HD11	0.54	2.43	6	1
1:A:184:ILE:HG23	1:A:185:ILE:HG23	0.54	1.80	5	2
1:A:40:ALA:O	1:A:43:ILE:HG23	0.54	2.03	8	1
1:A:84:LEU:HD13	1:A:84:LEU:N	0.53	2.18	6	1
1:A:79:THR:O	1:A:83:LEU:HD23	0.53	2.04	7	1
1:A:119:ALA:HB2	1:A:131:TRP:HB3	0.53	1.80	3	1
1:A:80:THR:HG23	1:A:176:TRP:CZ2	0.52	2.38	6	1
1:A:114:THR:O	1:A:118:ILE:HD12	0.52	2.04	4	1
1:A:46:TRP:CZ3	1:A:50:ALA:HB2	0.52	2.39	7	5
1:A:11:TYR:HH	1:A:207:PHE:HD1	0.52	1.49	8	1
1:A:112:VAL:HG22	1:A:138:ALA:HB3	0.51	1.82	5	3
1:A:138:ALA:O	1:A:142:ILE:HD12	0.51	2.05	5	1
2:A:301:RET:H161	2:A:301:RET:C8	0.51	2.36	1	10
1:A:41:MET:O	1:A:45:ILE:HG23	0.51	2.04	4	1
1:A:112:VAL:CG2	1:A:138:ALA:HB3	0.50	2.37	10	2
1:A:171:TYR:O	1:A:175:LEU:HD23	0.50	2.06	6	1
1:A:79:THR:O	1:A:83:LEU:HD12	0.49	2.07	8	1
1:A:146:ILE:HD12	1:A:165:TYR:OH	0.49	2.06	8	1
1:A:119:ALA:HB1	1:A:128:ARG:HA	0.49	1.84	3	1
1:A:124:ARG:O	1:A:127:VAL:HG12	0.49	2.07	3	1
1:A:59:GLY:HA3	1:A:71:ALA:HB2	0.49	1.83	8	2
1:A:85:LEU:HD12	1:A:89:TRP:CZ2	0.49	2.43	10	1
1:A:78:VAL:HA	1:A:82:LEU:HD23	0.49	1.82	3	1
1:A:108:THR:HB	1:A:142:ILE:HD12	0.49	1.83	7	1
1:A:43:ILE:HD11	1:A:82:LEU:CB	0.48	2.38	4	2
1:A:61:VAL:O	1:A:61:VAL:HG13	0.48	2.08	6	1
1:A:32:VAL:O	1:A:32:VAL:HG23	0.48	2.09	3	1
1:A:82:LEU:HD22	1:A:82:LEU:N	0.48	2.24	3	4
1:A:122:SER:CB	1:A:127:VAL:HG11	0.48	2.36	3	1
1:A:56:ILE:HG22	1:A:56:ILE:O	0.48	2.09	1	2
1:A:179:TYR:CD1	1:A:205:LEU:HD23	0.47	2.43	2	1
1:A:187:PRO:O	1:A:193:ILE:HD11	0.47	2.10	5	1
1:A:67:ILE:O	1:A:67:ILE:CG2	0.47	2.62	6	1
1:A:171:TYR:CZ	1:A:175:LEU:HD11	0.47	2.44	7	1
1:A:80:THR:HG22	1:A:176:TRP:CZ2	0.47	2.45	2	1
1:A:204:LEU:HD23	1:A:205:LEU:CD1	0.47	2.39	3	1
1:A:185:ILE:HD12	1:A:189:GLY:C	0.47	2.30	10	1
1:A:46:TRP:HH2	1:A:74:ILE:HD12	0.46	1.69	8	1
1:A:202:PHE:CG	1:A:206:PRO:HG2	0.46	2.46	7	1
1:A:59:GLY:CA	1:A:71:ALA:HB2	0.46	2.41	3	2
1:A:61:VAL:O	1:A:67:ILE:O	0.46	2.34	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:169:VAL:O	1:A:173:THR:HG23	0.46	2.09	5	1
1:A:53:ALA:HB1	1:A:58:GLN:O	0.45	2.11	3	1
1:A:34:GLN:O	1:A:38:LEU:HD12	0.45	2.11	9	1
1:A:142:ILE:HG23	1:A:143:LEU:N	0.45	2.27	9	2
1:A:116:GLY:CA	2:A:301:RET:H172	0.45	2.41	4	1
1:A:77:MET:O	1:A:81:PRO:CG	0.45	2.65	3	3
1:A:80:THR:HG21	1:A:113:ILE:CD1	0.45	2.42	4	1
1:A:76:TRP:O	1:A:80:THR:HG23	0.45	2.11	7	1
1:A:122:SER:HB2	1:A:127:VAL:CG1	0.45	2.42	2	2
1:A:85:LEU:HD12	1:A:89:TRP:CH2	0.44	2.47	10	1
1:A:190:PHE:CG	1:A:193:ILE:HD11	0.44	2.47	10	1
1:A:80:THR:HB	1:A:81:PRO:CD	0.44	2.43	5	3
1:A:71:ALA:HA	1:A:74:ILE:HD11	0.44	1.90	3	2
1:A:58:GLN:HG2	1:A:58:GLN:O	0.44	2.13	8	1
1:A:179:TYR:HB2	1:A:180:PRO:CD	0.44	2.43	9	4
1:A:182:VAL:HG23	1:A:183:TRP:CE3	0.44	2.46	9	3
1:A:7:LEU:HD12	1:A:203:CYS:HB3	0.44	1.90	4	1
1:A:181:ILE:O	1:A:184:ILE:HG22	0.44	2.12	5	2
1:A:146:ILE:HG22	1:A:146:ILE:O	0.44	2.13	8	1
1:A:139:PHE:CD1	1:A:142:ILE:HD11	0.43	2.48	4	1
1:A:154:THR:HG22	1:A:162:ALA:HB2	0.43	1.90	4	1
1:A:113:ILE:HD12	1:A:113:ILE:H	0.43	1.74	6	1
1:A:72:ARG:CZ	1:A:199:THR:HG23	0.43	2.42	4	1
1:A:67:ILE:HD13	1:A:67:ILE:N	0.43	2.29	9	2
1:A:12:VAL:HG23	1:A:48:GLY:O	0.43	2.13	7	1
1:A:43:ILE:HG23	1:A:44:PRO:HD2	0.43	1.89	1	1
1:A:61:VAL:HG12	1:A:70:TYR:HB3	0.43	1.90	6	1
1:A:179:TYR:O	1:A:182:VAL:HG22	0.43	2.13	2	1
1:A:164:LEU:HD12	1:A:164:LEU:O	0.43	2.13	4	1
1:A:221:LEU:O	1:A:221:LEU:HD13	0.42	2.14	2	1
1:A:87:LEU:HD21	1:A:213:PHE:CE1	0.42	2.49	2	1
1:A:158:SER:HB2	1:A:161:LEU:HB2	0.42	1.91	2	1
1:A:121:LEU:HD23	1:A:121:LEU:N	0.42	2.30	4	1
1:A:175:LEU:HD23	1:A:209:SER:OG	0.42	2.15	3	1
1:A:72:ARG:O	1:A:76:TRP:CD1	0.42	2.73	7	1
1:A:77:MET:HG3	1:A:113:ILE:HG21	0.42	1.91	5	1
1:A:202:PHE:O	1:A:206:PRO:CG	0.42	2.67	10	2
1:A:72:ARG:NH2	1:A:199:THR:HG23	0.42	2.30	7	1
1:A:73:TYR:CE2	2:A:301:RET:H172	0.42	2.49	9	1
1:A:52:MET:O	1:A:56:ILE:HD12	0.41	2.13	8	1
1:A:63:ALA:O	1:A:64:ALA:HB3	0.41	2.14	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:193:ILE:HG22	1:A:194:ASN:N	0.41	2.30	10	1
1:A:207:PHE:O	1:A:211:VAL:HG22	0.41	2.15	2	1
1:A:70:TYR:CE1	1:A:74:ILE:HD13	0.41	2.50	7	1
1:A:32:VAL:HG22	1:A:32:VAL:O	0.41	2.14	7	1
2:A:301:RET:H11	2:A:301:RET:H191	0.41	1.77	7	1
1:A:80:THR:HG23	1:A:176:TRP:CZ3	0.41	2.51	9	1
1:A:82:LEU:N	1:A:82:LEU:CD2	0.41	2.84	4	1
1:A:216:LEU:C	1:A:216:LEU:HD13	0.41	2.35	8	2
1:A:80:THR:OG1	1:A:81:PRO:HD3	0.41	2.16	7	1
1:A:84:LEU:HD23	1:A:84:LEU:N	0.41	2.31	7	1
1:A:32:VAL:HG12	1:A:36:GLU:CG	0.41	2.46	9	1
1:A:84:LEU:HD21	1:A:109:GLN:NE2	0.41	2.31	4	1
1:A:40:ALA:O	1:A:43:ILE:HB	0.40	2.16	5	2
1:A:32:VAL:HG11	1:A:89:TRP:HE3	0.40	1.76	6	1
1:A:60:LYS:HB3	1:A:68:ALA:HB1	0.40	1.92	6	1
1:A:32:VAL:HG11	1:A:90:THR:HA	0.40	1.92	9	1
1:A:139:PHE:CD1	2:A:301:RET:H182	0.40	2.51	1	1
1:A:216:LEU:HD13	1:A:216:LEU:C	0.40	2.37	3	1
1:A:154:THR:HG23	1:A:155:ARG:N	0.40	2.31	2	1
1:A:173:THR:HG22	1:A:174:VAL:N	0.40	2.31	8	1
1:A:183:TRP:O	1:A:189:GLY:CA	0.40	2.69	3	1
1:A:165:TYR:O	1:A:169:VAL:HG23	0.40	2.17	7	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/235 (88%)	178±3 (87±2%)	23±3 (11±1%)	5±2 (2±1%)	7	44
All	All	2060/2350 (88%)	1784 (87%)	227 (11%)	49 (2%)	7	44

All 19 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	29	PRO	6
1	A	151	ARG	6
1	A	192	TRP	6
1	A	190	PHE	5
1	A	59	GLY	4
1	A	191	GLY	3
1	A	186	GLY	3
1	A	149	PRO	2
1	A	184	ILE	2
1	A	30	ARG	2
1	A	222	ARG	2
1	A	62	GLU	1
1	A	157	GLN	1
1	A	185	ILE	1
1	A	150	LEU	1
1	A	57	ASP	1
1	A	69	HIS	1
1	A	33	PRO	1
1	A	189	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	175/204 (86%)	121±2 (69±1%)	54±2 (31±1%)	1	14
All	All	1750/2040 (86%)	1211 (69%)	539 (31%)	1	14

All 140 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	210	LYS	10
1	A	213	PHE	10
1	A	172	PHE	9
1	A	127	VAL	8
1	A	218	LEU	8
1	A	22	PHE	7
1	A	38	LEU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	42	PHE	7
1	A	46	TRP	7
1	A	67	ILE	7
1	A	128	ARG	7
1	A	134	CYS	7
1	A	20	LEU	7
1	A	115	SER	7
1	A	175	LEU	7
1	A	201	LEU	7
1	A	60	LYS	6
1	A	78	VAL	6
1	A	117	LEU	6
1	A	130	LEU	6
1	A	137	CYS	6
1	A	196	THR	6
1	A	198	ASP	6
1	A	200	PHE	6
1	A	208	PHE	6
1	A	72	ARG	6
1	A	120	ASP	6
1	A	147	TRP	6
1	A	148	ASN	6
1	A	105	LEU	6
1	A	32	VAL	6
1	A	30	ARG	5
1	A	43	ILE	5
1	A	66	GLN	5
1	A	84	LEU	5
1	A	88	SER	5
1	A	104	PHE	5
1	A	150	LEU	5
1	A	151	ARG	5
1	A	177	ILE	5
1	A	209	SER	5
1	A	140	LEU	5
1	A	159	SER	5
1	A	23	TRP	5
1	A	129	TYR	5
1	A	179	TYR	5
1	A	181	ILE	5
1	A	11	TYR	5
1	A	108	THR	5

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Mol	Chain	Res	Type	Models (Total)
1	A	37	TYR	5
1	A	17	ILE	4
1	A	39	VAL	4
1	A	47	SER	4
1	A	49	LEU	4
1	A	89	TRP	4
1	A	107	SER	4
1	A	199	THR	4
1	A	217	ASP	4
1	A	221	LEU	4
1	A	6	LEU	4
1	A	7	LEU	4
1	A	35	TYR	4
1	A	41	MET	4
1	A	56	ILE	4
1	A	87	LEU	4
1	A	160	GLU	4
1	A	164	LEU	4
1	A	193	ILE	4
1	A	195	GLN	4
1	A	204	LEU	4
1	A	144	TRP	4
1	A	184	ILE	4
1	A	118	ILE	4
1	A	190	PHE	4
1	A	70	TYR	4
1	A	157	GLN	4
1	A	27	ARG	3
1	A	106	MET	3
1	A	123	GLU	3
1	A	168	LEU	3
1	A	222	ARG	3
1	A	12	VAL	3
1	A	74	ILE	3
1	A	86	SER	3
1	A	90	THR	3
1	A	69	HIS	3
1	A	28	ASN	3
1	A	156	THR	3
1	A	109	GLN	3
1	A	25	LEU	2
1	A	34	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	139	PHE	2
1	A	166	ASP	2
1	A	205	LEU	2
1	A	214	SER	2
1	A	215	PHE	2
1	A	216	LEU	2
1	A	45	ILE	2
1	A	80	THR	2
1	A	142	ILE	2
1	A	153	LYS	2
1	A	52	MET	2
1	A	125	ASP	2
1	A	131	TRP	2
1	A	161	LEU	2
1	A	169	VAL	2
1	A	182	VAL	2
1	A	185	ILE	2
1	A	188	SER	2
1	A	15	MET	2
1	A	57	ASP	2
1	A	62	GLU	2
1	A	83	LEU	2
1	A	85	LEU	2
1	A	143	LEU	2
1	A	146	ILE	2
1	A	165	TYR	2
1	A	76	TRP	2
1	A	126	TRP	2
1	A	154	THR	2
1	A	155	ARG	2
1	A	171	TYR	2
1	A	114	THR	2
1	A	202	PHE	2
1	A	24	SER	2
1	A	36	GLU	2
1	A	113	ILE	2
1	A	16	THR	1
1	A	54	MET	1
1	A	207	PHE	1
1	A	77	MET	1
1	A	111	VAL	1
1	A	121	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	61	VAL	1
1	A	219	HIS	1
1	A	174	VAL	1
1	A	192	TRP	1
1	A	110	ILE	1
1	A	133	ILE	1
1	A	167	LYS	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 ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Counts	Bond lengths	
						RMSZ	#Z>2
2	RET	A	301	1	20,20,21	2.78±0.02	4±0 (20±0%)

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

considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	RET	A	301	1	27,27,28	1.66±0.00	6±0 (22±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RET	A	301	1	-	0±0,13,30,31	0±0,1,1,1

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
2	A	301	RET	C14-C13	10.71	1.41	1.33	8	10
2	A	301	RET	C1-C6	3.78	1.58	1.53	10	10
2	A	301	RET	C15-C14	3.17	1.37	1.49	6	10
2	A	301	RET	C12-C13	2.29	1.41	1.46	5	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
2	A	301	RET	C18-C5-C6	4.24	119.86	124.48	2	10
2	A	301	RET	C11-C10-C9	3.46	122.43	127.28	1	10
2	A	301	RET	C7-C8-C9	2.72	122.21	126.23	7	10
2	A	301	RET	C19-C9-C10	2.36	119.00	122.82	3	10
2	A	301	RET	C18-C5-C4	2.26	118.41	113.60	5	10
2	A	301	RET	C2-C1-C6	2.20	113.64	110.44	9	10

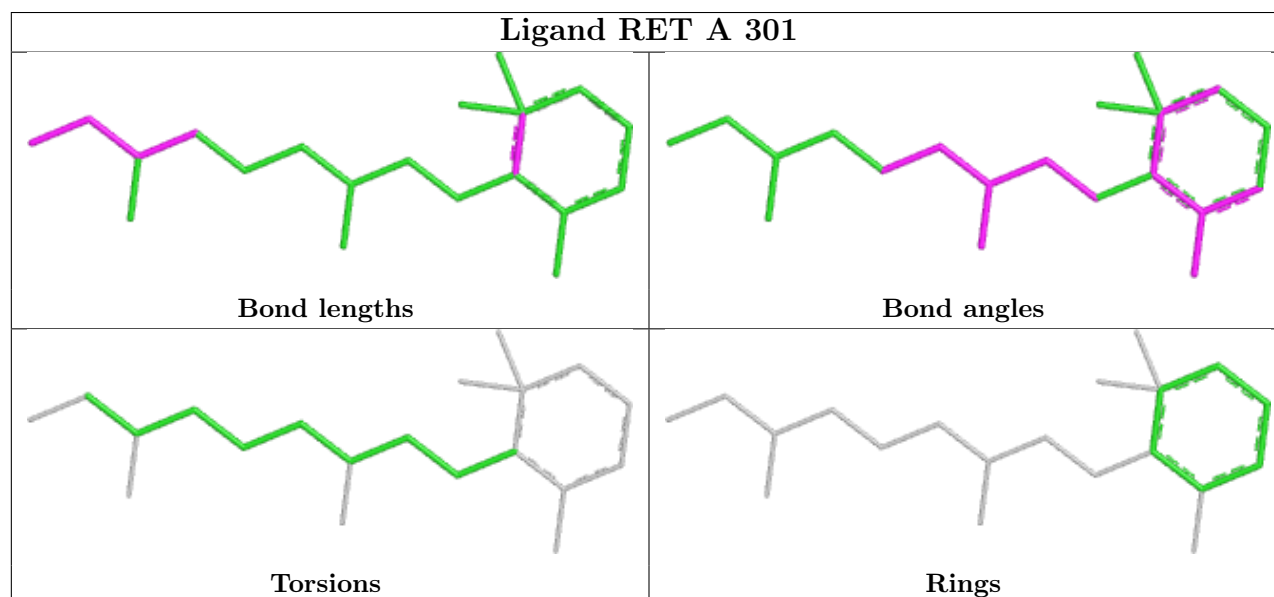
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 35% for the well-defined parts and 33% 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	1142
Number of shifts mapped to atoms	1142
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	205	$-1.33 \pm 0.20$	Should be checked
$^{13}\text{C}_\beta$	176	$0.53 \pm 0.10$	Should be checked
$^{13}\text{C}'$	203	$-0.40 \pm 0.24$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	205	$1.40 \pm 0.35$	Should be applied

#### 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 35%, i.e. 1041 atoms were assigned a chemical shift out of a possible 2948. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	581/1030 (56%)	0/420 (0%)	392/412 (95%)	189/198 (95%)
Sidechain	392/1523 (26%)	0/1018 (0%)	386/467 (83%)	6/38 (16%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	68/395 (17%)	0/192 (0%)	64/183 (35%)	4/20 (20%)
Overall	1041/2948 (35%)	0/1630 (0%)	842/1062 (79%)	199/256 (78%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 33%, i.e. 1085 atoms were assigned a chemical shift out of a possible 3288. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	605/1145 (53%)	0/466 (0%)	408/458 (89%)	197/221 (89%)
Sidechain	412/1726 (24%)	0/1148 (0%)	406/530 (77%)	6/48 (12%)
Aromatic	68/417 (16%)	0/203 (0%)	64/193 (33%)	4/21 (19%)
Overall	1085/3288 (33%)	0/1817 (0%)	878/1181 (74%)	207/290 (71%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

#### 7.1.4 Statistically unusual chemical shifts ⓘ

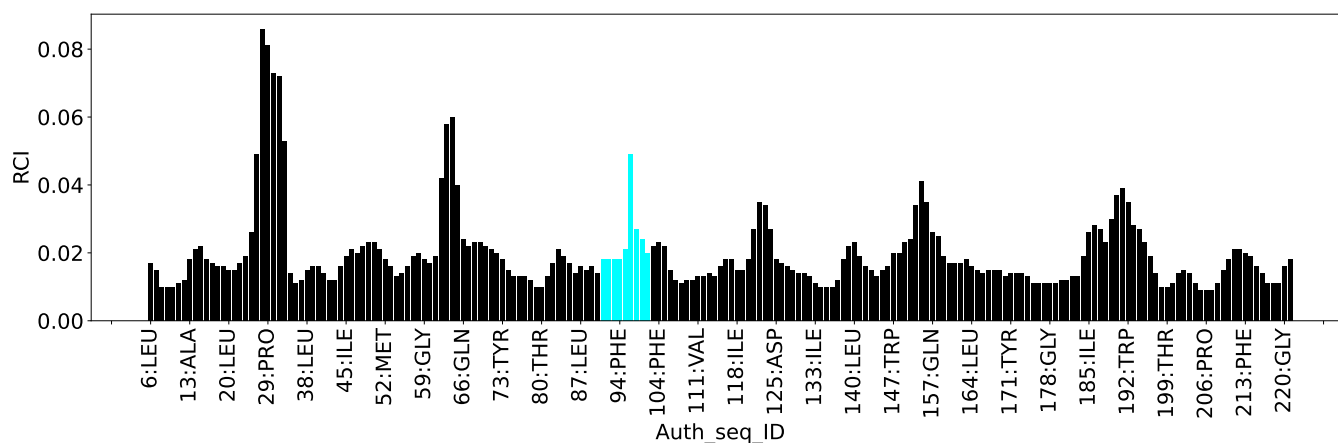
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	210	LYS	NZ	177.20	19.79 – 46.09	54.9
1	A	210	LYS	CE	55.67	37.57 – 46.21	15.9
1	A	109	GLN	NE2	98.30	103.38 – 120.35	-8.0
1	A	128	ARG	CD	37.40	38.57 – 47.75	-6.3

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

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:



## 7.2 Chemical shift list 2

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1\_dup*

### 7.2.1 Bookkeeping [i](#)

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

Total number of shifts	43
Number of shifts mapped to atoms	43
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

### 7.2.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

### 7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 1%, i.e. 28 atoms were assigned a chemical shift out of a possible 2948. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	18/1030 (2%)	0/420 (0%)	12/412 (3%)	6/198 (3%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Sidechain	6/1523 (0%)	0/1018 (0%)	6/467 (1%)	0/38 (0%)
Aromatic	4/395 (1%)	0/192 (0%)	4/183 (2%)	0/20 (0%)
Overall	28/2948 (1%)	0/1630 (0%)	22/1062 (2%)	6/256 (2%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 1%, i.e. 41 atoms were assigned a chemical shift out of a possible 3288. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	24/1145 (2%)	0/466 (0%)	16/458 (3%)	8/221 (4%)
Sidechain	13/1726 (1%)	0/1148 (0%)	13/530 (2%)	0/48 (0%)
Aromatic	4/417 (1%)	0/203 (0%)	4/193 (2%)	0/21 (0%)
Overall	41/3288 (1%)	0/1817 (0%)	33/1181 (3%)	8/290 (3%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

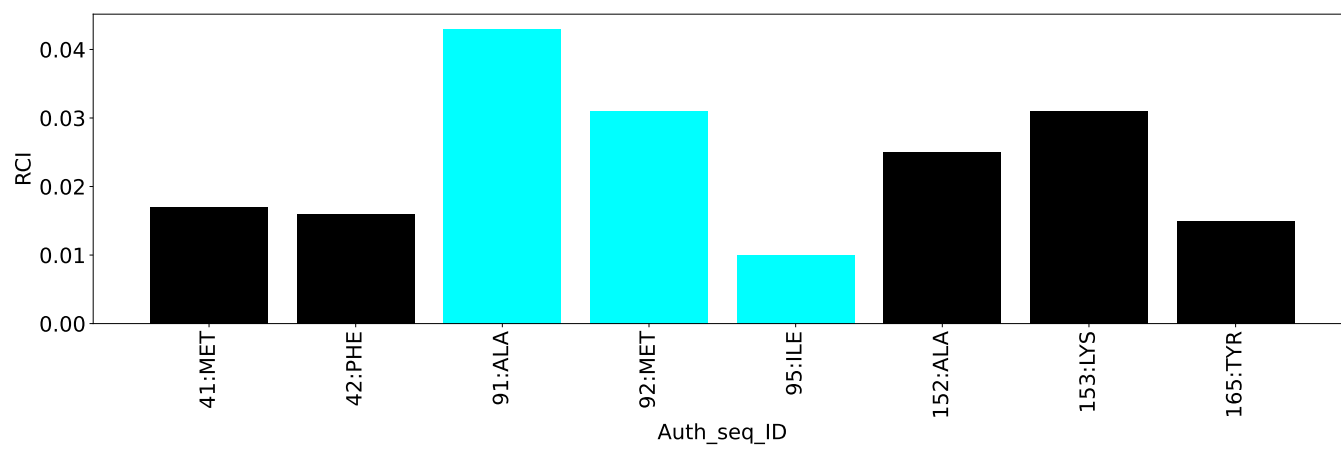
#### 7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	4093
Intra-residue ( $ i-j =0$ )	1702
Sequential ( $ i-j =1$ )	737
Medium range ( $ i-j >1$ and $ i-j <5$ )	725
Long range ( $ i-j \geq 5$ )	785
Inter-chain	0
Hydrogen bond restraints	144
Disulfide bond restraints	0
Total dihedral-angle restraints	372
Number of unmapped restraints	0
Number of restraints per residue	18.9
Number of long range restraints per residue <sup>1</sup>	3.3

<sup>1</sup>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)	24.0	0.19
0.2-0.5 (Medium)	34.6	0.5
>0.5 (Large)	144.0	31.32

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.1	1.08
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

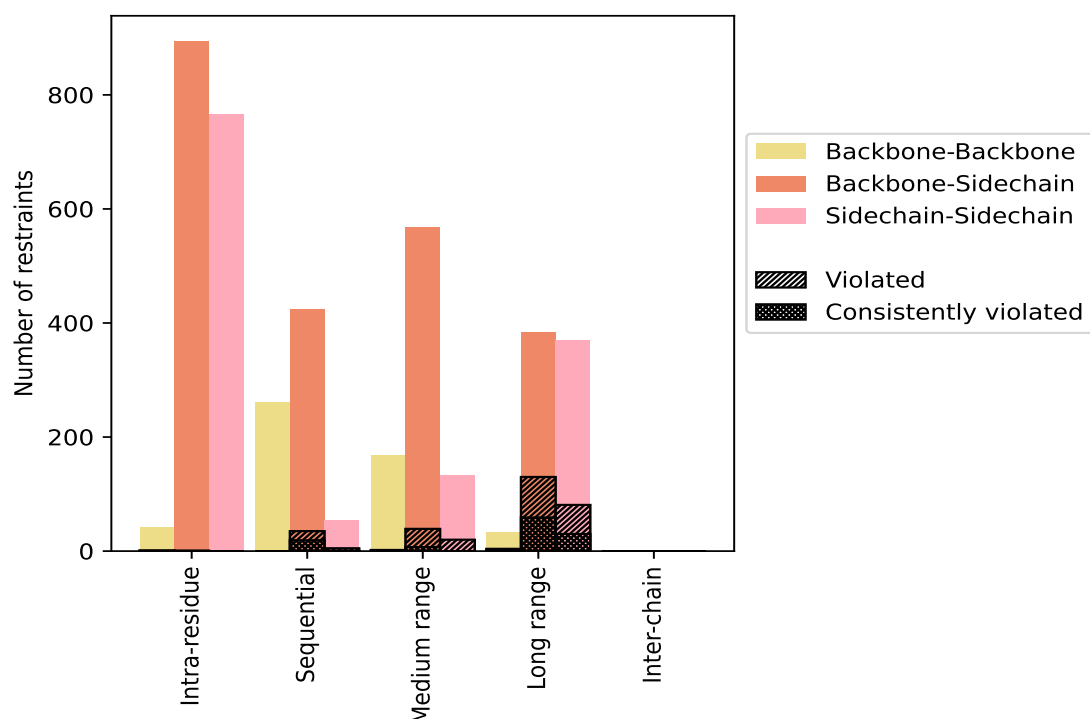
### 9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<a href="#">Intra-residue ( i-j =0)</a>	<a href="#">1702</a>	<a href="#">41.6</a>	<a href="#">2</a>	<a href="#">0.1</a>	<a href="#">0.0</a>	<a href="#">1</a>	<a href="#">0.1</a>	<a href="#">0.0</a>
Backbone-Backbone	42	1.0	1	2.4	0.0	1	2.4	0.0
Backbone-Sidechain	894	21.8	1	0.1	0.0	0	0.0	0.0
Sidechain-Sidechain	766	18.7	0	0.0	0.0	0	0.0	0.0
<a href="#">Sequential ( i-j =1)</a>	<a href="#">737</a>	<a href="#">18.0</a>	<a href="#">40</a>	<a href="#">5.4</a>	<a href="#">1.0</a>	<a href="#">20</a>	<a href="#">2.7</a>	<a href="#">0.5</a>
Backbone-Backbone	260	6.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	423	10.3	35	8.3	0.9	19	4.5	0.5
Sidechain-Sidechain	54	1.3	5	9.3	0.1	1	1.9	0.0
<a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a>	<a href="#">725</a>	<a href="#">17.7</a>	<a href="#">54</a>	<a href="#">7.4</a>	<a href="#">1.3</a>	<a href="#">3</a>	<a href="#">0.4</a>	<a href="#">0.1</a>
Backbone-Backbone	168	4.1	2	1.2	0.0	0	0.0	0.0
Backbone-Sidechain	424	10.4	32	7.5	0.8	3	0.7	0.1
Sidechain-Sidechain	133	3.2	20	15.0	0.5	0	0.0	0.0
<a href="#">Long range ( i-j ≥5)</a>	<a href="#">785</a>	<a href="#">19.2</a>	<a href="#">215</a>	<a href="#">27.4</a>	<a href="#">5.3</a>	<a href="#">90</a>	<a href="#">11.5</a>	<a href="#">2.2</a>
Backbone-Backbone	32	0.8	4	12.5	0.1	1	3.1	0.0
Backbone-Sidechain	384	9.4	130	33.9	3.2	59	15.4	1.4
Sidechain-Sidechain	369	9.0	81	22.0	2.0	30	8.1	0.7
<a href="#">Inter-chain</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
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
<a href="#">Hydrogen bond</a>	<a href="#">144</a>	<a href="#">3.5</a>	<a href="#">7</a>	<a href="#">4.9</a>	<a href="#">0.2</a>	<a href="#">4</a>	<a href="#">2.8</a>	<a href="#">0.1</a>
<a href="#">Disulfide bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Total</a>	<a href="#">4093</a>	<a href="#">100.0</a>	<a href="#">318</a>	<a href="#">7.8</a>	<a href="#">7.8</a>	<a href="#">118</a>	<a href="#">2.9</a>	<a href="#">2.9</a>
Backbone-Backbone	502	12.3	7	1.4	0.2	2	0.4	0.0
Backbone-Sidechain	2269	55.4	205	9.0	5.0	85	3.7	2.1
Sidechain-Sidechain	1322	32.3	106	8.0	2.6	31	2.3	0.8

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

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



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

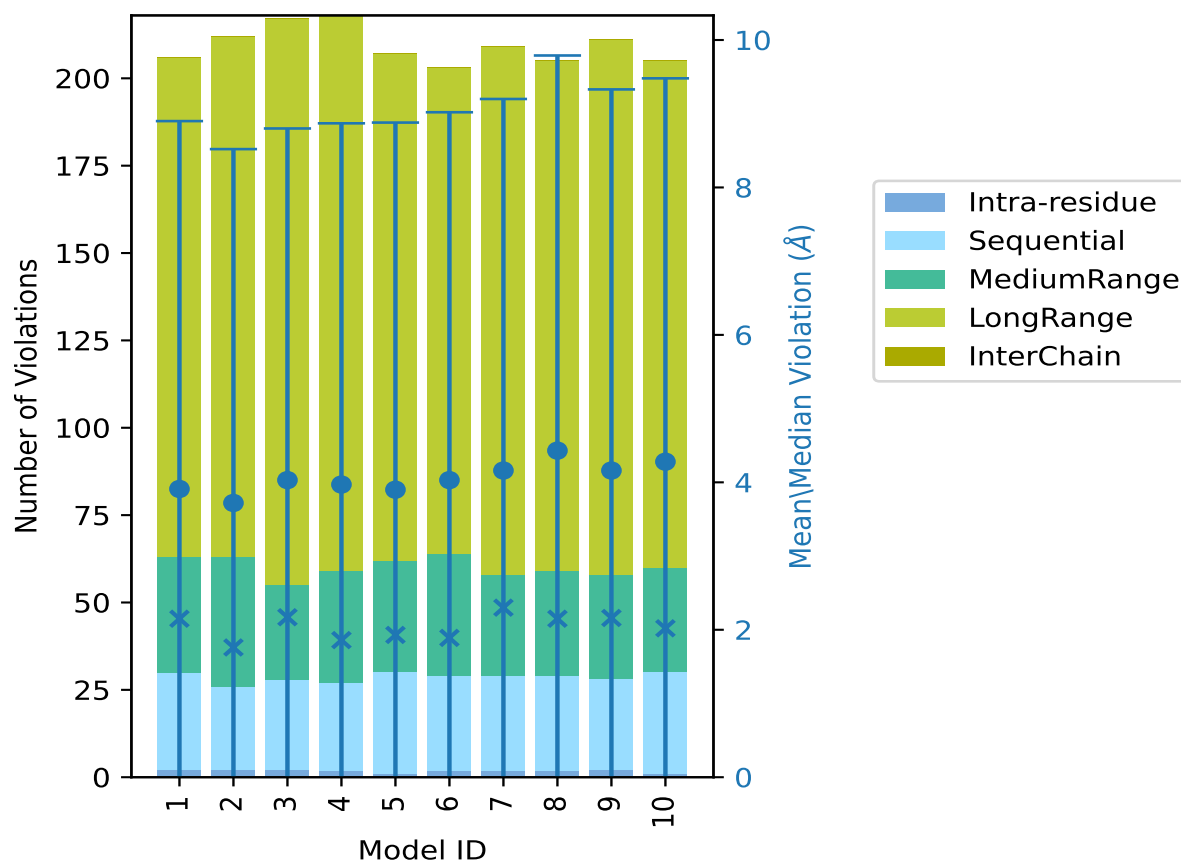
## 9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	2	28	33	143	0	206	3.91	27.26	4.99	2.15
2	2	24	37	149	0	212	3.72	27.17	4.8	1.76
3	2	26	27	162	0	217	4.03	28.64	4.77	2.17
4	2	25	32	159	0	218	3.97	27.15	4.9	1.86
5	1	29	32	145	0	207	3.9	31.32	4.98	1.93
6	2	27	35	139	0	203	4.03	26.54	4.99	1.89
7	2	27	29	151	0	209	4.16	29.26	5.04	2.3
8	2	27	30	146	0	205	4.43	27.72	5.36	2.15
9	2	26	30	153	0	211	4.16	28.9	5.17	2.16
10	1	29	30	145	0	205	4.28	29.0	5.2	2.02

