Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 06:09 pm BST

PDB ID	:	7P55
BMRB ID	:	34650
Title	:	NMR structure of human ACE2 21-42 fragment in HFIP/water 50/50 v/v
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Deposited on	:	2021-07-14

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

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

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

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

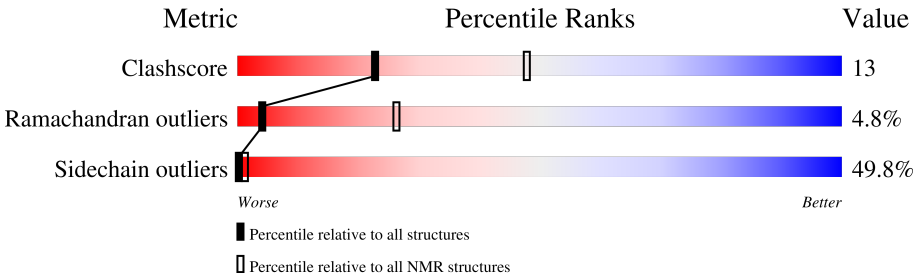
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 65%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	22	36% 50% 9% 5%

2 Ensemble composition and analysis (i)

This entry contains 50 models. Model 41 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:22-A:42 (21)	0.15	41

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 5 clusters and 5 single-model clusters were found.

Cluster number	Models
1	3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 17, 19, 20, 21
2	30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47
3	23, 24, 25, 26, 27
4	1, 2, 18
5	28, 29
Single-model clusters	16; 22; 48; 49; 50

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 365 atoms, of which 173 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Processed angiotensin-converting enzyme 2.

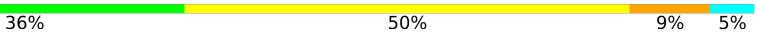
Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	22	365	124	173	29	39	0

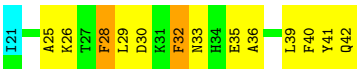
4 Residue-property plots (i)

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: Processed angiotensin-converting enzyme 2

Chain A: 

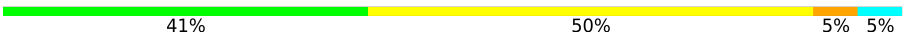


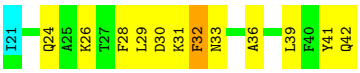
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

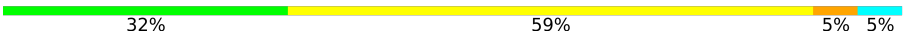
• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A: 

4.2.3 Score per residue for model 3

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.5 Score per residue for model 5

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.6 Score per residue for model 6

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.7 Score per residue for model 7

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.8 Score per residue for model 8

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.9 Score per residue for model 9

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.10 Score per residue for model 10

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.11 Score per residue for model 11

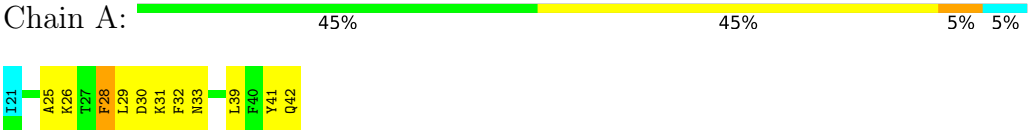
• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.12 Score per residue for model 12

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.14 Score per residue for model 14

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.15 Score per residue for model 15

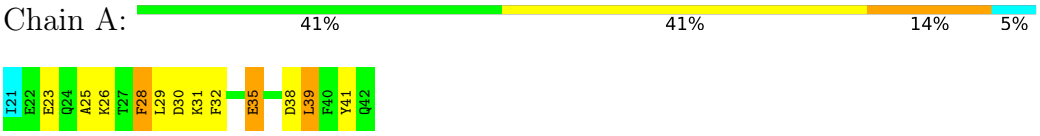
• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.16 Score per residue for model 16

• Molecule 1: Processed angiotensin-converting enzyme 2

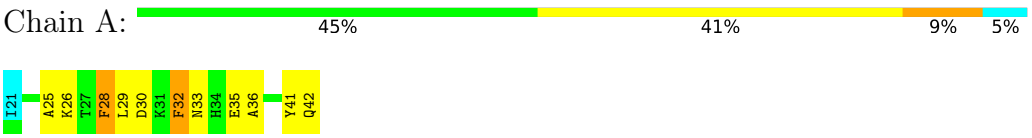
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Processed angiotensin-converting enzyme 2

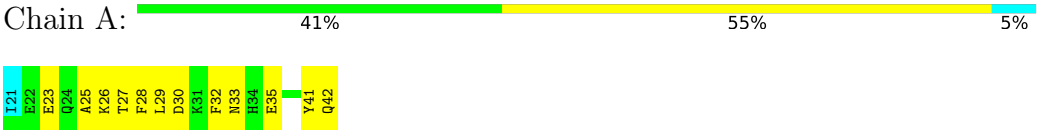
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.20 Score per residue for model 20

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.21 Score per residue for model 21

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.22 Score per residue for model 22

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.23 Score per residue for model 23

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.24 Score per residue for model 24

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.25 Score per residue for model 25

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.26 Score per residue for model 26

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.27 Score per residue for model 27

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.28 Score per residue for model 28

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.29 Score per residue for model 29

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.30 Score per residue for model 30

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.31 Score per residue for model 31

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.32 Score per residue for model 32

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.33 Score per residue for model 33

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.34 Score per residue for model 34

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.35 Score per residue for model 35

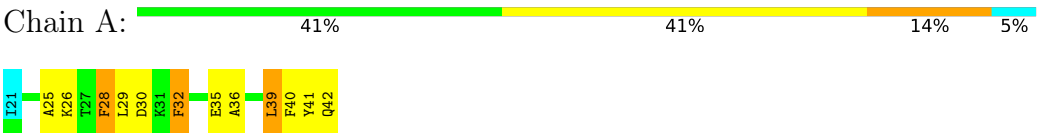
• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.36 Score per residue for model 36

