



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 4, 2023 – 04:02 AM EDT

PDB ID : 2LBX  
BMRB ID : 17579  
Title : Solution structure of the *S. cerevisiae* H/ACA RNP protein Nhp2p  
Authors : Koo, B.; Park, C.; Fernandez, C.F.; Chim, N.; Ding, Y.; Chanfreau, G.; Feigon, J.  
Deposited on : 2011-04-07

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  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.33

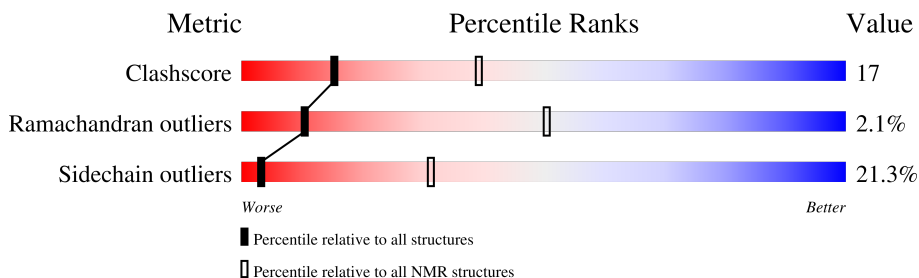
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 74%.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	121	

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:36-A:127, A:139-A:156 (110)	0.66	6

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

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

The models can be grouped into 4 clusters. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1933 atoms, of which 1006 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called H/ACA ribonucleoprotein complex subunit 2.

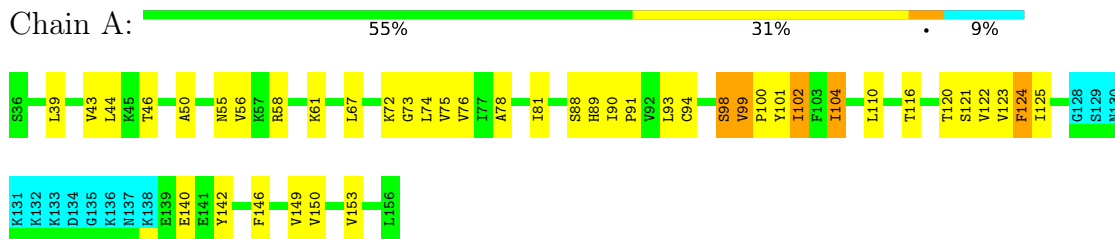
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	121	1933	592	1006	164	170	1	0

## 4 Residue-property plots [i](#)

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

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

- Molecule 1: H/ACA ribonucleoprotein complex subunit 2

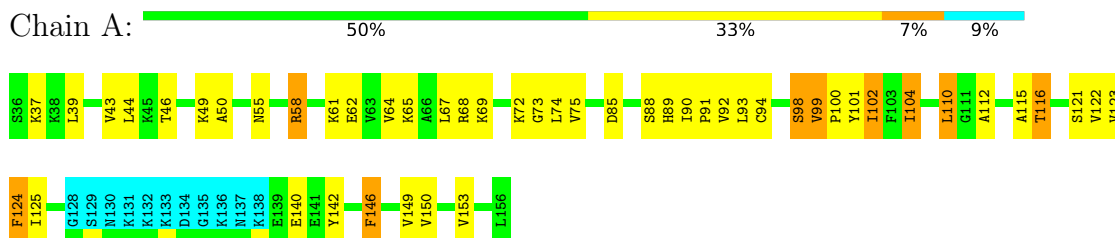


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

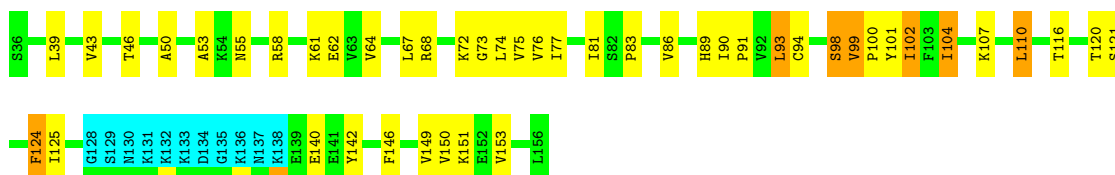
- Molecule 1: H/ACA ribonucleoprotein complex subunit 2



#### 4.2.2 Score per residue for model 2

- Molecule 1: H/ACA ribonucleoprotein complex subunit 2

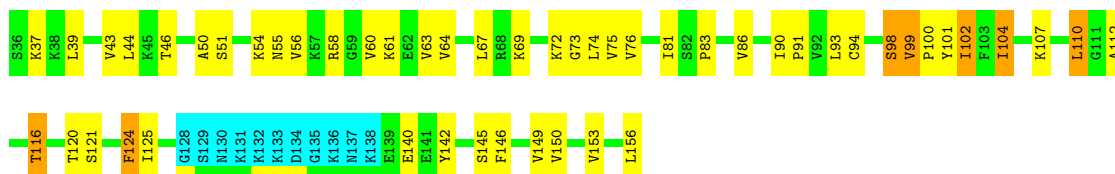




#### 4.2.3 Score per residue for model 3

- Molecule 1: H/ACA ribonucleoprotein complex subunit 2

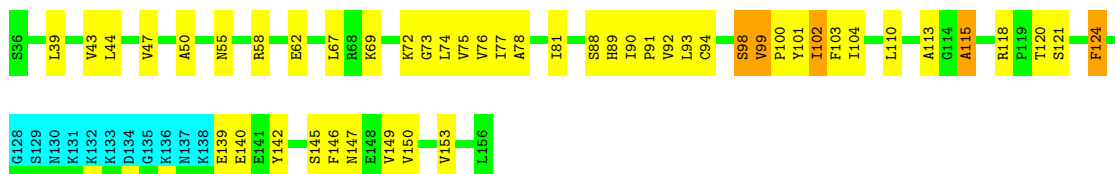
Chain A:



#### 4.2.4 Score per residue for model 4

- Molecule 1: H/ACA ribonucleoprotein complex subunit 2

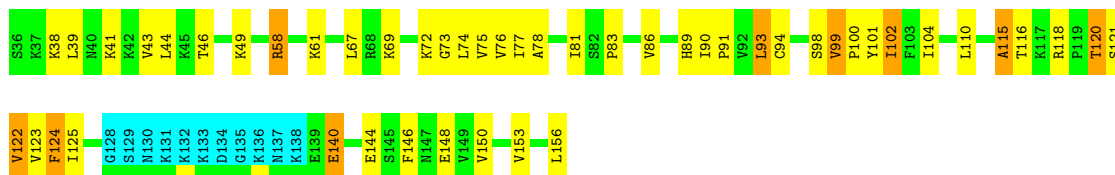
Chain A:



#### 4.2.5 Score per residue for model 5

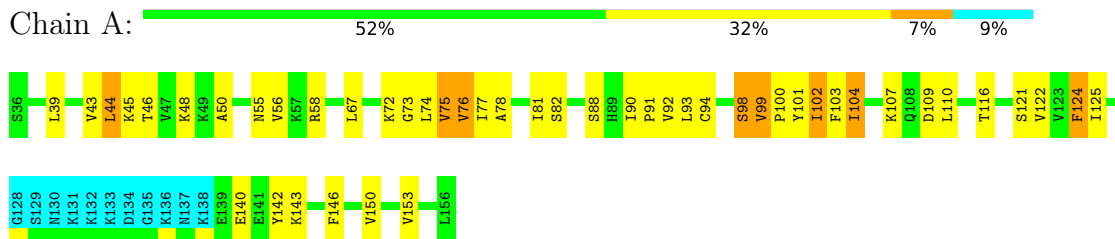
- Molecule 1: H/ACA ribonucleoprotein complex subunit 2

Chain A:



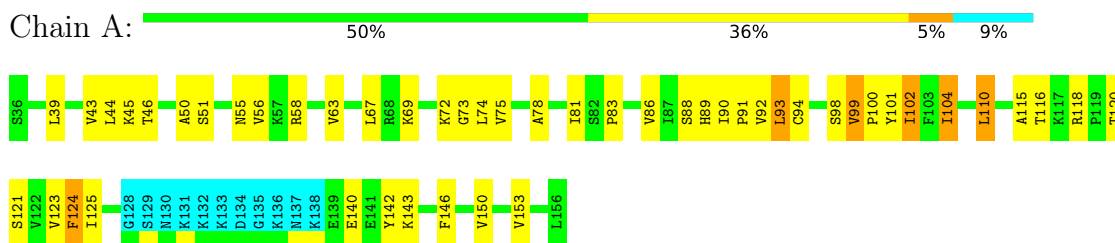
#### 4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: H/ACA ribonucleoprotein complex subunit 2



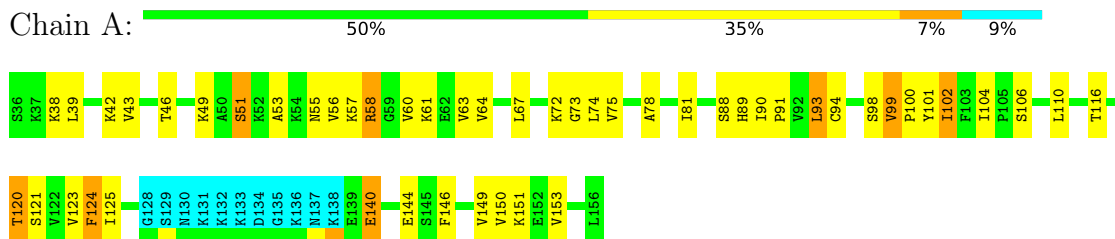
#### 4.2.7 Score per residue for model 7

- Molecule 1: H/ACA ribonucleoprotein complex subunit 2



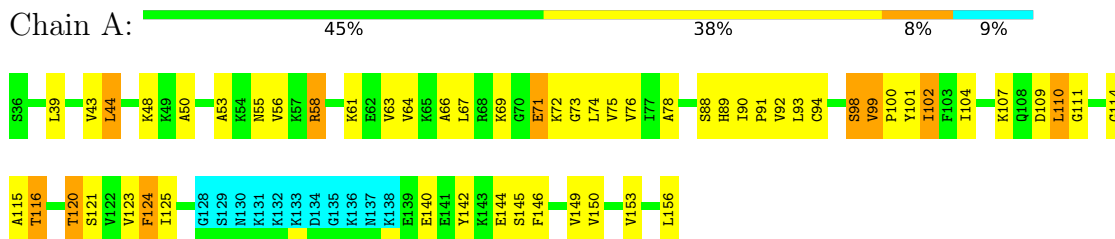
#### 4.2.8 Score per residue for model 8

- Molecule 1: H/ACA ribonucleoprotein complex subunit 2



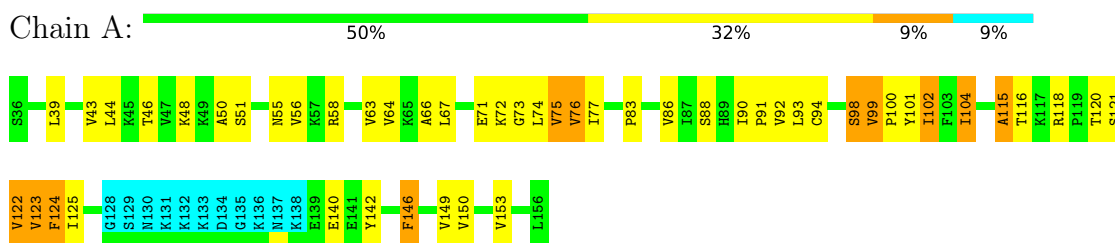
#### 4.2.9 Score per residue for model 9

- Molecule 1: H/ACA ribonucleoprotein complex subunit 2

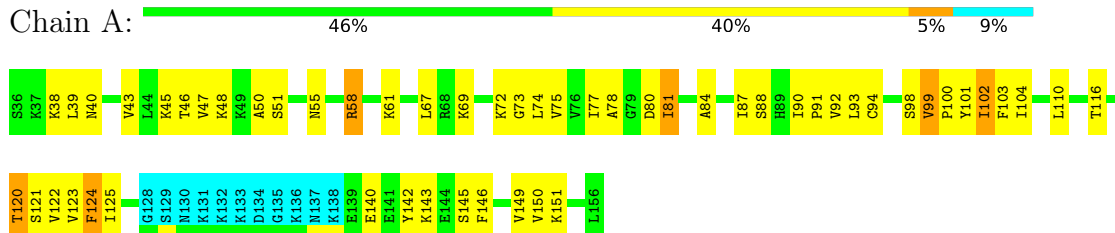


#### 4.2.10 Score per residue for model 10

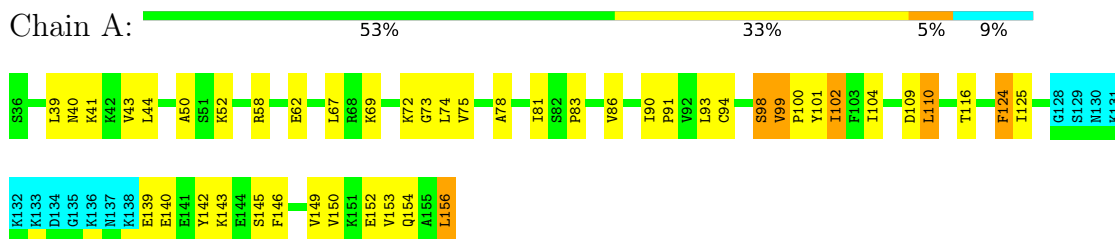
- Molecule 1: H/ACA ribonucleoprotein complex subunit 2