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

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



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

### 9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3638(IR:1700, SQ:697, MR:671, LR:570, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	7	10	38	0	55	1	10.0
0	3	6	9	0	18	2	20.0
0	3	8	9	0	20	3	30.0

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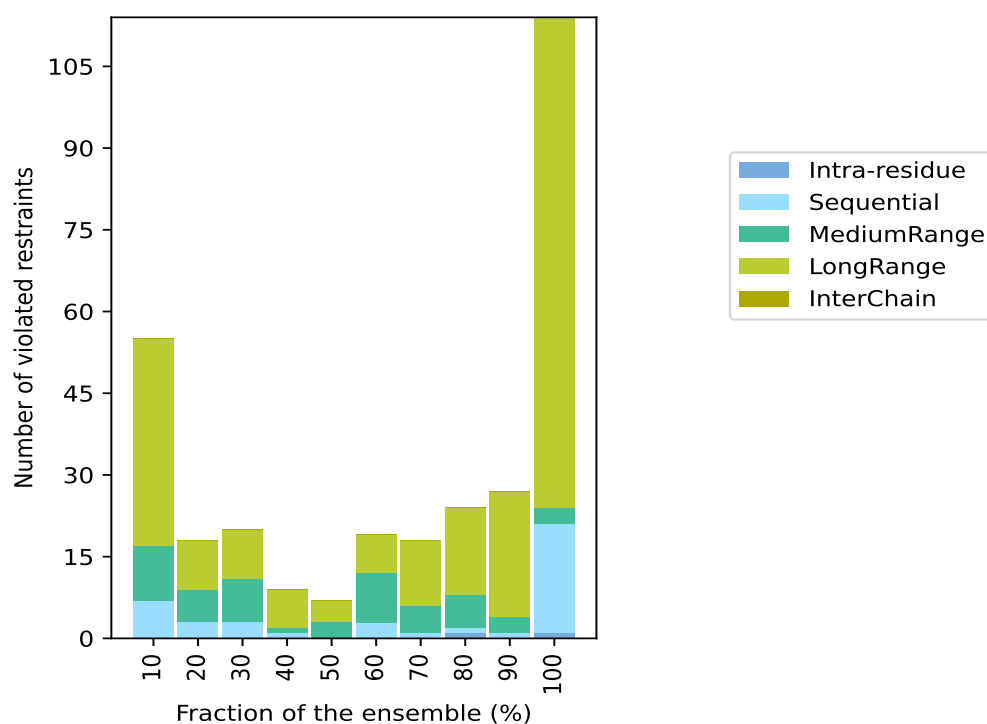
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	1	1	7	0	9	4	40.0
0	0	3	4	0	7	5	50.0
0	3	9	7	0	19	6	60.0
0	1	5	12	0	18	7	70.0
1	1	6	16	0	24	8	80.0
0	1	3	23	0	27	9	90.0
1	20	3	90	0	114	10	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

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



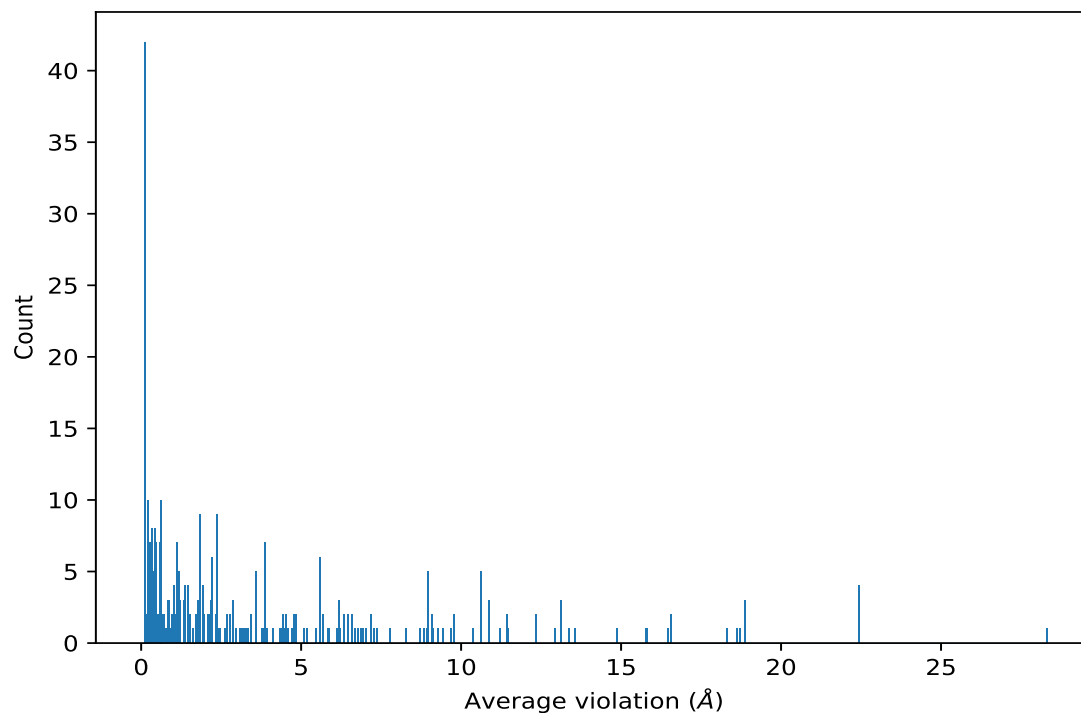
## 9.4 Most violated distance restraints in the ensemble [i](#)

### 9.4.1 Histogram : Distribution of mean distance violations [i](#)

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



in the ensemble



#### 9.4.2 Table: Most violated distance restraints [i](#)

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

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(4,93)	1:97:A:LYS:O	1:125:A:ASP:H	10	28.3	1.35	28.18
(5,79)	1:122:A:SER:OG	1:32:A:VAL:HG11	10	22.44	0.83	22.38
(5,79)	1:122:A:SER:OG	1:32:A:VAL:HG13	10	22.44	0.83	22.38
(5,79)	1:122:A:SER:OG	1:32:A:VAL:HG12	10	22.44	0.83	22.38
(5,79)	1:122:A:SER:OG	1:32:A:VAL:HG21	10	22.44	0.83	22.38
(5,58)	1:97:A:LYS:O	1:181:A:ILE:HD12	10	18.85	2.07	19.62
(5,58)	1:97:A:LYS:O	1:181:A:ILE:HD13	10	18.85	2.07	19.62
(5,58)	1:97:A:LYS:O	1:181:A:ILE:HD11	10	18.85	2.07	19.62
(4,145)	1:122:A:SER:OG	1:148:A:ASN:HA	10	18.73	0.67	18.92
(4,63)	1:92:A:MET:O	1:184:A:ILE:HA	10	18.6	2.14	18.94
(4,9)	1:5:A:SER:OG	1:126:A:TRP:HA	10	18.32	2.67	18.9
(4,8)	1:5:A:SER:OG	1:124:A:ARG:HA	10	16.58	2.42	16.82
(4,39)	1:58:A:GLN:NE2	1:130:A:LEU:HA	10	16.56	0.71	16.68
(4,40)	1:58:A:GLN:NE2	1:134:A:CYS:HA	10	16.46	0.33	16.44
(4,127)	1:122:A:SER:OG	1:15:A:MET:HA	10	15.8	0.38	15.83

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(4,38)	1:58:A:GLN:NE2	1:126:A:TRP:HA	10	15.75	1.68	15.86
(4,84)	1:97:A:LYS:O	1:19:A:ALA:H	10	14.86	1.39	14.84
(4,10)	1:5:A:SER:OG	1:172:A:PHE:HA	10	13.6	1.12	13.64
(4,128)	1:122:A:SER:OG	1:44:A:PRO:HA	10	13.36	0.53	13.2
(5,57)	1:97:A:LYS:O	1:177:A:ILE:HD11	10	13.11	1.94	13.86
(5,57)	1:97:A:LYS:O	1:177:A:ILE:HD13	10	13.11	1.94	13.86
(5,57)	1:97:A:LYS:O	1:177:A:ILE:HD12	10	13.11	1.94	13.86
(4,4)	1:5:A:SER:OG	1:64:A:ALA:HA	10	12.93	2.13	11.94
(5,3)	1:5:A:SER:OG	1:64:A:ALA:HB2	10	12.32	2.21	12.44
(5,3)	1:5:A:SER:OG	1:64:A:ALA:HB1	10	12.32	2.21	12.44
(4,37)	1:58:A:GLN:NE2	1:124:A:ARG:HA	10	11.46	1.57	11.72
(5,4)	1:5:A:SER:OG	1:119:A:ALA:HB2	10	11.42	2.32	11.36
(5,4)	1:5:A:SER:OG	1:119:A:ALA:HB1	10	11.42	2.32	11.36
(4,130)	1:122:A:SER:OG	1:52:A:MET:HA	10	11.21	0.33	11.36
(4,75)	1:97:A:LYS:O	1:28:A:ASN:H	10	10.88	1.95	10.8
(5,63)	1:122:A:SER:OG	1:55:A:ALA:HB2	10	10.86	0.62	11.1
(5,63)	1:122:A:SER:OG	1:55:A:ALA:HB1	10	10.86	0.62	11.1
(5,52)	1:97:A:LYS:O	1:25:A:LEU:HD21	10	10.61	1.68	10.99
(5,52)	1:97:A:LYS:O	1:25:A:LEU:HD22	10	10.61	1.68	10.99
(5,52)	1:97:A:LYS:O	1:25:A:LEU:HD13	10	10.61	1.68	10.99
(5,52)	1:97:A:LYS:O	1:25:A:LEU:HD11	10	10.61	1.68	10.99
(5,52)	1:97:A:LYS:O	1:25:A:LEU:HD12	10	10.61	1.68	10.99
(4,116)	1:122:A:SER:OG	1:47:A:SER:H	10	10.39	0.33	10.34
(5,49)	1:92:A:MET:O	1:177:A:ILE:HG12	10	9.78	1.89	10.28
(5,49)	1:92:A:MET:O	1:177:A:ILE:HG23	10	9.78	1.89	10.28
(4,87)	1:97:A:LYS:O	1:79:A:THR:H	10	9.68	1.01	10.01
(4,126)	1:122:A:SER:OG	1:8:A:HIS:HA	10	9.43	0.5	9.39
(4,131)	1:122:A:SER:OG	1:55:A:ALA:HA	10	9.25	0.63	9.28
(4,7)	1:5:A:SER:OG	1:120:A:ASP:HA	10	9.11	2.23	9.38
(5,62)	1:122:A:SER:OG	1:47:A:SER:HB3	10	9.07	0.62	9.03
(5,62)	1:122:A:SER:OG	1:47:A:SER:HB2	10	9.07	0.62	9.03
(4,96)	1:97:A:LYS:O	1:222:A:ARG:H	10	8.94	1.15	8.95
(4,100)	1:97:A:LYS:O	1:79:A:THR:HA	10	8.83	0.89	9.13
(4,148)	1:122:A:SER:OG	1:203:A:CYS:HA	10	8.71	0.9	8.66
(4,129)	1:122:A:SER:OG	1:47:A:SER:HA	10	8.29	0.31	8.21
(4,35)	1:58:A:GLN:NE2	1:119:A:ALA:HA	10	7.79	0.34	7.82
(4,97)	1:97:A:LYS:O	1:29:A:PRO:HA	10	7.36	1.73	7.17
(13,6)	1:210:A:LYS:C	1:80:A:THR:CG2	10	7.27	0.37	7.32
(5,25)	1:58:A:GLN:NE2	1:119:A:ALA:HB1	10	7.15	0.92	6.94
(5,25)	1:58:A:GLN:NE2	1:119:A:ALA:HB2	10	7.15	0.92	6.94
(4,86)	1:97:A:LYS:O	1:43:A:ILE:H	10	7.04	1.5	7.03
(4,99)	1:97:A:LYS:O	1:78:A:VAL:HA	10	6.94	1.16	7.07

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(6,8)	1:97:A:LYS:O	1:29:A:PRO:CA	10	6.89	1.79	6.76
(4,151)	1:122:A:SER:OG	1:78:A:VAL:HB	10	6.69	0.54	6.72
(4,11)	1:5:A:SER:OG	1:183:A:TRP:HA	10	6.59	1.91	6.86
(7,155)	1:124:A:ARG:O	1:114:A:THR:HA	10	6.56	0.7	6.67
(5,83)	1:124:A:ARG:O	1:179:A:TYR:HB3	10	6.47	1.56	6.8
(5,83)	1:124:A:ARG:O	1:179:A:TYR:HB2	10	6.47	1.56	6.8
(5,5)	1:5:A:SER:OG	1:179:A:TYR:HB3	10	6.31	1.73	6.25
(5,5)	1:5:A:SER:OG	1:179:A:TYR:HB2	10	6.31	1.73	6.25
(5,73)	1:122:A:SER:OG	1:176:A:TRP:HB3	10	6.22	0.8	6.35
(5,53)	1:97:A:LYS:O	1:43:A:ILE:HD12	10	6.16	1.6	5.74
(5,53)	1:97:A:LYS:O	1:43:A:ILE:HD13	10	6.16	1.6	5.74
(5,53)	1:97:A:LYS:O	1:43:A:ILE:HD11	10	6.16	1.6	5.74
(4,67)	1:92:A:MET:O	1:78:A:VAL:HB	10	6.14	1.0	6.08
(5,8)	1:5:A:SER:OG	1:62:A:GLU:HG3	10	5.65	2.78	5.08
(5,8)	1:5:A:SER:OG	1:62:A:GLU:HG2	10	5.65	2.78	5.08
(4,112)	1:97:A:LYS:O	1:29:A:PRO:HB3	10	5.59	1.88	5.4
(5,61)	1:97:A:LYS:O	1:43:A:ILE:HG21	10	5.57	1.18	5.63
(5,61)	1:97:A:LYS:O	1:43:A:ILE:HG12	10	5.57	1.18	5.63
(5,61)	1:97:A:LYS:O	1:43:A:ILE:HG13	10	5.57	1.18	5.63
(5,61)	1:97:A:LYS:O	1:43:A:ILE:HG23	10	5.57	1.18	5.63
(5,61)	1:97:A:LYS:O	1:43:A:ILE:HG22	10	5.57	1.18	5.63
(13,7)	1:210:A:LYS:C	1:179:A:TYR:CZ	10	5.48	1.37	4.72
(4,32)	1:58:A:GLN:NE2	1:64:A:ALA:HA	10	5.16	0.49	5.36
(4,154)	1:122:A:SER:OG	1:182:A:VAL:HB	10	5.06	1.73	5.32
(5,24)	1:58:A:GLN:NE2	1:64:A:ALA:HB2	10	4.84	0.96	5.08
(5,24)	1:58:A:GLN:NE2	1:64:A:ALA:HB1	10	4.84	0.96	5.08
(4,146)	1:122:A:SER:OG	1:182:A:VAL:HA	10	4.8	1.62	4.96
(4,70)	1:92:A:MET:O	1:100:A:THR:HB	10	4.77	1.8	5.01
(13,9)	1:210:A:LYS:C	1:80:A:THR:CB	10	4.71	0.34	4.7
(4,29)	1:58:A:GLN:NE2	1:120:A:ASP:H	10	4.58	0.46	4.5
(4,36)	1:58:A:GLN:NE2	1:120:A:ASP:HA	10	4.43	0.74	4.3
(4,54)	1:92:A:MET:O	1:44:A:PRO:HA	10	4.4	1.83	3.7
(4,92)	1:97:A:LYS:O	1:111:A:VAL:H	10	4.38	1.53	5.08
(4,105)	1:97:A:LYS:O	1:110:A:ILE:HA	10	4.35	1.38	5.05
(4,111)	1:97:A:LYS:O	1:161:A:LEU:HA	10	4.13	1.44	4.38
(4,56)	1:92:A:MET:O	1:100:A:THR:HA	10	3.92	1.42	3.92
(4,85)	1:97:A:LYS:O	1:31:A:GLY:H	10	3.9	1.68	4.4
(4,55)	1:92:A:MET:O	1:79:A:THR:HA	10	3.89	0.82	3.98
(4,74)	1:92:A:MET:O	1:79:A:THR:HA	10	3.89	0.82	3.98
(5,44)	1:92:A:MET:O	1:78:A:VAL:HG22	10	3.88	1.1	3.68
(5,44)	1:92:A:MET:O	1:78:A:VAL:HG21	10	3.88	1.1	3.68
(5,44)	1:92:A:MET:O	1:78:A:VAL:HG23	10	3.88	1.1	3.68

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(4,26)	1:58:A:GLN:NE2	1:65:A:GLY:H	10	3.82	0.66	3.74
(7,190)	1:124:A:ARG:O	1:76:A:TRP:CG	10	3.78	0.96	3.6
(6,6)	1:92:A:MET:O	1:100:A:THR:CA	10	3.59	1.53	3.98
(5,78)	1:122:A:SER:OG	1:180:A:PRO:HD3	10	3.57	1.39	3.75
(4,27)	1:58:A:GLN:NE2	1:66:A:GLN:H	10	3.56	0.46	3.62
(5,69)	1:122:A:SER:OG	1:75:A:ASP:HB3	10	3.21	0.22	3.2
(4,53)	1:92:A:MET:O	1:43:A:ILE:HA	10	3.14	1.51	2.76
(4,152)	1:122:A:SER:OG	1:111:A:VAL:HB	10	3.08	1.16	3.46
(7,13)	1:26:A:SER:OG	1:13:A:ALA:HA	10	2.95	0.68	2.79
(4,140)	1:122:A:SER:OG	1:77:A:MET:HA	10	2.46	0.4	2.57
(7,12)	1:26:A:SER:OG	1:12:A:VAL:HA	10	2.4	0.78	2.2
(7,48)	1:26:A:SER:OG	1:12:A:VAL:HA	10	2.4	0.78	2.2
(7,189)	1:124:A:ARG:O	1:76:A:TRP:HD1	10	2.37	1.48	1.54
(4,28)	1:58:A:GLN:NE2	1:78:A:VAL:H	10	2.2	0.76	2.08
(1,47)	1:32:A:VAL:HG23	1:33:A:PRO:HG3	10	1.81	0.5	1.9
(1,47)	1:32:A:VAL:HG21	1:33:A:PRO:HG2	10	1.81	0.5	1.9
(1,47)	1:32:A:VAL:HG21	1:33:A:PRO:HG3	10	1.81	0.5	1.9
(1,47)	1:32:A:VAL:HG22	1:33:A:PRO:HG2	10	1.81	0.5	1.9
(1,47)	1:32:A:VAL:HG22	1:33:A:PRO:HG3	10	1.81	0.5	1.9
(1,47)	1:32:A:VAL:HG23	1:33:A:PRO:HG2	10	1.81	0.5	1.9
(4,101)	1:97:A:LYS:O	1:91:A:ALA:HA	10	1.8	1.27	1.42
(4,153)	1:122:A:SER:OG	1:113:A:ILE:HB	10	1.48	0.62	1.63
(4,138)	1:122:A:SER:OG	1:72:A:ARG:HA	10	1.16	0.51	1.03
(5,68)	1:122:A:SER:OG	1:71:A:ALA:HB1	10	0.86	0.31	0.76
(5,68)	1:122:A:SER:OG	1:71:A:ALA:HB2	10	0.86	0.31	0.76
(3,772)	1:165:A:TYR:CE2	1:164:A:LEU:CA	10	0.8	0.21	0.92
(9,84)	1:79:A:THR:C	1:78:A:VAL:CG2	10	0.56	0.03	0.57
(9,61)	1:64:A:ALA:C	1:63:A:ALA:CB	10	0.53	0.03	0.54
(9,75)	1:72:A:ARG:C	1:71:A:ALA:CB	10	0.52	0.03	0.53
(9,177)	1:183:A:TRP:C	1:182:A:VAL:CG2	10	0.48	0.11	0.5
(9,133)	1:135:A:GLY:C	1:134:A:CYS:CB	10	0.46	0.01	0.47
(9,188)	1:198:A:ASP:C	1:197:A:ILE:CG2	10	0.46	0.09	0.45
(9,190)	1:199:A:THR:C	1:199:A:THR:CA	10	0.44	0.0	0.44
(9,143)	1:139:A:PHE:C	1:138:A:ALA:CB	10	0.44	0.06	0.44
(9,116)	1:120:A:ASP:C	1:119:A:ALA:CB	10	0.43	0.12	0.44
(9,139)	1:137:A:CYS:C	1:136:A:VAL:CG2	10	0.42	0.05	0.44
(9,111)	1:115:A:SER:C	1:114:A:THR:CG2	10	0.42	0.12	0.46
(9,203)	1:213:A:PHE:C	1:216:A:LEU:CD1	10	0.4	0.09	0.44
(9,163)	1:171:A:TYR:C	1:170:A:THR:CG2	10	0.39	0.07	0.42
(9,12)	1:14:A:GLY:C	1:13:A:ALA:CB	10	0.36	0.05	0.36
(9,71)	1:70:A:TYR:C	1:69:A:HIS:CB	10	0.35	0.08	0.33
(9,142)	1:138:A:ALA:C	1:137:A:CYS:CB	10	0.33	0.06	0.3

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(9,41)	1:51:A:TYR:C	1:50:A:ALA:CB	10	0.32	0.04	0.31
(9,50)	1:54:A:MET:C	1:53:A:ALA:CB	10	0.31	0.01	0.31
(10,25)	1:44:A:PRO:N	1:40:A:ALA:O	10	0.27	0.07	0.29
(9,175)	1:182:A:VAL:C	1:181:A:ILE:CG2	10	0.25	0.07	0.26
(9,62)	1:65:A:GLY:C	1:64:A:ALA:CB	10	0.23	0.07	0.24
(10,116)	1:180:A:PRO:N	1:176:A:TRP:O	10	0.22	0.07	0.18
(10,128)	1:206:A:PRO:N	1:202:A:PHE:O	10	0.2	0.06	0.17
(10,46)	1:81:A:PRO:N	1:77:A:MET:O	10	0.2	0.03	0.18
(12,55)	1:83:A:LEU:CA	1:176:A:TRP:CE3	10	0.13	0.01	0.13
(3,986)	1:208:A:PHE:CA	1:205:A:LEU:CG	10	0.12	0.01	0.12
(3,105)	1:29:A:PRO:CD	1:25:A:LEU:CA	10	0.11	0.01	0.11
(11,23)	1:53:A:ALA:CA	1:8:A:HIS:CA	10	0.11	0.0	0.11
(5,46)	1:92:A:MET:O	1:141:A:ILE:HG23	9	8.97	0.87	9.16
(5,46)	1:92:A:MET:O	1:141:A:ILE:HG21	9	8.97	0.87	9.16
(5,46)	1:92:A:MET:O	1:141:A:ILE:HG13	9	8.97	0.87	9.16
(5,46)	1:92:A:MET:O	1:141:A:ILE:HG22	9	8.97	0.87	9.16
(5,46)	1:92:A:MET:O	1:141:A:ILE:HG12	9	8.97	0.87	9.16
(4,58)	1:92:A:MET:O	1:144:A:TRP:HA	9	6.79	0.6	6.97
(4,57)	1:92:A:MET:O	1:142:A:ILE:HA	9	5.86	0.8	5.84
(4,43)	1:92:A:MET:O	1:145:A:GLY:H	9	5.83	0.57	6.17
(4,6)	1:5:A:SER:OG	1:71:A:ALA:HA	9	4.48	1.45	4.29
(6,11)	1:158:A:SER:OG	1:148:A:ASN:CA	9	3.85	1.43	4.48
(4,44)	1:92:A:MET:O	1:146:A:ILE:H	9	3.57	0.54	3.59
(4,125)	1:122:A:SER:OG	1:193:A:ILE:H	9	3.29	1.37	3.26
(4,42)	1:92:A:MET:O	1:100:A:THR:H	9	3.18	1.43	3.94
(4,5)	1:5:A:SER:OG	1:69:A:HIS:HA	9	2.9	1.62	2.86
(5,7)	1:5:A:SER:OG	1:58:A:GLN:HG3	9	2.9	1.42	2.34
(5,7)	1:5:A:SER:OG	1:58:A:GLN:HG2	9	2.9	1.42	2.34
(4,113)	1:97:A:LYS:O	1:32:A:VAL:HB	9	2.68	1.31	2.48
(4,52)	1:92:A:MET:O	1:41:A:MET:HA	9	2.66	2.4	1.95
(4,114)	1:97:A:LYS:O	1:39:A:VAL:HB	9	2.17	1.28	1.78
(5,56)	1:97:A:LYS:O	1:165:A:TYR:HD1	9	2.14	1.2	1.81
(5,56)	1:97:A:LYS:O	1:165:A:TYR:HD2	9	2.14	1.2	1.81
(4,167)	1:124:A:ARG:O	1:183:A:TRP:HA	9	1.83	0.99	1.96
(4,141)	1:122:A:SER:OG	1:111:A:VAL:HA	9	1.73	0.79	1.9
(4,16)	1:26:A:SER:OG	1:43:A:ILE:HA	9	1.49	0.79	1.39
(7,165)	1:124:A:ARG:O	1:110:A:ILE:HA	9	1.16	0.56	1.0
(4,73)	1:92:A:MET:O	1:169:A:VAL:HB	9	0.89	0.38	0.81
(5,75)	1:122:A:SER:OG	1:74:A:ILE:HD12	9	0.84	0.32	0.77
(5,75)	1:122:A:SER:OG	1:74:A:ILE:HD13	9	0.84	0.32	0.77
(4,137)	1:122:A:SER:OG	1:71:A:ALA:HA	9	0.67	0.28	0.56
(4,139)	1:122:A:SER:OG	1:74:A:ILE:HA	9	0.6	0.24	0.58

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(9,80)	1:76:A:TRP:C	1:80:A:THR:CG2	9	0.39	0.12	0.44
(9,17)	1:18:A:GLY:C	1:17:A:ILE:CD1	9	0.3	0.15	0.21
(3,423)	1:83:A:LEU:CG	1:87:A:LEU:CG	9	0.11	0.01	0.11
(3,115)	1:32:A:VAL:CA	1:35:A:TYR:CE1	9	0.11	0.0	0.11
(4,80)	1:97:A:LYS:O	1:145:A:GLY:H	8	4.54	1.72	4.97
(4,94)	1:97:A:LYS:O	1:145:A:GLY:H	8	4.54	1.72	4.97
(4,81)	1:97:A:LYS:O	1:146:A:ILE:H	8	3.42	1.39	3.76
(4,95)	1:97:A:LYS:O	1:146:A:ILE:H	8	3.42	1.39	3.76
(4,110)	1:97:A:LYS:O	1:158:A:SER:HA	8	3.32	1.27	3.46
(1,419)	1:181:A:ILE:HG23	1:185:A:ILE:HD12	8	2.23	1.16	2.42
(1,419)	1:181:A:ILE:HG22	1:185:A:ILE:HD11	8	2.23	1.16	2.42
(1,419)	1:181:A:ILE:HG23	1:185:A:ILE:HD13	8	2.23	1.16	2.42
(1,419)	1:181:A:ILE:HG21	1:185:A:ILE:HD12	8	2.23	1.16	2.42
(1,419)	1:181:A:ILE:HG21	1:185:A:ILE:HD11	8	2.23	1.16	2.42
(4,47)	1:92:A:MET:O	1:25:A:LEU:HA	8	2.16	3.33	0.99
(4,123)	1:122:A:SER:OG	1:186:A:GLY:H	8	1.73	1.0	1.8
(5,76)	1:122:A:SER:OG	1:113:A:ILE:HD11	8	1.4	0.87	1.12
(5,76)	1:122:A:SER:OG	1:113:A:ILE:HD13	8	1.4	0.87	1.12
(5,76)	1:122:A:SER:OG	1:113:A:ILE:HD12	8	1.4	0.87	1.12
(7,49)	1:26:A:SER:OG	1:12:A:VAL:HB	8	1.35	0.71	1.38
(7,121)	1:92:A:MET:O	1:46:A:TRP:HD1	8	1.23	0.72	1.13
(7,97)	1:92:A:MET:O	1:15:A:MET:HA	8	1.19	0.64	1.03
(4,33)	1:58:A:GLN:NE2	1:68:A:ALA:HA	8	1.13	0.44	1.2
(2,805)	1:127:A:VAL:CG1	1:124:A:ARG:CZ	8	1.03	0.6	0.8
(4,60)	1:92:A:MET:O	1:163:A:ASN:HA	8	0.67	0.34	0.48
(1,332)	1:143:A:LEU:HD11	1:146:A:ILE:HD13	8	0.61	0.32	0.55
(1,332)	1:143:A:LEU:HD13	1:146:A:ILE:HD12	8	0.61	0.32	0.55
(1,332)	1:143:A:LEU:HD12	1:146:A:ILE:HD13	8	0.61	0.32	0.55
(1,332)	1:143:A:LEU:HD13	1:146:A:ILE:HD11	8	0.61	0.32	0.55
(1,332)	1:143:A:LEU:HD11	1:146:A:ILE:HD12	8	0.61	0.32	0.55
(13,13)	1:210:A:LYS:HD2	1:47:A:SER:HB2	8	0.59	0.44	0.55
(13,13)	1:210:A:LYS:HD2	1:47:A:SER:HB3	8	0.59	0.44	0.55
(9,55)	1:61:A:VAL:C	1:67:A:ILE:CG2	8	0.44	0.09	0.46
(9,68)	1:69:A:HIS:C	1:71:A:ALA:CB	8	0.29	0.11	0.29
(2,506)	1:76:A:TRP:CH2	1:76:A:TRP:C	8	0.25	0.02	0.26
(11,35)	1:73:A:TYR:CA	1:116:A:GLY:CA	8	0.12	0.01	0.12
(3,322)	1:73:A:TYR:CA	1:72:A:ARG:CD	8	0.12	0.01	0.11
(3,383)	1:78:A:VAL:CB	1:75:A:ASP:CG	8	0.11	0.0	0.11
(3,982)	1:207:A:PHE:CG	1:211:A:VAL:CA	8	0.11	0.01	0.11
(5,55)	1:97:A:LYS:O	1:149:A:PRO:HD2	7	2.78	1.24	3.36
(5,55)	1:97:A:LYS:O	1:149:A:PRO:HD3	7	2.78	1.24	3.36
(4,108)	1:97:A:LYS:O	1:156:A:THR:HA	7	2.65	0.89	2.54

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,74)	1:45:A:ILE:HG23	1:49:A:LEU:HD11	7	2.36	1.68	2.38
(1,74)	1:45:A:ILE:HG23	1:49:A:LEU:HD13	7	2.36	1.68	2.38
(1,74)	1:45:A:ILE:HG22	1:49:A:LEU:HD12	7	2.36	1.68	2.38
(1,74)	1:45:A:ILE:HG22	1:49:A:LEU:HD11	7	2.36	1.68	2.38
(1,74)	1:45:A:ILE:HG23	1:49:A:LEU:HD12	7	2.36	1.68	2.38
(1,74)	1:45:A:ILE:HG22	1:49:A:LEU:HD13	7	2.36	1.68	2.38
(5,54)	1:97:A:LYS:O	1:146:A:ILE:HD13	7	1.97	1.06	2.37
(5,54)	1:97:A:LYS:O	1:146:A:ILE:HD11	7	1.97	1.06	2.37
(4,98)	1:97:A:LYS:O	1:32:A:VAL:HA	7	1.82	0.77	1.68
(5,36)	1:92:A:MET:O	1:43:A:ILE:HD11	7	1.75	1.46	0.98
(5,36)	1:92:A:MET:O	1:43:A:ILE:HD12	7	1.75	1.46	0.98
(5,36)	1:92:A:MET:O	1:43:A:ILE:HD13	7	1.75	1.46	0.98
(4,106)	1:97:A:LYS:O	1:146:A:ILE:HA	7	1.61	0.43	1.62
(2,643)	1:95:A:ILE:CG1	1:92:A:MET:CG	7	1.49	0.87	1.02
(5,27)	1:58:A:GLN:NE2	1:62:A:GLU:HG3	7	1.34	0.56	1.18
(5,51)	1:97:A:LYS:O	1:91:A:ALA:HB2	7	1.18	0.86	0.95
(5,51)	1:97:A:LYS:O	1:91:A:ALA:HB1	7	1.18	0.86	0.95
(4,88)	1:97:A:LYS:O	1:91:A:ALA:H	7	1.13	0.67	0.83
(5,60)	1:97:A:LYS:O	1:39:A:VAL:HG23	7	1.11	1.0	0.56
(5,60)	1:97:A:LYS:O	1:39:A:VAL:HG22	7	1.11	1.0	0.56
(5,60)	1:97:A:LYS:O	1:39:A:VAL:HG21	7	1.11	1.0	0.56
(9,144)	1:139:A:PHE:C	1:140:A:LEU:CD2	7	0.38	0.09	0.35
(10,57)	1:92:A:MET:H	1:88:A:SER:O	7	0.13	0.01	0.14
(3,337)	1:74:A:ILE:CB	1:76:A:TRP:CA	7	0.12	0.01	0.12
(3,410)	1:82:A:LEU:CG	1:85:A:LEU:CB	7	0.11	0.01	0.11
(11,33)	1:70:A:TYR:CA	1:59:A:GLY:CA	7	0.11	0.01	0.11
(11,74)	1:182:A:VAL:CB	1:201:A:LEU:CB	7	0.11	0.01	0.11
(12,82)	1:193:A:ILE:CG1	1:185:A:ILE:CD1	7	0.1	0.0	0.1
(4,107)	1:97:A:LYS:O	1:149:A:PRO:HA	6	3.59	1.35	3.8
(2,633)	1:92:A:MET:CE	1:95:A:ILE:CD1	6	2.44	1.31	2.48
(5,2)	1:5:A:SER:OG	1:60:A:LYS:HB3	6	2.06	1.27	2.11
(5,2)	1:5:A:SER:OG	1:60:A:LYS:HB2	6	2.06	1.27	2.11
(5,37)	1:92:A:MET:O	1:44:A:PRO:HD3	6	1.94	2.11	1.1
(5,37)	1:92:A:MET:O	1:44:A:PRO:HD2	6	1.94	2.11	1.1
(4,82)	1:97:A:LYS:O	1:155:A:ARG:H	6	1.52	1.02	1.38
(2,804)	1:127:A:VAL:CG2	1:124:A:ARG:CZ	6	1.51	1.21	1.3
(4,124)	1:122:A:SER:OG	1:189:A:GLY:H	6	1.08	0.5	1.04
(2,644)	1:95:A:ILE:CG1	1:92:A:MET:CB	6	0.95	0.67	0.7
(4,25)	1:58:A:GLN:NE2	1:63:A:ALA:H	6	0.74	0.32	0.74
(4,61)	1:92:A:MET:O	1:166:A:ASP:HA	6	0.61	0.25	0.61
(1,341)	1:146:A:ILE:HD13	1:143:A:LEU:HA	6	0.48	0.26	0.47
(1,341)	1:146:A:ILE:HD12	1:143:A:LEU:HA	6	0.48	0.26	0.47