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:



4.2.37 Score per residue for model 37

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.38 Score per residue for model 38

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.39 Score per residue for model 39

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.40 Score per residue for model 40

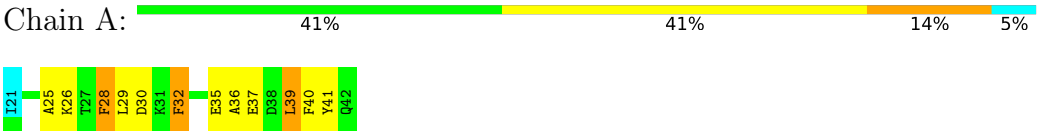
• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.41 Score per residue for model 41 (medoid)

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:



4.2.42 Score per residue for model 42

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.43 Score per residue for model 43

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.44 Score per residue for model 44

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.45 Score per residue for model 45

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.46 Score per residue for model 46

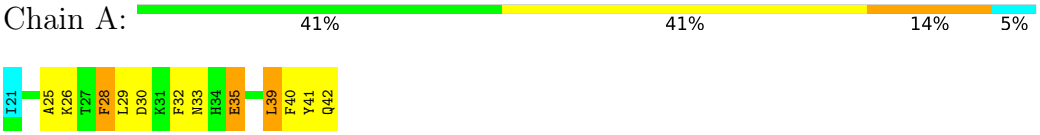
• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.47 Score per residue for model 47

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:



4.2.48 Score per residue for model 48

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.49 Score per residue for model 49

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

4.2.50 Score per residue for model 50

• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:

5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 50 calculated structures, 50 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
TALOS-N	refinement	
CYANA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	202
Number of shifts mapped to atoms	202
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	65%

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	184	162	162	4±3
All	All	9200	8100	8100	217

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LEU:HD13	1:A:40:PHE:N	0.86	1.85	50	25
1:A:39:LEU:O	1:A:39:LEU:HD22	0.78	1.79	34	25
1:A:39:LEU:HD13	1:A:39:LEU:C	0.62	2.14	50	25
1:A:35:GLU:CD	1:A:39:LEU:HD13	0.59	2.18	16	1
1:A:39:LEU:HD22	1:A:39:LEU:C	0.55	2.22	25	25
1:A:35:GLU:OE1	1:A:39:LEU:HD13	0.53	2.02	16	1
1:A:35:GLU:HG3	1:A:39:LEU:HD23	0.52	1.82	28	2
1:A:39:LEU:O	1:A:39:LEU:HD12	0.51	2.05	29	2
1:A:39:LEU:HD12	1:A:39:LEU:C	0.51	2.26	29	2
1:A:35:GLU:O	1:A:39:LEU:HD12	0.50	2.07	50	25
1:A:39:LEU:C	1:A:39:LEU:CD1	0.45	2.84	50	1
1:A:23:GLU:HA	1:A:27:THR:HG22	0.45	1.88	18	6
1:A:34:HIS:CG	1:A:35:GLU:N	0.45	2.82	49	2
1:A:32:PHE:O	1:A:36:ALA:HB2	0.45	2.11	21	30

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:HIS:ND1	1:A:35:GLU:N	0.43	2.66	50	1
1:A:28:PHE:O	1:A:28:PHE:CD1	0.42	2.73	16	43
1:A:39:LEU:C	1:A:39:LEU:CD2	0.40	2.90	32	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	20/22 (91%)	18±1 (89±4%)	1±1 (6±4%)	1±0 (5±1%)	4	26
All	All	1000/1100 (91%)	895 (90%)	57 (6%)	48 (5%)	4	26

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	25	ALA	48

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	19/20 (95%)	10±1 (50±6%)	9±1 (50±6%)	0	1
All	All	950/1000 (95%)	477 (50%)	473 (50%)	0	1

All 18 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	26	LYS	50
1	A	28	PHE	50

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Mol	Chain	Res	Type	Models (Total)
1	A	29	LEU	50
1	A	30	ASP	50
1	A	41	TYR	50
1	A	32	PHE	49
1	A	39	LEU	44
1	A	33	ASN	35
1	A	42	GLN	32
1	A	31	LYS	24
1	A	35	GLU	16
1	A	22	GLU	7
1	A	38	ASP	4
1	A	24	GLN	3
1	A	37	GLU	3
1	A	23	GLU	2
1	A	27	THR	2
1	A	34	HIS	2

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 65% for the well-defined parts and 64% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_ output*

7.1.1 Bookkeeping

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	202
Number of shifts mapped to atoms	202
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 65%, i.e. 191 atoms were assigned a chemical shift out of a possible 295. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	57/105 (54%)	42/42 (100%)	15/42 (36%)	0/21 (0%)
Sidechain	119/144 (83%)	81/90 (90%)	38/49 (78%)	0/5 (0%)
Aromatic	15/46 (33%)	15/23 (65%)	0/22 (0%)	0/1 (0%)
Overall	191/295 (65%)	138/155 (89%)	53/113 (47%)	0/27 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 64%, i.e. 201 atoms were assigned a chemical shift out of a possible 313. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	58/110 (53%)	43/44 (98%)	15/44 (34%)	0/22 (0%)
Sidechain	128/157 (82%)	88/99 (89%)	40/53 (75%)	0/5 (0%)
Aromatic	15/46 (33%)	15/23 (65%)	0/22 (0%)	0/1 (0%)
Overall	201/313 (64%)	146/166 (88%)	55/119 (46%)	0/28 (0%)