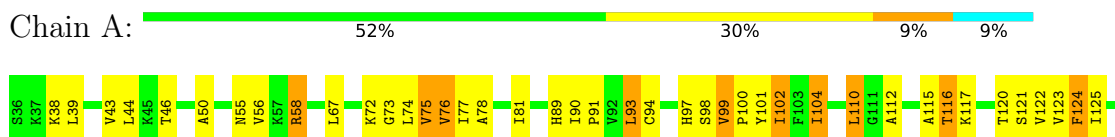
- Molecule 1: H/ACA ribonucleoprotein complex subunit 2



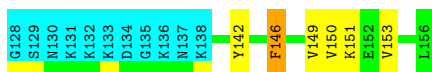
- Molecule 1: H/ACA ribonucleoprotein complex subunit 2



- Molecule 1: H/ACA ribonucleoprotein complex subunit 2



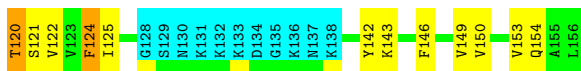




#### 4.2.14 Score per residue for model 14

- Molecule 1: H/ACA ribonucleoprotein complex subunit 2

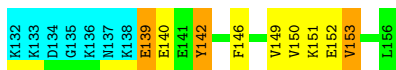
Chain A: 49% 36% 7% 9%



#### 4.2.15 Score per residue for model 15

- Molecule 1: H/ACA ribonucleoprotein complex subunit 2

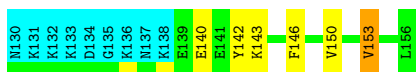
Chain A: 54% 30% 7% 9%



#### 4.2.16 Score per residue for model 16

- Molecule 1: H/ACA ribonucleoprotein complex subunit 2

Chain A: 56% 27% 7% 9%



#### 4.2.17 Score per residue for model 17

- Molecule 1: H/ACA ribonucleoprotein complex subunit 2

Chain A: 54% 31% 6% 9%



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
TALOS	geometry optimization	
CYANA	refinement	2.1

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1209
Number of shifts mapped to atoms	1209
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

## 6 Model quality

### 6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	844	914	913	29±3
All	All	16880	18280	18260	580

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:LEU:HD13	1:A:150:VAL:HG22	1.11	1.23	20	19
1:A:77:ILE:HD12	1:A:122:VAL:HG12	0.81	1.53	13	7
1:A:104:ILE:HD11	1:A:110:LEU:HD23	0.76	1.56	11	5
1:A:104:ILE:HD11	1:A:110:LEU:HD12	0.76	1.57	12	3
1:A:74:LEU:HD13	1:A:150:VAL:HG13	0.73	1.60	13	5
1:A:56:VAL:HG12	1:A:125:ILE:HD12	0.71	1.59	20	1
1:A:102:ILE:CD1	1:A:104:ILE:HG23	0.70	2.17	6	18
1:A:104:ILE:HD12	1:A:110:LEU:HD22	0.69	1.64	6	2
1:A:74:LEU:HD22	1:A:150:VAL:HG22	0.68	1.66	13	7
1:A:50:ALA:HB2	1:A:142:TYR:CE1	0.67	2.24	1	17
1:A:75:VAL:HG22	1:A:124:PHE:CZ	0.67	2.25	13	20
1:A:149:VAL:O	1:A:153:VAL:HG23	0.66	1.91	2	6
1:A:115:ALA:HB3	1:A:118:ARG:O	0.64	1.92	4	4
1:A:78:ALA:HB2	1:A:110:LEU:HD13	0.64	1.70	20	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:LEU:HD21	1:A:120:THR:O	0.64	1.93	14	2
1:A:102:ILE:CG1	1:A:153:VAL:HG21	0.63	2.24	17	9
1:A:56:VAL:CG1	1:A:125:ILE:HD12	0.63	2.23	20	1
1:A:39:LEU:O	1:A:43:VAL:HG23	0.62	1.94	7	20
1:A:50:ALA:HB1	1:A:55:ASN:HB2	0.62	1.70	13	9
1:A:74:LEU:CD1	1:A:150:VAL:HG22	0.62	2.23	12	7
1:A:74:LEU:HD22	1:A:146:PHE:CE1	0.61	2.31	20	9
1:A:75:VAL:HG12	1:A:77:ILE:HD11	0.61	1.72	4	1
1:A:74:LEU:HD13	1:A:150:VAL:CG2	0.60	2.19	14	9
1:A:110:LEU:HD22	1:A:120:THR:O	0.60	1.96	20	3
1:A:99:VAL:HG22	1:A:100:PRO:HD2	0.60	1.73	13	20
1:A:55:ASN:OD1	1:A:56:VAL:HG13	0.60	1.97	20	1
1:A:77:ILE:CD1	1:A:122:VAL:HG12	0.59	2.27	5	5
1:A:152:GLU:CD	1:A:156:LEU:HD21	0.58	2.19	12	1
1:A:82:SER:HB3	1:A:86:VAL:HG21	0.58	1.74	18	1
1:A:145:SER:O	1:A:149:VAL:HG22	0.57	1.98	19	4
1:A:110:LEU:HD12	1:A:120:THR:O	0.57	1.98	5	2
1:A:104:ILE:HD11	1:A:110:LEU:CD2	0.57	2.30	3	5
1:A:74:LEU:HD21	1:A:102:ILE:HG21	0.57	1.74	16	2
1:A:104:ILE:CD1	1:A:110:LEU:HD12	0.56	2.31	12	1
1:A:43:VAL:HG11	1:A:102:ILE:HD12	0.56	1.78	9	5
1:A:80:ASP:C	1:A:81:ILE:HD13	0.56	2.20	11	1
1:A:100:PRO:HB2	1:A:150:VAL:HG13	0.55	1.77	19	7
1:A:50:ALA:HB1	1:A:55:ASN:CG	0.55	2.22	15	3
1:A:104:ILE:HD11	1:A:110:LEU:HG	0.55	1.79	17	1
1:A:146:PHE:O	1:A:150:VAL:HG23	0.55	2.02	16	18
1:A:114:GLY:O	1:A:115:ALA:HB3	0.54	2.00	9	1
1:A:44:LEU:HD22	1:A:109:ASP:HB3	0.54	1.78	12	1
1:A:74:LEU:HD22	1:A:150:VAL:CG2	0.54	2.33	12	6
1:A:58:ARG:HB3	1:A:120:THR:HG21	0.54	1.80	19	1
1:A:78:ALA:HB2	1:A:110:LEU:CG	0.54	2.33	6	1
1:A:46:THR:HG21	1:A:146:PHE:CD1	0.54	2.38	14	6
1:A:63:VAL:HG12	1:A:124:PHE:HB2	0.53	1.78	10	6
1:A:58:ARG:HB3	1:A:123:VAL:HG22	0.53	1.80	8	5
1:A:46:THR:HG22	1:A:142:TYR:CD1	0.53	2.38	13	4
1:A:78:ALA:HB3	1:A:81:ILE:O	0.53	2.03	12	6
1:A:83:PRO:HG2	1:A:86:VAL:HG23	0.52	1.81	10	2
1:A:46:THR:HG22	1:A:142:TYR:CE1	0.52	2.39	3	6
1:A:104:ILE:CD1	1:A:110:LEU:HD22	0.52	2.33	5	2
1:A:86:VAL:HG12	1:A:90:ILE:CD1	0.52	2.35	18	1
1:A:125:ILE:HG21	1:A:146:PHE:CE1	0.52	2.40	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:SER:O	1:A:92:VAL:HG23	0.52	2.05	10	10
1:A:102:ILE:HG12	1:A:153:VAL:HG21	0.52	1.82	17	3
1:A:90:ILE:N	1:A:91:PRO:HD2	0.52	2.20	18	20
1:A:125:ILE:HG21	1:A:146:PHE:CZ	0.52	2.40	18	14
1:A:104:ILE:HD11	1:A:110:LEU:HD22	0.52	1.82	1	2
1:A:44:LEU:CD2	1:A:104:ILE:HD13	0.52	2.35	12	1
1:A:110:LEU:HD21	1:A:123:VAL:HG21	0.52	1.81	17	1
1:A:50:ALA:HB2	1:A:142:TYR:CD1	0.51	2.39	13	2
1:A:78:ALA:HB2	1:A:110:LEU:HG	0.51	1.83	6	1
1:A:44:LEU:HD22	1:A:109:ASP:CB	0.51	2.35	12	1
1:A:46:THR:HG21	1:A:146:PHE:CB	0.50	2.36	13	12
1:A:56:VAL:HG12	1:A:125:ILE:HG23	0.50	1.82	6	2
1:A:83:PRO:HG2	1:A:86:VAL:HG13	0.50	1.84	5	2
1:A:102:ILE:HG13	1:A:153:VAL:HG21	0.50	1.81	8	2
1:A:78:ALA:HB2	1:A:110:LEU:HD22	0.49	1.84	14	1
1:A:74:LEU:CD1	1:A:150:VAL:HG13	0.49	2.38	2	3
1:A:76:VAL:HG12	1:A:110:LEU:CD2	0.49	2.38	2	2
1:A:112:ALA:HA	1:A:116:THR:HG23	0.49	1.84	3	5
1:A:86:VAL:HG22	1:A:90:ILE:CD1	0.48	2.39	14	1
1:A:56:VAL:HG23	1:A:125:ILE:CD1	0.48	2.37	13	10
1:A:50:ALA:HB2	1:A:142:TYR:CZ	0.48	2.44	3	1
1:A:59:GLY:HA2	1:A:120:THR:HG21	0.48	1.84	14	1
1:A:50:ALA:HB2	1:A:142:TYR:CE2	0.48	2.44	15	1
1:A:74:LEU:HD13	1:A:150:VAL:CG1	0.48	2.39	2	4
1:A:44:LEU:HD21	1:A:104:ILE:HD13	0.48	1.85	12	2
1:A:84:ALA:O	1:A:87:ILE:HD12	0.47	2.09	11	1
1:A:58:ARG:CA	1:A:123:VAL:HG13	0.47	2.38	17	1
1:A:94:CYS:O	1:A:98:SER:HA	0.47	2.09	18	13
1:A:43:VAL:HG22	1:A:149:VAL:HB	0.47	1.86	15	6
1:A:89:HIS:O	1:A:93:LEU:HD23	0.47	2.09	9	14
1:A:66:ALA:HB1	1:A:71:GLU:O	0.47	2.09	10	2
1:A:81:ILE:HD11	1:A:107:LYS:CG	0.47	2.40	6	1
1:A:78:ALA:CB	1:A:110:LEU:HD13	0.47	2.40	12	2
1:A:76:VAL:HB	1:A:123:VAL:HG22	0.46	1.86	18	1
1:A:58:ARG:CA	1:A:123:VAL:HG23	0.46	2.40	13	1
1:A:46:THR:HG21	1:A:146:PHE:HB2	0.46	1.88	13	5
1:A:74:LEU:HD12	1:A:100:PRO:O	0.46	2.11	13	1
1:A:121:SER:O	1:A:122:VAL:HG13	0.46	2.11	18	1
1:A:41:LYS:HA	1:A:44:LEU:HD23	0.46	1.86	20	2
1:A:81:ILE:HD11	1:A:107:LYS:HB3	0.46	1.87	2	2
1:A:43:VAL:HG22	1:A:149:VAL:CG2	0.46	2.41	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:SER:O	1:A:149:VAL:HG13	0.46	2.11	3	3
1:A:94:CYS:O	1:A:98:SER:CA	0.45	2.65	11	20
1:A:76:VAL:HG12	1:A:104:ILE:HG12	0.45	1.86	13	4
1:A:86:VAL:HG12	1:A:90:ILE:HD11	0.45	1.87	18	1
1:A:76:VAL:HB	1:A:123:VAL:HG13	0.45	1.87	10	1
1:A:55:ASN:O	1:A:126:VAL:HG22	0.45	2.11	20	3
1:A:64:VAL:HG22	1:A:68:ARG:CD	0.45	2.42	2	2
1:A:83:PRO:O	1:A:86:VAL:HG12	0.45	2.12	7	1
1:A:43:VAL:HG22	1:A:149:VAL:HG21	0.45	1.89	3	1
1:A:60:VAL:O	1:A:64:VAL:HG23	0.45	2.11	3	2
1:A:102:ILE:HD11	1:A:104:ILE:HG23	0.44	1.89	2	2
1:A:104:ILE:CD1	1:A:110:LEU:HD23	0.44	2.36	11	1
1:A:104:ILE:HD11	1:A:110:LEU:CD1	0.44	2.38	12	1
1:A:58:ARG:CB	1:A:123:VAL:HG13	0.44	2.43	17	1
1:A:44:LEU:HD22	1:A:109:ASP:CG	0.44	2.33	9	1
1:A:58:ARG:HG3	1:A:123:VAL:HG13	0.44	1.88	11	1
1:A:104:ILE:HD13	1:A:104:ILE:H	0.43	1.72	14	2
1:A:58:ARG:HH21	1:A:115:ALA:HB2	0.43	1.74	5	1
1:A:110:LEU:CD2	1:A:123:VAL:HG21	0.43	2.42	17	1
1:A:110:LEU:O	1:A:110:LEU:HD13	0.43	2.13	7	1
1:A:87:ILE:HA	1:A:90:ILE:HD12	0.43	1.90	18	1
1:A:83:PRO:O	1:A:86:VAL:HG23	0.43	2.14	3	2
1:A:104:ILE:HD12	1:A:110:LEU:CD2	0.43	2.41	6	1
1:A:51:SER:HA	1:A:56:VAL:HG12	0.43	1.91	8	1
1:A:56:VAL:HG23	1:A:125:ILE:HD13	0.42	1.91	7	3
1:A:110:LEU:C	1:A:110:LEU:HD13	0.42	2.34	19	1
1:A:78:ALA:HB3	1:A:81:ILE:HG12	0.42	1.92	11	1
1:A:50:ALA:HB1	1:A:55:ASN:ND2	0.42	2.29	16	3
1:A:114:GLY:O	1:A:115:ALA:CB	0.42	2.65	9	1
1:A:47:VAL:CG1	1:A:113:ALA:HB1	0.42	2.44	14	1
1:A:67:LEU:HD12	1:A:67:LEU:O	0.42	2.15	14	1
1:A:76:VAL:O	1:A:77:ILE:HD12	0.42	2.14	2	1
1:A:78:ALA:N	1:A:110:LEU:HD13	0.42	2.30	14	1
1:A:47:VAL:HG22	1:A:113:ALA:HB1	0.42	1.92	4	1
1:A:39:LEU:HD23	1:A:40:ASN:N	0.42	2.30	11	1
1:A:78:ALA:HB3	1:A:81:ILE:CG1	0.42	2.44	11	1
1:A:58:ARG:HA	1:A:123:VAL:HG23	0.41	1.90	13	1
1:A:78:ALA:HB2	1:A:110:LEU:HD11	0.41	1.90	5	1
1:A:104:ILE:HD13	1:A:104:ILE:N	0.41	2.30	14	2
1:A:90:ILE:N	1:A:91:PRO:CD	0.41	2.83	18	4
1:A:111:GLY:O	1:A:115:ALA:N	0.41	2.53	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:VAL:O	1:A:77:ILE:HD13	0.41	2.15	5	1
1:A:146:PHE:O	1:A:149:VAL:HG22	0.41	2.15	20	1
1:A:43:VAL:HG21	1:A:102:ILE:CD1	0.41	2.46	11	1
1:A:40:ASN:OD1	1:A:44:LEU:HD11	0.41	2.16	12	1
1:A:81:ILE:HD11	1:A:107:LYS:HG2	0.41	1.91	16	1
1:A:110:LEU:HD22	1:A:120:THR:HG23	0.41	1.90	17	1
1:A:63:VAL:HG23	1:A:64:VAL:N	0.41	2.30	10	2
1:A:149:VAL:HG23	1:A:150:VAL:N	0.41	2.31	19	1
1:A:58:ARG:HB3	1:A:123:VAL:HG13	0.41	1.93	1	1
1:A:75:VAL:HG23	1:A:100:PRO:O	0.41	2.15	4	1
1:A:47:VAL:HG23	1:A:125:ILE:HD12	0.41	1.93	11	1
1:A:81:ILE:HD11	1:A:107:LYS:HG3	0.41	1.92	6	1
1:A:76:VAL:HG21	1:A:125:ILE:HD11	0.40	1.93	3	1
1:A:42:LYS:HB3	1:A:149:VAL:HG11	0.40	1.93	8	1
1:A:78:ALA:HB1	1:A:81:ILE:HD12	0.40	1.92	4	1
1:A:44:LEU:HD22	1:A:109:ASP:OD2	0.40	2.16	6	1
1:A:56:VAL:HB	1:A:125:ILE:HD12	0.40	1.94	9	1
1:A:76:VAL:HG12	1:A:110:LEU:HD21	0.40	1.93	2	1
1:A:63:VAL:HG12	1:A:124:PHE:N	0.40	2.32	10	1
1:A:102:ILE:HD13	1:A:104:ILE:HG23	0.40	1.91	11	1
1:A:89:HIS:CD2	1:A:93:LEU:HD23	0.40	2.51	18	1
1:A:90:ILE:CB	1:A:91:PRO:CD	0.40	3.00	19	1
1:A:39:LEU:HD21	1:A:153:VAL:HG22	0.40	1.94	13	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	108/121 (89%)	95±3 (88±3%)	11±3 (10±3%)	2±1 (2±1%)	10	50
All	All	2160/2420 (89%)	1896 (88%)	218 (10%)	46 (2%)	10	50