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,341)	1:146:A:ILE:HD11	1:143:A:LEU:HA	6	0.48	0.26	0.47
(9,35)	1:48:A:GLY:C	1:49:A:LEU:CD2	6	0.35	0.13	0.36
(9,117)	1:123:A:GLU:C	1:127:A:VAL:CG1	6	0.33	0.12	0.35
(9,46)	1:53:A:ALA:C	1:56:A:ILE:CD1	6	0.3	0.09	0.26
(2,131)	1:29:A:PRO:CB	1:26:A:SER:CB	6	0.12	0.03	0.12
(3,917)	1:187:A:PRO:C	1:191:A:GLY:CA	6	0.12	0.02	0.11
(3,885)	1:182:A:VAL:CA	1:179:A:TYR:CG	6	0.12	0.02	0.11
(3,729)	1:148:A:ASN:CA	1:147:A:TRP:CD2	6	0.12	0.02	0.11
(2,543)	1:79:A:THR:C	1:78:A:VAL:CG2	6	0.11	0.01	0.11
(1,185)	1:82:A:LEU:HD22	1:79:A:THR:HA	5	1.93	0.17	1.89
(1,185)	1:82:A:LEU:HD21	1:79:A:THR:HA	5	1.93	0.17	1.89
(4,59)	1:92:A:MET:O	1:156:A:THR:HA	5	1.34	0.73	1.43
(8,110)	1:124:A:ARG:O	1:75:A:ASP:HB2	5	1.31	1.21	0.86
(5,50)	1:97:A:LYS:O	1:85:A:LEU:HB3	5	0.76	0.75	0.41
(4,62)	1:92:A:MET:O	1:169:A:VAL:HA	5	0.43	0.15	0.33
(9,157)	1:165:A:TYR:C	1:168:A:LEU:CD2	5	0.39	0.13	0.4
(10,17)	1:26:A:SER:H	1:22:A:PHE:O	5	0.11	0.01	0.12
(3,567)	1:113:A:ILE:CB	1:117:A:LEU:CG	5	0.11	0.01	0.1
(4,115)	1:97:A:LYS:O	1:154:A:THR:HB	4	2.16	1.02	2.16
(6,13)	1:158:A:SER:OG	1:219:A:HIS:CA	4	0.97	0.74	0.67
(5,18)	1:26:A:SER:OG	1:39:A:VAL:HG23	4	0.63	0.33	0.64
(5,18)	1:26:A:SER:OG	1:39:A:VAL:HG21	4	0.63	0.33	0.64
(5,18)	1:26:A:SER:OG	1:39:A:VAL:HG22	4	0.63	0.33	0.64
(7,185)	1:124:A:ARG:O	1:141:A:ILE:HB	4	0.57	0.32	0.48
(5,33)	1:92:A:MET:O	1:163:A:ASN:HB2	4	0.45	0.17	0.37
(1,287)	1:117:A:LEU:HD13	1:114:A:THR:HB	4	0.23	0.15	0.16
(1,287)	1:117:A:LEU:HD11	1:114:A:THR:HB	4	0.23	0.15	0.16
(1,287)	1:117:A:LEU:HD12	1:114:A:THR:HB	4	0.23	0.15	0.16
(10,97)	1:158:A:SER:H	1:154:A:THR:O	4	0.15	0.03	0.16
(2,1106)	1:183:A:TRP:C	1:182:A:VAL:CG2	4	0.12	0.01	0.12
(12,53)	1:83:A:LEU:CA	1:176:A:TRP:CE2	4	0.11	0.0	0.11
(12,3)	1:8:A:HIS:CE1	1:69:A:HIS:CE1	4	0.1	0.0	0.1
(4,109)	1:97:A:LYS:O	1:157:A:GLN:HA	3	1.48	0.9	1.03
(2,634)	1:92:A:MET:CE	1:95:A:ILE:CA	3	1.23	0.23	1.25
(4,1)	1:5:A:SER:OG	1:52:A:MET:H	3	1.13	0.78	1.2
(4,83)	1:97:A:LYS:O	1:157:A:GLN:H	3	1.1	0.23	1.22
(7,192)	1:158:A:SER:OG	1:43:A:ILE:HB	3	1.06	0.45	0.96
(4,132)	1:122:A:SER:OG	1:61:A:VAL:HA	3	1.02	1.0	0.41
(6,15)	1:158:A:SER:OG	1:217:A:ASP:CA	3	0.74	0.28	0.87
(4,34)	1:58:A:GLN:NE2	1:74:A:ILE:HA	3	0.63	0.11	0.6
(4,71)	1:92:A:MET:O	1:102:A:ILE:HB	3	0.59	0.19	0.49
(9,148)	1:142:A:ILE:C	1:143:A:LEU:CD1	3	0.35	0.1	0.36

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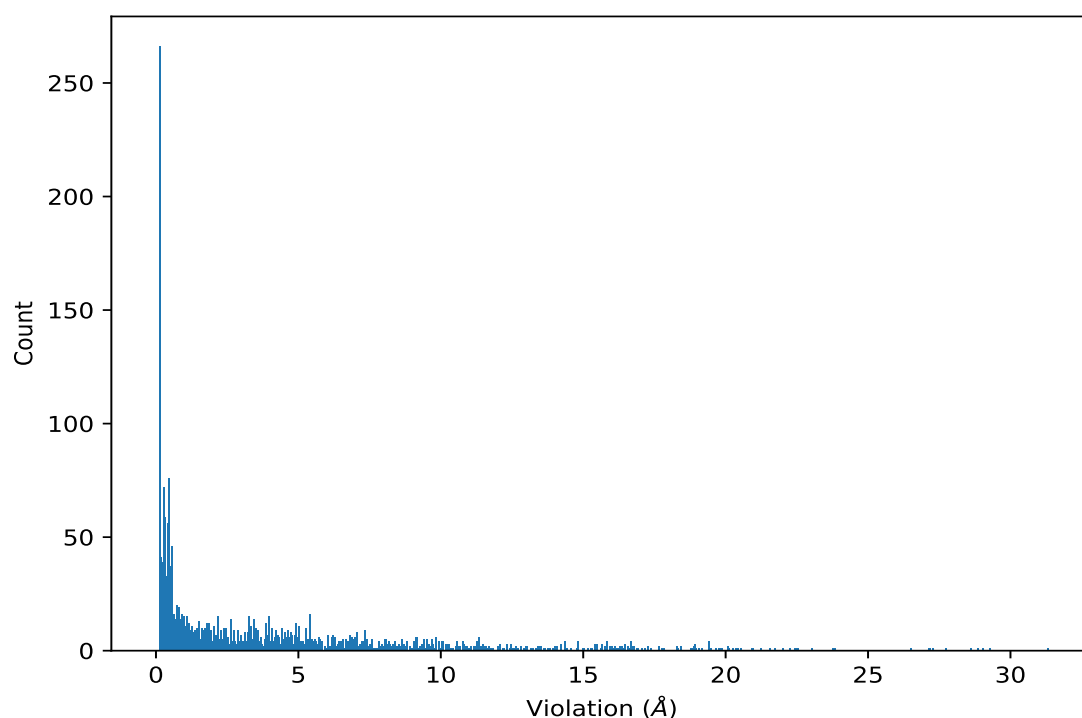
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(3,882)	1:181:A:ILE:CG1	1:182:A:VAL:CB	3	0.23	0.0	0.23
(9,130)	1:134:A:CYS:C	1:138:A:ALA:CB	3	0.21	0.06	0.22
(3,253)	1:58:A:GLN:CD	1:59:A:GLY:CA	3	0.16	0.06	0.15
(3,119)	1:32:A:VAL:CA	1:35:A:TYR:CE2	3	0.13	0.01	0.13
(3,360)	1:76:A:TRP:CA	1:73:A:TYR:CG	3	0.12	0.01	0.11
(1,173)	1:80:A:THR:HA	1:83:A:LEU:HA	3	0.11	0.01	0.11
(3,100)	1:26:A:SER:CA	1:22:A:PHE:CG	3	0.11	0.01	0.1
(3,705)	1:143:A:LEU:CG	1:146:A:ILE:CB	3	0.11	0.01	0.11
(11,50)	1:84:A:LEU:CG	1:176:A:TRP:CD2	3	0.1	0.0	0.1
(2,1070)	1:180:A:PRO:CB	1:183:A:TRP:CE2	3	0.1	0.0	0.1
(5,43)	1:92:A:MET:O	1:43:A:ILE:HG13	2	2.34	1.37	2.34
(5,43)	1:92:A:MET:O	1:43:A:ILE:HG23	2	2.34	1.37	2.34
(4,149)	1:122:A:SER:OG	1:61:A:VAL:HB	2	1.21	0.91	1.21
(4,45)	1:92:A:MET:O	1:154:A:THR:H	2	1.04	0.32	1.04
(4,30)	1:58:A:GLN:NE2	1:47:A:SER:HA	2	1.04	0.04	1.04
(4,46)	1:92:A:MET:O	1:156:A:THR:H	2	0.99	0.15	0.99
(6,14)	1:158:A:SER:OG	1:218:A:LEU:CA	2	0.56	0.16	0.56
(9,34)	1:48:A:GLY:C	1:50:A:ALA:CB	2	0.34	0.12	0.34
(4,76)	1:97:A:LYS:O	1:92:A:MET:H	2	0.29	0.12	0.29
(9,11)	1:14:A:GLY:C	1:15:A:MET:CE	2	0.21	0.1	0.21
(9,126)	1:132:A:TYR:C	1:136:A:VAL:CG1	2	0.16	0.06	0.16
(9,127)	1:132:A:TYR:C	1:134:A:CYS:CB	2	0.14	0.02	0.14
(9,40)	1:51:A:TYR:C	1:12:A:VAL:CG1	2	0.13	0.01	0.13
(1,193)	1:83:A:LEU:HD13	1:80:A:THR:HA	2	0.12	0.02	0.12
(2,779)	1:120:A:ASP:C	1:119:A:ALA:CB	2	0.11	0.01	0.11
(3,382)	1:78:A:VAL:CB	1:81:A:PRO:CD	2	0.11	0.0	0.11
(3,531)	1:109:A:GLN:CB	1:112:A:VAL:CA	2	0.11	0.01	0.11
(3,801)	1:169:A:VAL:CB	1:168:A:LEU:CG	2	0.11	0.0	0.11
(11,65)	1:119:A:ALA:CA	1:132:A:TYR:CA	2	0.11	0.0	0.11