7.1.4 Statistically unusual chemical shifts (i)

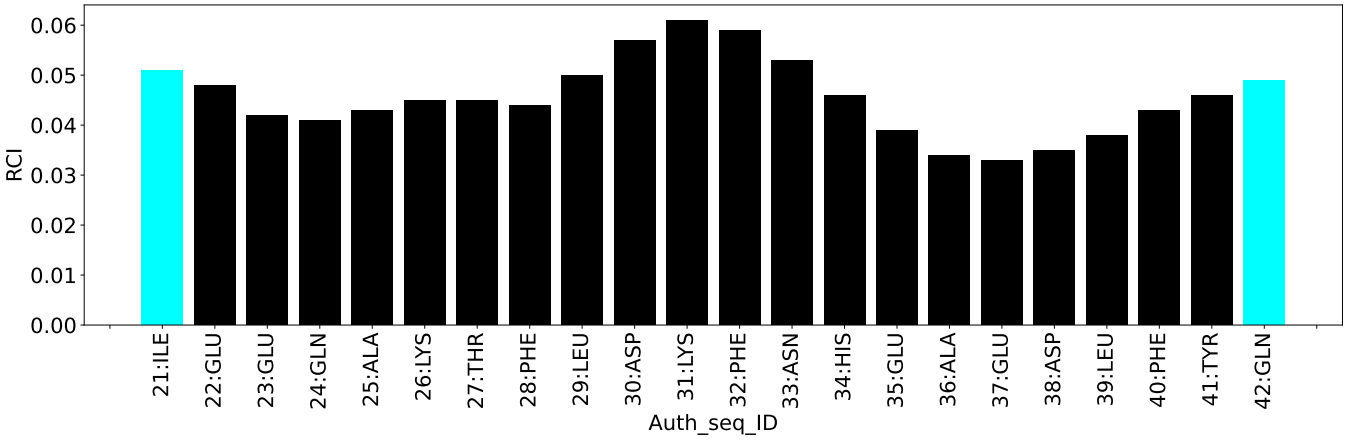
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	35	GLU	CG	30.15	30.20 – 42.01	-5.0

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	262
Intra-residue (|i-j|=0)	135
Sequential (|i-j|=1)	52
Medium range (|i-j|>1 and |i-j|<5)	75
Long range (|i-j|≥5)	0
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	3
Number of restraints per residue	11.9
Number of long range restraints per residue[1]	0.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	7.8	0.2
0.2-0.5 (Medium)	18.9	0.5
>0.5 (Large)	9.0	0.98

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

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

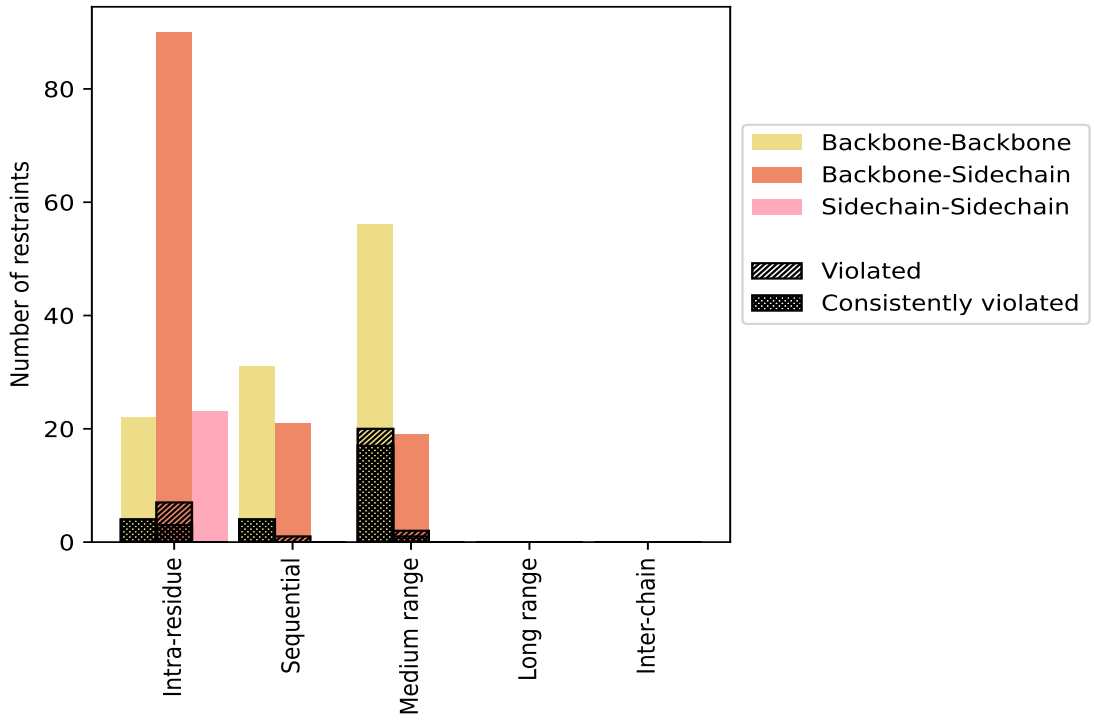
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	135	51.5	11	8.1	4.2	7	5.2	2.7
Backbone-Backbone	22	8.4	4	18.2	1.5	4	18.2	1.5
Backbone-Sidechain	90	34.4	7	7.8	2.7	3	3.3	1.1
Sidechain-Sidechain	23	8.8	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	52	19.8	5	9.6	1.9	4	7.7	1.5
Backbone-Backbone	31	11.8	4	12.9	1.5	4	12.9	1.5
Backbone-Sidechain	21	8.0	1	4.8	0.4	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	75	28.6	22	29.3	8.4	18	24.0	6.9
Backbone-Backbone	56	21.4	20	35.7	7.6	17	30.4	6.5
Backbone-Sidechain	19	7.3	2	10.5	0.8	1	5.3	0.4
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	262	100.0	38	14.5	14.5	29	11.1	11.1
Backbone-Backbone	109	41.6	28	25.7	10.7	25	22.9	9.5
Backbone-Sidechain	130	49.6	10	7.7	3.8	4	3.1	1.5
Sidechain-Sidechain	23	8.8	0	0.0	0.0	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	9	5	20	0	0	34	0.4	0.95	0.21	0.39
2	9	5	20	0	0	34	0.41	0.95	0.2	0.38
3	9	5	21	0	0	35	0.4	0.95	0.2	0.39
4	9	5	21	0	0	35	0.4	0.95	0.2	0.39
5	9	5	21	0	0	35	0.4	0.95	0.2	0.39
6	9	5	21	0	0	35	0.4	0.95	0.2	0.39
7	9	5	21	0	0	35	0.4	0.95	0.2	0.39
8	9	5	21	0	0	35	0.4	0.95	0.2	0.39
9	9	5	21	0	0	35	0.4	0.95	0.2	0.39
10	9	5	21	0	0	35	0.4	0.95	0.2	0.41
11	9	5	21	0	0	35	0.39	0.95	0.2	0.41