All 8 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	73	GLY	20
1	A	140	GLU	16
1	A	115	ALA	5
1	A	121	SER	1
1	A	116	THR	1
1	A	117	LYS	1
1	A	139	GLU	1
1	A	98	SER	1

### 6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	95/104 (91%)	75±2 (79±2%)	20±2 (21±2%)	3	31
All	All	1900/2080 (91%)	1495 (79%)	405 (21%)	3	31

All 59 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	67	LEU	20
1	A	72	LYS	20
1	A	99	VAL	20
1	A	101	TYR	20
1	A	102	ILE	20
1	A	124	PHE	20
1	A	58	ARG	19
1	A	116	THR	19
1	A	121	SER	16
1	A	93	LEU	14
1	A	120	THR	13
1	A	44	LEU	12
1	A	61	LYS	11
1	A	98	SER	11
1	A	104	ILE	11
1	A	110	LEU	11
1	A	69	LYS	9
1	A	51	SER	8

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Mol	Chain	Res	Type	Models (Total)
1	A	76	VAL	8
1	A	122	VAL	6
1	A	55	ASN	6
1	A	156	LEU	6
1	A	48	LYS	6
1	A	143	LYS	6
1	A	153	VAL	6
1	A	49	LYS	5
1	A	151	LYS	5
1	A	38	LYS	5
1	A	62	GLU	4
1	A	103	PHE	4
1	A	144	GLU	4
1	A	45	LYS	4
1	A	75	VAL	4
1	A	154	GLN	4
1	A	85	ASP	3
1	A	146	PHE	3
1	A	54	LYS	3
1	A	139	GLU	3
1	A	41	LYS	3
1	A	140	GLU	3
1	A	71	GLU	3
1	A	52	LYS	3
1	A	37	LYS	2
1	A	147	ASN	2
1	A	82	SER	2
1	A	88	SER	2
1	A	107	LYS	2
1	A	80	ASP	2
1	A	117	LYS	2
1	A	65	LYS	1
1	A	148	GLU	1
1	A	57	LYS	1
1	A	106	SER	1
1	A	123	VAL	1
1	A	81	ILE	1
1	A	97	HIS	1
1	A	142	TYR	1
1	A	152	GLU	1
1	A	68	ARG	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 74% for the well-defined parts and 72% 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 (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	1209
Number of shifts mapped to atoms	1209
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	115	$-0.69 \pm 0.16$	Should be checked
$^{13}\text{C}_\beta$	108	$-0.11 \pm 0.20$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	103	$-0.33 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	110	$0.54 \pm 0.27$	Should be applied

#### 7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 74%, i.e. 1120 atoms were assigned a chemical shift out of a possible 1522. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	508/544 (93%)	210/220 (95%)	198/220 (90%)	100/104 (96%)
Sidechain	604/916 (66%)	402/597 (67%)	199/287 (69%)	3/32 (9%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	8/62 (13%)	8/31 (26%)	0/29 (0%)	0/2 (0%)
Overall	1120/1522 (74%)	620/848 (73%)	397/536 (74%)	103/138 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 1205 atoms were assigned a chemical shift out of a possible 1665. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	560/601 (93%)	232/244 (95%)	218/242 (90%)	110/115 (96%)
Sidechain	637/1002 (64%)	421/649 (65%)	212/314 (68%)	4/39 (10%)
Aromatic	8/62 (13%)	8/31 (26%)	0/29 (0%)	0/2 (0%)
Overall	1205/1665 (72%)	661/924 (72%)	430/585 (74%)	114/156 (73%)

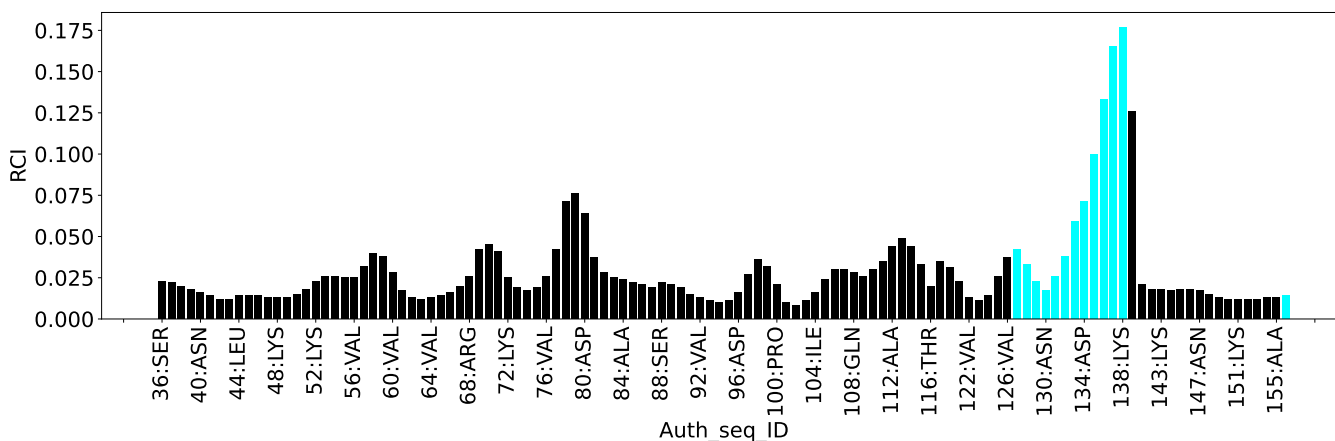
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1041
Intra-residue ( $ i-j =0$ )	298
Sequential ( $ i-j =1$ )	209
Medium range ( $ i-j >1$ and $ i-j <5$ )	91
Long range ( $ i-j \geq 5$ )	213
Inter-chain	0
Hydrogen bond restraints	230
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	8.6
Number of long range restraints per residue <sup>1</sup>	2.1

<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)	15.8	0.2
0.2-0.5 (Medium)	6.1	0.47
>0.5 (Large)	2.1	2.76

### 8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis [i](#)

### 9.1 Summary of distance violations [i](#)

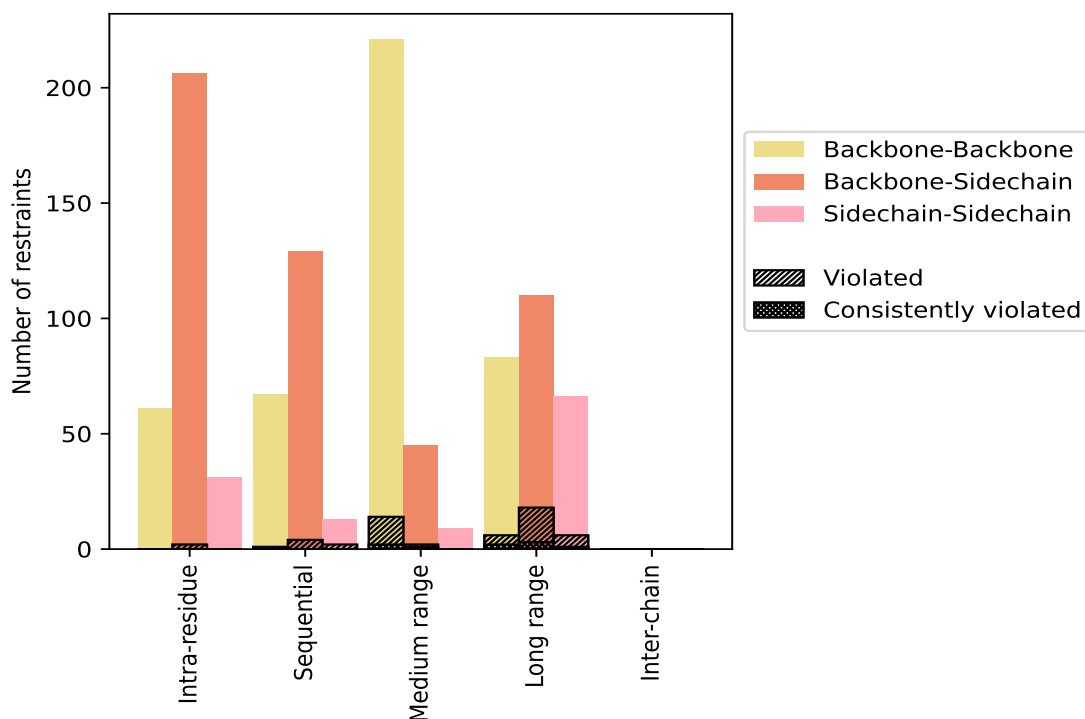
The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% <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>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>298</b>	<b>28.6</b>	<b>2</b>	<b>0.7</b>	<b>0.2</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	61	5.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	206	19.8	2	1.0	0.2	0	0.0	0.0
Sidechain-Sidechain	31	3.0	0	0.0	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>209</b>	<b>20.1</b>	<b>7</b>	<b>3.3</b>	<b>0.7</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	67	6.4	1	1.5	0.1	0	0.0	0.0
Backbone-Sidechain	129	12.4	4	3.1	0.4	0	0.0	0.0
Sidechain-Sidechain	13	1.2	2	15.4	0.2	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>91</b>	<b>8.7</b>	<b>3</b>	<b>3.3</b>	<b>0.3</b>	<b>1</b>	<b>1.1</b>	<b>0.1</b>
Backbone-Backbone	37	3.6	1	2.7	0.1	0	0.0	0.0
Backbone-Sidechain	45	4.3	2	4.4	0.2	1	2.2	0.1
Sidechain-Sidechain	9	0.9	0	0.0	0.0	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>213</b>	<b>20.5</b>	<b>26</b>	<b>12.2</b>	<b>2.5</b>	<b>5</b>	<b>2.3</b>	<b>0.5</b>
Backbone-Backbone	37	3.6	2	5.4	0.2	1	2.7	0.1
Backbone-Sidechain	110	10.6	18	16.4	1.7	3	2.7	0.3
Sidechain-Sidechain	66	6.3	6	9.1	0.6	1	1.5	0.1
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
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
<b>Hydrogen bond</b>	<b>230</b>	<b>22.1</b>	<b>17</b>	<b>7.4</b>	<b>1.6</b>	<b>3</b>	<b>1.3</b>	<b>0.3</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>1041</b>	<b>100.0</b>	<b>55</b>	<b>5.3</b>	<b>5.3</b>	<b>9</b>	<b>0.9</b>	<b>0.9</b>
Backbone-Backbone	432	41.5	21	4.9	2.0	4	0.9	0.4
Backbone-Sidechain	490	47.1	26	5.3	2.5	4	0.8	0.4
Sidechain-Sidechain	119	11.4	8	6.7	0.8	1	0.8	0.1