<sup>1</sup>Number of violated models, <sup>2</sup>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)
(4,93)	1:97:A:LYS:O	1:125:A:ASP:H	5	31.32
(4,93)	1:97:A:LYS:O	1:125:A:ASP:H	7	29.26
(4,93)	1:97:A:LYS:O	1:125:A:ASP:H	10	29.0
(4,93)	1:97:A:LYS:O	1:125:A:ASP:H	9	28.9
(4,93)	1:97:A:LYS:O	1:125:A:ASP:H	3	28.64
(4,93)	1:97:A:LYS:O	1:125:A:ASP:H	8	27.72
(4,93)	1:97:A:LYS:O	1:125:A:ASP:H	1	27.26
(4,93)	1:97:A:LYS:O	1:125:A:ASP:H	2	27.17
(4,93)	1:97:A:LYS:O	1:125:A:ASP:H	4	27.15
(4,93)	1:97:A:LYS:O	1:125:A:ASP:H	6	26.54
(5,79)	1:122:A:SER:OG	1:32:A:VAL:HG21	7	23.81
(5,79)	1:122:A:SER:OG	1:32:A:VAL:HG13	6	23.77
(5,79)	1:122:A:SER:OG	1:32:A:VAL:HG11	1	23.02
(5,79)	1:122:A:SER:OG	1:32:A:VAL:HG13	2	22.54
(5,79)	1:122:A:SER:OG	1:32:A:VAL:HG13	10	22.46
(4,9)	1:5:A:SER:OG	1:126:A:TRP:HA	8	22.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,79)	1:122:A:SER:OG	1:32:A:VAL:HG12	5	22.29
(5,79)	1:122:A:SER:OG	1:32:A:VAL:HG12	8	22.0
(5,79)	1:122:A:SER:OG	1:32:A:VAL:HG11	9	21.72
(5,79)	1:122:A:SER:OG	1:32:A:VAL:HG13	3	21.57
(5,79)	1:122:A:SER:OG	1:32:A:VAL:HG12	4	21.24
(5,58)	1:97:A:LYS:O	1:181:A:ILE:HD13	5	20.97
(5,58)	1:97:A:LYS:O	1:181:A:ILE:HD13	9	20.95
(4,9)	1:5:A:SER:OG	1:126:A:TRP:HA	10	20.5
(5,58)	1:97:A:LYS:O	1:181:A:ILE:HD12	1	20.43
(4,63)	1:92:A:MET:O	1:184:A:ILE:HA	1	20.37
(5,58)	1:97:A:LYS:O	1:181:A:ILE:HD13	10	20.25
(4,9)	1:5:A:SER:OG	1:126:A:TRP:HA	6	20.14
(4,63)	1:92:A:MET:O	1:184:A:ILE:HA	3	20.07
(4,63)	1:92:A:MET:O	1:184:A:ILE:HA	7	20.06
(4,9)	1:5:A:SER:OG	1:126:A:TRP:HA	9	19.9
(5,58)	1:97:A:LYS:O	1:181:A:ILE:HD13	3	19.82
(4,8)	1:5:A:SER:OG	1:124:A:ARG:HA	8	19.79
(4,63)	1:92:A:MET:O	1:184:A:ILE:HA	5	19.67
(4,9)	1:5:A:SER:OG	1:126:A:TRP:HA	1	19.46
(4,145)	1:122:A:SER:OG	1:148:A:ASN:HA	1	19.45
(4,8)	1:5:A:SER:OG	1:124:A:ARG:HA	10	19.45
(5,58)	1:97:A:LYS:O	1:181:A:ILE:HD13	7	19.43
(4,145)	1:122:A:SER:OG	1:148:A:ASN:HA	8	19.43
(4,145)	1:122:A:SER:OG	1:148:A:ASN:HA	10	19.17
(4,145)	1:122:A:SER:OG	1:148:A:ASN:HA	2	19.07
(4,63)	1:92:A:MET:O	1:184:A:ILE:HA	2	18.99
(4,8)	1:5:A:SER:OG	1:124:A:ARG:HA	9	18.94
(4,145)	1:122:A:SER:OG	1:148:A:ASN:HA	9	18.93
(4,145)	1:122:A:SER:OG	1:148:A:ASN:HA	5	18.92
(4,63)	1:92:A:MET:O	1:184:A:ILE:HA	6	18.9
(4,63)	1:92:A:MET:O	1:184:A:ILE:HA	10	18.89
(4,145)	1:122:A:SER:OG	1:148:A:ASN:HA	7	18.81
(4,63)	1:92:A:MET:O	1:184:A:ILE:HA	9	18.78
(5,58)	1:97:A:LYS:O	1:181:A:ILE:HD13	4	18.43
(4,145)	1:122:A:SER:OG	1:148:A:ASN:HA	6	18.43
(4,9)	1:5:A:SER:OG	1:126:A:TRP:HA	4	18.34
(4,8)	1:5:A:SER:OG	1:124:A:ARG:HA	6	18.28
(4,38)	1:58:A:GLN:NE2	1:126:A:TRP:HA	4	18.27
(5,58)	1:97:A:LYS:O	1:181:A:ILE:HD12	2	17.82
(4,145)	1:122:A:SER:OG	1:148:A:ASN:HA	4	17.79
(4,63)	1:92:A:MET:O	1:184:A:ILE:HA	8	17.68
(4,39)	1:58:A:GLN:NE2	1:130:A:LEU:HA	4	17.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,9)	1:5:A:SER:OG	1:126:A:TRP:HA	7	17.36
(4,145)	1:122:A:SER:OG	1:148:A:ASN:HA	3	17.29
(4,84)	1:97:A:LYS:O	1:19:A:ALA:H	8	17.25
(4,40)	1:58:A:GLN:NE2	1:134:A:CYS:HA	10	17.16
(4,39)	1:58:A:GLN:NE2	1:130:A:LEU:HA	6	17.09
(4,39)	1:58:A:GLN:NE2	1:130:A:LEU:HA	1	16.94
(4,8)	1:5:A:SER:OG	1:124:A:ARG:HA	1	16.86
(4,8)	1:5:A:SER:OG	1:124:A:ARG:HA	7	16.78
(4,39)	1:58:A:GLN:NE2	1:130:A:LEU:HA	5	16.77
(4,40)	1:58:A:GLN:NE2	1:134:A:CYS:HA	8	16.73
(4,84)	1:97:A:LYS:O	1:19:A:ALA:H	4	16.71
(4,39)	1:58:A:GLN:NE2	1:130:A:LEU:HA	10	16.69
(4,39)	1:58:A:GLN:NE2	1:130:A:LEU:HA	8	16.66
(4,38)	1:58:A:GLN:NE2	1:126:A:TRP:HA	6	16.66
(4,9)	1:5:A:SER:OG	1:126:A:TRP:HA	2	16.66
(4,38)	1:58:A:GLN:NE2	1:126:A:TRP:HA	1	16.63
(4,40)	1:58:A:GLN:NE2	1:134:A:CYS:HA	1	16.57
(4,40)	1:58:A:GLN:NE2	1:134:A:CYS:HA	6	16.55
(4,40)	1:58:A:GLN:NE2	1:134:A:CYS:HA	5	16.48
(4,39)	1:58:A:GLN:NE2	1:130:A:LEU:HA	9	16.47
(4,127)	1:122:A:SER:OG	1:15:A:MET:HA	9	16.45
(4,40)	1:58:A:GLN:NE2	1:134:A:CYS:HA	3	16.41
(4,40)	1:58:A:GLN:NE2	1:134:A:CYS:HA	4	16.4
(4,39)	1:58:A:GLN:NE2	1:130:A:LEU:HA	7	16.38
(4,40)	1:58:A:GLN:NE2	1:134:A:CYS:HA	7	16.27
(4,40)	1:58:A:GLN:NE2	1:134:A:CYS:HA	9	16.27
(4,127)	1:122:A:SER:OG	1:15:A:MET:HA	3	16.22
(4,38)	1:58:A:GLN:NE2	1:126:A:TRP:HA	8	16.17
(4,39)	1:58:A:GLN:NE2	1:130:A:LEU:HA	2	16.13
(4,4)	1:5:A:SER:OG	1:64:A:ALA:HA	8	16.12
(4,127)	1:122:A:SER:OG	1:15:A:MET:HA	7	16.06
(4,127)	1:122:A:SER:OG	1:15:A:MET:HA	8	16.03
(5,4)	1:5:A:SER:OG	1:119:A:ALA:HB2	8	16.01
(5,3)	1:5:A:SER:OG	1:64:A:ALA:HB2	8	15.95
(4,38)	1:58:A:GLN:NE2	1:126:A:TRP:HA	5	15.9
(4,4)	1:5:A:SER:OG	1:64:A:ALA:HA	9	15.84
(4,127)	1:122:A:SER:OG	1:15:A:MET:HA	1	15.83
(4,127)	1:122:A:SER:OG	1:15:A:MET:HA	2	15.83
(4,38)	1:58:A:GLN:NE2	1:126:A:TRP:HA	2	15.82
(4,40)	1:58:A:GLN:NE2	1:134:A:CYS:HA	2	15.79
(4,9)	1:5:A:SER:OG	1:126:A:TRP:HA	5	15.75
(5,57)	1:97:A:LYS:O	1:177:A:ILE:HD13	5	15.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,38)	1:58:A:GLN:NE2	1:126:A:TRP:HA	7	15.66
(4,38)	1:58:A:GLN:NE2	1:126:A:TRP:HA	9	15.66
(4,4)	1:5:A:SER:OG	1:64:A:ALA:HA	10	15.62
(4,84)	1:97:A:LYS:O	1:19:A:ALA:H	6	15.47
(4,127)	1:122:A:SER:OG	1:15:A:MET:HA	5	15.46
(4,38)	1:58:A:GLN:NE2	1:126:A:TRP:HA	10	15.46
(5,58)	1:97:A:LYS:O	1:181:A:ILE:HD11	8	15.43
(4,127)	1:122:A:SER:OG	1:15:A:MET:HA	4	15.42
(4,127)	1:122:A:SER:OG	1:15:A:MET:HA	6	15.4
(4,10)	1:5:A:SER:OG	1:172:A:PHE:HA	8	15.35
(4,127)	1:122:A:SER:OG	1:15:A:MET:HA	10	15.28
(4,84)	1:97:A:LYS:O	1:19:A:ALA:H	9	15.16
(5,3)	1:5:A:SER:OG	1:64:A:ALA:HB2	9	15.02
(5,58)	1:97:A:LYS:O	1:181:A:ILE:HD12	6	14.96
(4,84)	1:97:A:LYS:O	1:19:A:ALA:H	3	14.85
(4,10)	1:5:A:SER:OG	1:172:A:PHE:HA	1	14.85
(4,84)	1:97:A:LYS:O	1:19:A:ALA:H	5	14.84
(4,39)	1:58:A:GLN:NE2	1:130:A:LEU:HA	3	14.81
(4,8)	1:5:A:SER:OG	1:124:A:ARG:HA	2	14.79
(5,57)	1:97:A:LYS:O	1:177:A:ILE:HD13	3	14.58
(5,57)	1:97:A:LYS:O	1:177:A:ILE:HD11	9	14.41
(4,10)	1:5:A:SER:OG	1:172:A:PHE:HA	10	14.38
(4,128)	1:122:A:SER:OG	1:44:A:PRO:HA	7	14.36
(4,10)	1:5:A:SER:OG	1:172:A:PHE:HA	6	14.36
(4,8)	1:5:A:SER:OG	1:124:A:ARG:HA	5	14.36
(5,3)	1:5:A:SER:OG	1:64:A:ALA:HB2	10	14.24
(4,84)	1:97:A:LYS:O	1:19:A:ALA:H	10	14.24
(5,57)	1:97:A:LYS:O	1:177:A:ILE:HD12	7	14.21
(4,128)	1:122:A:SER:OG	1:44:A:PRO:HA	2	14.09
(5,57)	1:97:A:LYS:O	1:177:A:ILE:HD13	10	14.06
(4,84)	1:97:A:LYS:O	1:19:A:ALA:H	2	14.01
(4,8)	1:5:A:SER:OG	1:124:A:ARG:HA	4	14.01
(4,84)	1:97:A:LYS:O	1:19:A:ALA:H	7	13.97
(5,52)	1:97:A:LYS:O	1:25:A:LEU:HD13	4	13.9
(4,10)	1:5:A:SER:OG	1:172:A:PHE:HA	9	13.81
(4,128)	1:122:A:SER:OG	1:44:A:PRO:HA	1	13.76
(5,57)	1:97:A:LYS:O	1:177:A:ILE:HD11	1	13.65
(4,4)	1:5:A:SER:OG	1:64:A:ALA:HA	3	13.61
(4,75)	1:97:A:LYS:O	1:28:A:ASN:H	8	13.54
(4,75)	1:97:A:LYS:O	1:28:A:ASN:H	4	13.51
(4,128)	1:122:A:SER:OG	1:44:A:PRO:HA	9	13.48
(4,10)	1:5:A:SER:OG	1:172:A:PHE:HA	3	13.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,37)	1:58:A:GLN:NE2	1:124:A:ARG:HA	4	13.44
(5,4)	1:5:A:SER:OG	1:119:A:ALA:HB1	10	13.42
(4,10)	1:5:A:SER:OG	1:172:A:PHE:HA	7	13.3
(4,128)	1:122:A:SER:OG	1:44:A:PRO:HA	10	13.23
(4,128)	1:122:A:SER:OG	1:44:A:PRO:HA	8	13.17
(4,128)	1:122:A:SER:OG	1:44:A:PRO:HA	4	13.04
(4,128)	1:122:A:SER:OG	1:44:A:PRO:HA	6	13.04
(4,7)	1:5:A:SER:OG	1:120:A:ASP:HA	8	12.98
(5,57)	1:97:A:LYS:O	1:177:A:ILE:HD11	4	12.96
(5,3)	1:5:A:SER:OG	1:64:A:ALA:HB1	6	12.95
(5,4)	1:5:A:SER:OG	1:119:A:ALA:HB2	9	12.83
(4,128)	1:122:A:SER:OG	1:44:A:PRO:HA	3	12.83
(4,75)	1:97:A:LYS:O	1:28:A:ASN:H	6	12.71
(4,128)	1:122:A:SER:OG	1:44:A:PRO:HA	5	12.64
(4,9)	1:5:A:SER:OG	1:126:A:TRP:HA	3	12.64
(4,63)	1:92:A:MET:O	1:184:A:ILE:HA	4	12.6
(4,8)	1:5:A:SER:OG	1:124:A:ARG:HA	3	12.51
(4,10)	1:5:A:SER:OG	1:172:A:PHE:HA	2	12.49
(5,4)	1:5:A:SER:OG	1:119:A:ALA:HB2	1	12.48
(5,3)	1:5:A:SER:OG	1:64:A:ALA:HB1	3	12.46
(5,3)	1:5:A:SER:OG	1:64:A:ALA:HB1	7	12.41
(4,37)	1:58:A:GLN:NE2	1:124:A:ARG:HA	7	12.33
(4,37)	1:58:A:GLN:NE2	1:124:A:ARG:HA	5	12.31
(4,10)	1:5:A:SER:OG	1:172:A:PHE:HA	4	12.3
(4,4)	1:5:A:SER:OG	1:64:A:ALA:HA	4	12.22
(4,37)	1:58:A:GLN:NE2	1:124:A:ARG:HA	8	12.19
(5,52)	1:97:A:LYS:O	1:25:A:LEU:HD13	6	12.08
(4,84)	1:97:A:LYS:O	1:19:A:ALA:H	1	12.06
(5,57)	1:97:A:LYS:O	1:177:A:ILE:HD13	2	12.05
(4,75)	1:97:A:LYS:O	1:28:A:ASN:H	2	12.01
(5,49)	1:92:A:MET:O	1:177:A:ILE:HG12	10	12.0
(4,7)	1:5:A:SER:OG	1:120:A:ASP:HA	10	11.84
(4,37)	1:58:A:GLN:NE2	1:124:A:ARG:HA	1	11.75
(4,10)	1:5:A:SER:OG	1:172:A:PHE:HA	5	11.71
(4,37)	1:58:A:GLN:NE2	1:124:A:ARG:HA	2	11.68
(4,4)	1:5:A:SER:OG	1:64:A:ALA:HA	7	11.67
(4,4)	1:5:A:SER:OG	1:64:A:ALA:HA	1	11.61
(4,4)	1:5:A:SER:OG	1:64:A:ALA:HA	2	11.59
(4,37)	1:58:A:GLN:NE2	1:124:A:ARG:HA	6	11.56
(4,130)	1:122:A:SER:OG	1:52:A:MET:HA	7	11.54
(5,63)	1:122:A:SER:OG	1:55:A:ALA:HB2	7	11.51
(4,130)	1:122:A:SER:OG	1:52:A:MET:HA	3	11.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,130)	1:122:A:SER:OG	1:52:A:MET:HA	8	11.49
(5,4)	1:5:A:SER:OG	1:119:A:ALA:HB1	6	11.47
(5,63)	1:122:A:SER:OG	1:55:A:ALA:HB2	3	11.43
(4,130)	1:122:A:SER:OG	1:52:A:MET:HA	4	11.41
(5,63)	1:122:A:SER:OG	1:55:A:ALA:HB2	4	11.37
(4,130)	1:122:A:SER:OG	1:52:A:MET:HA	9	11.37
(5,52)	1:97:A:LYS:O	1:25:A:LEU:HD13	7	11.35
(4,130)	1:122:A:SER:OG	1:52:A:MET:HA	2	11.35
(4,37)	1:58:A:GLN:NE2	1:124:A:ARG:HA	9	11.35
(5,63)	1:122:A:SER:OG	1:55:A:ALA:HB2	9	11.32
(4,4)	1:5:A:SER:OG	1:64:A:ALA:HA	6	11.32
(4,38)	1:58:A:GLN:NE2	1:126:A:TRP:HA	3	11.3
(4,130)	1:122:A:SER:OG	1:52:A:MET:HA	1	11.26
(5,63)	1:122:A:SER:OG	1:55:A:ALA:HB1	8	11.25
(5,52)	1:97:A:LYS:O	1:25:A:LEU:HD12	8	11.25
(5,4)	1:5:A:SER:OG	1:119:A:ALA:HB1	3	11.25
(5,52)	1:97:A:LYS:O	1:25:A:LEU:HD13	9	11.23
(5,49)	1:92:A:MET:O	1:177:A:ILE:HG12	1	11.21
(4,96)	1:97:A:LYS:O	1:222:A:ARG:H	4	11.18
(5,49)	1:92:A:MET:O	1:177:A:ILE:HG12	3	11.16
(4,87)	1:97:A:LYS:O	1:79:A:THR:H	8	11.09
(4,75)	1:97:A:LYS:O	1:28:A:ASN:H	9	11.09
(5,63)	1:122:A:SER:OG	1:55:A:ALA:HB2	10	10.96
(5,3)	1:5:A:SER:OG	1:64:A:ALA:HB2	1	10.91
(4,47)	1:92:A:MET:O	1:25:A:LEU:HA	4	10.9
(4,116)	1:122:A:SER:OG	1:47:A:SER:H	2	10.87
(4,116)	1:122:A:SER:OG	1:47:A:SER:H	7	10.86
(5,3)	1:5:A:SER:OG	1:64:A:ALA:HB1	4	10.85
(5,63)	1:122:A:SER:OG	1:55:A:ALA:HB2	1	10.82
(4,37)	1:58:A:GLN:NE2	1:124:A:ARG:HA	10	10.82
(4,130)	1:122:A:SER:OG	1:52:A:MET:HA	10	10.79
(4,87)	1:97:A:LYS:O	1:79:A:THR:H	5	10.79
(4,130)	1:122:A:SER:OG	1:52:A:MET:HA	5	10.78
(5,52)	1:97:A:LYS:O	1:25:A:LEU:HD22	2	10.75
(5,49)	1:92:A:MET:O	1:177:A:ILE:HG23	9	10.7
(4,116)	1:122:A:SER:OG	1:47:A:SER:H	9	10.67
(5,57)	1:97:A:LYS:O	1:177:A:ILE:HD12	6	10.62
(4,11)	1:5:A:SER:OG	1:183:A:TRP:HA	8	10.61
(4,130)	1:122:A:SER:OG	1:52:A:MET:HA	6	10.58
(5,46)	1:92:A:MET:O	1:141:A:ILE:HG13	3	10.57
(5,49)	1:92:A:MET:O	1:177:A:ILE:HG12	8	10.56
(4,116)	1:122:A:SER:OG	1:47:A:SER:H	1	10.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,7)	1:5:A:SER:OG	1:120:A:ASP:HA	9	10.51
(4,75)	1:97:A:LYS:O	1:28:A:ASN:H	3	10.5
(4,116)	1:122:A:SER:OG	1:47:A:SER:H	4	10.41
(5,4)	1:5:A:SER:OG	1:119:A:ALA:HB2	4	10.37
(5,63)	1:122:A:SER:OG	1:55:A:ALA:HB1	2	10.31
(4,116)	1:122:A:SER:OG	1:47:A:SER:H	10	10.27
(4,131)	1:122:A:SER:OG	1:55:A:ALA:HA	3	10.25
(4,116)	1:122:A:SER:OG	1:47:A:SER:H	6	10.25
(4,97)	1:97:A:LYS:O	1:29:A:PRO:HA	4	10.24
(4,148)	1:122:A:SER:OG	1:203:A:CYS:HA	3	10.23
(4,87)	1:97:A:LYS:O	1:79:A:THR:H	7	10.23
(4,126)	1:122:A:SER:OG	1:8:A:HIS:HA	8	10.2
(4,116)	1:122:A:SER:OG	1:47:A:SER:H	5	10.2
(5,4)	1:5:A:SER:OG	1:119:A:ALA:HB2	7	10.18
(4,87)	1:97:A:LYS:O	1:79:A:THR:H	3	10.08
(5,62)	1:122:A:SER:OG	1:47:A:SER:HB2	2	10.06
(4,126)	1:122:A:SER:OG	1:8:A:HIS:HA	3	10.05
(4,100)	1:97:A:LYS:O	1:79:A:THR:HA	8	10.05
(4,131)	1:122:A:SER:OG	1:55:A:ALA:HA	8	10.03
(4,87)	1:97:A:LYS:O	1:79:A:THR:H	9	10.01
(4,87)	1:97:A:LYS:O	1:79:A:THR:H	10	10.01
(5,49)	1:92:A:MET:O	1:177:A:ILE:HG12	5	10.0
(4,75)	1:97:A:LYS:O	1:28:A:ASN:H	7	9.97
(4,116)	1:122:A:SER:OG	1:47:A:SER:H	3	9.93
(5,63)	1:122:A:SER:OG	1:55:A:ALA:HB2	6	9.92
(5,8)	1:5:A:SER:OG	1:62:A:GLU:HG3	8	9.92
(4,116)	1:122:A:SER:OG	1:47:A:SER:H	8	9.9
(4,126)	1:122:A:SER:OG	1:8:A:HIS:HA	9	9.85
(5,62)	1:122:A:SER:OG	1:47:A:SER:HB2	10	9.84
(4,148)	1:122:A:SER:OG	1:203:A:CYS:HA	8	9.84
(4,7)	1:5:A:SER:OG	1:120:A:ASP:HA	3	9.83
(5,3)	1:5:A:SER:OG	1:64:A:ALA:HB1	2	9.81
(4,96)	1:97:A:LYS:O	1:222:A:ARG:H	6	9.8
(4,126)	1:122:A:SER:OG	1:8:A:HIS:HA	7	9.79
(5,63)	1:122:A:SER:OG	1:55:A:ALA:HB2	5	9.74
(4,87)	1:97:A:LYS:O	1:79:A:THR:H	4	9.74
(4,86)	1:97:A:LYS:O	1:43:A:ILE:H	8	9.74
(6,8)	1:97:A:LYS:O	1:29:A:PRO:CA	4	9.69
(4,100)	1:97:A:LYS:O	1:79:A:THR:HA	5	9.68
(5,5)	1:5:A:SER:OG	1:179:A:TYR:HB2	8	9.67
(4,4)	1:5:A:SER:OG	1:64:A:ALA:HA	5	9.67
(5,49)	1:92:A:MET:O	1:177:A:ILE:HG12	2	9.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,131)	1:122:A:SER:OG	1:55:A:ALA:HA	7	9.64
(5,62)	1:122:A:SER:OG	1:47:A:SER:HB2	7	9.61
(5,52)	1:97:A:LYS:O	1:25:A:LEU:HD22	3	9.6
(4,96)	1:97:A:LYS:O	1:222:A:ARG:H	9	9.59
(4,7)	1:5:A:SER:OG	1:120:A:ASP:HA	6	9.56
(4,126)	1:122:A:SER:OG	1:8:A:HIS:HA	4	9.54
(4,131)	1:122:A:SER:OG	1:55:A:ALA:HA	9	9.52
(5,52)	1:97:A:LYS:O	1:25:A:LEU:HD11	10	9.51
(5,46)	1:92:A:MET:O	1:141:A:ILE:HG22	7	9.5
(4,96)	1:97:A:LYS:O	1:222:A:ARG:H	7	9.5
(5,8)	1:5:A:SER:OG	1:62:A:GLU:HG3	9	9.49
(5,46)	1:92:A:MET:O	1:141:A:ILE:HG23	5	9.44
(5,62)	1:122:A:SER:OG	1:47:A:SER:HB2	9	9.43
(5,53)	1:97:A:LYS:O	1:43:A:ILE:HD12	7	9.42
(4,75)	1:97:A:LYS:O	1:28:A:ASN:H	10	9.42
(4,148)	1:122:A:SER:OG	1:203:A:CYS:HA	10	9.4
(4,54)	1:92:A:MET:O	1:44:A:PRO:HA	4	9.39
(4,97)	1:97:A:LYS:O	1:29:A:PRO:HA	8	9.36
(5,46)	1:92:A:MET:O	1:141:A:ILE:HG12	9	9.31
(4,131)	1:122:A:SER:OG	1:55:A:ALA:HA	4	9.31
(4,100)	1:97:A:LYS:O	1:79:A:THR:HA	3	9.3
(4,96)	1:97:A:LYS:O	1:222:A:ARG:H	3	9.29
(4,131)	1:122:A:SER:OG	1:55:A:ALA:HA	10	9.26
(4,126)	1:122:A:SER:OG	1:8:A:HIS:HA	1	9.24
(4,7)	1:5:A:SER:OG	1:120:A:ASP:HA	1	9.2
(4,100)	1:97:A:LYS:O	1:79:A:THR:HA	4	9.19
(4,126)	1:122:A:SER:OG	1:8:A:HIS:HA	2	9.18
(4,99)	1:97:A:LYS:O	1:78:A:VAL:HA	8	9.18
(4,52)	1:92:A:MET:O	1:41:A:MET:HA	4	9.18
(5,46)	1:92:A:MET:O	1:141:A:ILE:HG21	2	9.16
(4,131)	1:122:A:SER:OG	1:55:A:ALA:HA	1	9.14
(4,100)	1:97:A:LYS:O	1:79:A:THR:HA	9	9.14
(5,62)	1:122:A:SER:OG	1:47:A:SER:HB2	8	9.13
(4,100)	1:97:A:LYS:O	1:79:A:THR:HA	7	9.12
(5,8)	1:5:A:SER:OG	1:62:A:GLU:HG3	10	9.1
(4,148)	1:122:A:SER:OG	1:203:A:CYS:HA	7	9.1
(6,8)	1:97:A:LYS:O	1:29:A:PRO:CA	8	9.08
(4,148)	1:122:A:SER:OG	1:203:A:CYS:HA	5	9.06
(5,49)	1:92:A:MET:O	1:177:A:ILE:HG12	7	9.05
(4,126)	1:122:A:SER:OG	1:8:A:HIS:HA	10	9.05
(4,100)	1:97:A:LYS:O	1:79:A:THR:HA	10	9.0
(4,97)	1:97:A:LYS:O	1:29:A:PRO:HA	6	8.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,62)	1:122:A:SER:OG	1:47:A:SER:HB3	1	8.93
(5,57)	1:97:A:LYS:O	1:177:A:ILE:HD11	8	8.91
(5,25)	1:58:A:GLN:NE2	1:119:A:ALA:HB1	4	8.83
(4,86)	1:97:A:LYS:O	1:43:A:ILE:H	4	8.83
(4,129)	1:122:A:SER:OG	1:47:A:SER:HA	7	8.81
(4,126)	1:122:A:SER:OG	1:8:A:HIS:HA	5	8.8
(5,83)	1:124:A:ARG:O	1:179:A:TYR:HB2	5	8.78
(4,131)	1:122:A:SER:OG	1:55:A:ALA:HA	2	8.77
(5,46)	1:92:A:MET:O	1:141:A:ILE:HG22	10	8.73
(5,62)	1:122:A:SER:OG	1:47:A:SER:HB3	4	8.72
(4,129)	1:122:A:SER:OG	1:47:A:SER:HA	9	8.72
(4,87)	1:97:A:LYS:O	1:79:A:THR:H	6	8.7
(4,126)	1:122:A:SER:OG	1:8:A:HIS:HA	6	8.65
(4,96)	1:97:A:LYS:O	1:222:A:ARG:H	8	8.62
(5,3)	1:5:A:SER:OG	1:64:A:ALA:HB1	5	8.61
(5,52)	1:97:A:LYS:O	1:25:A:LEU:HD11	5	8.6
(5,4)	1:5:A:SER:OG	1:119:A:ALA:HB1	2	8.6
(4,129)	1:122:A:SER:OG	1:47:A:SER:HA	2	8.6
(5,62)	1:122:A:SER:OG	1:47:A:SER:HB2	3	8.56
(5,46)	1:92:A:MET:O	1:141:A:ILE:HG23	1	8.55
(6,8)	1:97:A:LYS:O	1:29:A:PRO:CA	6	8.5
(5,49)	1:92:A:MET:O	1:177:A:ILE:HG23	6	8.5
(5,25)	1:58:A:GLN:NE2	1:119:A:ALA:HB2	8	8.5
(4,96)	1:97:A:LYS:O	1:222:A:ARG:H	2	8.48
(4,96)	1:97:A:LYS:O	1:222:A:ARG:H	5	8.48
(4,131)	1:122:A:SER:OG	1:55:A:ALA:HA	6	8.4
(5,83)	1:124:A:ARG:O	1:179:A:TYR:HB3	10	8.39
(4,112)	1:97:A:LYS:O	1:29:A:PRO:HB3	4	8.39
(5,53)	1:97:A:LYS:O	1:43:A:ILE:HD12	8	8.38
(4,129)	1:122:A:SER:OG	1:47:A:SER:HA	1	8.35
(4,112)	1:97:A:LYS:O	1:29:A:PRO:HB3	8	8.34
(4,35)	1:58:A:GLN:NE2	1:119:A:ALA:HA	4	8.34
(4,129)	1:122:A:SER:OG	1:47:A:SER:HA	4	8.33
(4,87)	1:97:A:LYS:O	1:79:A:THR:H	2	8.29
(4,148)	1:122:A:SER:OG	1:203:A:CYS:HA	6	8.25
(5,62)	1:122:A:SER:OG	1:47:A:SER:HB3	5	8.22
(4,100)	1:97:A:LYS:O	1:79:A:THR:HA	6	8.22
(5,62)	1:122:A:SER:OG	1:47:A:SER:HB2	6	8.21
(4,131)	1:122:A:SER:OG	1:55:A:ALA:HA	5	8.17
(5,46)	1:92:A:MET:O	1:141:A:ILE:HG21	6	8.16
(4,75)	1:97:A:LYS:O	1:28:A:ASN:H	1	8.16
(13,7)	1:210:A:LYS:C	1:179:A:TYR:CZ	5	8.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,35)	1:58:A:GLN:NE2	1:119:A:ALA:HA	10	8.13
(4,11)	1:5:A:SER:OG	1:183:A:TRP:HA	1	8.11
(4,97)	1:97:A:LYS:O	1:29:A:PRO:HA	2	8.1
(4,129)	1:122:A:SER:OG	1:47:A:SER:HA	8	8.09
(4,35)	1:58:A:GLN:NE2	1:119:A:ALA:HA	3	8.09
(4,148)	1:122:A:SER:OG	1:203:A:CYS:HA	2	8.07
(4,67)	1:92:A:MET:O	1:78:A:VAL:HB	4	8.07
(4,129)	1:122:A:SER:OG	1:47:A:SER:HA	10	8.05
(13,6)	1:210:A:LYS:C	1:80:A:THR:CG2	9	8.02
(4,99)	1:97:A:LYS:O	1:78:A:VAL:HA	5	8.02
(4,148)	1:122:A:SER:OG	1:203:A:CYS:HA	4	8.0
(4,129)	1:122:A:SER:OG	1:47:A:SER:HA	3	8.0
(4,129)	1:122:A:SER:OG	1:47:A:SER:HA	6	8.0
(4,35)	1:58:A:GLN:NE2	1:119:A:ALA:HA	1	7.99
(4,7)	1:5:A:SER:OG	1:120:A:ASP:HA	7	7.99
(5,25)	1:58:A:GLN:NE2	1:119:A:ALA:HB1	1	7.93
(4,129)	1:122:A:SER:OG	1:47:A:SER:HA	5	7.93
(4,75)	1:97:A:LYS:O	1:28:A:ASN:H	5	7.91
(7,155)	1:124:A:ARG:O	1:114:A:THR:HA	3	7.87
(6,8)	1:97:A:LYS:O	1:29:A:PRO:CA	2	7.87
(5,52)	1:97:A:LYS:O	1:25:A:LEU:HD21	1	7.85
(4,87)	1:97:A:LYS:O	1:79:A:THR:H	1	7.85
(4,35)	1:58:A:GLN:NE2	1:119:A:ALA:HA	8	7.85
(5,5)	1:5:A:SER:OG	1:179:A:TYR:HB3	1	7.83
(4,35)	1:58:A:GLN:NE2	1:119:A:ALA:HA	7	7.8
(5,73)	1:122:A:SER:OG	1:176:A:TRP:HB3	8	7.71
(5,5)	1:5:A:SER:OG	1:179:A:TYR:HB2	10	7.69
(4,35)	1:58:A:GLN:NE2	1:119:A:ALA:HA	5	7.61
(4,96)	1:97:A:LYS:O	1:222:A:ARG:H	1	7.59
(13,6)	1:210:A:LYS:C	1:80:A:THR:CG2	6	7.57
(4,148)	1:122:A:SER:OG	1:203:A:CYS:HA	1	7.57
(4,148)	1:122:A:SER:OG	1:203:A:CYS:HA	9	7.57
(4,154)	1:122:A:SER:OG	1:182:A:VAL:HB	3	7.56
(5,4)	1:5:A:SER:OG	1:119:A:ALA:HB2	5	7.55
(13,6)	1:210:A:LYS:C	1:80:A:THR:CG2	5	7.52
(4,99)	1:97:A:LYS:O	1:78:A:VAL:HA	7	7.51
(5,61)	1:97:A:LYS:O	1:43:A:ILE:HG22	8	7.49
(4,58)	1:92:A:MET:O	1:144:A:TRP:HA	9	7.49
(4,35)	1:58:A:GLN:NE2	1:119:A:ALA:HA	2	7.44
(13,7)	1:210:A:LYS:C	1:179:A:TYR:CZ	8	7.43
(4,100)	1:97:A:LYS:O	1:79:A:THR:HA	2	7.42
(4,151)	1:122:A:SER:OG	1:78:A:VAL:HB	2	7.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,35)	1:58:A:GLN:NE2	1:119:A:ALA:HA	6	7.41
(13,6)	1:210:A:LYS:C	1:80:A:THR:CG2	1	7.36
(4,151)	1:122:A:SER:OG	1:78:A:VAL:HB	6	7.36
(4,112)	1:97:A:LYS:O	1:29:A:PRO:HB3	6	7.35
(4,57)	1:92:A:MET:O	1:142:A:ILE:HA	3	7.34
(13,6)	1:210:A:LYS:C	1:80:A:THR:CG2	2	7.33
(5,46)	1:92:A:MET:O	1:141:A:ILE:HG23	8	7.33
(4,58)	1:92:A:MET:O	1:144:A:TRP:HA	8	7.32
(4,97)	1:97:A:LYS:O	1:29:A:PRO:HA	9	7.31
(4,86)	1:97:A:LYS:O	1:43:A:ILE:H	5	7.31
(4,70)	1:92:A:MET:O	1:100:A:THR:HB	9	7.31
(4,11)	1:5:A:SER:OG	1:183:A:TRP:HA	6	7.31
(13,6)	1:210:A:LYS:C	1:80:A:THR:CG2	4	7.3
(4,86)	1:97:A:LYS:O	1:43:A:ILE:H	6	7.3
(4,58)	1:92:A:MET:O	1:144:A:TRP:HA	10	7.27
(4,53)	1:92:A:MET:O	1:43:A:ILE:HA	4	7.26
(4,35)	1:58:A:GLN:NE2	1:119:A:ALA:HA	9	7.22
(7,155)	1:124:A:ARG:O	1:114:A:THR:HA	10	7.21
(4,37)	1:58:A:GLN:NE2	1:124:A:ARG:HA	3	7.21
(4,6)	1:5:A:SER:OG	1:71:A:ALA:HA	10	7.21
(5,83)	1:124:A:ARG:O	1:179:A:TYR:HB3	7	7.19
(5,25)	1:58:A:GLN:NE2	1:119:A:ALA:HB1	9	7.19
(5,83)	1:124:A:ARG:O	1:179:A:TYR:HB3	2	7.15
(4,100)	1:97:A:LYS:O	1:79:A:THR:HA	1	7.14
(4,99)	1:97:A:LYS:O	1:78:A:VAL:HA	10	7.14
(4,86)	1:97:A:LYS:O	1:43:A:ILE:H	9	7.1
(4,7)	1:5:A:SER:OG	1:120:A:ASP:HA	2	7.09
(5,83)	1:124:A:ARG:O	1:179:A:TYR:HB3	8	7.08
(4,146)	1:122:A:SER:OG	1:182:A:VAL:HA	3	7.08
(4,99)	1:97:A:LYS:O	1:78:A:VAL:HA	9	7.08
(13,6)	1:210:A:LYS:C	1:80:A:THR:CG2	3	7.07
(4,99)	1:97:A:LYS:O	1:78:A:VAL:HA	3	7.06
(4,67)	1:92:A:MET:O	1:78:A:VAL:HB	7	7.06
(5,5)	1:5:A:SER:OG	1:179:A:TYR:HB3	6	7.03
(4,97)	1:97:A:LYS:O	1:29:A:PRO:HA	7	7.03
(4,151)	1:122:A:SER:OG	1:78:A:VAL:HB	1	7.02
(5,53)	1:97:A:LYS:O	1:43:A:ILE:HD12	4	6.99
(4,58)	1:92:A:MET:O	1:144:A:TRP:HA	7	6.99
(5,25)	1:58:A:GLN:NE2	1:119:A:ALA:HB1	3	6.98
(6,8)	1:97:A:LYS:O	1:29:A:PRO:CA	9	6.97
(4,58)	1:92:A:MET:O	1:144:A:TRP:HA	3	6.97
(4,86)	1:97:A:LYS:O	1:43:A:ILE:H	3	6.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(13,7)	1:210:A:LYS:C	1:179:A:TYR:CZ	10	6.93
(13,6)	1:210:A:LYS:C	1:80:A:THR:CG2	10	6.92
(4,67)	1:92:A:MET:O	1:78:A:VAL:HB	5	6.92
(5,25)	1:58:A:GLN:NE2	1:119:A:ALA:HB1	10	6.9
(4,11)	1:5:A:SER:OG	1:183:A:TRP:HA	9	6.9
(4,151)	1:122:A:SER:OG	1:78:A:VAL:HB	5	6.89
(13,6)	1:210:A:LYS:C	1:80:A:THR:CG2	7	6.88
(5,61)	1:97:A:LYS:O	1:43:A:ILE:HG13	4	6.88
(4,99)	1:97:A:LYS:O	1:78:A:VAL:HA	4	6.88
(4,97)	1:97:A:LYS:O	1:29:A:PRO:HA	3	6.87
(4,11)	1:5:A:SER:OG	1:183:A:TRP:HA	10	6.87
(7,155)	1:124:A:ARG:O	1:114:A:THR:HA	1	6.85
(4,154)	1:122:A:SER:OG	1:182:A:VAL:HB	8	6.85
(4,96)	1:97:A:LYS:O	1:222:A:ARG:H	10	6.85
(4,58)	1:92:A:MET:O	1:144:A:TRP:HA	5	6.85
(7,155)	1:124:A:ARG:O	1:114:A:THR:HA	8	6.84
(4,11)	1:5:A:SER:OG	1:183:A:TRP:HA	3	6.84
(4,151)	1:122:A:SER:OG	1:78:A:VAL:HB	4	6.83
(4,86)	1:97:A:LYS:O	1:43:A:ILE:H	10	6.78
(5,73)	1:122:A:SER:OG	1:176:A:TRP:HB3	10	6.74
(4,92)	1:97:A:LYS:O	1:111:A:VAL:H	5	6.72
(13,6)	1:210:A:LYS:C	1:80:A:THR:CG2	8	6.7
(5,5)	1:5:A:SER:OG	1:179:A:TYR:HB3	9	6.7
(7,155)	1:124:A:ARG:O	1:114:A:THR:HA	5	6.68
(5,25)	1:58:A:GLN:NE2	1:119:A:ALA:HB2	7	6.68
(4,7)	1:5:A:SER:OG	1:120:A:ASP:HA	4	6.68
(7,155)	1:124:A:ARG:O	1:114:A:THR:HA	7	6.66
(4,86)	1:97:A:LYS:O	1:43:A:ILE:H	7	6.66
(4,151)	1:122:A:SER:OG	1:78:A:VAL:HB	8	6.62
(4,94)	1:97:A:LYS:O	1:145:A:GLY:H	3	6.6
(4,80)	1:97:A:LYS:O	1:145:A:GLY:H	3	6.6
(5,37)	1:92:A:MET:O	1:44:A:PRO:HD3	4	6.59
(6,8)	1:97:A:LYS:O	1:29:A:PRO:CA	3	6.56
(4,151)	1:122:A:SER:OG	1:78:A:VAL:HB	7	6.56
(5,34)	1:92:A:MET:O	1:29:A:PRO:HD2	4	6.54
(5,83)	1:124:A:ARG:O	1:179:A:TYR:HB3	6	6.52
(4,151)	1:122:A:SER:OG	1:78:A:VAL:HB	10	6.51
(4,85)	1:97:A:LYS:O	1:31:A:GLY:H	4	6.5
(4,57)	1:92:A:MET:O	1:142:A:ILE:HA	7	6.49
(4,43)	1:92:A:MET:O	1:145:A:GLY:H	3	6.49
(5,73)	1:122:A:SER:OG	1:176:A:TRP:HB3	5	6.47
(4,58)	1:92:A:MET:O	1:144:A:TRP:HA	2	6.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,73)	1:122:A:SER:OG	1:176:A:TRP:HB3	1	6.42
(5,73)	1:122:A:SER:OG	1:176:A:TRP:HB3	3	6.42
(5,44)	1:92:A:MET:O	1:78:A:VAL:HG23	4	6.41
(4,146)	1:122:A:SER:OG	1:182:A:VAL:HA	8	6.4
(7,155)	1:124:A:ARG:O	1:114:A:THR:HA	9	6.38
(4,105)	1:97:A:LYS:O	1:110:A:ILE:HA	5	6.38
(4,67)	1:92:A:MET:O	1:78:A:VAL:HB	10	6.37
(4,11)	1:5:A:SER:OG	1:183:A:TRP:HA	4	6.35
(5,25)	1:58:A:GLN:NE2	1:119:A:ALA:HB2	5	6.33
(4,43)	1:92:A:MET:O	1:145:A:GLY:H	9	6.3
(4,58)	1:92:A:MET:O	1:144:A:TRP:HA	1	6.29
(5,73)	1:122:A:SER:OG	1:176:A:TRP:HB3	7	6.28
(4,151)	1:122:A:SER:OG	1:78:A:VAL:HB	9	6.28
(6,8)	1:97:A:LYS:O	1:29:A:PRO:CA	7	6.26
(4,6)	1:5:A:SER:OG	1:71:A:ALA:HA	6	6.25
(4,43)	1:92:A:MET:O	1:145:A:GLY:H	10	6.24
(5,24)	1:58:A:GLN:NE2	1:64:A:ALA:HB2	8	6.23
(5,73)	1:122:A:SER:OG	1:176:A:TRP:HB3	2	6.22
(5,53)	1:97:A:LYS:O	1:43:A:ILE:HD11	3	6.21
(4,70)	1:92:A:MET:O	1:100:A:THR:HB	8	6.21
(4,57)	1:92:A:MET:O	1:142:A:ILE:HA	5	6.21
(4,57)	1:92:A:MET:O	1:142:A:ILE:HA	9	6.2
(5,61)	1:97:A:LYS:O	1:43:A:ILE:HG13	5	6.19
(5,25)	1:58:A:GLN:NE2	1:119:A:ALA:HB1	6	6.19
(4,125)	1:122:A:SER:OG	1:193:A:ILE:H	3	6.19
(4,43)	1:92:A:MET:O	1:145:A:GLY:H	2	6.19
(4,112)	1:97:A:LYS:O	1:29:A:PRO:HB3	2	6.18
(4,43)	1:92:A:MET:O	1:145:A:GLY:H	7	6.17
(7,155)	1:124:A:ARG:O	1:114:A:THR:HA	2	6.13
(4,67)	1:92:A:MET:O	1:78:A:VAL:HB	9	6.12
(4,111)	1:97:A:LYS:O	1:161:A:LEU:HA	4	6.1
(5,7)	1:5:A:SER:OG	1:58:A:GLN:HG2	10	6.09
(5,83)	1:124:A:ARG:O	1:179:A:TYR:HB3	9	6.05
(4,94)	1:97:A:LYS:O	1:145:A:GLY:H	5	6.05
(4,80)	1:97:A:LYS:O	1:145:A:GLY:H	5	6.05
(5,53)	1:97:A:LYS:O	1:43:A:ILE:HD13	2	6.03
(4,99)	1:97:A:LYS:O	1:78:A:VAL:HA	6	6.03
(4,67)	1:92:A:MET:O	1:78:A:VAL:HB	3	6.03
(4,70)	1:92:A:MET:O	1:100:A:THR:HB	10	6.02
(5,25)	1:58:A:GLN:NE2	1:119:A:ALA:HB1	2	5.99
(5,73)	1:122:A:SER:OG	1:176:A:TRP:HB3	6	5.91
(4,86)	1:97:A:LYS:O	1:43:A:ILE:H	2	5.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,32)	1:58:A:GLN:NE2	1:64:A:ALA:HA	8	5.85