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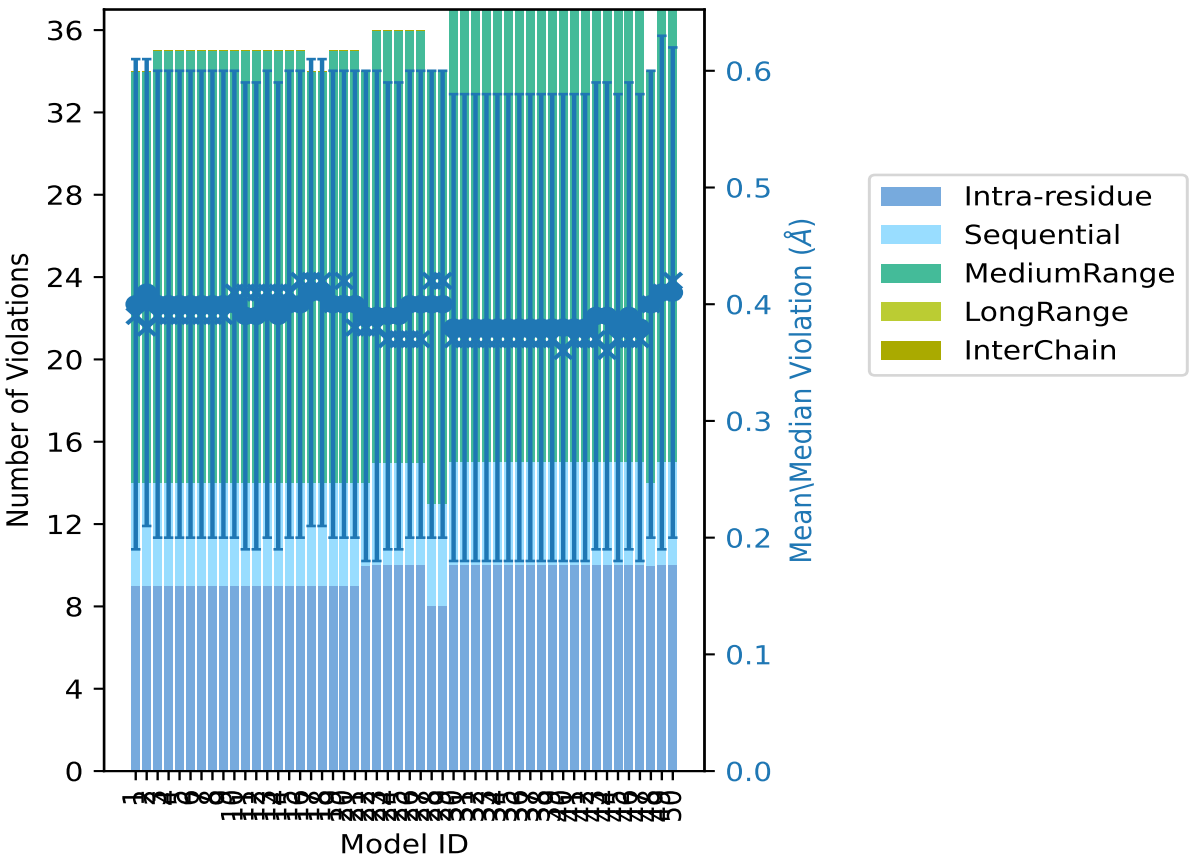
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	9	5	21	0	0	35	0.39	0.95	0.2	0.41
13	9	5	21	0	0	35	0.4	0.95	0.2	0.41
14	9	5	21	0	0	35	0.39	0.95	0.2	0.41
15	9	5	21	0	0	35	0.4	0.95	0.2	0.41
16	9	5	21	0	0	35	0.4	0.93	0.2	0.42
17	9	5	20	0	0	34	0.41	0.94	0.2	0.42
18	9	5	20	0	0	34	0.41	0.95	0.2	0.42
19	9	5	21	0	0	35	0.4	0.95	0.2	0.4
20	9	5	21	0	0	35	0.4	0.95	0.2	0.42
21	9	5	21	0	0	35	0.4	0.98	0.2	0.38
22	10	4	20	0	0	34	0.39	0.94	0.21	0.38
23	10	5	21	0	0	36	0.39	0.94	0.21	0.38
24	10	5	21	0	0	36	0.39	0.94	0.2	0.37
25	10	5	21	0	0	36	0.39	0.94	0.2	0.37
26	10	5	21	0	0	36	0.4	0.94	0.2	0.37
27	10	5	21	0	0	36	0.4	0.94	0.2	0.37
28	8	5	21	0	0	34	0.4	0.93	0.2	0.42
29	8	5	21	0	0	34	0.4	0.93	0.2	0.42
30	10	5	22	0	0	37	0.38	0.94	0.2	0.37
31	10	5	22	0	0	37	0.38	0.94	0.2	0.37
32	10	5	22	0	0	37	0.38	0.94	0.2	0.37
33	10	5	22	0	0	37	0.38	0.94	0.2	0.37
34	10	5	22	0	0	37	0.38	0.94	0.2	0.37
35	10	5	22	0	0	37	0.38	0.94	0.2	0.37
36	10	5	22	0	0	37	0.38	0.94	0.2	0.37
37	10	5	22	0	0	37	0.38	0.94	0.2	0.37
38	10	5	22	0	0	37	0.38	0.94	0.2	0.37
39	10	5	22	0	0	37	0.38	0.94	0.2	0.37
40	10	5	22	0	0	37	0.38	0.94	0.2	0.36
41	10	5	22	0	0	37	0.38	0.94	0.2	0.37
42	10	5	22	0	0	37	0.38	0.94	0.2	0.37
43	10	5	22	0	0	37	0.39	0.94	0.2	0.37
44	10	5	22	0	0	37	0.39	0.94	0.2	0.36
45	10	5	22	0	0	37	0.38	0.94	0.2	0.37
46	10	5	22	0	0	37	0.39	0.94	0.2	0.37
47	10	5	22	0	0	37	0.38	0.94	0.2	0.37
48	10	4	20	0	0	34	0.4	0.94	0.2	0.4
49	10	5	22	0	0	37	0.41	0.97	0.22	0.41
50	10	5	22	0	0	37	0.41	0.94	0.21	0.42