<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 disulfid bonds are counted in their appropriate category on the x-axis

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <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	1	4	6	12	0	23	0.26	1.5	0.3	0.18
2	1	2	5	14	0	22	0.26	1.51	0.3	0.16
3	1	4	5	15	0	25	0.29	2.59	0.48	0.18
4	0	5	6	12	0	23	0.19	0.4	0.08	0.17
5	1	3	6	15	0	25	0.32	2.13	0.46	0.15
6	1	3	9	16	0	29	0.26	1.5	0.28	0.15
7	2	4	5	14	0	25	0.36	2.59	0.54	0.17
8	1	4	5	15	0	25	0.34	2.29	0.48	0.16
9	1	2	8	9	0	20	0.33	2.45	0.49	0.21
10	1	3	8	13	0	25	0.34	2.1	0.46	0.17
11	2	3	5	13	0	23	0.24	0.93	0.17	0.18

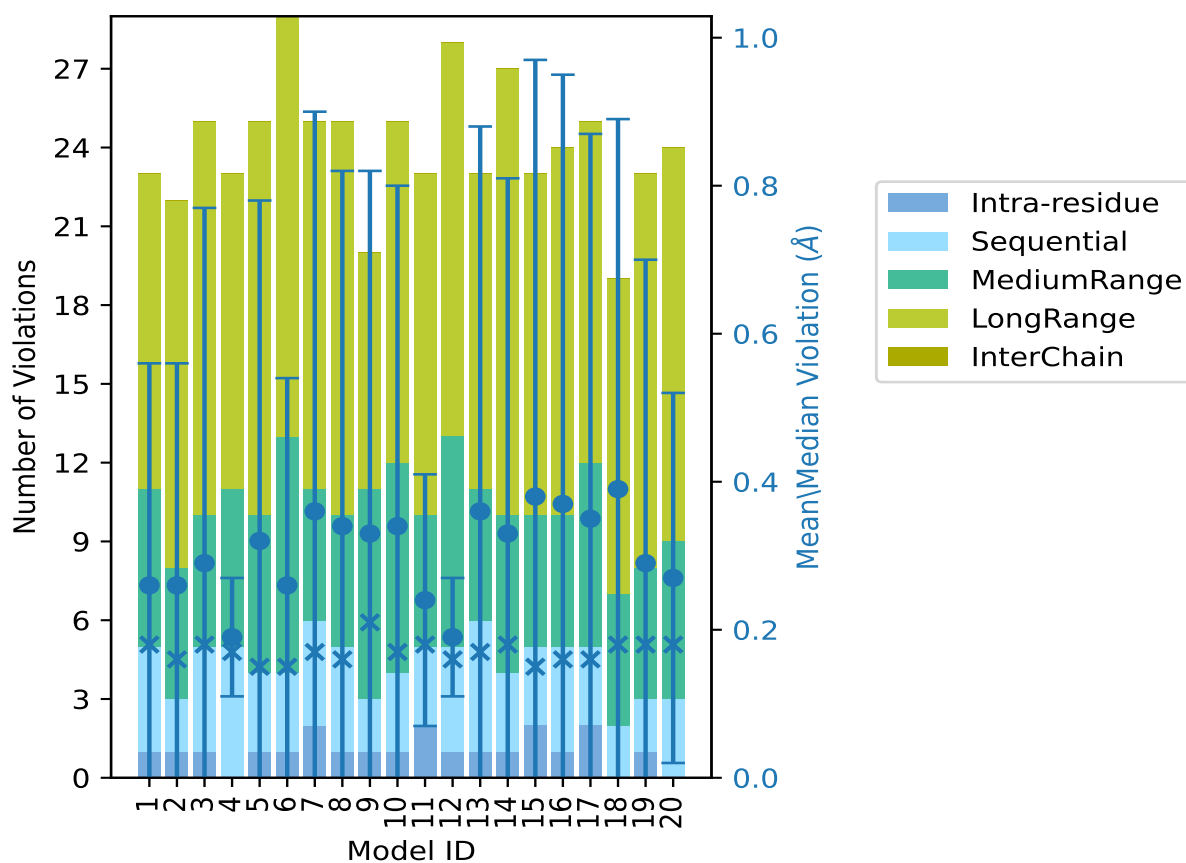
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>					
12	1	4	8	15	0	28	0.19	0.4	0.08	0.16
13	1	5	5	12	0	23	0.36	2.3	0.52	0.17
14	1	3	6	17	0	27	0.33	2.33	0.48	0.18
15	2	3	5	13	0	23	0.38	2.62	0.59	0.15
16	1	4	5	14	0	24	0.37	2.76	0.58	0.16
17	2	3	7	13	0	25	0.35	2.51	0.52	0.16
18	0	2	5	12	0	19	0.39	2.05	0.5	0.18
19	1	2	5	15	0	23	0.29	2.17	0.41	0.18
20	0	3	6	15	0	24	0.27	1.31	0.25	0.18

<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



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

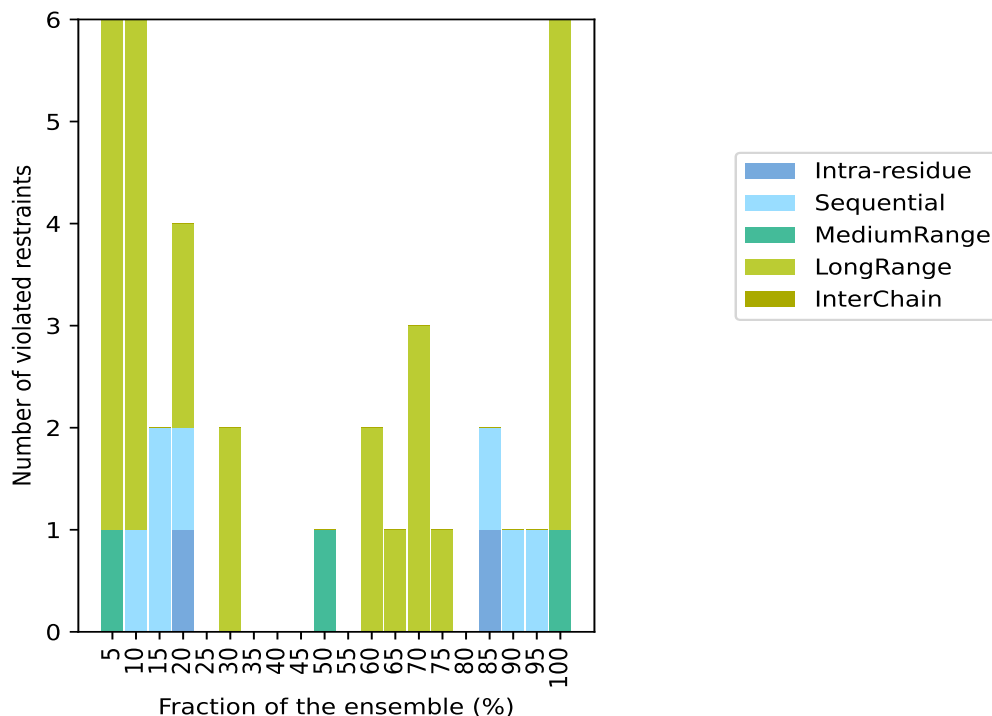
### 9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 773(IR:296, SQ:202, MR:88, LR:187, 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	0	1	5	0	6	1	5.0
0	1	0	5	0	6	2	10.0
0	2	0	0	0	2	3	15.0
1	1	0	2	0	4	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	2	0	2	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	1	0	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	2	0	2	12	60.0
0	0	0	1	0	1	13	65.0
0	0	0	3	0	3	14	70.0
0	0	0	1	0	1	15	75.0
0	0	0	0	0	0	16	80.0
1	1	0	0	0	2	17	85.0
0	1	0	0	0	1	18	90.0
0	1	0	0	0	1	19	95.0
0	0	1	5	0	6	20	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

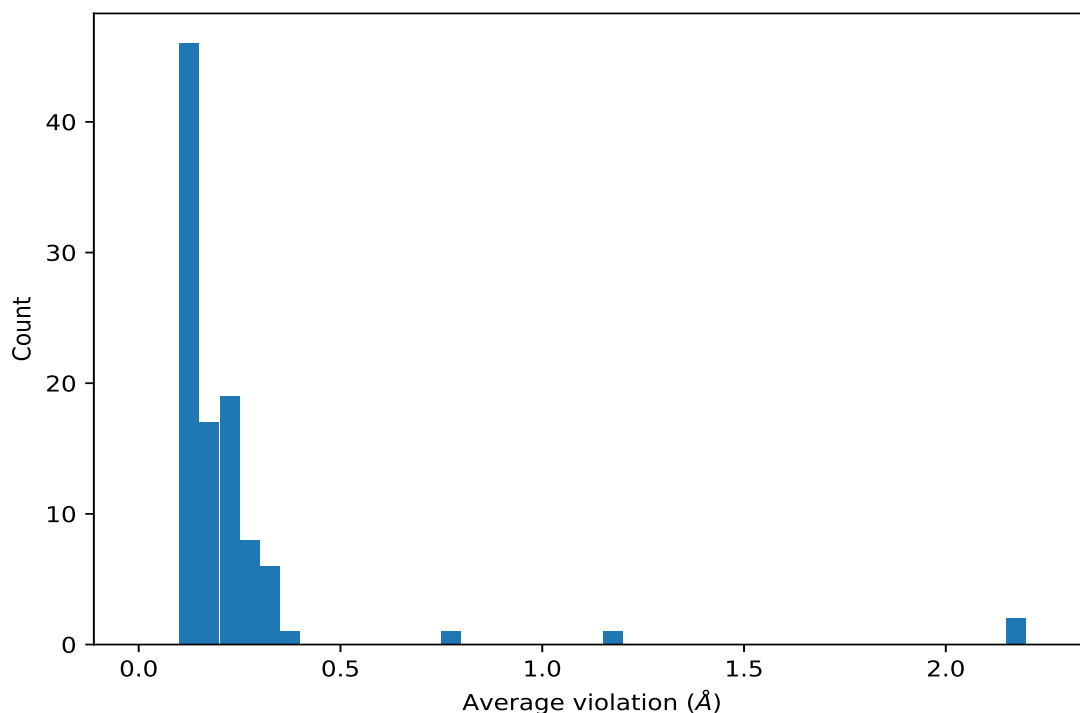
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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)
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	20	1.16	0.5	1.42
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	20	0.36	0.03	0.36
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	20	0.34	0.05	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	20	0.34	0.05	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	20	0.34	0.05	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	20	0.34	0.05	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	20	0.34	0.05	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	20	0.34	0.05	0.34
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	20	0.25	0.02	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	20	0.25	0.02	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	20	0.25	0.02	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	20	0.25	0.02	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	20	0.25	0.02	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	20	0.25	0.02	0.26
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	20	0.22	0.04	0.21
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	20	0.22	0.04	0.21