(4,57)	1:92:A:MET:O	1:142:A:ILE:HA	2	5.84
(4,57)	1:92:A:MET:O	1:142:A:ILE:HA	10	5.82
(4,36)	1:58:A:GLN:NE2	1:120:A:ASP:HA	8	5.81
(5,5)	1:5:A:SER:OG	1:179:A:TYR:HB3	7	5.8
(5,61)	1:97:A:LYS:O	1:43:A:ILE:HG12	9	5.78
(4,70)	1:92:A:MET:O	1:100:A:THR:HB	6	5.78
(7,155)	1:124:A:ARG:O	1:114:A:THR:HA	4	5.76
(5,24)	1:58:A:GLN:NE2	1:64:A:ALA:HB2	1	5.75
(4,97)	1:97:A:LYS:O	1:29:A:PRO:HA	10	5.74
(4,43)	1:92:A:MET:O	1:145:A:GLY:H	5	5.74
(4,32)	1:58:A:GLN:NE2	1:64:A:ALA:HA	1	5.73
(7,190)	1:124:A:ARG:O	1:76:A:TRP:CG	3	5.72
(4,94)	1:97:A:LYS:O	1:145:A:GLY:H	7	5.71
(4,80)	1:97:A:LYS:O	1:145:A:GLY:H	7	5.71
(5,61)	1:97:A:LYS:O	1:43:A:ILE:HG12	3	5.66
(4,154)	1:122:A:SER:OG	1:182:A:VAL:HB	2	5.66
(4,67)	1:92:A:MET:O	1:78:A:VAL:HB	1	5.66
(5,73)	1:122:A:SER:OG	1:176:A:TRP:HB3	9	5.64
(5,24)	1:58:A:GLN:NE2	1:64:A:ALA:HB1	7	5.64
(4,99)	1:97:A:LYS:O	1:78:A:VAL:HA	2	5.62
(6,6)	1:92:A:MET:O	1:100:A:THR:CA	9	5.61
(5,61)	1:97:A:LYS:O	1:43:A:ILE:HG13	6	5.6
(4,92)	1:97:A:LYS:O	1:111:A:VAL:H	3	5.59
(5,83)	1:124:A:ARG:O	1:179:A:TYR:HB2	3	5.57
(4,111)	1:97:A:LYS:O	1:161:A:LEU:HA	7	5.56
(4,56)	1:92:A:MET:O	1:100:A:THR:HA	7	5.56
(4,146)	1:122:A:SER:OG	1:182:A:VAL:HA	2	5.55
(4,5)	1:5:A:SER:OG	1:69:A:HIS:HA	10	5.52
(4,67)	1:92:A:MET:O	1:78:A:VAL:HB	6	5.51
(4,112)	1:97:A:LYS:O	1:29:A:PRO:HB3	7	5.5
(4,154)	1:122:A:SER:OG	1:182:A:VAL:HB	7	5.49
(4,32)	1:58:A:GLN:NE2	1:64:A:ALA:HA	5	5.47
(4,105)	1:97:A:LYS:O	1:110:A:ILE:HA	3	5.46
(5,5)	1:5:A:SER:OG	1:179:A:TYR:HB3	3	5.45
(4,151)	1:122:A:SER:OG	1:78:A:VAL:HB	3	5.45
(5,61)	1:97:A:LYS:O	1:43:A:ILE:HG23	7	5.44
(5,53)	1:97:A:LYS:O	1:43:A:ILE:HD12	1	5.44
(4,67)	1:92:A:MET:O	1:78:A:VAL:HB	2	5.44
(4,7)	1:5:A:SER:OG	1:120:A:ASP:HA	5	5.44
(5,78)	1:122:A:SER:OG	1:180:A:PRO:HD3	8	5.43
(4,111)	1:97:A:LYS:O	1:161:A:LEU:HA	9	5.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,74)	1:92:A:MET:O	1:79:A:THR:HA	4	5.43
(4,58)	1:92:A:MET:O	1:144:A:TRP:HA	6	5.43
(4,55)	1:92:A:MET:O	1:79:A:THR:HA	4	5.43
(4,57)	1:92:A:MET:O	1:142:A:ILE:HA	1	5.42
(4,56)	1:92:A:MET:O	1:100:A:THR:HA	9	5.42
(4,85)	1:97:A:LYS:O	1:31:A:GLY:H	6	5.41
(4,29)	1:58:A:GLN:NE2	1:120:A:ASP:H	8	5.41
(5,8)	1:5:A:SER:OG	1:62:A:GLU:HG2	7	5.4
(4,43)	1:92:A:MET:O	1:145:A:GLY:H	1	5.4
(4,32)	1:58:A:GLN:NE2	1:64:A:ALA:HA	7	5.4
(4,32)	1:58:A:GLN:NE2	1:64:A:ALA:HA	10	5.38
(4,5)	1:5:A:SER:OG	1:69:A:HIS:HA	8	5.38
(13,9)	1:210:A:LYS:C	1:80:A:THR:CB	2	5.37
(5,53)	1:97:A:LYS:O	1:43:A:ILE:HD11	9	5.37
(5,24)	1:58:A:GLN:NE2	1:64:A:ALA:HB2	9	5.36
(4,154)	1:122:A:SER:OG	1:182:A:VAL:HB	5	5.34
(4,36)	1:58:A:GLN:NE2	1:120:A:ASP:HA	4	5.34
(4,32)	1:58:A:GLN:NE2	1:64:A:ALA:HA	2	5.34
(4,6)	1:5:A:SER:OG	1:71:A:ALA:HA	9	5.32
(4,92)	1:97:A:LYS:O	1:111:A:VAL:H	8	5.31
(4,154)	1:122:A:SER:OG	1:182:A:VAL:HB	10	5.3
(5,61)	1:97:A:LYS:O	1:43:A:ILE:HG12	10	5.29
(4,112)	1:97:A:LYS:O	1:29:A:PRO:HB3	9	5.29
(4,105)	1:97:A:LYS:O	1:110:A:ILE:HA	10	5.29
(4,56)	1:92:A:MET:O	1:100:A:THR:HA	8	5.29
(6,8)	1:97:A:LYS:O	1:29:A:PRO:CA	10	5.27
(7,155)	1:124:A:ARG:O	1:114:A:THR:HA	6	5.26
(4,110)	1:97:A:LYS:O	1:158:A:SER:HA	6	5.25
(4,105)	1:97:A:LYS:O	1:110:A:ILE:HA	9	5.25
(4,92)	1:97:A:LYS:O	1:111:A:VAL:H	10	5.25
(5,24)	1:58:A:GLN:NE2	1:64:A:ALA:HB2	10	5.24
(4,43)	1:92:A:MET:O	1:145:A:GLY:H	8	5.23
(4,97)	1:97:A:LYS:O	1:29:A:PRO:HA	1	5.2
(4,92)	1:97:A:LYS:O	1:111:A:VAL:H	7	5.18
(4,85)	1:97:A:LYS:O	1:31:A:GLY:H	2	5.18
(4,42)	1:92:A:MET:O	1:100:A:THR:H	9	5.18
(5,8)	1:5:A:SER:OG	1:62:A:GLU:HG3	6	5.17
(4,154)	1:122:A:SER:OG	1:182:A:VAL:HB	9	5.14
(6,6)	1:92:A:MET:O	1:100:A:THR:CA	8	5.11
(4,70)	1:92:A:MET:O	1:100:A:THR:HB	7	5.11
(4,54)	1:92:A:MET:O	1:44:A:PRO:HA	5	5.11
(4,56)	1:92:A:MET:O	1:100:A:THR:HA	6	5.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,53)	1:97:A:LYS:O	1:43:A:ILE:HD12	10	5.07
(4,29)	1:58:A:GLN:NE2	1:120:A:ASP:H	4	5.07
(4,105)	1:97:A:LYS:O	1:110:A:ILE:HA	8	5.06
(4,105)	1:97:A:LYS:O	1:110:A:ILE:HA	7	5.04
(4,94)	1:97:A:LYS:O	1:145:A:GLY:H	10	5.04
(4,80)	1:97:A:LYS:O	1:145:A:GLY:H	10	5.04
(4,57)	1:92:A:MET:O	1:142:A:ILE:HA	6	5.03
(4,29)	1:58:A:GLN:NE2	1:120:A:ASP:H	3	5.03
(13,9)	1:210:A:LYS:C	1:80:A:THR:CB	7	5.02
(7,189)	1:124:A:ARG:O	1:76:A:TRP:HD1	10	5.02
(13,7)	1:210:A:LYS:C	1:179:A:TYR:CZ	1	5.0
(5,8)	1:5:A:SER:OG	1:62:A:GLU:HG3	2	5.0
(4,146)	1:122:A:SER:OG	1:182:A:VAL:HA	7	5.0
(4,36)	1:58:A:GLN:NE2	1:120:A:ASP:HA	3	5.0
(13,9)	1:210:A:LYS:C	1:80:A:THR:CB	9	4.99
(4,146)	1:122:A:SER:OG	1:182:A:VAL:HA	9	4.98
(4,92)	1:97:A:LYS:O	1:111:A:VAL:H	9	4.98
(6,11)	1:158:A:SER:OG	1:148:A:ASN:CA	2	4.97
(5,49)	1:92:A:MET:O	1:177:A:ILE:HG12	4	4.97
(4,11)	1:5:A:SER:OG	1:183:A:TRP:HA	7	4.97
(4,146)	1:122:A:SER:OG	1:182:A:VAL:HA	5	4.94
(4,107)	1:97:A:LYS:O	1:149:A:PRO:HA	7	4.94
(5,5)	1:5:A:SER:OG	1:179:A:TYR:HB3	4	4.93
(4,113)	1:97:A:LYS:O	1:32:A:VAL:HB	8	4.93
(4,111)	1:97:A:LYS:O	1:161:A:LEU:HA	3	4.93
(7,190)	1:124:A:ARG:O	1:76:A:TRP:CG	10	4.92
(5,24)	1:58:A:GLN:NE2	1:64:A:ALA:HB2	5	4.91
(4,94)	1:97:A:LYS:O	1:145:A:GLY:H	1	4.91
(4,80)	1:97:A:LYS:O	1:145:A:GLY:H	1	4.91
(4,70)	1:92:A:MET:O	1:100:A:THR:HB	3	4.91
(5,78)	1:122:A:SER:OG	1:180:A:PRO:HD3	10	4.9
(4,107)	1:97:A:LYS:O	1:149:A:PRO:HA	3	4.9
(4,125)	1:122:A:SER:OG	1:193:A:ILE:H	7	4.88
(13,9)	1:210:A:LYS:C	1:80:A:THR:CB	5	4.87
(6,11)	1:158:A:SER:OG	1:148:A:ASN:CA	6	4.86
(4,114)	1:97:A:LYS:O	1:39:A:VAL:HB	8	4.86
(4,95)	1:97:A:LYS:O	1:146:A:ILE:H	3	4.86
(4,81)	1:97:A:LYS:O	1:146:A:ILE:H	3	4.86
(4,32)	1:58:A:GLN:NE2	1:64:A:ALA:HA	3	4.86
(4,99)	1:97:A:LYS:O	1:78:A:VAL:HA	1	4.84
(4,85)	1:97:A:LYS:O	1:31:A:GLY:H	8	4.81
(1,74)	1:45:A:ILE:HG23	1:49:A:LEU:HD13	2	4.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,112)	1:97:A:LYS:O	1:29:A:PRO:HB3	3	4.8
(4,146)	1:122:A:SER:OG	1:182:A:VAL:HA	10	4.79
(4,54)	1:92:A:MET:O	1:44:A:PRO:HA	10	4.79
(13,7)	1:210:A:LYS:C	1:179:A:TYR:CZ	3	4.77
(4,70)	1:92:A:MET:O	1:100:A:THR:HB	1	4.76
(4,97)	1:97:A:LYS:O	1:29:A:PRO:HA	5	4.75
(4,50)	1:92:A:MET:O	1:39:A:VAL:HA	4	4.75
(4,29)	1:58:A:GLN:NE2	1:120:A:ASP:H	10	4.74
(4,74)	1:92:A:MET:O	1:79:A:THR:HA	5	4.72
(4,55)	1:92:A:MET:O	1:79:A:THR:HA	5	4.72
(13,9)	1:210:A:LYS:C	1:80:A:THR:CB	1	4.71
(5,53)	1:97:A:LYS:O	1:43:A:ILE:HD13	5	4.71
(4,54)	1:92:A:MET:O	1:44:A:PRO:HA	3	4.71
(4,152)	1:122:A:SER:OG	1:111:A:VAL:HB	6	4.7
(4,43)	1:92:A:MET:O	1:145:A:GLY:H	6	4.7
(6,6)	1:92:A:MET:O	1:100:A:THR:CA	7	4.69
(13,9)	1:210:A:LYS:C	1:80:A:THR:CB	8	4.68
(4,26)	1:58:A:GLN:NE2	1:65:A:GLY:H	6	4.68
(5,44)	1:92:A:MET:O	1:78:A:VAL:HG21	7	4.67
(13,7)	1:210:A:LYS:C	1:179:A:TYR:CZ	7	4.66
(5,78)	1:122:A:SER:OG	1:180:A:PRO:HD3	3	4.65
(6,11)	1:158:A:SER:OG	1:148:A:ASN:CA	8	4.64
(5,78)	1:122:A:SER:OG	1:180:A:PRO:HD3	5	4.64
(4,32)	1:58:A:GLN:NE2	1:64:A:ALA:HA	9	4.64
(6,11)	1:158:A:SER:OG	1:148:A:ASN:CA	10	4.63
(6,8)	1:97:A:LYS:O	1:29:A:PRO:CA	1	4.63
(4,95)	1:97:A:LYS:O	1:146:A:ILE:H	5	4.63
(4,81)	1:97:A:LYS:O	1:146:A:ILE:H	5	4.63
(13,7)	1:210:A:LYS:C	1:179:A:TYR:CZ	4	4.62
(1,74)	1:45:A:ILE:HG22	1:49:A:LEU:HD12	4	4.61
(13,7)	1:210:A:LYS:C	1:179:A:TYR:CZ	6	4.58
(4,85)	1:97:A:LYS:O	1:31:A:GLY:H	9	4.58
(4,26)	1:58:A:GLN:NE2	1:65:A:GLY:H	1	4.58
(4,51)	1:92:A:MET:O	1:40:A:ALA:HA	4	4.57
(4,36)	1:58:A:GLN:NE2	1:120:A:ASP:HA	1	4.57
(4,29)	1:58:A:GLN:NE2	1:120:A:ASP:H	1	4.57
(5,83)	1:124:A:ARG:O	1:179:A:TYR:HB3	1	4.53
(5,44)	1:92:A:MET:O	1:78:A:VAL:HG22	5	4.53
(6,6)	1:92:A:MET:O	1:100:A:THR:CA	6	4.52
(4,111)	1:97:A:LYS:O	1:161:A:LEU:HA	6	4.52
(4,11)	1:5:A:SER:OG	1:183:A:TRP:HA	5	4.52
(13,9)	1:210:A:LYS:C	1:80:A:THR:CB	6	4.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,26)	1:58:A:GLN:NE2	1:65:A:GLY:H	2	4.51
(4,154)	1:122:A:SER:OG	1:182:A:VAL:HB	6	4.5
(4,6)	1:5:A:SER:OG	1:71:A:ALA:HA	8	4.49
(6,11)	1:158:A:SER:OG	1:148:A:ASN:CA	7	4.48
(4,32)	1:58:A:GLN:NE2	1:64:A:ALA:HA	6	4.48
(4,94)	1:97:A:LYS:O	1:145:A:GLY:H	9	4.46
(4,80)	1:97:A:LYS:O	1:145:A:GLY:H	9	4.46
(7,190)	1:124:A:ARG:O	1:76:A:TRP:CG	8	4.44
(13,9)	1:210:A:LYS:C	1:80:A:THR:CB	10	4.42
(13,7)	1:210:A:LYS:C	1:179:A:TYR:CZ	2	4.42
(4,57)	1:92:A:MET:O	1:142:A:ILE:HA	8	4.42
(4,32)	1:58:A:GLN:NE2	1:64:A:ALA:HA	4	4.42
(4,29)	1:58:A:GLN:NE2	1:120:A:ASP:H	7	4.42
(4,56)	1:92:A:MET:O	1:100:A:THR:HA	3	4.41
(4,36)	1:58:A:GLN:NE2	1:120:A:ASP:HA	10	4.41
(13,9)	1:210:A:LYS:C	1:80:A:THR:CB	3	4.4
(5,73)	1:122:A:SER:OG	1:176:A:TRP:HB3	4	4.4
(4,146)	1:122:A:SER:OG	1:182:A:VAL:HA	6	4.38
(7,189)	1:124:A:ARG:O	1:76:A:TRP:HD1	3	4.36
(5,24)	1:58:A:GLN:NE2	1:64:A:ALA:HB2	3	4.36
(5,56)	1:97:A:LYS:O	1:165:A:TYR:HD1	4	4.35
(5,8)	1:5:A:SER:OG	1:62:A:GLU:HG3	3	4.34
(4,113)	1:97:A:LYS:O	1:32:A:VAL:HB	4	4.34
(5,61)	1:97:A:LYS:O	1:43:A:ILE:HG21	2	4.32
(4,95)	1:97:A:LYS:O	1:146:A:ILE:H	7	4.3
(4,81)	1:97:A:LYS:O	1:146:A:ILE:H	7	4.3
(7,48)	1:26:A:SER:OG	1:12:A:VAL:HA	5	4.29
(7,12)	1:26:A:SER:OG	1:12:A:VAL:HA	5	4.29
(4,26)	1:58:A:GLN:NE2	1:65:A:GLY:H	8	4.29
(4,6)	1:5:A:SER:OG	1:71:A:ALA:HA	1	4.29
(4,29)	1:58:A:GLN:NE2	1:120:A:ASP:H	6	4.27
(5,2)	1:5:A:SER:OG	1:60:A:LYS:HB2	10	4.26
(5,78)	1:122:A:SER:OG	1:180:A:PRO:HD3	7	4.25
(2,633)	1:92:A:MET:CE	1:95:A:ILE:CD1	8	4.24
(4,111)	1:97:A:LYS:O	1:161:A:LEU:HA	1	4.23
(4,67)	1:92:A:MET:O	1:78:A:VAL:HB	8	4.23
(4,85)	1:97:A:LYS:O	1:31:A:GLY:H	3	4.22
(13,7)	1:210:A:LYS:C	1:179:A:TYR:CZ	9	4.21
(4,29)	1:58:A:GLN:NE2	1:120:A:ASP:H	5	4.21
(4,146)	1:122:A:SER:OG	1:182:A:VAL:HA	1	4.2
(4,36)	1:58:A:GLN:NE2	1:120:A:ASP:HA	2	4.2
(4,29)	1:58:A:GLN:NE2	1:120:A:ASP:H	2	4.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,74)	1:92:A:MET:O	1:79:A:THR:HA	10	4.19
(4,55)	1:92:A:MET:O	1:79:A:THR:HA	10	4.19
(4,44)	1:92:A:MET:O	1:146:A:ILE:H	3	4.19
(4,107)	1:97:A:LYS:O	1:149:A:PRO:HA	10	4.18
(4,36)	1:58:A:GLN:NE2	1:120:A:ASP:HA	5	4.18
(13,9)	1:210:A:LYS:C	1:80:A:THR:CB	4	4.16
(4,27)	1:58:A:GLN:NE2	1:66:A:GLN:H	10	4.13
(7,189)	1:124:A:ARG:O	1:76:A:TRP:HD1	5	4.12
(4,44)	1:92:A:MET:O	1:146:A:ILE:H	9	4.12
(4,42)	1:92:A:MET:O	1:100:A:THR:H	6	4.12
(6,8)	1:97:A:LYS:O	1:29:A:PRO:CA	5	4.1
(4,42)	1:92:A:MET:O	1:100:A:THR:H	8	4.09
(7,190)	1:124:A:ARG:O	1:76:A:TRP:CG	5	4.08
(7,13)	1:26:A:SER:OG	1:13:A:ALA:HA	5	4.07
(6,11)	1:158:A:SER:OG	1:148:A:ASN:CA	3	4.07
(1,419)	1:181:A:ILE:HG22	1:185:A:ILE:HD11	8	4.07
(5,36)	1:92:A:MET:O	1:43:A:ILE:HD11	7	4.06
(5,5)	1:5:A:SER:OG	1:179:A:TYR:HB2	5	4.06
(5,24)	1:58:A:GLN:NE2	1:64:A:ALA:HB1	6	4.05
(4,27)	1:58:A:GLN:NE2	1:66:A:GLN:H	8	4.05
(5,36)	1:92:A:MET:O	1:43:A:ILE:HD11	4	4.0
(4,74)	1:92:A:MET:O	1:79:A:THR:HA	3	4.0
(4,55)	1:92:A:MET:O	1:79:A:THR:HA	3	4.0
(4,36)	1:58:A:GLN:NE2	1:120:A:ASP:HA	7	4.0
(6,6)	1:92:A:MET:O	1:100:A:THR:CA	3	3.99
(4,154)	1:122:A:SER:OG	1:182:A:VAL:HB	1	3.99
(4,27)	1:58:A:GLN:NE2	1:66:A:GLN:H	1	3.99
(4,74)	1:92:A:MET:O	1:79:A:THR:HA	1	3.98
(4,55)	1:92:A:MET:O	1:79:A:THR:HA	1	3.98
(4,42)	1:92:A:MET:O	1:100:A:THR:H	7	3.98
(4,110)	1:97:A:LYS:O	1:158:A:SER:HA	3	3.97
(4,74)	1:92:A:MET:O	1:79:A:THR:HA	7	3.97
(4,55)	1:92:A:MET:O	1:79:A:THR:HA	7	3.97
(6,6)	1:92:A:MET:O	1:100:A:THR:CA	10	3.96
(5,53)	1:97:A:LYS:O	1:43:A:ILE:HD12	6	3.96
(4,152)	1:122:A:SER:OG	1:111:A:VAL:HB	5	3.96
(4,54)	1:92:A:MET:O	1:44:A:PRO:HA	6	3.96
(4,95)	1:97:A:LYS:O	1:146:A:ILE:H	10	3.95
(4,81)	1:97:A:LYS:O	1:146:A:ILE:H	10	3.95
(4,42)	1:92:A:MET:O	1:100:A:THR:H	10	3.94
(4,26)	1:58:A:GLN:NE2	1:65:A:GLY:H	5	3.94
(5,44)	1:92:A:MET:O	1:78:A:VAL:HG22	10	3.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,5)	1:5:A:SER:OG	1:179:A:TYR:HB3	2	3.93
(4,44)	1:92:A:MET:O	1:146:A:ILE:H	10	3.92
(4,6)	1:5:A:SER:OG	1:71:A:ALA:HA	3	3.92
(5,24)	1:58:A:GLN:NE2	1:64:A:ALA:HB2	2	3.91
(5,55)	1:97:A:LYS:O	1:149:A:PRO:HD2	3	3.9
(4,108)	1:97:A:LYS:O	1:156:A:THR:HA	6	3.9
(4,101)	1:97:A:LYS:O	1:91:A:ALA:HA	6	3.9
(4,114)	1:97:A:LYS:O	1:39:A:VAL:HB	4	3.88
(4,27)	1:58:A:GLN:NE2	1:66:A:GLN:H	2	3.88
(5,55)	1:97:A:LYS:O	1:149:A:PRO:HD2	7	3.87
(7,13)	1:26:A:SER:OG	1:13:A:ALA:HA	8	3.86
(4,152)	1:122:A:SER:OG	1:111:A:VAL:HB	2	3.86
(4,112)	1:97:A:LYS:O	1:29:A:PRO:HB3	10	3.86
(4,44)	1:92:A:MET:O	1:146:A:ILE:H	7	3.86
(4,110)	1:97:A:LYS:O	1:158:A:SER:HA	4	3.85
(4,29)	1:58:A:GLN:NE2	1:120:A:ASP:H	9	3.85
(4,86)	1:97:A:LYS:O	1:43:A:ILE:H	1	3.84
(5,7)	1:5:A:SER:OG	1:58:A:GLN:HG3	6	3.83
(4,70)	1:92:A:MET:O	1:100:A:THR:HB	2	3.83
(6,11)	1:158:A:SER:OG	1:148:A:ASN:CA	9	3.82
(5,7)	1:5:A:SER:OG	1:58:A:GLN:HG3	9	3.82
(5,29)	1:92:A:MET:O	1:40:A:ALA:HB2	4	3.77
(4,152)	1:122:A:SER:OG	1:111:A:VAL:HB	7	3.77
(5,44)	1:92:A:MET:O	1:78:A:VAL:HG21	3	3.71
(5,43)	1:92:A:MET:O	1:43:A:ILE:HG13	4	3.71
(5,28)	1:92:A:MET:O	1:29:A:PRO:HB2	4	3.71
(7,190)	1:124:A:ARG:O	1:76:A:TRP:CG	1	3.68
(4,74)	1:92:A:MET:O	1:79:A:THR:HA	9	3.68
(4,55)	1:92:A:MET:O	1:79:A:THR:HA	9	3.68
(4,53)	1:92:A:MET:O	1:43:A:ILE:HA	7	3.68
(8,110)	1:124:A:ARG:O	1:75:A:ASP:HB2	3	3.67
(4,108)	1:97:A:LYS:O	1:156:A:THR:HA	3	3.66
(4,27)	1:58:A:GLN:NE2	1:66:A:GLN:H	5	3.65
(4,5)	1:5:A:SER:OG	1:69:A:HIS:HA	9	3.65
(5,44)	1:92:A:MET:O	1:78:A:VAL:HG22	9	3.64
(2,804)	1:127:A:VAL:CG2	1:124:A:ARG:CZ	3	3.63
(4,92)	1:97:A:LYS:O	1:111:A:VAL:H	1	3.59
(4,44)	1:92:A:MET:O	1:146:A:ILE:H	8	3.59
(4,27)	1:58:A:GLN:NE2	1:66:A:GLN:H	3	3.59
(2,633)	1:92:A:MET:CE	1:95:A:ILE:CD1	1	3.59
(5,69)	1:122:A:SER:OG	1:75:A:ASP:HB3	4	3.58
(4,95)	1:97:A:LYS:O	1:146:A:ILE:H	9	3.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,81)	1:97:A:LYS:O	1:146:A:ILE:H	9	3.58
(4,44)	1:92:A:MET:O	1:146:A:ILE:H	2	3.57
(4,115)	1:97:A:LYS:O	1:154:A:THR:HB	4	3.56
(4,26)	1:58:A:GLN:NE2	1:65:A:GLY:H	7	3.55
(4,152)	1:122:A:SER:OG	1:111:A:VAL:HB	10	3.54
(4,36)	1:58:A:GLN:NE2	1:120:A:ASP:HA	9	3.54
(5,8)	1:5:A:SER:OG	1:62:A:GLU:HG3	1	3.52
(5,8)	1:5:A:SER:OG	1:62:A:GLU:HG3	4	3.52
(4,26)	1:58:A:GLN:NE2	1:65:A:GLY:H	4	3.52
(7,190)	1:124:A:ARG:O	1:76:A:TRP:CG	9	3.51
(5,76)	1:122:A:SER:OG	1:113:A:ILE:HD12	6	3.51
(5,56)	1:97:A:LYS:O	1:165:A:TYR:HD2	3	3.5
(4,110)	1:97:A:LYS:O	1:158:A:SER:HA	7	3.5
(4,101)	1:97:A:LYS:O	1:91:A:ALA:HA	9	3.49
(4,6)	1:5:A:SER:OG	1:71:A:ALA:HA	2	3.48
(4,26)	1:58:A:GLN:NE2	1:65:A:GLY:H	10	3.46
(7,13)	1:26:A:SER:OG	1:13:A:ALA:HA	7	3.45
(4,54)	1:92:A:MET:O	1:44:A:PRO:HA	9	3.45
(4,28)	1:58:A:GLN:NE2	1:78:A:VAL:H	6	3.45
(5,44)	1:92:A:MET:O	1:78:A:VAL:HG22	1	3.44
(4,82)	1:97:A:LYS:O	1:155:A:ARG:H	4	3.44
(4,74)	1:92:A:MET:O	1:79:A:THR:HA	2	3.44
(4,55)	1:92:A:MET:O	1:79:A:THR:HA	2	3.44
(4,107)	1:97:A:LYS:O	1:149:A:PRO:HA	1	3.43
(5,83)	1:124:A:ARG:O	1:179:A:TYR:HB3	4	3.42
(5,69)	1:122:A:SER:OG	1:75:A:ASP:HB3	3	3.42
(5,55)	1:97:A:LYS:O	1:149:A:PRO:HD2	10	3.42
(4,56)	1:92:A:MET:O	1:100:A:THR:HA	10	3.42
(4,44)	1:92:A:MET:O	1:146:A:ILE:H	5	3.42
(4,125)	1:122:A:SER:OG	1:193:A:ILE:H	1	3.41
(4,110)	1:97:A:LYS:O	1:158:A:SER:HA	1	3.41
(4,54)	1:92:A:MET:O	1:44:A:PRO:HA	7	3.41
(4,11)	1:5:A:SER:OG	1:183:A:TRP:HA	2	3.41
(5,69)	1:122:A:SER:OG	1:75:A:ASP:HB3	7	3.4
(4,152)	1:122:A:SER:OG	1:111:A:VAL:HB	9	3.39
(1,419)	1:181:A:ILE:HG23	1:185:A:ILE:HD13	4	3.37
(5,55)	1:97:A:LYS:O	1:149:A:PRO:HD2	9	3.36
(4,105)	1:97:A:LYS:O	1:110:A:ILE:HA	4	3.36
(7,48)	1:26:A:SER:OG	1:12:A:VAL:HA	8	3.34
(7,13)	1:26:A:SER:OG	1:13:A:ALA:HA	10	3.34
(7,12)	1:26:A:SER:OG	1:12:A:VAL:HA	8	3.34
(5,69)	1:122:A:SER:OG	1:75:A:ASP:HB3	2	3.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,95)	1:97:A:LYS:O	1:146:A:ILE:H	1	3.34
(4,81)	1:97:A:LYS:O	1:146:A:ILE:H	1	3.34
(4,111)	1:97:A:LYS:O	1:161:A:LEU:HA	5	3.33
(5,60)	1:97:A:LYS:O	1:39:A:VAL:HG22	8	3.32
(4,152)	1:122:A:SER:OG	1:111:A:VAL:HB	1	3.32
(4,111)	1:97:A:LYS:O	1:161:A:LEU:HA	2	3.32
(4,27)	1:58:A:GLN:NE2	1:66:A:GLN:H	7	3.32
(4,74)	1:92:A:MET:O	1:79:A:THR:HA	6	3.3
(4,55)	1:92:A:MET:O	1:79:A:THR:HA	6	3.3
(4,27)	1:58:A:GLN:NE2	1:66:A:GLN:H	4	3.3
(4,36)	1:58:A:GLN:NE2	1:120:A:ASP:HA	6	3.29
(4,28)	1:58:A:GLN:NE2	1:78:A:VAL:H	10	3.29
(5,69)	1:122:A:SER:OG	1:75:A:ASP:HB3	8	3.28
(5,44)	1:92:A:MET:O	1:78:A:VAL:HG22	2	3.28
(4,113)	1:97:A:LYS:O	1:32:A:VAL:HB	2	3.28
(4,167)	1:124:A:ARG:O	1:183:A:TRP:HA	2	3.27
(4,125)	1:122:A:SER:OG	1:193:A:ILE:H	6	3.27
(4,85)	1:97:A:LYS:O	1:31:A:GLY:H	7	3.27
(4,54)	1:92:A:MET:O	1:44:A:PRO:HA	2	3.27
(4,125)	1:122:A:SER:OG	1:193:A:ILE:H	5	3.26
(4,56)	1:92:A:MET:O	1:100:A:THR:HA	1	3.26
(5,78)	1:122:A:SER:OG	1:180:A:PRO:HD3	2	3.25
(4,101)	1:97:A:LYS:O	1:91:A:ALA:HA	4	3.24
(4,70)	1:92:A:MET:O	1:100:A:THR:HB	5	3.23
(4,49)	1:92:A:MET:O	1:33:A:PRO:HA	4	3.23
(4,42)	1:92:A:MET:O	1:100:A:THR:H	3	3.23
(2,633)	1:92:A:MET:CE	1:95:A:ILE:CD1	5	3.23
(4,52)	1:92:A:MET:O	1:41:A:MET:HA	7	3.22
(5,44)	1:92:A:MET:O	1:78:A:VAL:HG22	6	3.21
(4,54)	1:92:A:MET:O	1:44:A:PRO:HA	1	3.21
(6,6)	1:92:A:MET:O	1:100:A:THR:CA	1	3.17
(4,112)	1:97:A:LYS:O	1:29:A:PRO:HB3	1	3.17
(4,44)	1:92:A:MET:O	1:146:A:ILE:H	1	3.17
(4,53)	1:92:A:MET:O	1:43:A:ILE:HA	10	3.16
(4,98)	1:97:A:LYS:O	1:32:A:VAL:HA	4	3.15
(4,53)	1:92:A:MET:O	1:43:A:ILE:HA	5	3.15
(5,69)	1:122:A:SER:OG	1:75:A:ASP:HB3	9	3.13
(4,110)	1:97:A:LYS:O	1:158:A:SER:HA	9	3.13
(5,69)	1:122:A:SER:OG	1:75:A:ASP:HB3	6	3.12
(4,56)	1:92:A:MET:O	1:100:A:THR:HA	2	3.12
(5,56)	1:97:A:LYS:O	1:165:A:TYR:HD1	9	3.1
(4,108)	1:97:A:LYS:O	1:156:A:THR:HA	4	3.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,54)	1:97:A:LYS:O	1:146:A:ILE:HD13	7	3.09
(4,107)	1:97:A:LYS:O	1:149:A:PRO:HA	9	3.09
(5,69)	1:122:A:SER:OG	1:75:A:ASP:HB3	1	3.07
(4,27)	1:58:A:GLN:NE2	1:66:A:GLN:H	6	3.06
(5,61)	1:97:A:LYS:O	1:43:A:ILE:HG21	1	3.04
(4,110)	1:97:A:LYS:O	1:158:A:SER:HA	2	3.04
(4,26)	1:58:A:GLN:NE2	1:65:A:GLY:H	3	3.04
(7,190)	1:124:A:ARG:O	1:76:A:TRP:CG	4	3.01
(6,11)	1:158:A:SER:OG	1:148:A:ASN:CA	1	2.99
(4,112)	1:97:A:LYS:O	1:29:A:PRO:HB3	5	2.99
(4,123)	1:122:A:SER:OG	1:186:A:GLY:H	3	2.98
(2,643)	1:95:A:ILE:CG1	1:92:A:MET:CG	8	2.98
(7,190)	1:124:A:ARG:O	1:76:A:TRP:CG	7	2.97
(5,54)	1:97:A:LYS:O	1:146:A:ILE:HD11	4	2.97
(4,92)	1:97:A:LYS:O	1:111:A:VAL:H	4	2.95
(5,69)	1:122:A:SER:OG	1:75:A:ASP:HB3	10	2.94
(5,55)	1:97:A:LYS:O	1:149:A:PRO:HD2	1	2.94
(5,24)	1:58:A:GLN:NE2	1:64:A:ALA:HB2	4	2.91
(4,140)	1:122:A:SER:OG	1:77:A:MET:HA	2	2.91
(7,13)	1:26:A:SER:OG	1:13:A:ALA:HA	1	2.88
(4,140)	1:122:A:SER:OG	1:77:A:MET:HA	6	2.88
(4,105)	1:97:A:LYS:O	1:110:A:ILE:HA	1	2.88
(4,5)	1:5:A:SER:OG	1:69:A:HIS:HA	3	2.88
(4,28)	1:58:A:GLN:NE2	1:78:A:VAL:H	3	2.86
(4,5)	1:5:A:SER:OG	1:69:A:HIS:HA	6	2.86
(5,78)	1:122:A:SER:OG	1:180:A:PRO:HD3	9	2.85
(5,69)	1:122:A:SER:OG	1:75:A:ASP:HB3	5	2.85
(5,7)	1:5:A:SER:OG	1:58:A:GLN:HG3	4	2.85
(7,49)	1:26:A:SER:OG	1:12:A:VAL:HB	5	2.81
(4,140)	1:122:A:SER:OG	1:77:A:MET:HA	8	2.81
(4,53)	1:92:A:MET:O	1:43:A:ILE:HA	1	2.81
(4,123)	1:122:A:SER:OG	1:186:A:GLY:H	7	2.78
(4,105)	1:97:A:LYS:O	1:110:A:ILE:HA	2	2.78
(4,6)	1:5:A:SER:OG	1:71:A:ALA:HA	7	2.76
(4,140)	1:122:A:SER:OG	1:77:A:MET:HA	7	2.75
(7,190)	1:124:A:ARG:O	1:76:A:TRP:CG	2	2.73
(7,190)	1:124:A:ARG:O	1:76:A:TRP:CG	6	2.73
(4,109)	1:97:A:LYS:O	1:157:A:GLN:HA	6	2.73
(4,111)	1:97:A:LYS:O	1:161:A:LEU:HA	10	2.72
(4,53)	1:92:A:MET:O	1:43:A:ILE:HA	9	2.71
(7,13)	1:26:A:SER:OG	1:13:A:ALA:HA	3	2.7
(4,167)	1:124:A:ARG:O	1:183:A:TRP:HA	5	2.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,141)	1:122:A:SER:OG	1:111:A:VAL:HA	6	2.7
(4,113)	1:97:A:LYS:O	1:32:A:VAL:HB	3	2.7
(7,13)	1:26:A:SER:OG	1:13:A:ALA:HA	2	2.69
(4,123)	1:122:A:SER:OG	1:186:A:GLY:H	6	2.69
(4,53)	1:92:A:MET:O	1:43:A:ILE:HA	2	2.68
(4,54)	1:92:A:MET:O	1:44:A:PRO:HA	8	2.67
(7,189)	1:124:A:ARG:O	1:76:A:TRP:HD1	8	2.65
(4,167)	1:124:A:ARG:O	1:183:A:TRP:HA	10	2.65
(4,92)	1:97:A:LYS:O	1:111:A:VAL:H	2	2.65
(4,56)	1:92:A:MET:O	1:100:A:THR:HA	5	2.64
(4,27)	1:58:A:GLN:NE2	1:66:A:GLN:H	9	2.64
(4,6)	1:5:A:SER:OG	1:71:A:ALA:HA	4	2.64
(4,53)	1:92:A:MET:O	1:43:A:ILE:HA	3	2.63
(4,26)	1:58:A:GLN:NE2	1:65:A:GLY:H	9	2.63
(5,51)	1:97:A:LYS:O	1:91:A:ALA:HB1	4	2.61
(4,140)	1:122:A:SER:OG	1:77:A:MET:HA	5	2.61
(1,419)	1:181:A:ILE:HG23	1:185:A:ILE:HD13	5	2.61
(1,74)	1:45:A:ILE:HG22	1:49:A:LEU:HD13	9	2.61
(2,643)	1:95:A:ILE:CG1	1:92:A:MET:CG	4	2.6
(1,419)	1:181:A:ILE:HG22	1:185:A:ILE:HD11	3	2.6
(4,125)	1:122:A:SER:OG	1:193:A:ILE:H	2	2.59
(5,2)	1:5:A:SER:OG	1:60:A:LYS:HB2	8	2.57
(5,78)	1:122:A:SER:OG	1:180:A:PRO:HD3	1	2.56
(4,115)	1:97:A:LYS:O	1:154:A:THR:HB	5	2.54
(4,108)	1:97:A:LYS:O	1:156:A:THR:HA	1	2.54
(5,6)	1:5:A:SER:OG	1:194:A:ASN:HB3	8	2.53
(4,140)	1:122:A:SER:OG	1:77:A:MET:HA	1	2.53
(4,16)	1:26:A:SER:OG	1:43:A:ILE:HA	2	2.53
(4,5)	1:5:A:SER:OG	1:69:A:HIS:HA	1	2.51
(5,27)	1:58:A:GLN:NE2	1:62:A:GLU:HG3	2	2.49
(6,6)	1:92:A:MET:O	1:100:A:THR:CA	2	2.48
(5,54)	1:97:A:LYS:O	1:146:A:ILE:HD11	5	2.48
(4,141)	1:122:A:SER:OG	1:111:A:VAL:HA	5	2.48
(4,114)	1:97:A:LYS:O	1:39:A:VAL:HB	6	2.48
(4,113)	1:97:A:LYS:O	1:32:A:VAL:HB	6	2.48
(7,97)	1:92:A:MET:O	1:15:A:MET:HA	8	2.46
(7,48)	1:26:A:SER:OG	1:12:A:VAL:HA	10	2.45
(7,12)	1:26:A:SER:OG	1:12:A:VAL:HA	10	2.45
(5,78)	1:122:A:SER:OG	1:180:A:PRO:HD3	6	2.45
(4,132)	1:122:A:SER:OG	1:61:A:VAL:HA	4	2.44
(5,2)	1:5:A:SER:OG	1:60:A:LYS:HB2	9	2.43
(4,28)	1:58:A:GLN:NE2	1:78:A:VAL:H	9	2.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,13)	1:26:A:SER:OG	1:13:A:ALA:HA	9	2.42
(4,167)	1:124:A:ARG:O	1:183:A:TRP:HA	7	2.41
(4,95)	1:97:A:LYS:O	1:146:A:ILE:H	4	2.41
(4,81)	1:97:A:LYS:O	1:146:A:ILE:H	4	2.41
(4,98)	1:97:A:LYS:O	1:32:A:VAL:HA	8	2.4
(7,121)	1:92:A:MET:O	1:46:A:TRP:HD1	8	2.39
(1,74)	1:45:A:ILE:HG22	1:49:A:LEU:HD11	5	2.38
(1,47)	1:32:A:VAL:HG21	1:33:A:PRO:HG3	9	2.38
(5,54)	1:97:A:LYS:O	1:146:A:ILE:HD11	3	2.37
(4,28)	1:58:A:GLN:NE2	1:78:A:VAL:H	8	2.37
(4,140)	1:122:A:SER:OG	1:77:A:MET:HA	10	2.36
(4,113)	1:97:A:LYS:O	1:32:A:VAL:HB	7	2.36
(4,88)	1:97:A:LYS:O	1:91:A:ALA:H	9	2.35
(4,42)	1:92:A:MET:O	1:100:A:THR:H	1	2.35
(5,7)	1:5:A:SER:OG	1:58:A:GLN:HG3	8	2.34
(4,125)	1:122:A:SER:OG	1:193:A:ILE:H	9	2.33
(4,59)	1:92:A:MET:O	1:156:A:THR:HA	8	2.32
(4,108)	1:97:A:LYS:O	1:156:A:THR:HA	7	2.31
(4,44)	1:92:A:MET:O	1:146:A:ILE:H	6	2.31
(7,48)	1:26:A:SER:OG	1:12:A:VAL:HA	1	2.3
(7,48)	1:26:A:SER:OG	1:12:A:VAL:HA	7	2.3
(7,12)	1:26:A:SER:OG	1:12:A:VAL:HA	1	2.3
(7,12)	1:26:A:SER:OG	1:12:A:VAL:HA	7	2.3
(4,123)	1:122:A:SER:OG	1:186:A:GLY:H	1	2.29
(5,7)	1:5:A:SER:OG	1:58:A:GLN:HG3	1	2.28
(1,47)	1:32:A:VAL:HG21	1:33:A:PRO:HG3	5	2.27
(4,141)	1:122:A:SER:OG	1:111:A:VAL:HA	2	2.26
(4,16)	1:26:A:SER:OG	1:43:A:ILE:HA	7	2.25
(1,419)	1:181:A:ILE:HG23	1:185:A:ILE:HD12	2	2.24
(1,185)	1:82:A:LEU:HD21	1:79:A:THR:HA	7	2.24
(4,153)	1:122:A:SER:OG	1:113:A:ILE:HB	7	2.23
(5,50)	1:97:A:LYS:O	1:85:A:LEU:HB3	8	2.22
(4,113)	1:97:A:LYS:O	1:32:A:VAL:HB	9	2.21
(7,165)	1:124:A:ARG:O	1:110:A:ILE:HA	3	2.19
(2,804)	1:127:A:VAL:CG2	1:124:A:ARG:CZ	2	2.19
(6,13)	1:158:A:SER:OG	1:219:A:HIS:CA	8	2.18
(4,106)	1:97:A:LYS:O	1:146:A:ILE:HA	3	2.18
(4,52)	1:92:A:MET:O	1:41:A:MET:HA	2	2.18
(4,16)	1:26:A:SER:OG	1:43:A:ILE:HA	3	2.18
(5,54)	1:97:A:LYS:O	1:146:A:ILE:HD13	1	2.17
(5,7)	1:5:A:SER:OG	1:58:A:GLN:HG3	3	2.17
(4,153)	1:122:A:SER:OG	1:113:A:ILE:HB	2	2.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,140)	1:122:A:SER:OG	1:77:A:MET:HA	9	2.16
(4,66)	1:92:A:MET:O	1:39:A:VAL:HB	4	2.16
(4,159)	1:124:A:ARG:O	1:64:A:ALA:HA	4	2.15
(4,125)	1:122:A:SER:OG	1:193:A:ILE:H	8	2.15
(4,74)	1:92:A:MET:O	1:79:A:THR:HA	8	2.15
(4,55)	1:92:A:MET:O	1:79:A:THR:HA	8	2.15
(4,98)	1:97:A:LYS:O	1:32:A:VAL:HA	2	2.14
(4,85)	1:97:A:LYS:O	1:31:A:GLY:H	1	2.13
(4,16)	1:26:A:SER:OG	1:43:A:ILE:HA	1	2.13
(4,149)	1:122:A:SER:OG	1:61:A:VAL:HB	4	2.12
(7,48)	1:26:A:SER:OG	1:12:A:VAL:HA	3	2.1
(7,12)	1:26:A:SER:OG	1:12:A:VAL:HA	3	2.1
(5,51)	1:97:A:LYS:O	1:91:A:ALA:HB1	9	2.1
(7,13)	1:26:A:SER:OG	1:13:A:ALA:HA	6	2.09
(4,101)	1:97:A:LYS:O	1:91:A:ALA:HA	7	2.09
(1,47)	1:32:A:VAL:HG22	1:33:A:PRO:HG3	8	2.09
(2,805)	1:127:A:VAL:CG1	1:124:A:ARG:CZ	3	2.08
(4,141)	1:122:A:SER:OG	1:111:A:VAL:HA	7	2.06
(4,53)	1:92:A:MET:O	1:43:A:ILE:HA	6	2.06
(4,52)	1:92:A:MET:O	1:41:A:MET:HA	3	2.06
(7,121)	1:92:A:MET:O	1:46:A:TRP:HD1	9	2.05
(4,1)	1:5:A:SER:OG	1:52:A:MET:H	10	2.05
(6,6)	1:92:A:MET:O	1:100:A:THR:CA	5	2.04
(7,48)	1:26:A:SER:OG	1:12:A:VAL:HA	2	2.03
(7,12)	1:26:A:SER:OG	1:12:A:VAL:HA	2	2.03
(4,101)	1:97:A:LYS:O	1:91:A:ALA:HA	3	2.03
(5,44)	1:92:A:MET:O	1:78:A:VAL:HG21	8	2.02