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 224(IR:124, SQ:47, MR:53, LR:0, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	1	2.0
1	0	0	0	0	1	2	4.0
0	0	0	0	0	0	3	6.0
0	0	0	0	0	0	4	8.0
0	0	0	0	0	0	5	10.0
0	0	0	0	0	0	6	12.0

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Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	7	14.0
0	0	0	0	0	0	8	16.0
0	0	0	0	0	0	9	18.0
0	0	0	0	0	0	10	20.0
0	0	0	0	0	0	11	22.0
0	0	0	0	0	0	12	24.0
0	0	0	0	0	0	13	26.0
0	0	0	0	0	0	14	28.0
0	0	0	0	0	0	15	30.0
0	0	0	0	0	0	16	32.0
0	0	0	0	0	0	17	34.0
0	0	0	0	0	0	18	36.0
0	0	0	0	0	0	19	38.0
0	0	0	0	0	0	20	40.0
0	0	0	0	0	0	21	42.0
0	0	0	0	0	0	22	44.0
0	0	0	0	0	0	23	46.0
0	0	0	0	0	0	24	48.0
0	0	0	0	0	0	25	50.0
1	0	1	0	0	2	26	52.0
0	0	0	0	0	0	27	54.0
0	0	0	0	0	0	28	56.0
0	0	0	0	0	0	29	58.0
0	0	0	0	0	0	30	60.0
0	0	0	0	0	0	31	62.0
0	0	0	0	0	0	32	64.0
0	0	0	0	0	0	33	66.0
0	0	0	0	0	0	34	68.0
0	0	0	0	0	0	35	70.0
0	0	0	0	0	0	36	72.0
0	0	0	0	0	0	37	74.0
0	0	0	0	0	0	38	76.0
0	0	0	0	0	0	39	78.0
0	0	0	0	0	0	40	80.0
0	0	0	0	0	0	41	82.0
0	0	1	0	0	1	42	84.0
0	0	0	0	0	0	43	86.0
0	0	0	0	0	0	44	88.0
0	0	0	0	0	0	45	90.0
0	0	0	0	0	0	46	92.0
0	0	1	0	0	1	47	94.0

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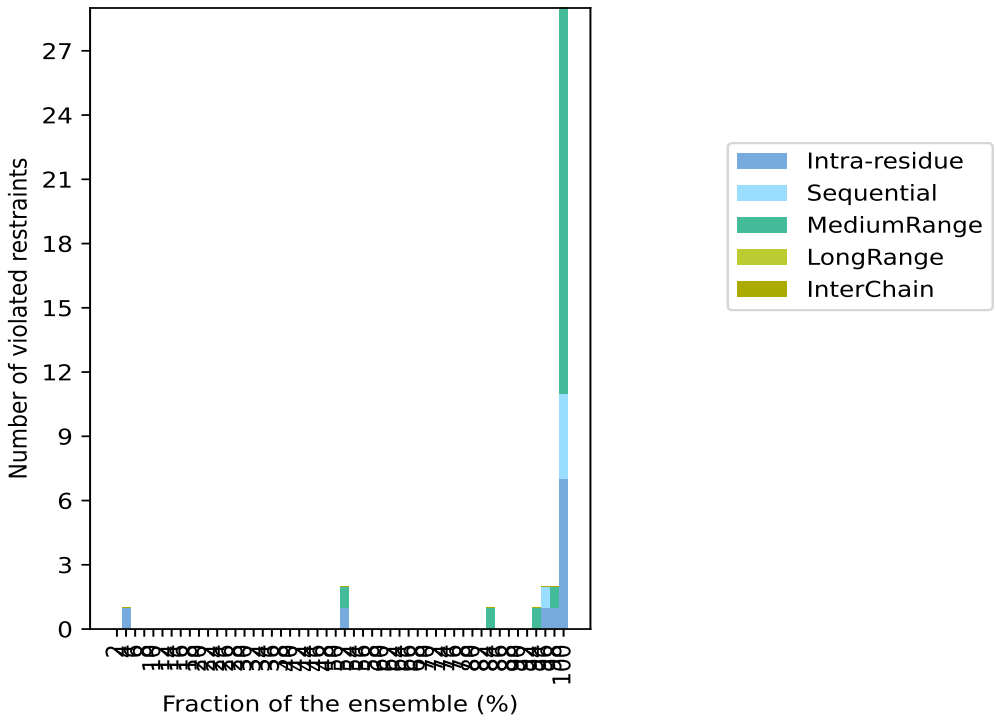
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	1	0	0	0	2	48	96.0
1	0	1	0	0	2	49	98.0
7	4	18	0	0	29	50	100.0