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	20	0.22	0.04	0.21
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	20	0.18	0.04	0.18
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	20	0.18	0.03	0.18
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	20	0.18	0.03	0.18
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	20	0.18	0.03	0.18
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	20	0.18	0.04	0.18
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	20	0.15	0.02	0.16
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	19	0.21	0.06	0.19
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	19	0.21	0.06	0.19
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	18	0.16	0.03	0.16
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	18	0.16	0.03	0.16
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	18	0.16	0.03	0.16
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	17	0.19	0.06	0.16
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	17	0.16	0.02	0.15
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	17	0.14	0.02	0.14
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	17	0.14	0.02	0.14
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	15	2.17	0.58	2.3
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	15	2.17	0.58	2.3
(1,331)	1:A:125:ILE:HB	1:A:146:PHE:HD1	14	0.79	0.06	0.8
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG2	14	0.15	0.03	0.16
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG3	14	0.15	0.03	0.16
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG2	14	0.15	0.03	0.16
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG3	14	0.15	0.03	0.16
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG2	14	0.15	0.03	0.16
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG3	14	0.15	0.03	0.16
(1,422)	1:A:72:LYS:HA	1:A:126:VAL:HA	14	0.13	0.02	0.12
(4,103)	1:A:74:LEU:O	1:A:125:ILE:H	14	0.12	0.01	0.12
(1,475)	1:A:46:THR:HG21	1:A:143:LYS:HA	13	0.18	0.04	0.18
(1,475)	1:A:46:THR:HG22	1:A:143:LYS:HA	13	0.18	0.04	0.18
(1,475)	1:A:46:THR:HG23	1:A:143:LYS:HA	13	0.18	0.04	0.18
(1,452)	1:A:56:VAL:HB	1:A:125:ILE:HB	12	0.14	0.04	0.13
(1,397)	1:A:75:VAL:H	1:A:125:ILE:HB	12	0.12	0.01	0.12
(1,235)	1:A:99:VAL:HB	1:A:101:TYR:H	10	0.12	0.01	0.12
(3,95)	1:A:57:LYS:H	1:A:124:PHE:O	9	0.12	0.01	0.12
(3,35)	1:A:85:ASP:O	1:A:89:HIS:H	7	0.18	0.03	0.18
(3,21)	1:A:59:GLY:O	1:A:63:VAL:H	7	0.14	0.02	0.13
(1,476)	1:A:46:THR:H	1:A:146:PHE:HD1	6	0.26	0.03	0.26
(1,476)	1:A:46:THR:H	1:A:146:PHE:HD2	6	0.26	0.03	0.26
(1,428)	1:A:60:VAL:HA	1:A:122:VAL:HB	6	0.13	0.01	0.12
(3,29)	1:A:63:VAL:O	1:A:67:LEU:H	6	0.12	0.01	0.12
(1,583)	1:A:58:ARG:HA	1:A:58:ARG:HD2	4	0.2	0.06	0.2
(1,583)	1:A:58:ARG:HA	1:A:58:ARG:HD3	4	0.2	0.06	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(3,61)	1:A:111:GLY:O	1:A:115:ALA:H	4	0.16	0.07	0.12
(1,132)	1:A:60:VAL:H	1:A:61:LYS:HB2	4	0.13	0.02	0.13
(1,132)	1:A:60:VAL:H	1:A:61:LYS:HB3	4	0.13	0.02	0.13
(1,414)	1:A:73:GLY:HA2	1:A:125:ILE:HD11	4	0.13	0.02	0.12
(1,414)	1:A:73:GLY:HA2	1:A:125:ILE:HD12	4	0.13	0.02	0.12
(1,414)	1:A:73:GLY:HA2	1:A:125:ILE:HD13	4	0.13	0.02	0.12
(1,414)	1:A:73:GLY:HA3	1:A:125:ILE:HD11	4	0.13	0.02	0.12
(1,414)	1:A:73:GLY:HA3	1:A:125:ILE:HD12	4	0.13	0.02	0.12
(1,414)	1:A:73:GLY:HA3	1:A:125:ILE:HD13	4	0.13	0.02	0.12
(1,495)	1:A:100:PRO:HA	1:A:153:VAL:HG21	4	0.12	0.02	0.12
(1,495)	1:A:100:PRO:HA	1:A:153:VAL:HG22	4	0.12	0.02	0.12
(1,495)	1:A:100:PRO:HA	1:A:153:VAL:HG23	4	0.12	0.02	0.12
(1,107)	1:A:37:LYS:HB2	1:A:38:LYS:HA	3	0.2	0.01	0.2
(1,107)	1:A:37:LYS:HB3	1:A:38:LYS:HA	3	0.2	0.01	0.2
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG11	3	0.12	0.01	0.12
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG12	3	0.12	0.01	0.12
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG13	3	0.12	0.01	0.12
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG21	3	0.12	0.01	0.12
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG22	3	0.12	0.01	0.12
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG23	3	0.12	0.01	0.12
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG11	3	0.12	0.01	0.12
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG12	3	0.12	0.01	0.12
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG13	3	0.12	0.01	0.12
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG21	3	0.12	0.01	0.12
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG22	3	0.12	0.01	0.12
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG23	3	0.12	0.01	0.12
(3,17)	1:A:46:THR:O	1:A:50:ALA:H	3	0.11	0.0	0.11
(1,334)	1:A:76:VAL:H	1:A:101:TYR:HD1	2	0.2	0.0	0.2
(1,334)	1:A:76:VAL:H	1:A:101:TYR:HD2	2	0.2	0.0	0.2
(1,357)	1:A:78:ALA:HB1	1:A:104:ILE:HG12	2	0.2	0.02	0.2
(1,357)	1:A:78:ALA:HB1	1:A:104:ILE:HG13	2	0.2	0.02	0.2
(1,357)	1:A:78:ALA:HB2	1:A:104:ILE:HG12	2	0.2	0.02	0.2
(1,357)	1:A:78:ALA:HB2	1:A:104:ILE:HG13	2	0.2	0.02	0.2
(1,357)	1:A:78:ALA:HB3	1:A:104:ILE:HG12	2	0.2	0.02	0.2
(1,357)	1:A:78:ALA:HB3	1:A:104:ILE:HG13	2	0.2	0.02	0.2
(1,459)	1:A:55:ASN:HB2	1:A:126:VAL:HA	2	0.2	0.02	0.2
(1,459)	1:A:55:ASN:HB3	1:A:126:VAL:HA	2	0.2	0.02	0.2
(1,471)	1:A:49:LYS:H	1:A:142:TYR:HD1	2	0.16	0.02	0.16
(1,471)	1:A:49:LYS:H	1:A:142:TYR:HD2	2	0.16	0.02	0.16
(1,468)	1:A:50:ALA:H	1:A:138:LYS:HG2	2	0.14	0.02	0.14
(1,468)	1:A:50:ALA:H	1:A:138:LYS:HG3	2	0.14	0.02	0.14
(1,163)	1:A:87:ILE:H	1:A:88:SER:HA	2	0.12	0.01	0.12

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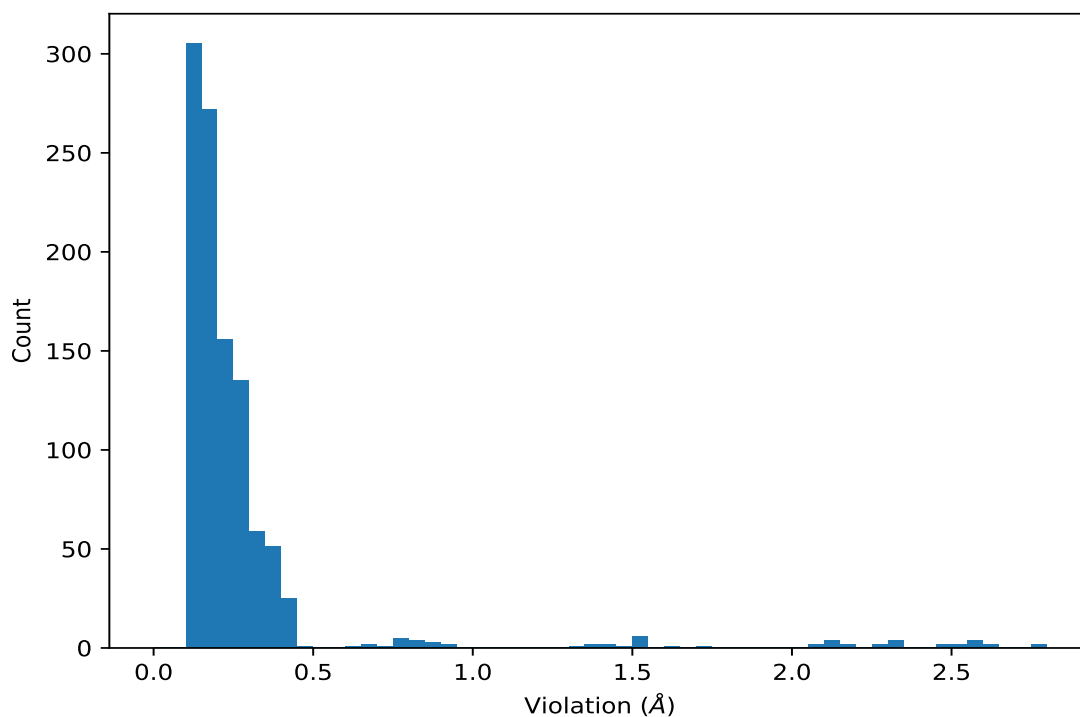
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(3,99)	1:A:78:ALA:H	1:A:121:SER:O	2	0.12	0.01	0.12