(4,105)	1:97:A:LYS:O	1:110:A:ILE:HA	6	2.02
(4,82)	1:97:A:LYS:O	1:155:A:ARG:H	5	2.02
(1,47)	1:32:A:VAL:HG23	1:33:A:PRO:HG2	10	2.02
(4,106)	1:97:A:LYS:O	1:146:A:ILE:HA	5	2.01
(7,165)	1:124:A:ARG:O	1:110:A:ILE:HA	10	1.98
(7,13)	1:26:A:SER:OG	1:13:A:ALA:HA	4	1.97
(2,804)	1:127:A:VAL:CG2	1:124:A:ARG:CZ	1	1.97
(4,167)	1:124:A:ARG:O	1:183:A:TRP:HA	9	1.96
(4,52)	1:92:A:MET:O	1:41:A:MET:HA	5	1.95
(4,153)	1:122:A:SER:OG	1:113:A:ILE:HB	6	1.94
(4,140)	1:122:A:SER:OG	1:77:A:MET:HA	4	1.94
(5,56)	1:97:A:LYS:O	1:165:A:TYR:HD2	5	1.93
(4,138)	1:122:A:SER:OG	1:72:A:ARG:HA	8	1.92
(4,52)	1:92:A:MET:O	1:41:A:MET:HA	1	1.92
(1,47)	1:32:A:VAL:HG21	1:33:A:PRO:HG3	4	1.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,644)	1:95:A:ILE:CG1	1:92:A:MET:CB	8	1.91
(1,185)	1:82:A:LEU:HD21	1:79:A:THR:HA	10	1.91
(4,141)	1:122:A:SER:OG	1:111:A:VAL:HA	10	1.9
(8,75)	1:92:A:MET:O	1:180:A:PRO:HB3	4	1.89
(1,185)	1:82:A:LEU:HD22	1:79:A:THR:HA	6	1.89
(5,76)	1:122:A:SER:OG	1:113:A:ILE:HD12	7	1.88
(1,47)	1:32:A:VAL:HG21	1:33:A:PRO:HG3	6	1.88
(4,124)	1:122:A:SER:OG	1:189:A:GLY:H	2	1.87
(4,85)	1:97:A:LYS:O	1:31:A:GLY:H	10	1.87
(1,185)	1:82:A:LEU:HD22	1:79:A:THR:HA	1	1.87
(7,110)	1:92:A:MET:O	1:137:A:CYS:HA	4	1.86
(4,152)	1:122:A:SER:OG	1:111:A:VAL:HB	4	1.86
(1,47)	1:32:A:VAL:HG23	1:33:A:PRO:HG3	1	1.86
(4,138)	1:122:A:SER:OG	1:72:A:ARG:HA	3	1.85
(4,141)	1:122:A:SER:OG	1:111:A:VAL:HA	1	1.84
(2,644)	1:95:A:ILE:CG1	1:92:A:MET:CB	4	1.83
(1,47)	1:32:A:VAL:HG23	1:33:A:PRO:HG3	3	1.83
(1,419)	1:181:A:ILE:HG21	1:185:A:ILE:HD11	10	1.82
(5,56)	1:97:A:LYS:O	1:165:A:TYR:HD1	1	1.81
(4,94)	1:97:A:LYS:O	1:145:A:GLY:H	2	1.81
(4,80)	1:97:A:LYS:O	1:145:A:GLY:H	2	1.81
(4,114)	1:97:A:LYS:O	1:39:A:VAL:HB	7	1.8
(7,48)	1:26:A:SER:OG	1:12:A:VAL:HA	9	1.79
(7,12)	1:26:A:SER:OG	1:12:A:VAL:HA	9	1.79
(5,2)	1:5:A:SER:OG	1:60:A:LYS:HB3	6	1.79
(4,59)	1:92:A:MET:O	1:156:A:THR:HA	3	1.79
(4,28)	1:58:A:GLN:NE2	1:78:A:VAL:H	1	1.79
(7,48)	1:26:A:SER:OG	1:12:A:VAL:HA	6	1.78
(7,12)	1:26:A:SER:OG	1:12:A:VAL:HA	6	1.78
(5,27)	1:58:A:GLN:NE2	1:62:A:GLU:HG3	8	1.78
(4,114)	1:97:A:LYS:O	1:39:A:VAL:HB	5	1.78
(4,115)	1:97:A:LYS:O	1:154:A:THR:HB	9	1.77
(5,7)	1:5:A:SER:OG	1:58:A:GLN:HG2	2	1.76
(2,805)	1:127:A:VAL:CG1	1:124:A:ARG:CZ	2	1.75
(5,60)	1:97:A:LYS:O	1:39:A:VAL:HG22	4	1.74
(4,153)	1:122:A:SER:OG	1:113:A:ILE:HB	9	1.74
(5,55)	1:97:A:LYS:O	1:149:A:PRO:HD3	5	1.73
(4,167)	1:124:A:ARG:O	1:183:A:TRP:HA	6	1.73
(4,106)	1:97:A:LYS:O	1:146:A:ILE:HA	7	1.73
(2,633)	1:92:A:MET:CE	1:95:A:ILE:CD1	4	1.73
(4,94)	1:97:A:LYS:O	1:145:A:GLY:H	4	1.72
(4,80)	1:97:A:LYS:O	1:145:A:GLY:H	4	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,185)	1:82:A:LEU:HD21	1:79:A:THR:HA	8	1.72
(4,138)	1:122:A:SER:OG	1:72:A:ARG:HA	4	1.71
(5,56)	1:97:A:LYS:O	1:165:A:TYR:HD2	10	1.69
(4,98)	1:97:A:LYS:O	1:32:A:VAL:HA	3	1.68
(7,49)	1:26:A:SER:OG	1:12:A:VAL:HB	10	1.67
(5,37)	1:92:A:MET:O	1:44:A:PRO:HD3	5	1.67
(4,98)	1:97:A:LYS:O	1:32:A:VAL:HA	6	1.67
(4,88)	1:97:A:LYS:O	1:91:A:ALA:H	6	1.67
(4,33)	1:58:A:GLN:NE2	1:68:A:ALA:HA	8	1.67
(4,140)	1:122:A:SER:OG	1:77:A:MET:HA	3	1.66
(4,28)	1:58:A:GLN:NE2	1:78:A:VAL:H	7	1.66
(7,192)	1:158:A:SER:OG	1:43:A:ILE:HB	4	1.65
(7,49)	1:26:A:SER:OG	1:12:A:VAL:HB	3	1.65
(7,49)	1:26:A:SER:OG	1:12:A:VAL:HB	8	1.65
(4,153)	1:122:A:SER:OG	1:113:A:ILE:HB	10	1.65
(7,121)	1:92:A:MET:O	1:46:A:TRP:HD1	2	1.64
(4,108)	1:97:A:LYS:O	1:156:A:THR:HA	9	1.63
(4,106)	1:97:A:LYS:O	1:146:A:ILE:HA	4	1.62
(4,153)	1:122:A:SER:OG	1:113:A:ILE:HB	5	1.61
(7,97)	1:92:A:MET:O	1:15:A:MET:HA	7	1.6
(7,97)	1:92:A:MET:O	1:15:A:MET:HA	9	1.6
(13,13)	1:210:A:LYS:HD2	1:47:A:SER:HB2	6	1.59
(7,48)	1:26:A:SER:OG	1:12:A:VAL:HA	4	1.59
(7,12)	1:26:A:SER:OG	1:12:A:VAL:HA	4	1.59
(4,106)	1:97:A:LYS:O	1:146:A:ILE:HA	10	1.57
(7,189)	1:124:A:ARG:O	1:76:A:TRP:HD1	1	1.55
(7,189)	1:124:A:ARG:O	1:76:A:TRP:HD1	7	1.54
(4,92)	1:97:A:LYS:O	1:111:A:VAL:H	6	1.53
(4,47)	1:92:A:MET:O	1:25:A:LEU:HA	7	1.53
(5,51)	1:97:A:LYS:O	1:91:A:ALA:HB1	6	1.52
(4,153)	1:122:A:SER:OG	1:113:A:ILE:HB	1	1.52
(4,134)	1:122:A:SER:OG	1:63:A:ALA:HA	4	1.52
(4,125)	1:122:A:SER:OG	1:193:A:ILE:H	10	1.52
(4,82)	1:97:A:LYS:O	1:155:A:ARG:H	9	1.52
(5,68)	1:122:A:SER:OG	1:71:A:ALA:HB1	1	1.51
(4,141)	1:122:A:SER:OG	1:111:A:VAL:HA	9	1.51
(4,113)	1:97:A:LYS:O	1:32:A:VAL:HB	10	1.51
(4,28)	1:58:A:GLN:NE2	1:78:A:VAL:H	4	1.5
(2,634)	1:92:A:MET:CE	1:95:A:ILE:CA	1	1.5
(2,643)	1:95:A:ILE:CG1	1:92:A:MET:CG	6	1.49
(5,75)	1:122:A:SER:OG	1:74:A:ILE:HD13	9	1.48
(4,138)	1:122:A:SER:OG	1:72:A:ARG:HA	7	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,47)	1:92:A:MET:O	1:25:A:LEU:HA	2	1.47
(4,124)	1:122:A:SER:OG	1:189:A:GLY:H	9	1.46
(4,106)	1:97:A:LYS:O	1:146:A:ILE:HA	9	1.45
(4,33)	1:58:A:GLN:NE2	1:68:A:ALA:HA	1	1.45
(4,152)	1:122:A:SER:OG	1:111:A:VAL:HB	8	1.44
(4,28)	1:58:A:GLN:NE2	1:78:A:VAL:H	2	1.44
(4,59)	1:92:A:MET:O	1:156:A:THR:HA	2	1.43
(4,52)	1:92:A:MET:O	1:41:A:MET:HA	10	1.43
(4,60)	1:92:A:MET:O	1:163:A:ASN:HA	2	1.42
(4,33)	1:58:A:GLN:NE2	1:68:A:ALA:HA	5	1.42
(2,805)	1:127:A:VAL:CG1	1:124:A:ARG:CZ	1	1.42
(4,108)	1:97:A:LYS:O	1:156:A:THR:HA	2	1.41
(7,189)	1:124:A:ARG:O	1:76:A:TRP:HD1	9	1.4
(7,181)	1:124:A:ARG:O	1:79:A:THR:HB	3	1.4
(4,114)	1:97:A:LYS:O	1:39:A:VAL:HB	2	1.39
(4,16)	1:26:A:SER:OG	1:43:A:ILE:HA	9	1.39
(4,88)	1:97:A:LYS:O	1:91:A:ALA:H	4	1.37
(4,73)	1:92:A:MET:O	1:169:A:VAL:HB	2	1.37
(4,73)	1:92:A:MET:O	1:169:A:VAL:HB	10	1.36
(4,45)	1:92:A:MET:O	1:154:A:THR:H	5	1.36
(7,97)	1:92:A:MET:O	1:15:A:MET:HA	6	1.35
(5,56)	1:97:A:LYS:O	1:165:A:TYR:HD1	6	1.33
(5,42)	1:92:A:MET:O	1:39:A:VAL:HG12	4	1.33
(4,33)	1:58:A:GLN:NE2	1:68:A:ALA:HA	3	1.33
(7,165)	1:124:A:ARG:O	1:110:A:ILE:HA	9	1.3
(4,123)	1:122:A:SER:OG	1:186:A:GLY:H	2	1.3
(4,83)	1:97:A:LYS:O	1:157:A:GLN:H	4	1.3
(4,52)	1:92:A:MET:O	1:41:A:MET:HA	6	1.3
(1,74)	1:45:A:ILE:HG23	1:49:A:LEU:HD12	10	1.3
(7,121)	1:92:A:MET:O	1:46:A:TRP:HD1	1	1.29
(5,56)	1:97:A:LYS:O	1:165:A:TYR:HD1	7	1.29
(4,137)	1:122:A:SER:OG	1:71:A:ALA:HA	4	1.29
(5,76)	1:122:A:SER:OG	1:113:A:ILE:HD13	8	1.28
(4,16)	1:26:A:SER:OG	1:43:A:ILE:HA	6	1.28
(4,114)	1:97:A:LYS:O	1:39:A:VAL:HB	10	1.27
(5,75)	1:122:A:SER:OG	1:74:A:ILE:HD13	10	1.26
(4,114)	1:97:A:LYS:O	1:39:A:VAL:HB	3	1.26
(1,47)	1:32:A:VAL:HG21	1:33:A:PRO:HG2	2	1.26
(5,36)	1:92:A:MET:O	1:43:A:ILE:HD13	3	1.25
(2,634)	1:92:A:MET:CE	1:95:A:ILE:CA	5	1.25
(5,47)	1:92:A:MET:O	1:146:A:ILE:HG22	7	1.24
(4,82)	1:97:A:LYS:O	1:155:A:ARG:H	3	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,165)	1:124:A:ARG:O	1:110:A:ILE:HA	1	1.22
(4,83)	1:97:A:LYS:O	1:157:A:GLN:H	6	1.22
(4,28)	1:58:A:GLN:NE2	1:78:A:VAL:H	5	1.22
(4,104)	1:97:A:LYS:O	1:106:A:MET:HA	5	1.21
(4,73)	1:92:A:MET:O	1:169:A:VAL:HB	9	1.21
(4,53)	1:92:A:MET:O	1:43:A:ILE:HA	8	1.21
(1,332)	1:143:A:LEU:HD12	1:146:A:ILE:HD13	8	1.21
(5,65)	1:122:A:SER:OG	1:63:A:ALA:HB2	4	1.2
(5,37)	1:92:A:MET:O	1:44:A:PRO:HD3	10	1.2
(5,27)	1:58:A:GLN:NE2	1:62:A:GLU:HG3	4	1.2
(4,1)	1:5:A:SER:OG	1:52:A:MET:H	6	1.2
(5,68)	1:122:A:SER:OG	1:71:A:ALA:HB2	3	1.19
(4,42)	1:92:A:MET:O	1:100:A:THR:H	2	1.19
(5,27)	1:58:A:GLN:NE2	1:62:A:GLU:HG3	1	1.18
(5,2)	1:5:A:SER:OG	1:60:A:LYS:HB3	3	1.18
(5,76)	1:122:A:SER:OG	1:113:A:ILE:HD13	2	1.17
(4,138)	1:122:A:SER:OG	1:72:A:ARG:HA	2	1.17
(4,124)	1:122:A:SER:OG	1:189:A:GLY:H	7	1.17
(4,25)	1:58:A:GLN:NE2	1:63:A:ALA:H	8	1.17
(5,68)	1:122:A:SER:OG	1:71:A:ALA:HB2	4	1.15
(4,73)	1:92:A:MET:O	1:169:A:VAL:HB	8	1.15
(4,47)	1:92:A:MET:O	1:25:A:LEU:HA	6	1.15
(4,111)	1:97:A:LYS:O	1:161:A:LEU:HA	8	1.14
(4,46)	1:92:A:MET:O	1:156:A:THR:H	8	1.14
(4,5)	1:5:A:SER:OG	1:69:A:HIS:HA	7	1.13
(4,5)	1:5:A:SER:OG	1:69:A:HIS:HA	4	1.11
(7,49)	1:26:A:SER:OG	1:12:A:VAL:HB	9	1.1
(2,633)	1:92:A:MET:CE	1:95:A:ILE:CD1	2	1.1
(5,8)	1:5:A:SER:OG	1:62:A:GLU:HG2	5	1.08
(4,118)	1:122:A:SER:OG	1:64:A:ALA:H	4	1.08
(4,33)	1:58:A:GLN:NE2	1:68:A:ALA:HA	7	1.08
(4,30)	1:58:A:GLN:NE2	1:47:A:SER:HA	10	1.08
(7,189)	1:124:A:ARG:O	1:76:A:TRP:HD1	2	1.07
(7,189)	1:124:A:ARG:O	1:76:A:TRP:HD1	6	1.07
(7,185)	1:124:A:ARG:O	1:141:A:ILE:HB	7	1.07
(5,18)	1:26:A:SER:OG	1:39:A:VAL:HG21	3	1.07
(6,10)	1:122:A:SER:OG	1:62:A:GLU:CA	4	1.06
(5,76)	1:122:A:SER:OG	1:113:A:ILE:HD11	1	1.06
(4,139)	1:122:A:SER:OG	1:74:A:ILE:HA	2	1.06
(4,77)	1:97:A:LYS:O	1:93:A:GLN:H	6	1.06
(4,33)	1:58:A:GLN:NE2	1:68:A:ALA:HA	10	1.06
(8,110)	1:124:A:ARG:O	1:75:A:ASP:HB2	8	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,5)	1:5:A:SER:OG	1:69:A:HIS:HA	2	1.05
(5,27)	1:58:A:GLN:NE2	1:62:A:GLU:HG3	6	1.04
(4,61)	1:92:A:MET:O	1:166:A:ASP:HA	2	1.04
(4,109)	1:97:A:LYS:O	1:157:A:GLN:HA	3	1.03
(4,25)	1:58:A:GLN:NE2	1:63:A:ALA:H	1	1.03
(2,643)	1:95:A:ILE:CG1	1:92:A:MET:CG	2	1.02
(5,37)	1:92:A:MET:O	1:44:A:PRO:HD3	3	1.01
(4,98)	1:97:A:LYS:O	1:32:A:VAL:HA	9	1.01
(7,165)	1:124:A:ARG:O	1:110:A:ILE:HA	7	1.0
(6,15)	1:158:A:SER:OG	1:217:A:ASP:CA	3	1.0
(4,30)	1:58:A:GLN:NE2	1:47:A:SER:HA	6	1.0
(3,772)	1:165:A:TYR:CE2	1:164:A:LEU:CA	3	1.0
(4,152)	1:122:A:SER:OG	1:111:A:VAL:HB	3	0.99
(4,107)	1:97:A:LYS:O	1:149:A:PRO:HA	5	0.99
(4,85)	1:97:A:LYS:O	1:31:A:GLY:H	5	0.99
(5,36)	1:92:A:MET:O	1:43:A:ILE:HD12	10	0.98
(4,56)	1:92:A:MET:O	1:100:A:THR:HA	4	0.98
(3,772)	1:165:A:TYR:CE2	1:164:A:LEU:CA	2	0.98
(3,772)	1:165:A:TYR:CE2	1:164:A:LEU:CA	5	0.98
(3,772)	1:165:A:TYR:CE2	1:164:A:LEU:CA	6	0.98
(2,643)	1:95:A:ILE:CG1	1:92:A:MET:CG	5	0.98
(1,341)	1:146:A:ILE:HD13	1:143:A:LEU:HA	8	0.98
(7,121)	1:92:A:MET:O	1:46:A:TRP:HD1	3	0.97
(5,43)	1:92:A:MET:O	1:43:A:ILE:HG23	5	0.97
(4,16)	1:26:A:SER:OG	1:43:A:ILE:HA	4	0.97
(7,192)	1:158:A:SER:OG	1:43:A:ILE:HB	5	0.96
(6,13)	1:158:A:SER:OG	1:219:A:HIS:CA	3	0.96
(5,51)	1:97:A:LYS:O	1:91:A:ALA:HB2	3	0.95
(5,27)	1:58:A:GLN:NE2	1:62:A:GLU:HG3	10	0.95
(4,59)	1:92:A:MET:O	1:156:A:THR:HA	5	0.95
(5,76)	1:122:A:SER:OG	1:113:A:ILE:HD13	5	0.94
(5,75)	1:122:A:SER:OG	1:74:A:ILE:HD12	4	0.94
(5,7)	1:5:A:SER:OG	1:58:A:GLN:HG3	7	0.94
(4,25)	1:58:A:GLN:NE2	1:63:A:ALA:H	7	0.94
(3,772)	1:165:A:TYR:CE2	1:164:A:LEU:CA	9	0.94
(2,634)	1:92:A:MET:CE	1:95:A:ILE:CA	8	0.94
(4,60)	1:92:A:MET:O	1:163:A:ASN:HA	8	0.93
(7,165)	1:124:A:ARG:O	1:110:A:ILE:HA	8	0.92
(4,137)	1:122:A:SER:OG	1:71:A:ALA:HA	7	0.92
(4,124)	1:122:A:SER:OG	1:189:A:GLY:H	1	0.92
(7,189)	1:124:A:ARG:O	1:76:A:TRP:HD1	4	0.9
(3,772)	1:165:A:TYR:CE2	1:164:A:LEU:CA	10	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,805)	1:127:A:VAL:CG1	1:124:A:ARG:CZ	10	0.9
(4,153)	1:122:A:SER:OG	1:113:A:ILE:HB	4	0.89
(4,138)	1:122:A:SER:OG	1:72:A:ARG:HA	9	0.89
(4,72)	1:92:A:MET:O	1:154:A:THR:HB	5	0.89
(4,167)	1:124:A:ARG:O	1:183:A:TRP:HA	1	0.88
(7,121)	1:92:A:MET:O	1:46:A:TRP:HD1	6	0.87
(6,15)	1:158:A:SER:OG	1:217:A:ASP:CA	8	0.87
(5,68)	1:122:A:SER:OG	1:71:A:ALA:HB2	5	0.87
(8,110)	1:124:A:ARG:O	1:75:A:ASP:HB2	1	0.86
(7,49)	1:26:A:SER:OG	1:12:A:VAL:HB	1	0.86
(5,75)	1:122:A:SER:OG	1:74:A:ILE:HD12	8	0.86
(4,153)	1:122:A:SER:OG	1:113:A:ILE:HB	8	0.86
(4,71)	1:92:A:MET:O	1:102:A:ILE:HB	9	0.86
(1,419)	1:181:A:ILE:HG21	1:185:A:ILE:HD12	9	0.86
(1,332)	1:143:A:LEU:HD13	1:146:A:ILE:HD11	9	0.86
(4,137)	1:122:A:SER:OG	1:71:A:ALA:HA	3	0.85
(4,60)	1:92:A:MET:O	1:163:A:ASN:HA	3	0.84
(4,46)	1:92:A:MET:O	1:156:A:THR:H	5	0.84
(7,165)	1:124:A:ARG:O	1:110:A:ILE:HA	5	0.83
(4,88)	1:97:A:LYS:O	1:91:A:ALA:H	3	0.83
(4,47)	1:92:A:MET:O	1:25:A:LEU:HA	1	0.83
(4,33)	1:58:A:GLN:NE2	1:68:A:ALA:HA	9	0.83
(5,64)	1:122:A:SER:OG	1:60:A:LYS:HB3	4	0.82
(4,88)	1:97:A:LYS:O	1:91:A:ALA:H	7	0.82
(2,644)	1:95:A:ILE:CG1	1:92:A:MET:CB	5	0.82
(5,68)	1:122:A:SER:OG	1:71:A:ALA:HB1	7	0.81
(4,73)	1:92:A:MET:O	1:169:A:VAL:HB	1	0.81
(4,73)	1:92:A:MET:O	1:169:A:VAL:HB	3	0.81
(13,13)	1:210:A:LYS:HD2	1:47:A:SER:HB2	9	0.8
(5,36)	1:92:A:MET:O	1:43:A:ILE:HD11	1	0.8
(4,139)	1:122:A:SER:OG	1:74:A:ILE:HA	6	0.8
(4,114)	1:97:A:LYS:O	1:39:A:VAL:HB	9	0.8
(4,101)	1:97:A:LYS:O	1:91:A:ALA:HA	10	0.8
(1,332)	1:143:A:LEU:HD13	1:146:A:ILE:HD11	6	0.8
(5,76)	1:122:A:SER:OG	1:113:A:ILE:HD12	10	0.79
(4,115)	1:97:A:LYS:O	1:154:A:THR:HB	3	0.79
(4,101)	1:97:A:LYS:O	1:91:A:ALA:HA	2	0.79
(5,75)	1:122:A:SER:OG	1:74:A:ILE:HD13	2	0.77
(4,154)	1:122:A:SER:OG	1:182:A:VAL:HB	4	0.77
(4,83)	1:97:A:LYS:O	1:157:A:GLN:H	3	0.77
(4,34)	1:58:A:GLN:NE2	1:74:A:ILE:HA	6	0.77
(2,633)	1:92:A:MET:CE	1:95:A:ILE:CD1	6	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,60)	1:97:A:LYS:O	1:39:A:VAL:HG23	3	0.74
(5,40)	1:92:A:MET:O	1:146:A:ILE:HD11	3	0.74
(5,33)	1:92:A:MET:O	1:163:A:ASN:HB2	2	0.74
(4,139)	1:122:A:SER:OG	1:74:A:ILE:HA	7	0.74
(4,124)	1:122:A:SER:OG	1:189:A:GLY:H	10	0.73
(4,106)	1:97:A:LYS:O	1:146:A:ILE:HA	1	0.73
(4,101)	1:97:A:LYS:O	1:91:A:ALA:HA	8	0.73
(4,88)	1:97:A:LYS:O	1:91:A:ALA:H	8	0.73
(4,45)	1:92:A:MET:O	1:154:A:THR:H	8	0.73
(2,643)	1:95:A:ILE:CG1	1:92:A:MET:CG	1	0.73
(6,14)	1:158:A:SER:OG	1:218:A:LEU:CA	8	0.72
(5,18)	1:26:A:SER:OG	1:39:A:VAL:HG21	2	0.72
(4,98)	1:97:A:LYS:O	1:32:A:VAL:HA	7	0.72
(4,61)	1:92:A:MET:O	1:166:A:ASP:HA	3	0.72
(7,97)	1:92:A:MET:O	1:15:A:MET:HA	3	0.71
(5,68)	1:122:A:SER:OG	1:71:A:ALA:HB1	9	0.71
(5,27)	1:58:A:GLN:NE2	1:62:A:GLU:HG3	9	0.71
(3,772)	1:165:A:TYR:CE2	1:164:A:LEU:CA	1	0.71
(2,805)	1:127:A:VAL:CG1	1:124:A:ARG:CZ	7	0.71
(1,332)	1:143:A:LEU:HD11	1:146:A:ILE:HD13	2	0.71
(8,110)	1:124:A:ARG:O	1:75:A:ASP:HB2	10	0.7
(7,97)	1:92:A:MET:O	1:15:A:MET:HA	1	0.7
(5,50)	1:97:A:LYS:O	1:85:A:LEU:HB3	3	0.7
(4,62)	1:92:A:MET:O	1:169:A:VAL:HA	10	0.69
(3,772)	1:165:A:TYR:CE2	1:164:A:LEU:CA	8	0.69
(7,49)	1:26:A:SER:OG	1:12:A:VAL:HB	7	0.68
(5,78)	1:122:A:SER:OG	1:180:A:PRO:HD3	4	0.68
(5,36)	1:92:A:MET:O	1:43:A:ILE:HD12	9	0.68
(5,68)	1:122:A:SER:OG	1:71:A:ALA:HB2	6	0.67
(4,109)	1:97:A:LYS:O	1:157:A:GLN:HA	4	0.67
(4,61)	1:92:A:MET:O	1:166:A:ASP:HA	7	0.66
(4,52)	1:92:A:MET:O	1:41:A:MET:HA	9	0.66
(7,97)	1:92:A:MET:O	1:15:A:MET:HA	2	0.65
(4,138)	1:122:A:SER:OG	1:72:A:ARG:HA	10	0.65
(5,68)	1:122:A:SER:OG	1:71:A:ALA:HB1	10	0.64
(5,51)	1:97:A:LYS:O	1:91:A:ALA:HB2	7	0.64
(4,146)	1:122:A:SER:OG	1:182:A:VAL:HA	4	0.64
(4,138)	1:122:A:SER:OG	1:72:A:ARG:HA	5	0.64
(4,137)	1:122:A:SER:OG	1:71:A:ALA:HA	2	0.64
(4,123)	1:122:A:SER:OG	1:186:A:GLY:H	9	0.64
(2,804)	1:127:A:VAL:CG2	1:124:A:ARG:CZ	6	0.64
(13,13)	1:210:A:LYS:HD2	1:47:A:SER:HB2	4	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,139)	1:122:A:SER:OG	1:74:A:ILE:HA	5	0.63
(2,643)	1:95:A:ILE:CG1	1:92:A:MET:CG	10	0.63
(7,185)	1:124:A:ARG:O	1:141:A:ILE:HB	2	0.62
(4,138)	1:122:A:SER:OG	1:72:A:ARG:HA	1	0.62
(4,138)	1:122:A:SER:OG	1:72:A:ARG:HA	6	0.62
(13,13)	1:210:A:LYS:HD2	1:47:A:SER:HB2	7	0.61
(5,75)	1:122:A:SER:OG	1:74:A:ILE:HD12	5	0.61
(5,75)	1:122:A:SER:OG	1:74:A:ILE:HD13	6	0.61
(9,177)	1:183:A:TRP:C	1:182:A:VAL:CG2	2	0.6
(4,167)	1:124:A:ARG:O	1:183:A:TRP:HA	3	0.6
(4,34)	1:58:A:GLN:NE2	1:74:A:ILE:HA	3	0.6
(9,177)	1:183:A:TRP:C	1:182:A:VAL:CG2	5	0.59
(9,177)	1:183:A:TRP:C	1:182:A:VAL:CG2	9	0.59
(9,116)	1:120:A:ASP:C	1:119:A:ALA:CB	4	0.59
(9,84)	1:79:A:THR:C	1:78:A:VAL:CG2	9	0.59
(9,84)	1:79:A:THR:C	1:78:A:VAL:CG2	10	0.59
(5,76)	1:122:A:SER:OG	1:113:A:ILE:HD11	3	0.59
(5,37)	1:92:A:MET:O	1:44:A:PRO:HD2	7	0.59
(4,101)	1:97:A:LYS:O	1:91:A:ALA:HA	5	0.59
(9,177)	1:183:A:TRP:C	1:182:A:VAL:CG2	10	0.58
(9,111)	1:115:A:SER:C	1:114:A:THR:CG2	5	0.58
(9,84)	1:79:A:THR:C	1:78:A:VAL:CG2	5	0.58
(9,84)	1:79:A:THR:C	1:78:A:VAL:CG2	6	0.58
(9,84)	1:79:A:THR:C	1:78:A:VAL:CG2	7	0.58
(4,139)	1:122:A:SER:OG	1:74:A:ILE:HA	4	0.58
(4,123)	1:122:A:SER:OG	1:186:A:GLY:H	8	0.58
(1,47)	1:32:A:VAL:HG22	1:33:A:PRO:HG2	7	0.58
(9,188)	1:198:A:ASP:C	1:197:A:ILE:CG2	1	0.57
(9,188)	1:198:A:ASP:C	1:197:A:ILE:CG2	3	0.57
(9,157)	1:165:A:TYR:C	1:168:A:LEU:CD2	1	0.57
(9,116)	1:120:A:ASP:C	1:119:A:ALA:CB	10	0.57
(9,84)	1:79:A:THR:C	1:78:A:VAL:CG2	1	0.57
(9,55)	1:61:A:VAL:C	1:67:A:ILE:CG2	6	0.57
(7,192)	1:158:A:SER:OG	1:43:A:ILE:HB	9	0.57
(5,75)	1:122:A:SER:OG	1:74:A:ILE:HD12	1	0.57
(5,37)	1:92:A:MET:O	1:44:A:PRO:HD3	6	0.57
(5,18)	1:26:A:SER:OG	1:39:A:VAL:HG23	1	0.57
(2,644)	1:95:A:ILE:CG1	1:92:A:MET:CB	6	0.57
(9,84)	1:79:A:THR:C	1:78:A:VAL:CG2	8	0.56
(9,75)	1:72:A:ARG:C	1:71:A:ALA:CB	1	0.56
(9,61)	1:64:A:ALA:C	1:63:A:ALA:CB	1	0.56
(9,61)	1:64:A:ALA:C	1:63:A:ALA:CB	6	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,60)	1:97:A:LYS:O	1:39:A:VAL:HG23	2	0.56
(4,137)	1:122:A:SER:OG	1:71:A:ALA:HA	10	0.56
(4,61)	1:92:A:MET:O	1:166:A:ASP:HA	9	0.56
(4,42)	1:92:A:MET:O	1:100:A:THR:H	5	0.56
(9,188)	1:198:A:ASP:C	1:197:A:ILE:CG2	4	0.55
(9,177)	1:183:A:TRP:C	1:182:A:VAL:CG2	8	0.55
(9,75)	1:72:A:ARG:C	1:71:A:ALA:CB	10	0.55
(9,61)	1:64:A:ALA:C	1:63:A:ALA:CB	3	0.55
(4,137)	1:122:A:SER:OG	1:71:A:ALA:HA	1	0.55
(4,123)	1:122:A:SER:OG	1:186:A:GLY:H	5	0.55
(4,82)	1:97:A:LYS:O	1:155:A:ARG:H	1	0.55
(2,805)	1:127:A:VAL:CG1	1:124:A:ARG:CZ	6	0.55
(9,143)	1:139:A:PHE:C	1:138:A:ALA:CB	9	0.54
(9,116)	1:120:A:ASP:C	1:119:A:ALA:CB	1	0.54
(9,75)	1:72:A:ARG:C	1:71:A:ALA:CB	9	0.54
(9,61)	1:64:A:ALA:C	1:63:A:ALA:CB	5	0.54
(9,61)	1:64:A:ALA:C	1:63:A:ALA:CB	7	0.54
(4,139)	1:122:A:SER:OG	1:74:A:ILE:HA	1	0.54
(4,139)	1:122:A:SER:OG	1:74:A:ILE:HA	10	0.54
(4,70)	1:92:A:MET:O	1:100:A:THR:HB	4	0.54
(9,111)	1:115:A:SER:C	1:114:A:THR:CG2	2	0.53
(9,84)	1:79:A:THR:C	1:78:A:VAL:CG2	2	0.53
(9,75)	1:72:A:ARG:C	1:71:A:ALA:CB	3	0.53
(9,75)	1:72:A:ARG:C	1:71:A:ALA:CB	5	0.53
(9,75)	1:72:A:ARG:C	1:71:A:ALA:CB	7	0.53
(9,61)	1:64:A:ALA:C	1:63:A:ALA:CB	2	0.53
(9,61)	1:64:A:ALA:C	1:63:A:ALA:CB	10	0.53
(5,68)	1:122:A:SER:OG	1:71:A:ALA:HB1	8	0.53
(4,25)	1:58:A:GLN:NE2	1:63:A:ALA:H	10	0.53
(7,165)	1:124:A:ARG:O	1:110:A:ILE:HA	2	0.52
(4,47)	1:92:A:MET:O	1:25:A:LEU:HA	9	0.52
(9,188)	1:198:A:ASP:C	1:197:A:ILE:CG2	2	0.51
(9,84)	1:79:A:THR:C	1:78:A:VAL:CG2	3	0.51
(7,121)	1:92:A:MET:O	1:46:A:TRP:HD1	10	0.51
(4,62)	1:92:A:MET:O	1:169:A:VAL:HA	9	0.51
(4,60)	1:92:A:MET:O	1:163:A:ASN:HA	9	0.51
(4,34)	1:58:A:GLN:NE2	1:74:A:ILE:HA	10	0.51
(1,341)	1:146:A:ILE:HD12	1:143:A:LEU:HA	4	0.51
(9,143)	1:139:A:PHE:C	1:138:A:ALA:CB	1	0.5
(9,116)	1:120:A:ASP:C	1:119:A:ALA:CB	7	0.5
(9,111)	1:115:A:SER:C	1:114:A:THR:CG2	8	0.5
(9,84)	1:79:A:THR:C	1:78:A:VAL:CG2	4	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,75)	1:72:A:ARG:C	1:71:A:ALA:CB	6	0.5
(9,75)	1:72:A:ARG:C	1:71:A:ALA:CB	8	0.5
(9,61)	1:64:A:ALA:C	1:63:A:ALA:CB	9	0.5
(5,75)	1:122:A:SER:OG	1:74:A:ILE:HD13	7	0.5
(5,54)	1:97:A:LYS:O	1:146:A:ILE:HD11	10	0.5
(4,155)	1:124:A:ARG:O	1:68:A:ALA:H	4	0.5
(1,74)	1:45:A:ILE:HG23	1:49:A:LEU:HD12	6	0.5
(13,13)	1:210:A:LYS:HD2	1:47:A:SER:HB3	8	0.49
(9,116)	1:120:A:ASP:C	1:119:A:ALA:CB	5	0.49
(9,111)	1:115:A:SER:C	1:114:A:THR:CG2	4	0.49
(9,111)	1:115:A:SER:C	1:114:A:THR:CG2	7	0.49
(9,80)	1:76:A:TRP:C	1:80:A:THR:CG2	5	0.49
(9,75)	1:72:A:ARG:C	1:71:A:ALA:CB	4	0.49
(9,71)	1:70:A:TYR:C	1:69:A:HIS:CB	6	0.49
(9,61)	1:64:A:ALA:C	1:63:A:ALA:CB	8	0.49
(4,71)	1:92:A:MET:O	1:102:A:ILE:HB	8	0.49
(9,203)	1:213:A:PHE:C	1:216:A:LEU:CD1	5	0.48
(9,144)	1:139:A:PHE:C	1:140:A:LEU:CD2	6	0.48
(9,144)	1:139:A:PHE:C	1:140:A:LEU:CD2	7	0.48
(9,143)	1:139:A:PHE:C	1:138:A:ALA:CB	3	0.48
(9,143)	1:139:A:PHE:C	1:138:A:ALA:CB	6	0.48
(9,143)	1:139:A:PHE:C	1:138:A:ALA:CB	7	0.48
(9,139)	1:137:A:CYS:C	1:136:A:VAL:CG2	4	0.48
(9,133)	1:135:A:GLY:C	1:134:A:CYS:CB	1	0.48
(9,80)	1:76:A:TRP:C	1:80:A:THR:CG2	3	0.48
(9,80)	1:76:A:TRP:C	1:80:A:THR:CG2	10	0.48
(9,75)	1:72:A:ARG:C	1:71:A:ALA:CB	2	0.48
(9,35)	1:48:A:GLY:C	1:49:A:LEU:CD2	3	0.48
(9,35)	1:48:A:GLY:C	1:49:A:LEU:CD2	6	0.48
(5,60)	1:97:A:LYS:O	1:39:A:VAL:HG22	6	0.48
(5,60)	1:97:A:LYS:O	1:39:A:VAL:HG22	9	0.48
(5,36)	1:92:A:MET:O	1:43:A:ILE:HD12	2	0.48
(4,73)	1:92:A:MET:O	1:169:A:VAL:HB	7	0.48
(4,47)	1:92:A:MET:O	1:25:A:LEU:HA	10	0.48
(3,772)	1:165:A:TYR:CE2	1:164:A:LEU:CA	7	0.48
(1,341)	1:146:A:ILE:HD12	1:143:A:LEU:HA	9	0.48
(1,287)	1:117:A:LEU:HD11	1:114:A:THR:HB	4	0.48
(9,203)	1:213:A:PHE:C	1:216:A:LEU:CD1	1	0.47
(9,203)	1:213:A:PHE:C	1:216:A:LEU:CD1	2	0.47
(9,203)	1:213:A:PHE:C	1:216:A:LEU:CD1	10	0.47
(9,188)	1:198:A:ASP:C	1:197:A:ILE:CG2	7	0.47
(9,163)	1:171:A:TYR:C	1:170:A:THR:CG2	7	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,163)	1:171:A:TYR:C	1:170:A:THR:CG2	8	0.47
(9,163)	1:171:A:TYR:C	1:170:A:THR:CG2	10	0.47
(9,157)	1:165:A:TYR:C	1:168:A:LEU:CD2	5	0.47
(9,148)	1:142:A:ILE:C	1:143:A:LEU:CD1	7	0.47
(9,139)	1:137:A:CYS:C	1:136:A:VAL:CG2	3	0.47
(9,139)	1:137:A:CYS:C	1:136:A:VAL:CG2	7	0.47
(9,133)	1:135:A:GLY:C	1:134:A:CYS:CB	2	0.47
(9,133)	1:135:A:GLY:C	1:134:A:CYS:CB	5	0.47
(9,133)	1:135:A:GLY:C	1:134:A:CYS:CB	6	0.47
(9,133)	1:135:A:GLY:C	1:134:A:CYS:CB	7	0.47
(9,133)	1:135:A:GLY:C	1:134:A:CYS:CB	8	0.47
(9,133)	1:135:A:GLY:C	1:134:A:CYS:CB	9	0.47
(9,133)	1:135:A:GLY:C	1:134:A:CYS:CB	10	0.47
(9,117)	1:123:A:GLU:C	1:127:A:VAL:CG1	7	0.47
(9,117)	1:123:A:GLU:C	1:127:A:VAL:CG1	8	0.47
(9,80)	1:76:A:TRP:C	1:80:A:THR:CG2	9	0.47
(9,68)	1:69:A:HIS:C	1:71:A:ALA:CB	1	0.47
(9,61)	1:64:A:ALA:C	1:63:A:ALA:CB	4	0.47
(9,55)	1:61:A:VAL:C	1:67:A:ILE:CG2	1	0.47
(9,55)	1:61:A:VAL:C	1:67:A:ILE:CG2	3	0.47
(9,55)	1:61:A:VAL:C	1:67:A:ILE:CG2	7	0.47
(9,46)	1:53:A:ALA:C	1:56:A:ILE:CD1	10	0.47
(9,34)	1:48:A:GLY:C	1:50:A:ALA:CB	3	0.47
(9,17)	1:18:A:GLY:C	1:17:A:ILE:CD1	1	0.47
(9,17)	1:18:A:GLY:C	1:17:A:ILE:CD1	3	0.47
(9,17)	1:18:A:GLY:C	1:17:A:ILE:CD1	5	0.47
(5,68)	1:122:A:SER:OG	1:71:A:ALA:HB2	2	0.47
(2,805)	1:127:A:VAL:CG1	1:124:A:ARG:CZ	5	0.47
(9,203)	1:213:A:PHE:C	1:216:A:LEU:CD1	8	0.46
(9,55)	1:61:A:VAL:C	1:67:A:ILE:CG2	8	0.46
(9,17)	1:18:A:GLY:C	1:17:A:ILE:CD1	2	0.46
(9,12)	1:14:A:GLY:C	1:13:A:ALA:CB	9	0.46
(4,137)	1:122:A:SER:OG	1:71:A:ALA:HA	8	0.46
(1,341)	1:146:A:ILE:HD11	1:143:A:LEU:HA	6	0.46
(9,190)	1:199:A:THR:C	1:199:A:THR:CA	3	0.45
(9,190)	1:199:A:THR:C	1:199:A:THR:CA	7	0.45
(9,144)	1:139:A:PHE:C	1:140:A:LEU:CD2	8	0.45
(9,142)	1:138:A:ALA:C	1:137:A:CYS:CB	9	0.45
(9,139)	1:137:A:CYS:C	1:136:A:VAL:CG2	2	0.45
(9,71)	1:70:A:TYR:C	1:69:A:HIS:CB	4	0.45
(7,165)	1:124:A:ARG:O	1:110:A:ILE:HA	4	0.45
(9,190)	1:199:A:THR:C	1:199:A:THR:CA	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,190)	1:199:A:THR:C	1:199:A:THR:CA	2	0.44
(9,190)	1:199:A:THR:C	1:199:A:THR:CA	4	0.44
(9,190)	1:199:A:THR:C	1:199:A:THR:CA	5	0.44
(9,190)	1:199:A:THR:C	1:199:A:THR:CA	6	0.44
(9,190)	1:199:A:THR:C	1:199:A:THR:CA	8	0.44
(9,190)	1:199:A:THR:C	1:199:A:THR:CA	9	0.44
(9,190)	1:199:A:THR:C	1:199:A:THR:CA	10	0.44
(9,177)	1:183:A:TRP:C	1:182:A:VAL:CG2	1	0.44
(9,177)	1:183:A:TRP:C	1:182:A:VAL:CG2	3	0.44
(9,139)	1:137:A:CYS:C	1:136:A:VAL:CG2	5	0.44
(9,133)	1:135:A:GLY:C	1:134:A:CYS:CB	3	0.44
(9,133)	1:135:A:GLY:C	1:134:A:CYS:CB	4	0.44
(9,80)	1:76:A:TRP:C	1:80:A:THR:CG2	6	0.44
(9,55)	1:61:A:VAL:C	1:67:A:ILE:CG2	10	0.44
(4,79)	1:97:A:LYS:O	1:107:A:SER:H	5	0.44
(4,60)	1:92:A:MET:O	1:163:A:ASN:HA	5	0.44
(4,60)	1:92:A:MET:O	1:163:A:ASN:HA	10	0.44
(9,188)	1:198:A:ASP:C	1:197:A:ILE:CG2	5	0.43
(9,188)	1:198:A:ASP:C	1:197:A:ILE:CG2	9	0.43
(9,163)	1:171:A:TYR:C	1:170:A:THR:CG2	1	0.43
(9,142)	1:138:A:ALA:C	1:137:A:CYS:CB	7	0.43
(9,139)	1:137:A:CYS:C	1:136:A:VAL:CG2	10	0.43
(9,111)	1:115:A:SER:C	1:114:A:THR:CG2	3	0.43
(7,97)	1:92:A:MET:O	1:15:A:MET:HA	10	0.43
(5,60)	1:97:A:LYS:O	1:39:A:VAL:HG21	7	0.43
(4,110)	1:97:A:LYS:O	1:158:A:SER:HA	5	0.43
(4,71)	1:92:A:MET:O	1:102:A:ILE:HB	7	0.43
(4,47)	1:92:A:MET:O	1:25:A:LEU:HA	3	0.43
(9,163)	1:171:A:TYR:C	1:170:A:THR:CG2	3	0.42
(9,139)	1:137:A:CYS:C	1:136:A:VAL:CG2	9	0.42
(9,80)	1:76:A:TRP:C	1:80:A:THR:CG2	4	0.42
(9,41)	1:51:A:TYR:C	1:50:A:ALA:CB	3	0.42
(8,64)	1:92:A:MET:O	1:15:A:MET:HB2	8	0.42
(4,141)	1:122:A:SER:OG	1:111:A:VAL:HA	4	0.42
(4,137)	1:122:A:SER:OG	1:71:A:ALA:HA	9	0.42
(4,25)	1:58:A:GLN:NE2	1:63:A:ALA:H	2	0.42
(9,203)	1:213:A:PHE:C	1:216:A:LEU:CD1	6	0.41
(9,163)	1:171:A:TYR:C	1:170:A:THR:CG2	5	0.41
(9,143)	1:139:A:PHE:C	1:138:A:ALA:CB	2	0.41
(9,68)	1:69:A:HIS:C	1:71:A:ALA:CB	6	0.41
(6,14)	1:158:A:SER:OG	1:218:A:LEU:CA	3	0.41
(5,50)	1:97:A:LYS:O	1:85:A:LEU:HB3	9	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,132)	1:122:A:SER:OG	1:61:A:VAL:HA	3	0.41
(4,76)	1:97:A:LYS:O	1:92:A:MET:H	6	0.41