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

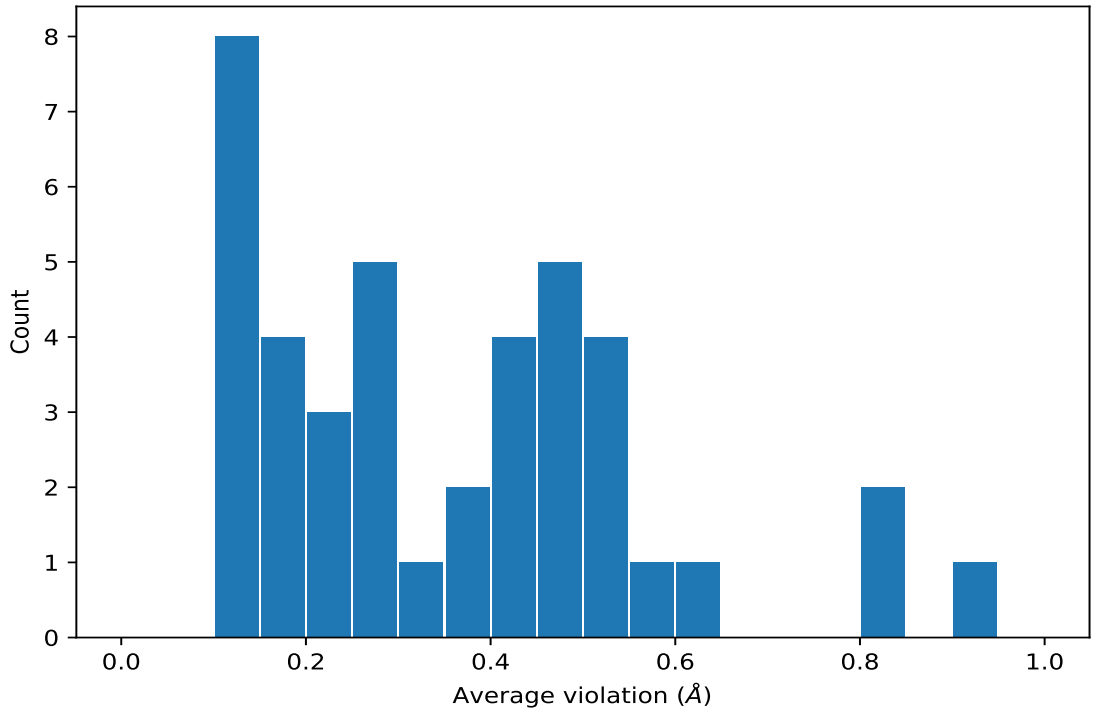
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	50	0.94	0.01	0.94
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	50	0.83	0.01	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	50	0.83	0.01	0.83
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	50	0.63	0.02	0.63
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	50	0.56	0.01	0.56
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	50	0.54	0.01	0.54
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	50	0.53	0.0	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	50	0.51	0.04	0.53
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	50	0.51	0.02	0.51
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	50	0.49	0.0	0.49
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	50	0.48	0.01	0.48
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	50	0.46	0.02	0.45
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	50	0.45	0.05	0.47
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	50	0.44	0.04	0.42
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	50	0.44	0.02	0.43
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	50	0.43	0.1	0.4