<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)
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	16	2.76
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	16	2.76
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	15	2.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	15	2.62
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	3	2.59
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	3	2.59
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	7	2.59
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	7	2.59
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	17	2.51
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	17	2.51
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	9	2.45
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	9	2.45
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	14	2.33
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	14	2.33
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	13	2.3
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	13	2.3
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	8	2.29
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	8	2.29
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	19	2.17
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	19	2.17
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	5	2.13
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	5	2.13
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	10	2.1
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	10	2.1
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	18	2.05
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	18	2.05
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	15	1.7
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	13	1.63
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	16	1.54
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	10	1.53
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	2	1.51
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	1	1.5
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	6	1.5
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	7	1.5
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	14	1.46
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	8	1.44
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	18	1.4
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	5	1.38
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	17	1.37
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	20	1.31
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	11	0.93
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	11	0.93
(1,331)	1:A:125:ILE:HB	1:A:146:PHE:HD1	7	0.86
(1,331)	1:A:125:ILE:HB	1:A:146:PHE:HD1	15	0.85
(1,331)	1:A:125:ILE:HB	1:A:146:PHE:HD1	17	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,331)	1:A:125:ILE:HB	1:A:146:PHE:HD1	14	0.84
(1,331)	1:A:125:ILE:HB	1:A:146:PHE:HD1	18	0.84
(1,331)	1:A:125:ILE:HB	1:A:146:PHE:HD1	16	0.83
(1,331)	1:A:125:ILE:HB	1:A:146:PHE:HD1	6	0.81
(1,331)	1:A:125:ILE:HB	1:A:146:PHE:HD1	1	0.79
(1,331)	1:A:125:ILE:HB	1:A:146:PHE:HD1	10	0.79
(1,331)	1:A:125:ILE:HB	1:A:146:PHE:HD1	20	0.78
(1,331)	1:A:125:ILE:HB	1:A:146:PHE:HD1	5	0.76
(1,331)	1:A:125:ILE:HB	1:A:146:PHE:HD1	8	0.76
(1,331)	1:A:125:ILE:HB	1:A:146:PHE:HD1	2	0.72
(1,330)	1:A:79:GLY:HA2	1:A:103:PHE:HD1	6	0.66
(1,330)	1:A:79:GLY:HA3	1:A:103:PHE:HD1	6	0.66
(1,331)	1:A:125:ILE:HB	1:A:146:PHE:HD1	13	0.62
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	3	0.47
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	13	0.43
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	13	0.43
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	13	0.43
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	13	0.43
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	13	0.43
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	13	0.43
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	14	0.42
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	14	0.42
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	14	0.42
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	14	0.42
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	14	0.42
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	14	0.42
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	9	0.42
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	19	0.41
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	10	0.4
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	10	0.4
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	10	0.4
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	10	0.4
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	10	0.4
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	10	0.4
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	4	0.4
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	11	0.4
(1,277)	1:A:143:LYS:HA	1:A:146:PHE:HD1	12	0.4
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	11	0.4
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	11	0.4
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	5	0.39
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	10	0.39
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	19	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	19	0.39
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	19	0.39
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	19	0.39
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	19	0.39
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	19	0.39
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	6	0.38
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	7	0.38
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	11	0.38
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	2	0.38
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	2	0.38
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	2	0.38
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	2	0.38
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	2	0.38
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	2	0.38
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	2	0.37
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	8	0.37
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	12	0.37
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	3	0.36
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	13	0.36
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	19	0.36
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	20	0.36
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	15	0.36
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	15	0.36
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	15	0.36
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	15	0.36
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	15	0.36
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	15	0.36
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	4	0.35
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	16	0.35
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	18	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	1	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	1	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	1	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	1	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	1	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	1	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	7	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	7	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	7	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	7	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	7	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	16	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	16	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	16	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	16	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	16	0.35
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	16	0.35
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	1	0.34
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	9	0.34
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	14	0.34
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	17	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	8	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	8	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	8	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	8	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	8	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	8	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	18	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	18	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	18	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	18	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	18	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	18	0.34
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	4	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	4	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	4	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	4	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	4	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	4	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	6	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	6	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	6	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	6	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	6	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	6	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	9	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	9	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	9	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	9	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	9	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	9	0.33
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	20	0.32
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	20	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	20	0.32
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	20	0.32
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	20	0.32
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	20	0.32
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	12	0.31
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	12	0.31
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	12	0.31
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	18	0.31
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	12	0.31
(1,476)	1:A:46:THR:H	1:A:146:PHE:HD1	12	0.3
(1,476)	1:A:46:THR:H	1:A:146:PHE:HD2	12	0.3
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	17	0.3
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	17	0.3
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	17	0.3
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	17	0.3
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	17	0.3
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	17	0.3
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	15	0.3
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	15	0.3
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	15	0.3
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	15	0.3
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	15	0.3
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	15	0.3
(1,476)	1:A:46:THR:H	1:A:146:PHE:HD1	9	0.29
(1,476)	1:A:46:THR:H	1:A:146:PHE:HD2	9	0.29
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	3	0.29
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	3	0.29
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	3	0.29
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	3	0.29
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	3	0.29
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	3	0.29
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	6	0.28
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	6	0.28
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	6	0.28
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	18	0.28
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	18	0.28
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	18	0.28
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	5	0.28
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	5	0.28
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	5	0.28
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	5	0.28
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	5	0.28
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	10	0.28
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	10	0.28
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	10	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	9	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	9	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	9	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	9	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	9	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	9	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	12	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	12	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	12	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	12	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	12	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	12	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	17	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	17	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	17	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	17	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	17	0.28
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	17	0.28
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	9	0.28
(3,61)	1:A:111:GLY:O	1:A:115:ALA:H	9	0.27
(1,583)	1:A:58:ARG:HA	1:A:58:ARG:HD2	15	0.27
(1,583)	1:A:58:ARG:HA	1:A:58:ARG:HD3	15	0.27
(1,476)	1:A:46:THR:H	1:A:146:PHE:HD1	19	0.27
(1,476)	1:A:46:THR:H	1:A:146:PHE:HD2	19	0.27
(1,452)	1:A:56:VAL:HB	1:A:125:ILE:HB	20	0.27
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	11	0.27
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	11	0.27
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	11	0.27
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	11	0.27
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	11	0.27
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	11	0.27
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG11	12	0.27
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG12	12	0.27
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG13	12	0.27
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG21	12	0.27
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG22	12	0.27
(1,388)	1:A:102:ILE:H	1:A:150:VAL:HG23	12	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	4	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	4	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	4	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	4	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	4	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	13	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	13	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	13	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	13	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	13	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	13	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	20	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	20	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	20	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	20	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	20	0.27
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	20	0.27
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	3	0.27
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	11	0.27
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	7	0.27
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	7	0.27
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	13	0.26
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	13	0.26
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	13	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	6	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	6	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	6	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	6	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	6	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	6	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	14	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	14	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	14	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	14	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	14	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	14	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	19	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	19	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	19	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	19	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	19	0.26
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	19	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	19	0.26
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	5	0.26
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	5	0.26
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	6	0.26
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	6	0.26
(3,49)	1:A:94:CYS:O	1:A:98:SER:H	15	0.25
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	9	0.25
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	20	0.25
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	20	0.25
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	20	0.25
(1,476)	1:A:46:THR:H	1:A:146:PHE:HD1	4	0.25
(1,476)	1:A:46:THR:H	1:A:146:PHE:HD2	4	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	1	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	1	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	1	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	1	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	1	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	1	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	8	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	8	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	8	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	8	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	8	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	8	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	16	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	16	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	16	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	16	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	16	0.25
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	16	0.25
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	20	0.25
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	20	0.25
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	14	0.24
(1,583)	1:A:58:ARG:HA	1:A:58:ARG:HD2	11	0.24
(1,583)	1:A:58:ARG:HA	1:A:58:ARG:HD3	11	0.24
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	17	0.24
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	17	0.24
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	17	0.24
(1,475)	1:A:46:THR:HG21	1:A:143:LYS:HA	16	0.24
(1,475)	1:A:46:THR:HG22	1:A:143:LYS:HA	16	0.24