(4,73)	1:92:A:MET:O	1:169:A:VAL:HB	5	0.41
(4,61)	1:92:A:MET:O	1:166:A:ASP:HA	10	0.41
(9,203)	1:213:A:PHE:C	1:216:A:LEU:CD1	3	0.4
(9,188)	1:198:A:ASP:C	1:197:A:ILE:CG2	6	0.4
(9,175)	1:182:A:VAL:C	1:181:A:ILE:CG2	10	0.4
(9,157)	1:165:A:TYR:C	1:168:A:LEU:CD2	4	0.4
(9,71)	1:70:A:TYR:C	1:69:A:HIS:CB	8	0.4
(9,12)	1:14:A:GLY:C	1:13:A:ALA:CB	6	0.4
(7,49)	1:26:A:SER:OG	1:12:A:VAL:HB	2	0.4
(2,804)	1:127:A:VAL:CG2	1:124:A:ARG:CZ	5	0.4
(1,332)	1:143:A:LEU:HD12	1:146:A:ILE:HD13	5	0.4
(9,143)	1:139:A:PHE:C	1:138:A:ALA:CB	5	0.39
(9,142)	1:138:A:ALA:C	1:137:A:CYS:CB	4	0.39
(9,116)	1:120:A:ASP:C	1:119:A:ALA:CB	9	0.39
(9,111)	1:115:A:SER:C	1:114:A:THR:CG2	10	0.39
(9,55)	1:61:A:VAL:C	1:67:A:ILE:CG2	5	0.39
(9,35)	1:48:A:GLY:C	1:49:A:LEU:CD2	5	0.39
(9,12)	1:14:A:GLY:C	1:13:A:ALA:CB	2	0.39
(5,33)	1:92:A:MET:O	1:163:A:ASN:HB2	3	0.39
(4,60)	1:92:A:MET:O	1:163:A:ASN:HA	1	0.39
(4,60)	1:92:A:MET:O	1:163:A:ASN:HA	7	0.39
(3,772)	1:165:A:TYR:CE2	1:164:A:LEU:CA	4	0.39
(9,177)	1:183:A:TRP:C	1:182:A:VAL:CG2	6	0.38
(9,143)	1:139:A:PHE:C	1:138:A:ALA:CB	4	0.38
(9,143)	1:139:A:PHE:C	1:138:A:ALA:CB	8	0.38
(9,117)	1:123:A:GLU:C	1:127:A:VAL:CG1	2	0.38
(9,12)	1:14:A:GLY:C	1:13:A:ALA:CB	4	0.38
(6,13)	1:158:A:SER:OG	1:219:A:HIS:CA	5	0.38
(4,82)	1:97:A:LYS:O	1:155:A:ARG:H	7	0.38
(10,25)	1:44:A:PRO:N	1:40:A:ALA:O	8	0.37
(9,143)	1:139:A:PHE:C	1:138:A:ALA:CB	10	0.37
(4,73)	1:92:A:MET:O	1:169:A:VAL:HB	6	0.37
(10,25)	1:44:A:PRO:N	1:40:A:ALA:O	6	0.36
(9,203)	1:213:A:PHE:C	1:216:A:LEU:CD1	4	0.36
(9,148)	1:142:A:ILE:C	1:143:A:LEU:CD1	4	0.36
(9,139)	1:137:A:CYS:C	1:136:A:VAL:CG2	1	0.36
(9,139)	1:137:A:CYS:C	1:136:A:VAL:CG2	6	0.36
(9,139)	1:137:A:CYS:C	1:136:A:VAL:CG2	8	0.36
(9,116)	1:120:A:ASP:C	1:119:A:ALA:CB	3	0.36
(9,71)	1:70:A:TYR:C	1:69:A:HIS:CB	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,62)	1:65:A:GLY:C	1:64:A:ALA:CB	6	0.36
(9,12)	1:14:A:GLY:C	1:13:A:ALA:CB	10	0.36
(4,141)	1:122:A:SER:OG	1:111:A:VAL:HA	8	0.36
(2,805)	1:127:A:VAL:CG1	1:124:A:ARG:CZ	9	0.36
(9,157)	1:165:A:TYR:C	1:168:A:LEU:CD2	2	0.35
(9,144)	1:139:A:PHE:C	1:140:A:LEU:CD2	2	0.35
(9,144)	1:139:A:PHE:C	1:140:A:LEU:CD2	10	0.35
(9,116)	1:120:A:ASP:C	1:119:A:ALA:CB	8	0.35
(9,80)	1:76:A:TRP:C	1:80:A:THR:CG2	1	0.35
(9,46)	1:53:A:ALA:C	1:56:A:ILE:CD1	6	0.35
(9,12)	1:14:A:GLY:C	1:13:A:ALA:CB	3	0.35
(9,12)	1:14:A:GLY:C	1:13:A:ALA:CB	7	0.35
(6,15)	1:158:A:SER:OG	1:217:A:ASP:CA	2	0.35
(6,13)	1:158:A:SER:OG	1:219:A:HIS:CA	2	0.35
(5,33)	1:92:A:MET:O	1:163:A:ASN:HB2	8	0.35
(4,137)	1:122:A:SER:OG	1:71:A:ALA:HA	5	0.35
(4,16)	1:26:A:SER:OG	1:43:A:ILE:HA	8	0.35
(1,186)	1:82:A:LEU:HA	1:85:A:LEU:HD21	1	0.35
(10,116)	1:180:A:PRO:N	1:176:A:TRP:O	5	0.34
(10,25)	1:44:A:PRO:N	1:40:A:ALA:O	5	0.34
(9,188)	1:198:A:ASP:C	1:197:A:ILE:CG2	10	0.34
(9,177)	1:183:A:TRP:C	1:182:A:VAL:CG2	7	0.34
(9,68)	1:69:A:HIS:C	1:71:A:ALA:CB	10	0.34
(9,50)	1:54:A:MET:C	1:53:A:ALA:CB	3	0.34
(9,41)	1:51:A:TYR:C	1:50:A:ALA:CB	2	0.34
(9,35)	1:48:A:GLY:C	1:49:A:LEU:CD2	1	0.34
(9,12)	1:14:A:GLY:C	1:13:A:ALA:CB	5	0.34
(7,185)	1:124:A:ARG:O	1:141:A:ILE:HB	4	0.34
(4,101)	1:97:A:LYS:O	1:91:A:ALA:HA	1	0.34
(4,65)	1:92:A:MET:O	1:32:A:VAL:HB	4	0.34
(4,25)	1:58:A:GLN:NE2	1:63:A:ALA:H	5	0.34
(1,332)	1:143:A:LEU:HD11	1:146:A:ILE:HD12	10	0.34
(10,116)	1:180:A:PRO:N	1:176:A:TRP:O	7	0.33
(9,163)	1:171:A:TYR:C	1:170:A:THR:CG2	2	0.33
(9,71)	1:70:A:TYR:C	1:69:A:HIS:CB	3	0.33
(9,71)	1:70:A:TYR:C	1:69:A:HIS:CB	7	0.33
(9,50)	1:54:A:MET:C	1:53:A:ALA:CB	8	0.33
(5,33)	1:92:A:MET:O	1:163:A:ASN:HB2	7	0.33
(4,147)	1:122:A:SER:OG	1:187:A:PRO:HA	3	0.33
(4,62)	1:92:A:MET:O	1:169:A:VAL:HA	8	0.33
(9,177)	1:183:A:TRP:C	1:182:A:VAL:CG2	4	0.32
(9,142)	1:138:A:ALA:C	1:137:A:CYS:CB	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,117)	1:123:A:GLU:C	1:127:A:VAL:CG1	3	0.32
(9,71)	1:70:A:TYR:C	1:69:A:HIS:CB	5	0.32
(9,50)	1:54:A:MET:C	1:53:A:ALA:CB	5	0.32
(9,50)	1:54:A:MET:C	1:53:A:ALA:CB	6	0.32
(9,41)	1:51:A:TYR:C	1:50:A:ALA:CB	5	0.32
(9,41)	1:51:A:TYR:C	1:50:A:ALA:CB	9	0.32
(4,124)	1:122:A:SER:OG	1:189:A:GLY:H	5	0.32
(1,74)	1:45:A:ILE:HG23	1:49:A:LEU:HD11	1	0.32
(10,128)	1:206:A:PRO:N	1:202:A:PHE:O	2	0.31
(9,188)	1:198:A:ASP:C	1:197:A:ILE:CG2	8	0.31
(9,163)	1:171:A:TYR:C	1:170:A:THR:CG2	4	0.31
(9,163)	1:171:A:TYR:C	1:170:A:THR:CG2	6	0.31
(9,144)	1:139:A:PHE:C	1:140:A:LEU:CD2	3	0.31
(9,68)	1:69:A:HIS:C	1:71:A:ALA:CB	3	0.31
(9,50)	1:54:A:MET:C	1:53:A:ALA:CB	1	0.31
(9,50)	1:54:A:MET:C	1:53:A:ALA:CB	2	0.31
(9,41)	1:51:A:TYR:C	1:50:A:ALA:CB	1	0.31
(9,41)	1:51:A:TYR:C	1:50:A:ALA:CB	4	0.31
(9,11)	1:14:A:GLY:C	1:15:A:MET:CE	1	0.31
(4,113)	1:97:A:LYS:O	1:32:A:VAL:HB	5	0.31
(4,62)	1:92:A:MET:O	1:169:A:VAL:HA	3	0.31
(10,128)	1:206:A:PRO:N	1:202:A:PHE:O	9	0.3
(9,175)	1:182:A:VAL:C	1:181:A:ILE:CG2	4	0.3
(9,142)	1:138:A:ALA:C	1:137:A:CYS:CB	1	0.3
(9,142)	1:138:A:ALA:C	1:137:A:CYS:CB	10	0.3
(9,71)	1:70:A:TYR:C	1:69:A:HIS:CB	10	0.3
(9,50)	1:54:A:MET:C	1:53:A:ALA:CB	4	0.3
(9,50)	1:54:A:MET:C	1:53:A:ALA:CB	9	0.3
(9,50)	1:54:A:MET:C	1:53:A:ALA:CB	10	0.3
(9,41)	1:51:A:TYR:C	1:50:A:ALA:CB	10	0.3
(9,12)	1:14:A:GLY:C	1:13:A:ALA:CB	8	0.3
(4,149)	1:122:A:SER:OG	1:61:A:VAL:HB	2	0.3
(4,95)	1:97:A:LYS:O	1:146:A:ILE:H	2	0.3
(4,81)	1:97:A:LYS:O	1:146:A:ILE:H	2	0.3
(2,644)	1:95:A:ILE:CG1	1:92:A:MET:CB	1	0.3
(1,419)	1:181:A:ILE:HG23	1:185:A:ILE:HD12	6	0.3
(1,341)	1:146:A:ILE:HD13	1:143:A:LEU:HA	2	0.3
(10,25)	1:44:A:PRO:N	1:40:A:ALA:O	4	0.29
(10,25)	1:44:A:PRO:N	1:40:A:ALA:O	9	0.29
(9,142)	1:138:A:ALA:C	1:137:A:CYS:CB	5	0.29
(9,142)	1:138:A:ALA:C	1:137:A:CYS:CB	6	0.29
(9,142)	1:138:A:ALA:C	1:137:A:CYS:CB	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,111)	1:115:A:SER:C	1:114:A:THR:CG2	6	0.29
(9,62)	1:65:A:GLY:C	1:64:A:ALA:CB	7	0.29
(9,50)	1:54:A:MET:C	1:53:A:ALA:CB	7	0.29
(9,41)	1:51:A:TYR:C	1:50:A:ALA:CB	6	0.29
(9,35)	1:48:A:GLY:C	1:49:A:LEU:CD2	4	0.29
(9,12)	1:14:A:GLY:C	1:13:A:ALA:CB	1	0.29
(6,6)	1:92:A:MET:O	1:100:A:THR:CA	4	0.29
(4,62)	1:92:A:MET:O	1:169:A:VAL:HA	5	0.29
(4,16)	1:26:A:SER:OG	1:43:A:ILE:HA	10	0.29
(10,25)	1:44:A:PRO:N	1:40:A:ALA:O	10	0.28
(9,203)	1:213:A:PHE:C	1:216:A:LEU:CD1	7	0.28
(9,175)	1:182:A:VAL:C	1:181:A:ILE:CG2	8	0.28
(9,71)	1:70:A:TYR:C	1:69:A:HIS:CB	1	0.28
(9,62)	1:65:A:GLY:C	1:64:A:ALA:CB	9	0.28
(9,41)	1:51:A:TYR:C	1:50:A:ALA:CB	7	0.28
(9,41)	1:51:A:TYR:C	1:50:A:ALA:CB	8	0.28
(8,110)	1:124:A:ARG:O	1:75:A:ASP:HB2	9	0.28
(2,644)	1:95:A:ILE:CG1	1:92:A:MET:CB	10	0.28
(1,332)	1:143:A:LEU:HD13	1:146:A:ILE:HD11	7	0.28
(10,128)	1:206:A:PRO:N	1:202:A:PHE:O	1	0.27
(10,116)	1:180:A:PRO:N	1:176:A:TRP:O	10	0.27
(10,46)	1:81:A:PRO:N	1:77:A:MET:O	7	0.27
(9,175)	1:182:A:VAL:C	1:181:A:ILE:CG2	7	0.27
(9,163)	1:171:A:TYR:C	1:170:A:THR:CG2	9	0.27
(9,142)	1:138:A:ALA:C	1:137:A:CYS:CB	2	0.27
(9,130)	1:134:A:CYS:C	1:138:A:ALA:CB	10	0.27
(9,116)	1:120:A:ASP:C	1:119:A:ALA:CB	2	0.27
(9,111)	1:115:A:SER:C	1:114:A:THR:CG2	1	0.27
(9,80)	1:76:A:TRP:C	1:80:A:THR:CG2	8	0.27
(9,68)	1:69:A:HIS:C	1:71:A:ALA:CB	5	0.27
(9,62)	1:65:A:GLY:C	1:64:A:ALA:CB	10	0.27
(9,46)	1:53:A:ALA:C	1:56:A:ILE:CD1	7	0.27
(7,180)	1:124:A:ARG:O	1:78:A:VAL:HB	3	0.27
(7,159)	1:124:A:ARG:O	1:81:A:PRO:HA	3	0.27
(5,51)	1:97:A:LYS:O	1:91:A:ALA:HB2	10	0.27
(1,342)	1:146:A:ILE:HG23	1:143:A:LEU:HA	8	0.27
(9,175)	1:182:A:VAL:C	1:181:A:ILE:CG2	2	0.26
(9,175)	1:182:A:VAL:C	1:181:A:ILE:CG2	5	0.26
(4,139)	1:122:A:SER:OG	1:74:A:ILE:HA	9	0.26
(2,506)	1:76:A:TRP:CH2	1:76:A:TRP:C	3	0.26
(2,506)	1:76:A:TRP:CH2	1:76:A:TRP:C	4	0.26
(2,506)	1:76:A:TRP:CH2	1:76:A:TRP:C	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,506)	1:76:A:TRP:CH2	1:76:A:TRP:C	9	0.26
(1,332)	1:143:A:LEU:HD13	1:146:A:ILE:HD12	4	0.26
(10,25)	1:44:A:PRO:N	1:40:A:ALA:O	3	0.25
(9,175)	1:182:A:VAL:C	1:181:A:ILE:CG2	1	0.25
(9,175)	1:182:A:VAL:C	1:181:A:ILE:CG2	9	0.25
(9,116)	1:120:A:ASP:C	1:119:A:ALA:CB	6	0.25
(9,62)	1:65:A:GLY:C	1:64:A:ALA:CB	3	0.25
(4,167)	1:124:A:ARG:O	1:183:A:TRP:HA	8	0.25
(2,506)	1:76:A:TRP:CH2	1:76:A:TRP:C	1	0.25
(9,46)	1:53:A:ALA:C	1:56:A:ILE:CD1	1	0.24
(7,185)	1:124:A:ARG:O	1:141:A:ILE:HB	6	0.24
(6,3)	1:92:A:MET:O	1:31:A:GLY:CA	4	0.24
(5,50)	1:97:A:LYS:O	1:85:A:LEU:HB3	4	0.24
(4,64)	1:92:A:MET:O	1:218:A:LEU:HA	4	0.24
(4,61)	1:92:A:MET:O	1:166:A:ASP:HA	8	0.24
(3,882)	1:181:A:ILE:CG1	1:182:A:VAL:CB	6	0.24
(3,253)	1:58:A:GLN:CD	1:59:A:GLY:CA	8	0.24
(13,13)	1:210:A:LYS:HD2	1:47:A:SER:HB2	2	0.23
(9,55)	1:61:A:VAL:C	1:67:A:ILE:CG2	9	0.23
(9,46)	1:53:A:ALA:C	1:56:A:ILE:CD1	2	0.23
(9,46)	1:53:A:ALA:C	1:56:A:ILE:CD1	9	0.23
(5,56)	1:97:A:LYS:O	1:165:A:TYR:HD1	2	0.23
(5,55)	1:97:A:LYS:O	1:149:A:PRO:HD3	4	0.23
(5,54)	1:97:A:LYS:O	1:146:A:ILE:HD13	9	0.23
(5,50)	1:97:A:LYS:O	1:85:A:LEU:HB3	5	0.23
(3,882)	1:181:A:ILE:CG1	1:182:A:VAL:CB	3	0.23
(3,882)	1:181:A:ILE:CG1	1:182:A:VAL:CB	7	0.23
(2,506)	1:76:A:TRP:CH2	1:76:A:TRP:C	7	0.23
(2,506)	1:76:A:TRP:CH2	1:76:A:TRP:C	8	0.23
(10,46)	1:81:A:PRO:N	1:77:A:MET:O	2	0.22
(10,46)	1:81:A:PRO:N	1:77:A:MET:O	8	0.22
(9,148)	1:142:A:ILE:C	1:143:A:LEU:CD1	8	0.22
(9,130)	1:134:A:CYS:C	1:138:A:ALA:CB	3	0.22
(9,126)	1:132:A:TYR:C	1:136:A:VAL:CG1	9	0.22
(9,68)	1:69:A:HIS:C	1:71:A:ALA:CB	7	0.22
(9,62)	1:65:A:GLY:C	1:64:A:ALA:CB	8	0.22
(9,34)	1:48:A:GLY:C	1:50:A:ALA:CB	9	0.22
(4,139)	1:122:A:SER:OG	1:74:A:ILE:HA	8	0.22
(4,132)	1:122:A:SER:OG	1:61:A:VAL:HA	2	0.22
(2,804)	1:127:A:VAL:CG2	1:124:A:ARG:CZ	10	0.22
(2,506)	1:76:A:TRP:CH2	1:76:A:TRP:C	2	0.22
(13,13)	1:210:A:LYS:HD2	1:47:A:SER:HB2	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(10,116)	1:180:A:PRO:N	1:176:A:TRP:O	6	0.21
(10,46)	1:81:A:PRO:N	1:77:A:MET:O	9	0.21
(9,144)	1:139:A:PHE:C	1:140:A:LEU:CD2	1	0.21
(9,117)	1:123:A:GLU:C	1:127:A:VAL:CG1	9	0.21
(9,71)	1:70:A:TYR:C	1:69:A:HIS:CB	9	0.21
(9,17)	1:18:A:GLY:C	1:17:A:ILE:CD1	8	0.21
(10,97)	1:158:A:SER:H	1:154:A:THR:O	6	0.19
(10,46)	1:81:A:PRO:N	1:77:A:MET:O	5	0.19
(9,111)	1:115:A:SER:C	1:114:A:THR:CG2	9	0.19
(9,68)	1:69:A:HIS:C	1:71:A:ALA:CB	9	0.19
(5,81)	1:124:A:ARG:O	1:68:A:ALA:HB1	6	0.19
(4,59)	1:92:A:MET:O	1:156:A:THR:HA	6	0.19
(10,128)	1:206:A:PRO:N	1:202:A:PHE:O	7	0.18
(10,116)	1:180:A:PRO:N	1:176:A:TRP:O	1	0.18
(10,116)	1:180:A:PRO:N	1:176:A:TRP:O	2	0.18
(10,116)	1:180:A:PRO:N	1:176:A:TRP:O	3	0.18
(10,116)	1:180:A:PRO:N	1:176:A:TRP:O	4	0.18
(10,46)	1:81:A:PRO:N	1:77:A:MET:O	4	0.18
(9,203)	1:213:A:PHE:C	1:216:A:LEU:CD1	9	0.18
(9,115)	1:120:A:ASP:C	1:121:A:LEU:CD2	8	0.18
(9,62)	1:65:A:GLY:C	1:64:A:ALA:CB	1	0.18
(9,17)	1:18:A:GLY:C	1:17:A:ILE:CD1	7	0.18
(4,33)	1:58:A:GLN:NE2	1:68:A:ALA:HA	2	0.18
(2,131)	1:29:A:PRO:CB	1:26:A:SER:CB	9	0.18
(1,287)	1:117:A:LEU:HD13	1:114:A:THR:HB	2	0.18
(10,128)	1:206:A:PRO:N	1:202:A:PHE:O	3	0.17
(10,128)	1:206:A:PRO:N	1:202:A:PHE:O	6	0.17
(10,97)	1:158:A:SER:H	1:154:A:THR:O	7	0.17
(10,46)	1:81:A:PRO:N	1:77:A:MET:O	1	0.17
(10,46)	1:81:A:PRO:N	1:77:A:MET:O	3	0.17
(10,46)	1:81:A:PRO:N	1:77:A:MET:O	6	0.17
(10,46)	1:81:A:PRO:N	1:77:A:MET:O	10	0.17
(10,25)	1:44:A:PRO:N	1:40:A:ALA:O	1	0.17
(10,25)	1:44:A:PRO:N	1:40:A:ALA:O	2	0.17
(10,25)	1:44:A:PRO:N	1:40:A:ALA:O	7	0.17
(9,157)	1:165:A:TYR:C	1:168:A:LEU:CD2	10	0.17
(4,76)	1:97:A:LYS:O	1:92:A:MET:H	9	0.17
(10,128)	1:206:A:PRO:N	1:202:A:PHE:O	4	0.16
(10,128)	1:206:A:PRO:N	1:202:A:PHE:O	10	0.16
(10,116)	1:180:A:PRO:N	1:176:A:TRP:O	8	0.16
(10,116)	1:180:A:PRO:N	1:176:A:TRP:O	9	0.16
(9,127)	1:132:A:TYR:C	1:134:A:CYS:CB	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(9,62)	1:65:A:GLY:C	1:64:A:ALA:CB	2	0.16
(9,62)	1:65:A:GLY:C	1:64:A:ALA:CB	5	0.16
(6,11)	1:158:A:SER:OG	1:148:A:ASN:CA	4	0.16
(5,51)	1:97:A:LYS:O	1:91:A:ALA:HB2	1	0.16
(5,2)	1:5:A:SER:OG	1:60:A:LYS:HB3	1	0.16
(12,55)	1:83:A:LEU:CA	1:176:A:TRP:CE3	4	0.15
(12,55)	1:83:A:LEU:CA	1:176:A:TRP:CE3	6	0.15
(10,128)	1:206:A:PRO:N	1:202:A:PHE:O	5	0.15
(10,128)	1:206:A:PRO:N	1:202:A:PHE:O	8	0.15
(10,57)	1:92:A:MET:H	1:88:A:SER:O	7	0.15
(9,175)	1:182:A:VAL:C	1:181:A:ILE:CG2	3	0.15
(9,117)	1:123:A:GLU:C	1:127:A:VAL:CG1	4	0.15
(9,88)	1:81:A:PRO:C	1:84:A:LEU:CD2	8	0.15
(9,17)	1:18:A:GLY:C	1:17:A:ILE:CD1	4	0.15
(9,17)	1:18:A:GLY:C	1:17:A:ILE:CD1	9	0.15
(5,18)	1:26:A:SER:OG	1:39:A:VAL:HG22	7	0.15
(4,1)	1:5:A:SER:OG	1:52:A:MET:H	9	0.15
(3,885)	1:182:A:VAL:CA	1:179:A:TYR:CG	3	0.15
(3,729)	1:148:A:ASN:CA	1:147:A:TRP:CD2	4	0.15
(3,253)	1:58:A:GLN:CD	1:59:A:GLY:CA	6	0.15
(12,55)	1:83:A:LEU:CA	1:176:A:TRP:CE3	2	0.14
(10,97)	1:158:A:SER:H	1:154:A:THR:O	1	0.14
(10,57)	1:92:A:MET:H	1:88:A:SER:O	3	0.14
(10,57)	1:92:A:MET:H	1:88:A:SER:O	5	0.14
(10,57)	1:92:A:MET:H	1:88:A:SER:O	9	0.14
(9,62)	1:65:A:GLY:C	1:64:A:ALA:CB	4	0.14
(9,40)	1:51:A:TYR:C	1:12:A:VAL:CG1	8	0.14
(4,153)	1:122:A:SER:OG	1:113:A:ILE:HB	3	0.14
(4,88)	1:97:A:LYS:O	1:91:A:ALA:H	10	0.14
(3,986)	1:208:A:PHE:CA	1:205:A:LEU:CG	5	0.14
(3,917)	1:187:A:PRO:C	1:191:A:GLY:CA	4	0.14
(3,917)	1:187:A:PRO:C	1:191:A:GLY:CA	8	0.14
(3,337)	1:74:A:ILE:CB	1:76:A:TRP:CA	8	0.14
(3,119)	1:32:A:VAL:CA	1:35:A:TYR:CE2	2	0.14
(1,193)	1:83:A:LEU:HD13	1:80:A:THR:HA	4	0.14
(13,13)	1:210:A:LYS:HD2	1:47:A:SER:HB2	10	0.13
(12,55)	1:83:A:LEU:CA	1:176:A:TRP:CE3	1	0.13
(12,55)	1:83:A:LEU:CA	1:176:A:TRP:CE3	3	0.13
(12,55)	1:83:A:LEU:CA	1:176:A:TRP:CE3	5	0.13
(12,55)	1:83:A:LEU:CA	1:176:A:TRP:CE3	8	0.13
(12,55)	1:83:A:LEU:CA	1:176:A:TRP:CE3	9	0.13
(11,35)	1:73:A:TYR:CA	1:116:A:GLY:CA	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(11,35)	1:73:A:TYR:CA	1:116:A:GLY:CA	6	0.13
(11,35)	1:73:A:TYR:CA	1:116:A:GLY:CA	10	0.13
(10,57)	1:92:A:MET:H	1:88:A:SER:O	2	0.13
(9,130)	1:134:A:CYS:C	1:138:A:ALA:CB	8	0.13
(4,135)	1:122:A:SER:OG	1:64:A:ALA:HA	4	0.13
(3,986)	1:208:A:PHE:CA	1:205:A:LEU:CG	3	0.13
(3,986)	1:208:A:PHE:CA	1:205:A:LEU:CG	4	0.13
(3,982)	1:207:A:PHE:CG	1:211:A:VAL:CA	8	0.13
(3,729)	1:148:A:ASN:CA	1:147:A:TRP:CD2	5	0.13
(3,567)	1:113:A:ILE:CB	1:117:A:LEU:CG	6	0.13
(3,423)	1:83:A:LEU:CG	1:87:A:LEU:CG	8	0.13
(3,360)	1:76:A:TRP:CA	1:73:A:TYR:CG	7	0.13
(3,337)	1:74:A:ILE:CB	1:76:A:TRP:CA	7	0.13
(3,322)	1:73:A:TYR:CA	1:72:A:ARG:CD	2	0.13
(3,119)	1:32:A:VAL:CA	1:35:A:TYR:CE2	10	0.13
(3,105)	1:29:A:PRO:CD	1:25:A:LEU:CA	9	0.13
(3,105)	1:29:A:PRO:CD	1:25:A:LEU:CA	10	0.13
(3,100)	1:26:A:SER:CA	1:22:A:PHE:CG	9	0.13
(2,1106)	1:183:A:TRP:C	1:182:A:VAL:CG2	2	0.13
(1,287)	1:117:A:LEU:HD13	1:114:A:THR:HB	8	0.13
(1,173)	1:80:A:THR:HA	1:83:A:LEU:HA	7	0.13
(12,55)	1:83:A:LEU:CA	1:176:A:TRP:CE3	7	0.12
(11,74)	1:182:A:VAL:CB	1:201:A:LEU:CB	9	0.12
(11,35)	1:73:A:TYR:CA	1:116:A:GLY:CA	3	0.12
(11,35)	1:73:A:TYR:CA	1:116:A:GLY:CA	7	0.12
(11,33)	1:70:A:TYR:CA	1:59:A:GLY:CA	2	0.12
(11,23)	1:53:A:ALA:CA	1:8:A:HIS:CA	1	0.12
(10,57)	1:92:A:MET:H	1:88:A:SER:O	4	0.12
(10,57)	1:92:A:MET:H	1:88:A:SER:O	10	0.12
(10,17)	1:26:A:SER:H	1:22:A:PHE:O	2	0.12
(10,17)	1:26:A:SER:H	1:22:A:PHE:O	5	0.12
(10,17)	1:26:A:SER:H	1:22:A:PHE:O	8	0.12
(9,175)	1:182:A:VAL:C	1:181:A:ILE:CG2	6	0.12
(9,166)	1:174:A:VAL:C	1:177:A:ILE:CG2	2	0.12
(9,40)	1:51:A:TYR:C	1:12:A:VAL:CG1	4	0.12
(9,17)	1:18:A:GLY:C	1:17:A:ILE:CD1	6	0.12
(7,121)	1:92:A:MET:O	1:46:A:TRP:HD1	5	0.12
(3,986)	1:208:A:PHE:CA	1:205:A:LEU:CG	1	0.12
(3,986)	1:208:A:PHE:CA	1:205:A:LEU:CG	7	0.12
(3,986)	1:208:A:PHE:CA	1:205:A:LEU:CG	8	0.12
(3,885)	1:182:A:VAL:CA	1:179:A:TYR:CG	7	0.12
(3,762)	1:165:A:TYR:CG	1:164:A:LEU:CG	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,705)	1:143:A:LEU:CG	1:146:A:ILE:CB	7	0.12
(3,567)	1:113:A:ILE:CB	1:117:A:LEU:CG	10	0.12
(3,531)	1:109:A:GLN:CB	1:112:A:VAL:CA	7	0.12
(3,410)	1:82:A:LEU:CG	1:85:A:LEU:CB	1	0.12
(3,383)	1:78:A:VAL:CB	1:75:A:ASP:CG	6	0.12
(3,337)	1:74:A:ILE:CB	1:76:A:TRP:CA	2	0.12
(3,337)	1:74:A:ILE:CB	1:76:A:TRP:CA	9	0.12
(3,322)	1:73:A:TYR:CA	1:72:A:ARG:CD	6	0.12
(3,322)	1:73:A:TYR:CA	1:72:A:ARG:CD	7	0.12
(3,105)	1:29:A:PRO:CD	1:25:A:LEU:CA	3	0.12
(2,1106)	1:183:A:TRP:C	1:182:A:VAL:CG2	5	0.12
(2,1106)	1:183:A:TRP:C	1:182:A:VAL:CG2	9	0.12
(2,779)	1:120:A:ASP:C	1:119:A:ALA:CB	4	0.12
(2,543)	1:79:A:THR:C	1:78:A:VAL:CG2	9	0.12
(2,543)	1:79:A:THR:C	1:78:A:VAL:CG2	10	0.12
(2,131)	1:29:A:PRO:CB	1:26:A:SER:CB	1	0.12
(2,131)	1:29:A:PRO:CB	1:26:A:SER:CB	2	0.12
(1,341)	1:146:A:ILE:HD13	1:143:A:LEU:HA	5	0.12
(1,287)	1:117:A:LEU:HD12	1:114:A:THR:HB	5	0.12
(12,82)	1:193:A:ILE:CG1	1:185:A:ILE:CD1	3	0.11
(12,82)	1:193:A:ILE:CG1	1:185:A:ILE:CD1	10	0.11
(12,55)	1:83:A:LEU:CA	1:176:A:TRP:CE3	10	0.11
(12,53)	1:83:A:LEU:CA	1:176:A:TRP:CE2	1	0.11
(12,53)	1:83:A:LEU:CA	1:176:A:TRP:CE2	2	0.11
(12,53)	1:83:A:LEU:CA	1:176:A:TRP:CE2	4	0.11
(12,53)	1:83:A:LEU:CA	1:176:A:TRP:CE2	9	0.11
(11,95)	1:203:A:CYS:CA	1:11:A:TYR:CE2	2	0.11
(11,92)	1:202:A:PHE:CG	1:179:A:TYR:CG	4	0.11
(11,74)	1:182:A:VAL:CB	1:201:A:LEU:CB	1	0.11
(11,74)	1:182:A:VAL:CB	1:201:A:LEU:CB	2	0.11
(11,74)	1:182:A:VAL:CB	1:201:A:LEU:CB	8	0.11
(11,65)	1:119:A:ALA:CA	1:132:A:TYR:CA	6	0.11
(11,50)	1:84:A:LEU:CG	1:176:A:TRP:CD2	5	0.11
(11,35)	1:73:A:TYR:CA	1:116:A:GLY:CA	4	0.11
(11,35)	1:73:A:TYR:CA	1:116:A:GLY:CA	8	0.11
(11,33)	1:70:A:TYR:CA	1:59:A:GLY:CA	3	0.11
(11,33)	1:70:A:TYR:CA	1:59:A:GLY:CA	4	0.11
(11,33)	1:70:A:TYR:CA	1:59:A:GLY:CA	5	0.11
(11,33)	1:70:A:TYR:CA	1:59:A:GLY:CA	7	0.11
(11,33)	1:70:A:TYR:CA	1:59:A:GLY:CA	8	0.11
(11,23)	1:53:A:ALA:CA	1:8:A:HIS:CA	2	0.11
(11,23)	1:53:A:ALA:CA	1:8:A:HIS:CA	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(11,23)	1:53:A:ALA:CA	1:8:A:HIS:CA	4	0.11
(11,23)	1:53:A:ALA:CA	1:8:A:HIS:CA	5	0.11
(11,23)	1:53:A:ALA:CA	1:8:A:HIS:CA	6	0.11
(11,23)	1:53:A:ALA:CA	1:8:A:HIS:CA	7	0.11
(11,23)	1:53:A:ALA:CA	1:8:A:HIS:CA	8	0.11
(11,23)	1:53:A:ALA:CA	1:8:A:HIS:CA	9	0.11
(11,23)	1:53:A:ALA:CA	1:8:A:HIS:CA	10	0.11
(10,17)	1:26:A:SER:H	1:22:A:PHE:O	1	0.11
(9,127)	1:132:A:TYR:C	1:134:A:CYS:CB	5	0.11
(9,80)	1:76:A:TRP:C	1:80:A:THR:CG2	2	0.11
(9,11)	1:14:A:GLY:C	1:15:A:MET:CE	9	0.11
(3,986)	1:208:A:PHE:CA	1:205:A:LEU:CG	2	0.11
(3,986)	1:208:A:PHE:CA	1:205:A:LEU:CG	6	0.11
(3,986)	1:208:A:PHE:CA	1:205:A:LEU:CG	9	0.11
(3,986)	1:208:A:PHE:CA	1:205:A:LEU:CG	10	0.11
(3,982)	1:207:A:PHE:CG	1:211:A:VAL:CA	1	0.11
(3,982)	1:207:A:PHE:CG	1:211:A:VAL:CA	3	0.11
(3,982)	1:207:A:PHE:CG	1:211:A:VAL:CA	5	0.11
(3,982)	1:207:A:PHE:CG	1:211:A:VAL:CA	6	0.11
(3,982)	1:207:A:PHE:CG	1:211:A:VAL:CA	9	0.11
(3,917)	1:187:A:PRO:C	1:191:A:GLY:CA	2	0.11
(3,917)	1:187:A:PRO:C	1:191:A:GLY:CA	5	0.11
(3,917)	1:187:A:PRO:C	1:191:A:GLY:CA	7	0.11
(3,885)	1:182:A:VAL:CA	1:179:A:TYR:CG	4	0.11
(3,885)	1:182:A:VAL:CA	1:179:A:TYR:CG	6	0.11
(3,885)	1:182:A:VAL:CA	1:179:A:TYR:CG	10	0.11
(3,801)	1:169:A:VAL:CB	1:168:A:LEU:CG	10	0.11
(3,729)	1:148:A:ASN:CA	1:147:A:TRP:CD2	1	0.11
(3,705)	1:143:A:LEU:CG	1:146:A:ILE:CB	1	0.11
(3,646)	1:131:A:TRP:CZ3	1:132:A:TYR:CA	10	0.11
(3,423)	1:83:A:LEU:CG	1:87:A:LEU:CG	2	0.11
(3,423)	1:83:A:LEU:CG	1:87:A:LEU:CG	3	0.11
(3,423)	1:83:A:LEU:CG	1:87:A:LEU:CG	4	0.11
(3,423)	1:83:A:LEU:CG	1:87:A:LEU:CG	5	0.11
(3,423)	1:83:A:LEU:CG	1:87:A:LEU:CG	6	0.11
(3,423)	1:83:A:LEU:CG	1:87:A:LEU:CG	7	0.11
(3,410)	1:82:A:LEU:CG	1:85:A:LEU:CB	2	0.11
(3,410)	1:82:A:LEU:CG	1:85:A:LEU:CB	4	0.11
(3,410)	1:82:A:LEU:CG	1:85:A:LEU:CB	6	0.11
(3,410)	1:82:A:LEU:CG	1:85:A:LEU:CB	7	0.11
(3,410)	1:82:A:LEU:CG	1:85:A:LEU:CB	10	0.11
(3,383)	1:78:A:VAL:CB	1:75:A:ASP:CG	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,383)	1:78:A:VAL:CB	1:75:A:ASP:CG	3	0.11
(3,383)	1:78:A:VAL:CB	1:75:A:ASP:CG	4	0.11
(3,383)	1:78:A:VAL:CB	1:75:A:ASP:CG	7	0.11
(3,383)	1:78:A:VAL:CB	1:75:A:ASP:CG	9	0.11
(3,383)	1:78:A:VAL:CB	1:75:A:ASP:CG	10	0.11
(3,382)	1:78:A:VAL:CB	1:81:A:PRO:CD	3	0.11
(3,382)	1:78:A:VAL:CB	1:81:A:PRO:CD	10	0.11
(3,360)	1:76:A:TRP:CA	1:73:A:TYR:CG	3	0.11
(3,360)	1:76:A:TRP:CA	1:73:A:TYR:CG	9	0.11
(3,337)	1:74:A:ILE:CB	1:76:A:TRP:CA	3	0.11
(3,337)	1:74:A:ILE:CB	1:76:A:TRP:CA	6	0.11
(3,322)	1:73:A:TYR:CA	1:72:A:ARG:CD	1	0.11
(3,322)	1:73:A:TYR:CA	1:72:A:ARG:CD	3	0.11
(3,322)	1:73:A:TYR:CA	1:72:A:ARG:CD	5	0.11
(3,322)	1:73:A:TYR:CA	1:72:A:ARG:CD	9	0.11
(3,322)	1:73:A:TYR:CA	1:72:A:ARG:CD	10	0.11
(3,119)	1:32:A:VAL:CA	1:35:A:TYR:CE2	9	0.11
(3,115)	1:32:A:VAL:CA	1:35:A:TYR:CE1	2	0.11
(3,115)	1:32:A:VAL:CA	1:35:A:TYR:CE1	7	0.11
(3,115)	1:32:A:VAL:CA	1:35:A:TYR:CE1	8	0.11
(3,115)	1:32:A:VAL:CA	1:35:A:TYR:CE1	9	0.11
(3,115)	1:32:A:VAL:CA	1:35:A:TYR:CE1	10	0.11
(3,105)	1:29:A:PRO:CD	1:25:A:LEU:CA	1	0.11
(3,105)	1:29:A:PRO:CD	1:25:A:LEU:CA	2	0.11
(3,105)	1:29:A:PRO:CD	1:25:A:LEU:CA	5	0.11
(3,105)	1:29:A:PRO:CD	1:25:A:LEU:CA	6	0.11
(3,105)	1:29:A:PRO:CD	1:25:A:LEU:CA	7	0.11
(3,105)	1:29:A:PRO:CD	1:25:A:LEU:CA	8	0.11
(2,1106)	1:183:A:TRP:C	1:182:A:VAL:CG2	10	0.11
(2,746)	1:115:A:SER:C	1:114:A:THR:CG2	5	0.11
(2,543)	1:79:A:THR:C	1:78:A:VAL:CG2	5	0.11
(2,543)	1:79:A:THR:C	1:78:A:VAL:CG2	6	0.11
(2,543)	1:79:A:THR:C	1:78:A:VAL:CG2	7	0.11
(2,131)	1:29:A:PRO:CB	1:26:A:SER:CB	3	0.11
(2,131)	1:29:A:PRO:CB	1:26:A:SER:CB	8	0.11
(1,173)	1:80:A:THR:HA	1:83:A:LEU:HA	4	0.11
(12,82)	1:193:A:ILE:CG1	1:185:A:ILE:CD1	2	0.1
(12,82)	1:193:A:ILE:CG1	1:185:A:ILE:CD1	4	0.1
(12,82)	1:193:A:ILE:CG1	1:185:A:ILE:CD1	6	0.1
(12,82)	1:193:A:ILE:CG1	1:185:A:ILE:CD1	8	0.1
(12,82)	1:193:A:ILE:CG1	1:185:A:ILE:CD1	9	0.1
(12,4)	1:11:A:TYR:CZ	1:54:A:MET:CE	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(12,3)	1:8:A:HIS:CE1	1:69:A:HIS:CE1	1	0.1
(12,3)	1:8:A:HIS:CE1	1:69:A:HIS:CE1	2	0.1
(12,3)	1:8:A:HIS:CE1	1:69:A:HIS:CE1	3	0.1
(12,3)	1:8:A:HIS:CE1	1:69:A:HIS:CE1	7	0.1
(11,85)	1:189:A:GLY:CA	1:183:A:TRP:CZ3	1	0.1
(11,74)	1:182:A:VAL:CB	1:201:A:LEU:CB	4	0.1
(11,74)	1:182:A:VAL:CB	1:201:A:LEU:CB	5	0.1
(11,74)	1:182:A:VAL:CB	1:201:A:LEU:CB	6	0.1
(11,65)	1:119:A:ALA:CA	1:132:A:TYR:CA	5	0.1
(11,50)	1:84:A:LEU:CG	1:176:A:TRP:CD2	2	0.1
(11,50)	1:84:A:LEU:CG	1:176:A:TRP:CD2	8	0.1
(11,35)	1:73:A:TYR:CA	1:116:A:GLY:CA	1	0.1
(11,33)	1:70:A:TYR:CA	1:59:A:GLY:CA	9	0.1
(11,28)	1:55:A:ALA:CA	1:9:A:TRP:CZ3	8	0.1
(10,97)	1:158:A:SER:H	1:154:A:THR:O	4	0.1
(10,17)	1:26:A:SER:H	1:22:A:PHE:O	6	0.1
(9,126)	1:132:A:TYR:C	1:136:A:VAL:CG1	2	0.1
(9,68)	1:69:A:HIS:C	1:71:A:ALA:CB	8	0.1
(9,35)	1:48:A:GLY:C	1:49:A:LEU:CD2	8	0.1
(3,1010)	1:216:A:LEU:CG	1:218:A:LEU:C	6	0.1
(3,982)	1:207:A:PHE:CG	1:211:A:VAL:CA	2	0.1
(3,982)	1:207:A:PHE:CG	1:211:A:VAL:CA	4	0.1
(3,952)	1:201:A:LEU:CG	1:204:A:LEU:CB	2	0.1
(3,917)	1:187:A:PRO:C	1:191:A:GLY:CA	6	0.1
(3,885)	1:182:A:VAL:CA	1:179:A:TYR:CG	2	0.1
(3,801)	1:169:A:VAL:CB	1:168:A:LEU:CG	5	0.1
(3,729)	1:148:A:ASN:CA	1:147:A:TRP:CD2	3	0.1
(3,729)	1:148:A:ASN:CA	1:147:A:TRP:CD2	8	0.1
(3,729)	1:148:A:ASN:CA	1:147:A:TRP:CD2	9	0.1
(3,705)	1:143:A:LEU:CG	1:146:A:ILE:CB	5	0.1
(3,567)	1:113:A:ILE:CB	1:117:A:LEU:CG	4	0.1
(3,567)	1:113:A:ILE:CB	1:117:A:LEU:CG	5	0.1
(3,567)	1:113:A:ILE:CB	1:117:A:LEU:CG	7	0.1
(3,531)	1:109:A:GLN:CB	1:112:A:VAL:CA	9	0.1
(3,512)	1:106:A:MET:CG	1:105:A:LEU:CB	5	0.1
(3,423)	1:83:A:LEU:CG	1:87:A:LEU:CG	1	0.1
(3,423)	1:83:A:LEU:CG	1:87:A:LEU:CG	10	0.1
(3,410)	1:82:A:LEU:CG	1:85:A:LEU:CB	5	0.1
(3,383)	1:78:A:VAL:CB	1:75:A:ASP:CG	5	0.1
(3,337)	1:74:A:ILE:CB	1:76:A:TRP:CA	1	0.1
(3,253)	1:58:A:GLN:CD	1:59:A:GLY:CA	10	0.1
(3,191)	1:47:A:SER:CA	1:46:A:TRP:CD1	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,115)	1:32:A:VAL:CA	1:35:A:TYR:CE1	3	0.1
(3,115)	1:32:A:VAL:CA	1:35:A:TYR:CE1	4	0.1
(3,115)	1:32:A:VAL:CA	1:35:A:TYR:CE1	5	0.1
(3,115)	1:32:A:VAL:CA	1:35:A:TYR:CE1	6	0.1
(3,105)	1:29:A:PRO:CD	1:25:A:LEU:CA	4	0.1
(3,100)	1:26:A:SER:CA	1:22:A:PHE:CG	3	0.1
(3,100)	1:26:A:SER:CA	1:22:A:PHE:CG	7	0.1
(3,45)	1:12:A:VAL:CA	1:9:A:TRP:CD2	1	0.1
(2,1175)	1:198:A:ASP:C	1:197:A:ILE:CG2	1	0.1
(2,1070)	1:180:A:PRO:CB	1:183:A:TRP:CE2	1	0.1
(2,1070)	1:180:A:PRO:CB	1:183:A:TRP:CE2	2	0.1
(2,1070)	1:180:A:PRO:CB	1:183:A:TRP:CE2	9	0.1
(2,987)	1:165:A:TYR:C	1:168:A:LEU:CD2	1	0.1
(2,779)	1:120:A:ASP:C	1:119:A:ALA:CB	10	0.1
(2,590)	1:84:A:LEU:CD1	1:81:A:PRO:CB	4	0.1
(2,543)	1:79:A:THR:C	1:78:A:VAL:CG2	1	0.1
(2,131)	1:29:A:PRO:CB	1:26:A:SER:CB	6	0.1
(1,193)	1:83:A:LEU:HD13	1:80:A:THR:HA	7	0.1
(1,173)	1:80:A:THR:HA	1:83:A:LEU:HA	2	0.1