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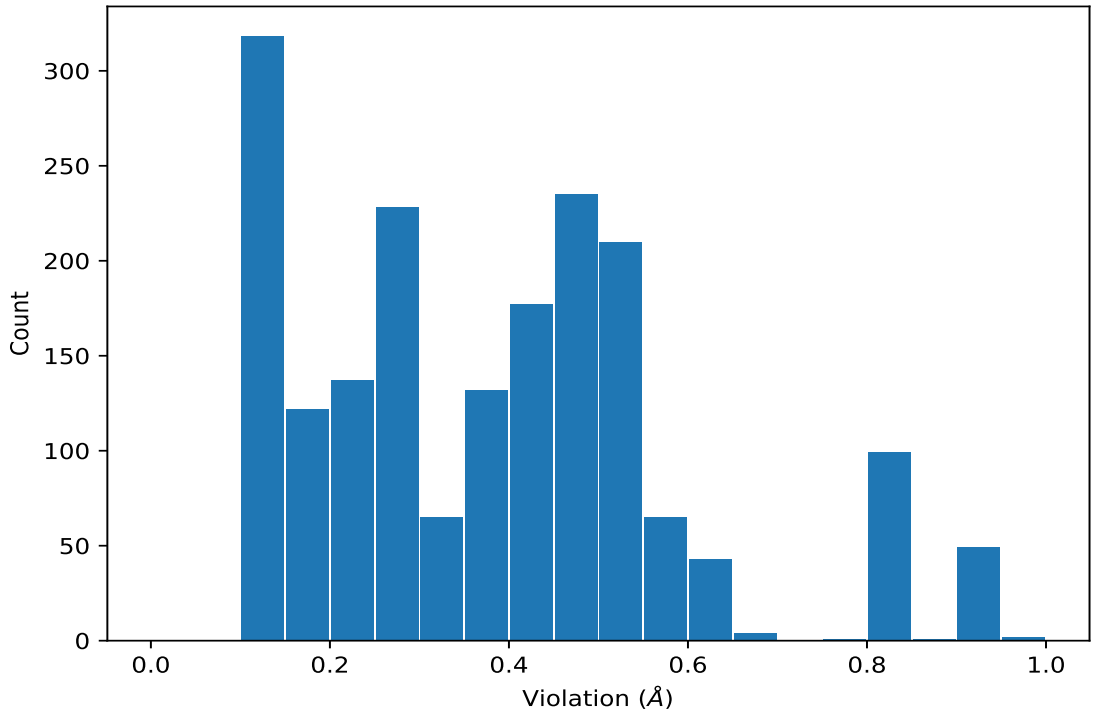
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	50	0.43	0.0	0.43
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	50	0.37	0.01	0.37
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	50	0.36	0.0	0.36
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	50	0.34	0.03	0.33
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	50	0.3	0.03	0.29
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	50	0.28	0.01	0.28
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	50	0.27	0.03	0.27
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	50	0.26	0.04	0.28
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	50	0.24	0.01	0.24
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	50	0.17	0.04	0.16
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	50	0.16	0.01	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	50	0.16	0.01	0.17
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	50	0.15	0.0	0.15
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	50	0.13	0.0	0.13
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	49	0.24	0.02	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	49	0.24	0.02	0.24
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	49	0.16	0.09	0.13
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	48	0.48	0.01	0.48
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	48	0.3	0.05	0.33
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	47	0.13	0.01	0.13
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	42	0.14	0.0	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	26	0.14	0.0	0.14
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	26	0.13	0.0	0.13
(1,36)	1:A:32:PHE:HA	1:A:32:PHE:HB2	2	0.11	0.0	0.11
(1,36)	1:A:32:PHE:HA	1:A:32:PHE:HB3	2	0.11	0.0	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	21	0.98
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	49	0.97
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	1	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	2	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	3	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	4	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	5	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	6	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	7	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	8	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	9	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	10	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	11	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	12	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	13	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	14	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	15	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	18	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	19	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	20	0.95
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	49	0.95
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	17	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	22	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	23	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	24	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	25	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	26	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	27	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	30	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	31	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	32	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	33	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	34	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	35	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	36	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	37	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	38	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	39	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	40	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	41	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	42	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	43	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	44	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	45	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	46	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	47	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	48	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	50	0.94
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	16	0.93
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	28	0.93
(1,59)	1:A:37:GLU:HA	1:A:38:ASP:H	29	0.93
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	50	0.87
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	17	0.84
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	22	0.84
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	48	0.84
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	1	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	2	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	3	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	4	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	5	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	6	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	7	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	8	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	9	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	10	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	11	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	12	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	13	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	14	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	15	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	16	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	18	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	19	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	20	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	23	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	24	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	25	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	26	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	27	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	28	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	29	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	30	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	31	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	32	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	33	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	34	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	35	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	36	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	37	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	38	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	39	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	40	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	41	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	42	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	43	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	44	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	45	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	46	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	47	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	3	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	4	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	5	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	6	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	7	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	8	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	9	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	10	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	11	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	12	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	13	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	14	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	15	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	16	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	19	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	20	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	21	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	28	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	29	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	30	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	31	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	32	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	33	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	34	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	35	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	36	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	37	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	38	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	39	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	40	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	41	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	42	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	43	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	44	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	45	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	46	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	47	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	49	0.83
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	50	0.83
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	17	0.82
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	21	0.82
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	1	0.82
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	23	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	49	0.81
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	50	0.81
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	2	0.81
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	18	0.81
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	24	0.81
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	25	0.81
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	26	0.81
(1,104)	1:A:27:THR:HA	1:A:29:LEU:H	27	0.81
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	48	0.8
(1,39)	1:A:32:PHE:HA	1:A:33:ASN:H	22	0.79
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	16	0.66
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	18	0.66
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	19	0.65
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	20	0.65
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	26	0.64
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	27	0.64
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	30	0.64
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	32	0.64
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	34	0.64
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	35	0.64
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	43	0.64
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	44	0.64
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	45	0.64
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	46	0.64
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	47	0.64
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	48	0.64
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	23	0.63
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	24	0.63
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	25	0.63
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	31	0.63
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	33	0.63
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	36	0.63
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	37	0.63
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	38	0.63
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	39	0.63
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	40	0.63
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	41	0.63
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	42	0.63
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	50	0.63
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	1	0.62
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	2	0.62
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	3	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	4	0.62
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	5	0.62
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	6	0.62
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	7	0.62
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	8	0.62
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	9	0.62
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	17	0.62
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	49	0.61
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	10	0.61
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	11	0.61
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	12	0.61
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	13	0.61
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	14	0.61
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	15	0.61
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	22	0.61
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	50	0.6
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	21	0.6
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	28	0.6
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	29	0.6
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	21	0.6
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	22	0.6
(1,156)	1:A:36:ALA:HA	1:A:39:LEU:H	49	0.58
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	48	0.58
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	1	0.57
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	23	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	1	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	2	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	3	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	4	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	5	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	6	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	7	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	8	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	9	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	10	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	11	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	12	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	13	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	14	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	15	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	16	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	17	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	18	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	19	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	20	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	22	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	49	0.57
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	28	0.56
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	29	0.56
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	50	0.56
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	2	0.55
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	18	0.55
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	24	0.55
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	25	0.55
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	26	0.55
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	27	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	23	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	24	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	25	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	26	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	27	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	30	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	31	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	32	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	33	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	34	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	35	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	36	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	37	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	38	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	39	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	40	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	41	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	42	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	43	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	44	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	45	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	46	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	47	0.55
(1,150)	1:A:35:GLU:HA	1:A:38:ASP:H	48	0.55
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	3	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	4	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	5	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	7	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	8	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	9	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	10	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	11	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	12	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	13	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	14	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	15	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	16	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	17	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	19	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	20	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	21	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	28	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	29	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	30	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	31	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	32	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	33	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	34	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	35	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	36	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	37	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	38	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	39	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	40	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	41	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	42	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	43	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	44	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	45	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	46	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	47	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	49	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	50	0.54
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	1	0.54
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	23	0.54
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	28	0.54
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	29	0.54
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	22	0.53
(1,96)	1:A:25:ALA:HA	1:A:28:PHE:H	48	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	1	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	2	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	3	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	4	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	5	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	6	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	7	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	8	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	9	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	10	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	11	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	12	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	13	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	14	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	15	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	16	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	17	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	18	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	19	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	20	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	22	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	23	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	24	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	25	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	26	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	27	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	30	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	31	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	32	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	33	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	34	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	35	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	36	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	37	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	38	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	39	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	40	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	41	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	42	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	43	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	44	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	45	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	46	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	47	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	48	0.53