(1,475)	1:A:46:THR:HG23	1:A:143:LYS:HA	16	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	2	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	2	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	2	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	2	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	2	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	7	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	7	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	7	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	7	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	7	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	7	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	10	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	10	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	10	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	10	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	10	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	10	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	18	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	18	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	18	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	18	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	18	0.24
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	18	0.24
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	4	0.24
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	17	0.23
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	9	0.23
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	9	0.23
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	9	0.23
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	16	0.23
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	16	0.23
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	16	0.23
(1,476)	1:A:46:THR:H	1:A:146:PHE:HD1	11	0.23
(1,476)	1:A:46:THR:H	1:A:146:PHE:HD2	11	0.23
(1,475)	1:A:46:THR:HG21	1:A:143:LYS:HA	6	0.23
(1,475)	1:A:46:THR:HG22	1:A:143:LYS:HA	6	0.23
(1,475)	1:A:46:THR:HG23	1:A:143:LYS:HA	6	0.23
(1,475)	1:A:46:THR:HG21	1:A:143:LYS:HA	8	0.23
(1,475)	1:A:46:THR:HG22	1:A:143:LYS:HA	8	0.23
(1,475)	1:A:46:THR:HG23	1:A:143:LYS:HA	8	0.23
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	11	0.23
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	11	0.23
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	11	0.23
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	11	0.23
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	11	0.23
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	3	0.22
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	19	0.22
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	11	0.22
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	11	0.22
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	19	0.22
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	19	0.22
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	19	0.22
(1,475)	1:A:46:THR:HG21	1:A:143:LYS:HA	7	0.22
(1,475)	1:A:46:THR:HG22	1:A:143:LYS:HA	7	0.22
(1,475)	1:A:46:THR:HG23	1:A:143:LYS:HA	7	0.22
(1,459)	1:A:55:ASN:HB2	1:A:126:VAL:HA	17	0.22
(1,459)	1:A:55:ASN:HB3	1:A:126:VAL:HA	17	0.22
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	1	0.22
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	12	0.22
(1,357)	1:A:78:ALA:HB1	1:A:104:ILE:HG12	14	0.22
(1,357)	1:A:78:ALA:HB1	1:A:104:ILE:HG13	14	0.22
(1,357)	1:A:78:ALA:HB2	1:A:104:ILE:HG12	14	0.22
(1,357)	1:A:78:ALA:HB2	1:A:104:ILE:HG13	14	0.22
(1,357)	1:A:78:ALA:HB3	1:A:104:ILE:HG12	14	0.22
(1,357)	1:A:78:ALA:HB3	1:A:104:ILE:HG13	14	0.22
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	5	0.22
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	5	0.22
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	5	0.22
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	5	0.22
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	5	0.22
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	5	0.22
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	17	0.22
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	17	0.22
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	6	0.22
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	6	0.22
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	6	0.22
(3,35)	1:A:85:ASP:O	1:A:89:HIS:H	8	0.21
(3,35)	1:A:85:ASP:O	1:A:89:HIS:H	13	0.21
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	15	0.21
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	8	0.21
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	8	0.21
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	8	0.21
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	15	0.21
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	15	0.21
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG2	20	0.21
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG3	20	0.21
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG2	20	0.21
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG3	20	0.21
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG2	20	0.21
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG3	20	0.21
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	5	0.21
(1,334)	1:A:76:VAL:H	1:A:101:TYR:HD1	20	0.21
(1,334)	1:A:76:VAL:H	1:A:101:TYR:HD2	20	0.21
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	4	0.21
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	4	0.21
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	4	0.21
(1,107)	1:A:37:LYS:HB2	1:A:38:LYS:HA	12	0.21
(1,107)	1:A:37:LYS:HB3	1:A:38:LYS:HA	12	0.21
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	7	0.2
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	16	0.2
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	5	0.2
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	5	0.2
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	5	0.2
(1,476)	1:A:46:THR:H	1:A:146:PHE:HD1	3	0.2
(1,476)	1:A:46:THR:H	1:A:146:PHE:HD2	3	0.2
(1,475)	1:A:46:THR:HG21	1:A:143:LYS:HA	1	0.2
(1,475)	1:A:46:THR:HG22	1:A:143:LYS:HA	1	0.2
(1,475)	1:A:46:THR:HG23	1:A:143:LYS:HA	1	0.2
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG2	18	0.2
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG3	18	0.2
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG2	18	0.2
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG3	18	0.2
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG2	18	0.2
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG3	18	0.2
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	2	0.2
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	4	0.2
(1,334)	1:A:76:VAL:H	1:A:101:TYR:HD1	4	0.2
(1,334)	1:A:76:VAL:H	1:A:101:TYR:HD2	4	0.2
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	3	0.2
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	3	0.2
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	3	0.2
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	8	0.2
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	8	0.2
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	8	0.2
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	17	0.2
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	17	0.2
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG11	3	0.2
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG12	3	0.2
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG13	3	0.2
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG21	3	0.2
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG22	3	0.2
(1,314)	1:A:93:LEU:HG	1:A:99:VAL:HG23	3	0.2
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	3	0.2
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	3	0.2
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	8	0.2
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	8	0.2
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	7	0.2
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	7	0.2
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	7	0.2
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	10	0.2
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	10	0.2
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	10	0.2
(1,107)	1:A:37:LYS:HB2	1:A:38:LYS:HA	3	0.2
(1,107)	1:A:37:LYS:HB3	1:A:38:LYS:HA	3	0.2
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	9	0.19
(3,35)	1:A:85:ASP:O	1:A:89:HIS:H	2	0.19
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	8	0.19
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	3	0.19
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	3	0.19
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	3	0.19
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	4	0.19
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	4	0.19
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	4	0.19
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	11	0.19
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	11	0.19
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	11	0.19
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG2	12	0.19
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG3	12	0.19
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG2	12	0.19
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG3	12	0.19
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG2	12	0.19
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG3	12	0.19
(1,422)	1:A:72:LYS:HA	1:A:126:VAL:HA	2	0.19
(1,421)	1:A:101:TYR:H	1:A:154:GLN:HG2	12	0.19
(1,421)	1:A:101:TYR:H	1:A:154:GLN:HG3	12	0.19
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	6	0.19
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	6	0.19
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	7	0.19
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	7	0.19
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	7	0.19
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	9	0.19
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	9	0.19
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	9	0.19
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	15	0.19
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	15	0.19
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	19	0.19
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	19	0.19
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	1	0.19
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	1	0.19
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	1	0.19
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	20	0.19
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	20	0.19
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	20	0.19
(1,107)	1:A:37:LYS:HB2	1:A:38:LYS:HA	1	0.19
(1,107)	1:A:37:LYS:HB3	1:A:38:LYS:HA	1	0.19
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	3	0.18
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	11	0.18
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	19	0.18
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	5	0.18
(3,35)	1:A:85:ASP:O	1:A:89:HIS:H	3	0.18
(3,35)	1:A:85:ASP:O	1:A:89:HIS:H	20	0.18
(3,21)	1:A:59:GLY:O	1:A:63:VAL:H	6	0.18
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	1	0.18
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	20	0.18
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	1	0.18
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	1	0.18
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	1	0.18
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	2	0.18
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	2	0.18
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	2	0.18
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	14	0.18
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	14	0.18
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	14	0.18
(1,475)	1:A:46:THR:HG21	1:A:143:LYS:HA	13	0.18
(1,475)	1:A:46:THR:HG22	1:A:143:LYS:HA	13	0.18
(1,475)	1:A:46:THR:HG23	1:A:143:LYS:HA	13	0.18
(1,475)	1:A:46:THR:HG21	1:A:143:LYS:HA	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:A:46:THR:HG22	1:A:143:LYS:HA	14	0.18
(1,475)	1:A:46:THR:HG23	1:A:143:LYS:HA	14	0.18
(1,475)	1:A:46:THR:HG21	1:A:143:LYS:HA	20	0.18
(1,475)	1:A:46:THR:HG22	1:A:143:LYS:HA	20	0.18
(1,475)	1:A:46:THR:HG23	1:A:143:LYS:HA	20	0.18
(1,471)	1:A:49:LYS:H	1:A:142:TYR:HD1	5	0.18
(1,471)	1:A:49:LYS:H	1:A:142:TYR:HD2	5	0.18
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	7	0.18
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	11	0.18
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	14	0.18
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	15	0.18
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	19	0.18
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	20	0.18
(1,357)	1:A:78:ALA:HB1	1:A:104:ILE:HG12	19	0.18
(1,357)	1:A:78:ALA:HB1	1:A:104:ILE:HG13	19	0.18
(1,357)	1:A:78:ALA:HB2	1:A:104:ILE:HG12	19	0.18
(1,357)	1:A:78:ALA:HB2	1:A:104:ILE:HG13	19	0.18
(1,357)	1:A:78:ALA:HB3	1:A:104:ILE:HG12	19	0.18
(1,357)	1:A:78:ALA:HB3	1:A:104:ILE:HG13	19	0.18
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	12	0.18
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	12	0.18
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	12	0.18
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	14	0.18
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	14	0.18
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	14	0.18
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	18	0.18
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	18	0.18
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	18	0.18
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	1	0.18
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	1	0.18
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	4	0.18
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	4	0.18
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	9	0.18
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	9	0.18
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	12	0.18
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	12	0.18
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	14	0.18
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	14	0.18
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	14	0.18
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	14	0.18
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	14	0.18
(4,62)	1:A:111:GLY:O	1:A:115:ALA:N	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	4	0.17
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	12	0.17
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	20	0.17
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	3	0.17
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	6	0.17
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	7	0.17
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	10	0.17
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	18	0.17
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	7	0.17
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	7	0.17
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	7	0.17
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG11	10	0.17
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG12	10	0.17
(1,485)	1:A:125:ILE:H	1:A:76:VAL:HG13	10	0.17
(1,475)	1:A:46:THR:HG21	1:A:143:LYS:HA	2	0.17
(1,475)	1:A:46:THR:HG22	1:A:143:LYS:HA	2	0.17
(1,475)	1:A:46:THR:HG23	1:A:143:LYS:HA	2	0.17
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG2	1	0.17
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG3	1	0.17
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG2	1	0.17
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG3	1	0.17
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG2	1	0.17
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG3	1	0.17
(1,459)	1:A:55:ASN:HB2	1:A:126:VAL:HA	3	0.17
(1,459)	1:A:55:ASN:HB3	1:A:126:VAL:HA	3	0.17
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	3	0.17
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	10	0.17
(1,414)	1:A:73:GLY:HA2	1:A:125:ILE:HD11	13	0.17
(1,414)	1:A:73:GLY:HA2	1:A:125:ILE:HD12	13	0.17
(1,414)	1:A:73:GLY:HA2	1:A:125:ILE:HD13	13	0.17
(1,414)	1:A:73:GLY:HA3	1:A:125:ILE:HD11	13	0.17
(1,414)	1:A:73:GLY:HA3	1:A:125:ILE:HD12	13	0.17
(1,414)	1:A:73:GLY:HA3	1:A:125:ILE:HD13	13	0.17
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	1	0.17
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	1	0.17
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	1	0.17
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	13	0.17
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	13	0.17
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	13	0.17
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	20	0.17
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	20	0.17
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	2	0.17
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	10	0.17
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	10	0.17
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	10	0.17
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	13	0.17
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	13	0.17
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	16	0.17
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	16	0.17
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	16	0.17
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	16	0.17
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	16	0.17
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	18	0.17
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	18	0.17
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	18	0.17
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	8	0.16
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	2	0.16
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	8	0.16
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	11	0.16
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	20	0.16
(3,25)	1:A:61:LYS:O	1:A:65:LYS:H	10	0.16
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	10	0.16
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	18	0.16
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	6	0.16
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	6	0.16
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	12	0.16
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	12	0.16
(1,475)	1:A:46:THR:HG21	1:A:143:LYS:HA	10	0.16
(1,475)	1:A:46:THR:HG22	1:A:143:LYS:HA	10	0.16
(1,475)	1:A:46:THR:HG23	1:A:143:LYS:HA	10	0.16
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG2	13	0.16
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG3	13	0.16
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG2	13	0.16
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG3	13	0.16
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG2	13	0.16
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG3	13	0.16
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG2	16	0.16
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG3	16	0.16
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG2	16	0.16
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG3	16	0.16
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG2	16	0.16
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG3	16	0.16
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG2	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG3	17	0.16
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG2	17	0.16
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG3	17	0.16
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG2	17	0.16
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG3	17	0.16
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	8	0.16
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	13	0.16
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	17	0.16
(1,422)	1:A:72:LYS:HA	1:A:126:VAL:HA	8	0.16
(1,397)	1:A:75:VAL:H	1:A:125:ILE:HB	20	0.16
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	5	0.16
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	5	0.16
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	5	0.16
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	11	0.16
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	11	0.16
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	11	0.16
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	13	0.16