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

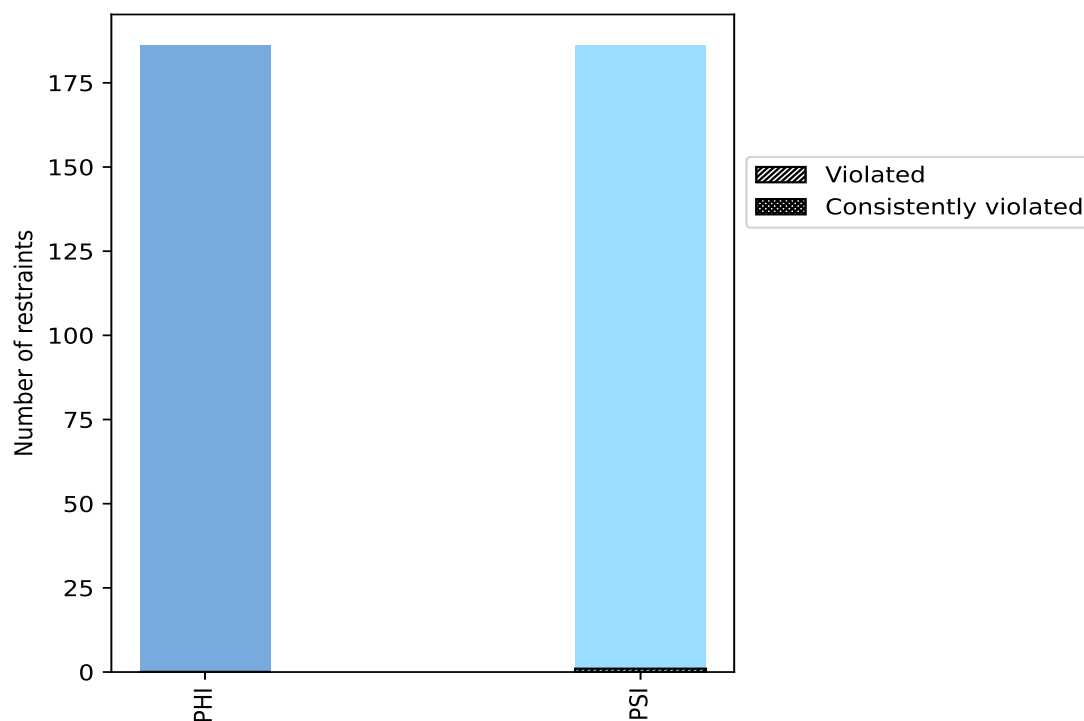
### 10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PHI	186	50.0	0	0.0	0.0	0	0.0	0.0
PSI	186	50.0	1	0.5	0.3	0	0.0	0.0
Total	372	100.0	1	0.3	0.3	0	0.0	0.0

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

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



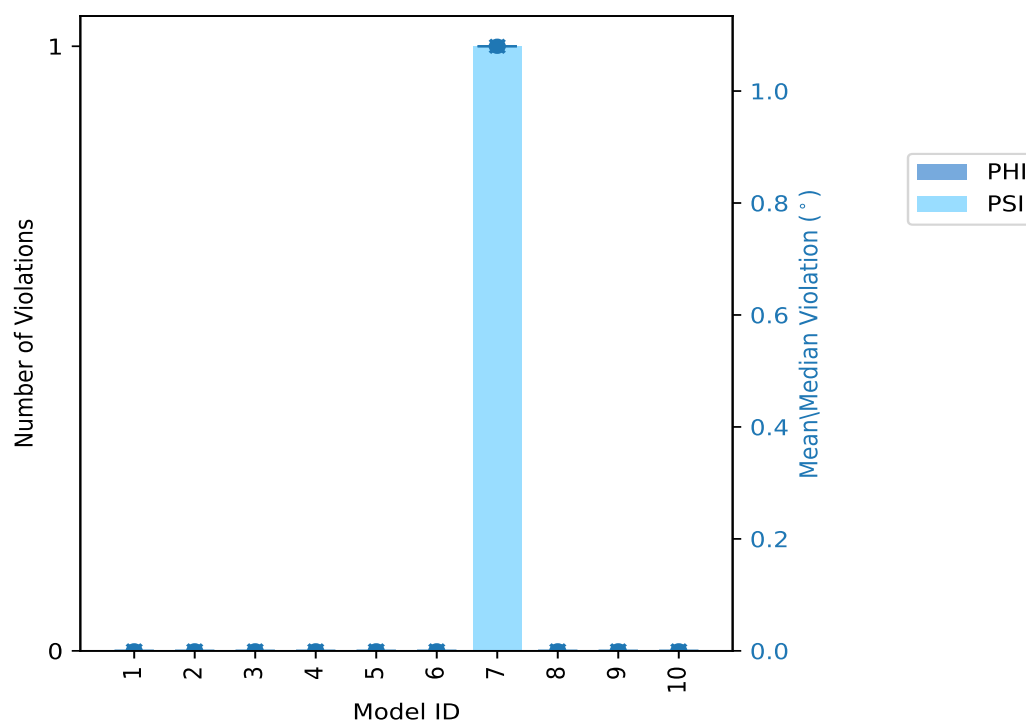
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0.0	0.0	0.0	0.0
7	0	1	1	1.08	1.08	0.0	1.08
8	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0.0	0.0	0.0	0.0

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



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

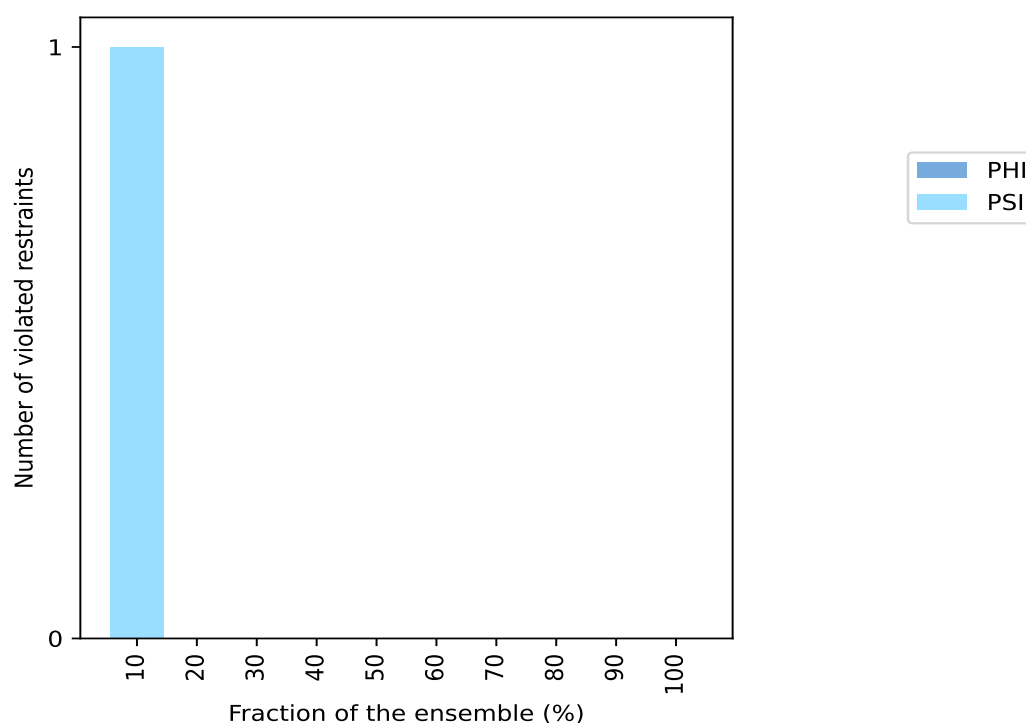
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count <sup>1</sup>	%
0	1	1	1	10.0
0	0	0	2	20.0
0	0	0	3	30.0
0	0	0	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

<sup>1</sup> Number of models with violations

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



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

No violations found

## 10.5 All violated dihedral-angle restraints [i](#)

### 10.5.1 Histogram : Distribution of violations [i](#)

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

Data insufficient to plot histogram

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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,342)	1:205:A:LEU:N	1:205:A:LEU:CA	1:205:A:LEU:C	1:206:A:PRO:N	7	1.08