(1,151)	1:A:77:ILE:HG12	1:A:78:ALA:H	18	0.16
(1,151)	1:A:77:ILE:HG13	1:A:78:ALA:H	18	0.16
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	8	0.16
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	8	0.16
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	8	0.16
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	11	0.16
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	11	0.16
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	11	0.16
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	12	0.16
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	12	0.16
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	12	0.16
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	17	0.16
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	17	0.16
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	17	0.16
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	5	0.15
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	6	0.15
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	7	0.15
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	16	0.15
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	12	0.15
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	13	0.15
(3,35)	1:A:85:ASP:O	1:A:89:HIS:H	16	0.15
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	2	0.15
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	2	0.15
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	8	0.15
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	14	0.15
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	14	0.15
(1,583)	1:A:58:ARG:HA	1:A:58:ARG:HD2	17	0.15
(1,583)	1:A:58:ARG:HA	1:A:58:ARG:HD3	17	0.15
(1,495)	1:A:100:PRO:HA	1:A:153:VAL:HG21	13	0.15
(1,495)	1:A:100:PRO:HA	1:A:153:VAL:HG22	13	0.15
(1,495)	1:A:100:PRO:HA	1:A:153:VAL:HG23	13	0.15
(1,475)	1:A:46:THR:HG21	1:A:143:LYS:HA	15	0.15
(1,475)	1:A:46:THR:HG22	1:A:143:LYS:HA	15	0.15
(1,475)	1:A:46:THR:HG23	1:A:143:LYS:HA	15	0.15
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG2	10	0.15
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG3	10	0.15
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG2	10	0.15
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG3	10	0.15
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG2	10	0.15
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG3	10	0.15
(1,468)	1:A:50:ALA:H	1:A:138:LYS:HG2	8	0.15
(1,468)	1:A:50:ALA:H	1:A:138:LYS:HG3	8	0.15
(1,452)	1:A:56:VAL:HB	1:A:125:ILE:HB	18	0.15
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	6	0.15
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	9	0.15
(1,428)	1:A:60:VAL:HA	1:A:122:VAL:HB	10	0.15
(1,422)	1:A:72:LYS:HA	1:A:126:VAL:HA	5	0.15
(1,422)	1:A:72:LYS:HA	1:A:126:VAL:HA	12	0.15
(1,422)	1:A:72:LYS:HA	1:A:126:VAL:HA	16	0.15
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	15	0.15
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	15	0.15
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	15	0.15
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	19	0.15
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	19	0.15
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	19	0.15
(1,256)	1:A:47:VAL:HA	1:A:50:ALA:HA	17	0.15
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	5	0.15
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	8	0.15
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	14	0.15
(1,132)	1:A:60:VAL:H	1:A:61:LYS:HB2	13	0.15
(1,132)	1:A:60:VAL:H	1:A:61:LYS:HB3	13	0.15
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	2	0.15
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	2	0.15
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	2	0.15
(4,103)	1:A:74:LEU:O	1:A:125:ILE:H	14	0.14
(4,103)	1:A:74:LEU:O	1:A:125:ILE:H	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,95)	1:A:57:LYS:H	1:A:124:PHE:O	18	0.14
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	1	0.14
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	14	0.14
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	1	0.14
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	4	0.14
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	9	0.14
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	16	0.14
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	17	0.14
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	19	0.14
(3,29)	1:A:63:VAL:O	1:A:67:LEU:H	14	0.14
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	2	0.14
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	4	0.14
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	6	0.14
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	11	0.14
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	1	0.14
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	1	0.14
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	3	0.14
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	3	0.14
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	19	0.14
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	19	0.14
(1,475)	1:A:46:THR:HG21	1:A:143:LYS:HA	17	0.14
(1,475)	1:A:46:THR:HG22	1:A:143:LYS:HA	17	0.14
(1,475)	1:A:46:THR:HG23	1:A:143:LYS:HA	17	0.14
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG2	6	0.14
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG3	6	0.14
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG2	6	0.14
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG3	6	0.14
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG2	6	0.14
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG3	6	0.14
(1,452)	1:A:56:VAL:HB	1:A:125:ILE:HB	7	0.14
(1,425)	1:A:56:VAL:HG11	1:A:113:ALA:HB1	11	0.14
(1,425)	1:A:56:VAL:HG11	1:A:113:ALA:HB2	11	0.14
(1,425)	1:A:56:VAL:HG11	1:A:113:ALA:HB3	11	0.14
(1,425)	1:A:56:VAL:HG12	1:A:113:ALA:HB1	11	0.14
(1,425)	1:A:56:VAL:HG12	1:A:113:ALA:HB2	11	0.14
(1,425)	1:A:56:VAL:HG12	1:A:113:ALA:HB3	11	0.14
(1,425)	1:A:56:VAL:HG13	1:A:113:ALA:HB1	11	0.14
(1,425)	1:A:56:VAL:HG13	1:A:113:ALA:HB2	11	0.14
(1,425)	1:A:56:VAL:HG13	1:A:113:ALA:HB3	11	0.14
(1,425)	1:A:56:VAL:HG21	1:A:113:ALA:HB1	11	0.14
(1,425)	1:A:56:VAL:HG21	1:A:113:ALA:HB2	11	0.14
(1,425)	1:A:56:VAL:HG21	1:A:113:ALA:HB3	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,425)	1:A:56:VAL:HG22	1:A:113:ALA:HB1	11	0.14
(1,425)	1:A:56:VAL:HG22	1:A:113:ALA:HB2	11	0.14
(1,425)	1:A:56:VAL:HG22	1:A:113:ALA:HB3	11	0.14
(1,425)	1:A:56:VAL:HG23	1:A:113:ALA:HB1	11	0.14
(1,425)	1:A:56:VAL:HG23	1:A:113:ALA:HB2	11	0.14
(1,425)	1:A:56:VAL:HG23	1:A:113:ALA:HB3	11	0.14
(1,422)	1:A:72:LYS:HA	1:A:126:VAL:HA	3	0.14
(1,397)	1:A:75:VAL:H	1:A:125:ILE:HB	4	0.14
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	2	0.14
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	2	0.14
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	2	0.14
(1,318)	1:A:66:ALA:HB1	1:A:73:GLY:HA3	16	0.14
(1,318)	1:A:66:ALA:HB2	1:A:73:GLY:HA3	16	0.14
(1,318)	1:A:66:ALA:HB3	1:A:73:GLY:HA3	16	0.14
(1,235)	1:A:99:VAL:HB	1:A:101:TYR:H	4	0.14
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	1	0.14
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	6	0.14
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	15	0.14
(1,132)	1:A:60:VAL:H	1:A:61:LYS:HB2	17	0.14
(1,132)	1:A:60:VAL:H	1:A:61:LYS:HB3	17	0.14
(4,103)	1:A:74:LEU:O	1:A:125:ILE:H	3	0.13
(4,103)	1:A:74:LEU:O	1:A:125:ILE:H	7	0.13
(4,103)	1:A:74:LEU:O	1:A:125:ILE:H	9	0.13
(4,103)	1:A:74:LEU:O	1:A:125:ILE:H	15	0.13
(4,103)	1:A:74:LEU:O	1:A:125:ILE:H	16	0.13
(3,99)	1:A:78:ALA:H	1:A:121:SER:O	14	0.13
(3,95)	1:A:57:LYS:H	1:A:124:PHE:O	10	0.13
(3,95)	1:A:57:LYS:H	1:A:124:PHE:O	12	0.13
(3,83)	1:A:148:GLU:O	1:A:152:GLU:H	12	0.13
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	2	0.13
(3,61)	1:A:111:GLY:O	1:A:115:ALA:H	5	0.13
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	14	0.13
(3,29)	1:A:63:VAL:O	1:A:67:LEU:H	9	0.13
(3,29)	1:A:63:VAL:O	1:A:67:LEU:H	10	0.13
(3,21)	1:A:59:GLY:O	1:A:63:VAL:H	5	0.13
(3,21)	1:A:59:GLY:O	1:A:63:VAL:H	12	0.13
(3,21)	1:A:59:GLY:O	1:A:63:VAL:H	15	0.13
(3,21)	1:A:59:GLY:O	1:A:63:VAL:H	19	0.13
(3,21)	1:A:59:GLY:O	1:A:63:VAL:H	20	0.13
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	13	0.13
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	7	0.13
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	9	0.13
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	9	0.13
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	15	0.13
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	15	0.13
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	17	0.13
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	17	0.13
(1,471)	1:A:49:LYS:H	1:A:142:TYR:HD1	8	0.13
(1,471)	1:A:49:LYS:H	1:A:142:TYR:HD2	8	0.13
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG2	15	0.13
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG3	15	0.13
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG2	15	0.13
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG3	15	0.13
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG2	15	0.13
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG3	15	0.13
(1,452)	1:A:56:VAL:HB	1:A:125:ILE:HB	3	0.13
(1,452)	1:A:56:VAL:HB	1:A:125:ILE:HB	12	0.13
(1,452)	1:A:56:VAL:HB	1:A:125:ILE:HB	15	0.13
(1,452)	1:A:56:VAL:HB	1:A:125:ILE:HB	16	0.13
(1,452)	1:A:56:VAL:HB	1:A:125:ILE:HB	19	0.13
(1,434)	1:A:58:ARG:H	1:A:123:VAL:HA	16	0.13
(1,428)	1:A:60:VAL:HA	1:A:122:VAL:HB	6	0.13
(1,428)	1:A:60:VAL:HA	1:A:122:VAL:HB	14	0.13
(1,422)	1:A:72:LYS:HA	1:A:126:VAL:HA	7	0.13
(1,397)	1:A:75:VAL:H	1:A:125:ILE:HB	2	0.13
(1,300)	1:A:50:ALA:HB1	1:A:55:ASN:H	20	0.13
(1,300)	1:A:50:ALA:HB2	1:A:55:ASN:H	20	0.13
(1,300)	1:A:50:ALA:HB3	1:A:55:ASN:H	20	0.13
(1,235)	1:A:99:VAL:HB	1:A:101:TYR:H	9	0.13
(1,235)	1:A:99:VAL:HB	1:A:101:TYR:H	11	0.13
(1,235)	1:A:99:VAL:HB	1:A:101:TYR:H	12	0.13
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	7	0.13
(1,198)	1:A:146:PHE:HD1	1:A:147:ASN:H	16	0.13
(1,163)	1:A:87:ILE:H	1:A:88:SER:HA	4	0.13
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG11	8	0.13
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG12	8	0.13
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG13	8	0.13
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG21	8	0.13
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG22	8	0.13
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG23	8	0.13
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG11	8	0.13
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG12	8	0.13
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG13	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG21	8	0.13
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG22	8	0.13
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG23	8	0.13
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	15	0.13
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	15	0.13
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	15	0.13
(4,103)	1:A:74:LEU:O	1:A:125:ILE:H	2	0.12
(4,103)	1:A:74:LEU:O	1:A:125:ILE:H	8	0.12
(4,103)	1:A:74:LEU:O	1:A:125:ILE:H	12	0.12
(4,103)	1:A:74:LEU:O	1:A:125:ILE:H	17	0.12
(3,95)	1:A:57:LYS:H	1:A:124:PHE:O	5	0.12
(3,95)	1:A:57:LYS:H	1:A:124:PHE:O	6	0.12
(3,95)	1:A:57:LYS:H	1:A:124:PHE:O	8	0.12
(3,95)	1:A:57:LYS:H	1:A:124:PHE:O	20	0.12
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	10	0.12
(3,29)	1:A:63:VAL:O	1:A:67:LEU:H	7	0.12
(3,21)	1:A:59:GLY:O	1:A:63:VAL:H	18	0.12
(3,17)	1:A:46:THR:O	1:A:50:ALA:H	17	0.12
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	5	0.12
(3,107)	1:A:74:LEU:H	1:A:125:ILE:O	12	0.12
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	5	0.12
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	5	0.12
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	10	0.12
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	10	0.12
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	13	0.12
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	13	0.12
(1,583)	1:A:58:ARG:HA	1:A:58:ARG:HD2	7	0.12
(1,583)	1:A:58:ARG:HA	1:A:58:ARG:HD3	7	0.12
(1,495)	1:A:100:PRO:HA	1:A:153:VAL:HG21	19	0.12
(1,495)	1:A:100:PRO:HA	1:A:153:VAL:HG22	19	0.12
(1,495)	1:A:100:PRO:HA	1:A:153:VAL:HG23	19	0.12
(1,475)	1:A:46:THR:HG21	1:A:143:LYS:HA	5	0.12
(1,475)	1:A:46:THR:HG22	1:A:143:LYS:HA	5	0.12
(1,475)	1:A:46:THR:HG23	1:A:143:LYS:HA	5	0.12
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG2	2	0.12
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG3	2	0.12
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG2	2	0.12
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG3	2	0.12
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG2	2	0.12
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG3	2	0.12
(1,468)	1:A:50:ALA:H	1:A:138:LYS:HG2	5	0.12
(1,468)	1:A:50:ALA:H	1:A:138:LYS:HG3	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:A:56:VAL:HB	1:A:125:ILE:HB	2	0.12
(1,452)	1:A:56:VAL:HB	1:A:125:ILE:HB	5	0.12
(1,428)	1:A:60:VAL:HA	1:A:122:VAL:HB	1	0.12
(1,428)	1:A:60:VAL:HA	1:A:122:VAL:HB	16	0.12
(1,422)	1:A:72:LYS:HA	1:A:126:VAL:HA	10	0.12
(1,422)	1:A:72:LYS:HA	1:A:126:VAL:HA	14	0.12
(1,422)	1:A:72:LYS:HA	1:A:126:VAL:HA	17	0.12
(1,414)	1:A:73:GLY:HA2	1:A:125:ILE:HD11	4	0.12
(1,414)	1:A:73:GLY:HA2	1:A:125:ILE:HD12	4	0.12
(1,414)	1:A:73:GLY:HA2	1:A:125:ILE:HD13	4	0.12
(1,414)	1:A:73:GLY:HA3	1:A:125:ILE:HD11	4	0.12
(1,414)	1:A:73:GLY:HA3	1:A:125:ILE:HD12	4	0.12
(1,414)	1:A:73:GLY:HA3	1:A:125:ILE:HD13	4	0.12
(1,414)	1:A:73:GLY:HA2	1:A:125:ILE:HD11	6	0.12
(1,414)	1:A:73:GLY:HA2	1:A:125:ILE:HD12	6	0.12
(1,414)	1:A:73:GLY:HA2	1:A:125:ILE:HD13	6	0.12
(1,414)	1:A:73:GLY:HA3	1:A:125:ILE:HD11	6	0.12
(1,414)	1:A:73:GLY:HA3	1:A:125:ILE:HD12	6	0.12
(1,414)	1:A:73:GLY:HA3	1:A:125:ILE:HD13	6	0.12
(1,397)	1:A:75:VAL:H	1:A:125:ILE:HB	3	0.12
(1,397)	1:A:75:VAL:H	1:A:125:ILE:HB	8	0.12
(1,397)	1:A:75:VAL:H	1:A:125:ILE:HB	11	0.12
(1,397)	1:A:75:VAL:H	1:A:125:ILE:HB	12	0.12
(1,235)	1:A:99:VAL:HB	1:A:101:TYR:H	10	0.12
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG11	13	0.12
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG12	13	0.12
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG13	13	0.12
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG21	13	0.12
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG22	13	0.12
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG23	13	0.12
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG11	13	0.12
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG12	13	0.12
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG13	13	0.12
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG21	13	0.12
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG22	13	0.12
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG23	13	0.12
(1,132)	1:A:60:VAL:H	1:A:61:LYS:HB2	4	0.12
(1,132)	1:A:60:VAL:H	1:A:61:LYS:HB3	4	0.12
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	3	0.12
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	3	0.12
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	3	0.12
(4,103)	1:A:74:LEU:O	1:A:125:ILE:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,103)	1:A:74:LEU:O	1:A:125:ILE:H	4	0.11
(4,103)	1:A:74:LEU:O	1:A:125:ILE:H	11	0.11
(3,99)	1:A:78:ALA:H	1:A:121:SER:O	19	0.11
(3,95)	1:A:57:LYS:H	1:A:124:PHE:O	3	0.11
(3,95)	1:A:57:LYS:H	1:A:124:PHE:O	7	0.11
(3,75)	1:A:144:GLU:O	1:A:148:GLU:H	13	0.11
(3,69)	1:A:141:GLU:O	1:A:145:SER:H	15	0.11
(3,61)	1:A:111:GLY:O	1:A:115:ALA:H	4	0.11
(3,61)	1:A:111:GLY:O	1:A:115:ALA:H	6	0.11
(3,45)	1:A:92:VAL:O	1:A:96:ASP:H	10	0.11
(3,41)	1:A:90:ILE:O	1:A:94:CYS:H	15	0.11
(3,35)	1:A:85:ASP:O	1:A:89:HIS:H	12	0.11
(3,29)	1:A:63:VAL:O	1:A:67:LEU:H	6	0.11
(3,29)	1:A:63:VAL:O	1:A:67:LEU:H	17	0.11
(3,17)	1:A:46:THR:O	1:A:50:ALA:H	1	0.11
(3,17)	1:A:46:THR:O	1:A:50:ALA:H	6	0.11
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE1	16	0.11
(1,703)	1:A:101:TYR:H	1:A:101:TYR:HE2	16	0.11
(1,495)	1:A:100:PRO:HA	1:A:153:VAL:HG21	2	0.11
(1,495)	1:A:100:PRO:HA	1:A:153:VAL:HG22	2	0.11
(1,495)	1:A:100:PRO:HA	1:A:153:VAL:HG23	2	0.11
(1,495)	1:A:100:PRO:HA	1:A:153:VAL:HG21	12	0.11
(1,495)	1:A:100:PRO:HA	1:A:153:VAL:HG22	12	0.11
(1,495)	1:A:100:PRO:HA	1:A:153:VAL:HG23	12	0.11
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG2	3	0.11
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG3	3	0.11
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG2	3	0.11
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG3	3	0.11
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG2	3	0.11
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG3	3	0.11
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG2	14	0.11
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG3	14	0.11
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG2	14	0.11
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG3	14	0.11
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG2	14	0.11
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG3	14	0.11
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG2	19	0.11
(1,469)	1:A:50:ALA:HB1	1:A:138:LYS:HG3	19	0.11
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG2	19	0.11
(1,469)	1:A:50:ALA:HB2	1:A:138:LYS:HG3	19	0.11
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG2	19	0.11
(1,469)	1:A:50:ALA:HB3	1:A:138:LYS:HG3	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:A:56:VAL:HB	1:A:125:ILE:HB	6	0.11
(1,452)	1:A:56:VAL:HB	1:A:125:ILE:HB	14	0.11
(1,428)	1:A:60:VAL:HA	1:A:122:VAL:HB	5	0.11
(1,422)	1:A:72:LYS:HA	1:A:126:VAL:HA	4	0.11
(1,422)	1:A:72:LYS:HA	1:A:126:VAL:HA	6	0.11
(1,422)	1:A:72:LYS:HA	1:A:126:VAL:HA	11	0.11
(1,422)	1:A:72:LYS:HA	1:A:126:VAL:HA	19	0.11
(1,414)	1:A:73:GLY:HA2	1:A:125:ILE:HD11	18	0.11
(1,414)	1:A:73:GLY:HA2	1:A:125:ILE:HD12	18	0.11
(1,414)	1:A:73:GLY:HA2	1:A:125:ILE:HD13	18	0.11
(1,414)	1:A:73:GLY:HA3	1:A:125:ILE:HD11	18	0.11
(1,414)	1:A:73:GLY:HA3	1:A:125:ILE:HD12	18	0.11
(1,414)	1:A:73:GLY:HA3	1:A:125:ILE:HD13	18	0.11
(1,397)	1:A:75:VAL:H	1:A:125:ILE:HB	1	0.11
(1,397)	1:A:75:VAL:H	1:A:125:ILE:HB	6	0.11
(1,397)	1:A:75:VAL:H	1:A:125:ILE:HB	7	0.11
(1,397)	1:A:75:VAL:H	1:A:125:ILE:HB	14	0.11
(1,397)	1:A:75:VAL:H	1:A:125:ILE:HB	15	0.11
(1,367)	1:A:81:ILE:HG21	1:A:121:SER:H	11	0.11
(1,367)	1:A:81:ILE:HG22	1:A:121:SER:H	11	0.11
(1,367)	1:A:81:ILE:HG23	1:A:121:SER:H	11	0.11
(1,307)	1:A:51:SER:H	1:A:56:VAL:HB	20	0.11
(1,235)	1:A:99:VAL:HB	1:A:101:TYR:H	1	0.11
(1,235)	1:A:99:VAL:HB	1:A:101:TYR:H	6	0.11
(1,235)	1:A:99:VAL:HB	1:A:101:TYR:H	14	0.11
(1,235)	1:A:99:VAL:HB	1:A:101:TYR:H	17	0.11
(1,235)	1:A:99:VAL:HB	1:A:101:TYR:H	18	0.11
(1,163)	1:A:87:ILE:H	1:A:88:SER:HA	7	0.11
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG11	20	0.11
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG12	20	0.11
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG13	20	0.11
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG21	20	0.11
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG22	20	0.11
(1,159)	1:A:85:ASP:HB2	1:A:86:VAL:HG23	20	0.11
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG11	20	0.11
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG12	20	0.11
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG13	20	0.11
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG21	20	0.11
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG22	20	0.11
(1,159)	1:A:85:ASP:HB3	1:A:86:VAL:HG23	20	0.11
(1,132)	1:A:60:VAL:H	1:A:61:LYS:HB2	16	0.11
(1,132)	1:A:60:VAL:H	1:A:61:LYS:HB3	16	0.11

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<b>Key</b>	<b>Atom-1</b>	<b>Atom-2</b>	<b>Model ID</b>	<b>Violation (Å)</b>
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	4	0.11
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	4	0.11
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	4	0.11
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	5	0.11
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	5	0.11
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	5	0.11
(1,117)	1:A:46:THR:HG21	1:A:47:VAL:HB	13	0.11
(1,117)	1:A:46:THR:HG22	1:A:47:VAL:HB	13	0.11
(1,117)	1:A:46:THR:HG23	1:A:47:VAL:HB	13	0.11

## 10 Dihedral-angle violation analysis

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value