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	50	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	1	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	3	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	4	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	5	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	6	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	7	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	8	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	9	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	10	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	11	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	12	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	13	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	14	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	15	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	19	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	23	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	24	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	25	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	30	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	31	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	32	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	33	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	34	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	35	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	36	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	37	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	38	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	39	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	40	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	41	0.53
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	42	0.53
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	2	0.52
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	18	0.52
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	24	0.52
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	25	0.52
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	26	0.52
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	27	0.52
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	21	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:A:38:ASP:H	1:A:38:ASP:HA	49	0.52
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	2	0.52
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	20	0.52
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	26	0.52
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	27	0.52
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	28	0.52
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	29	0.52
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	43	0.52
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	44	0.52
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	45	0.52
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	46	0.52
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	47	0.52
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	17	0.52
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	18	0.52
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	26	0.52
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	27	0.52
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	2	0.51
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	18	0.51
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	24	0.51
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	25	0.51
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	26	0.51
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	27	0.51
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	49	0.51
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	50	0.51
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	16	0.51
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	18	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	1	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	2	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	6	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	7	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	8	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	9	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	10	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	12	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	13	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	14	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	15	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	16	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	19	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	20	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	21	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	23	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	24	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	25	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	28	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	29	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	35	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	36	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	37	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	40	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	41	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	43	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	44	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	45	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	46	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	47	0.51
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	49	0.51
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	22	0.5
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	48	0.5
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	22	0.5
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	48	0.5
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	21	0.5
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	3	0.5
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	4	0.5
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	5	0.5
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	11	0.5
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	30	0.5
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	31	0.5
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	32	0.5
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	33	0.5
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	34	0.5
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	38	0.5
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	39	0.5
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	42	0.5
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	2	0.5
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	18	0.5
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	24	0.5
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	25	0.5
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	26	0.5
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	27	0.5
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	17	0.49
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	21	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	1	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	3	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	4	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	5	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	6	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	7	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	8	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	9	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	10	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	11	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	12	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	13	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	14	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	15	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	16	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	17	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	18	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	19	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	20	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	21	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	23	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	24	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	25	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	26	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	27	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	28	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	29	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	30	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	31	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	32	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	33	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	34	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	35	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	36	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	37	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	38	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	39	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	40	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	41	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	42	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	43	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	44	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	45	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	46	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	47	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	49	0.49
(1,15)	1:A:31:LYS:H	1:A:31:LYS:HA	50	0.49
(1,112)	1:A:28:PHE:HA	1:A:30:ASP:H	50	0.49
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	3	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	5	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	7	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	10	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	11	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	13	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	15	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	16	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	21	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	30	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	31	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	32	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	33	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	34	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	36	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	43	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	46	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	50	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	1	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	3	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	4	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	5	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	6	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	7	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	8	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	9	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	10	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	11	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	12	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	13	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	14	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	15	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	16	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	17	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	19	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	20	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	21	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	23	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	28	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	29	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	30	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	31	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	32	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	33	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	34	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	35	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	36	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	37	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	38	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	39	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	40	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	41	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	42	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	43	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	44	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	45	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	46	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	47	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	49	0.48
(1,52)	1:A:27:THR:HA	1:A:30:ASP:HB3	50	0.48
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	1	0.48
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	23	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	1	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	2	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	3	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	4	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	5	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	6	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	7	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	8	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	9	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	10	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	11	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	12	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	13	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	14	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	15	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	16	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	18	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	19	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	20	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	23	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	24	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	25	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	26	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	27	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	28	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	29	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	30	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	31	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	32	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	33	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	34	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	35	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	36	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	37	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	38	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	39	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	40	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	41	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	42	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	43	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	44	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	45	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	46	0.48
(1,38)	1:A:32:PHE:HB2	1:A:33:ASN:H	47	0.48
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	4	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	6	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	8	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	9	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	12	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	14	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	17	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	19	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	20	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	22	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	28	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	29	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	35	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	37	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	38	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	39	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	40	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	41	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	42	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	44	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	45	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	47	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	48	0.47
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	49	0.47
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	2	0.47
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	18	0.47
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	24	0.47
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	25	0.47
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	26	0.47
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	27	0.47
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	16	0.47
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	1	0.47
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	23	0.47
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	18	0.46
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	9	0.46
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	20	0.46
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	29	0.46
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	40	0.46
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	44	0.46
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	17	0.45
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	28	0.45
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	29	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	3	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	4	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	5	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	6	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	7	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	8	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	10	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	11	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	12	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	13	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	14	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	15	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	16	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	17	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	19	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	21	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	22	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	28	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	30	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	31	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	32	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	33	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	34	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	35	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	36	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	37	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	38	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	39	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	41	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	42	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	43	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	45	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	46	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	47	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	49	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	50	0.45
(1,106)	1:A:27:THR:H	1:A:29:LEU:H	48	0.44
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	3	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	4	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	5	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	6	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	7	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	8	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	9	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	10	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	11	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	12	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	13	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	14	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	15	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	16	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	17	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	19	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	20	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	21	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	22	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	28	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	29	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	30	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	31	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	32	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	33	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	34	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	35	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	36	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	37	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	38	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	39	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	40	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	41	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	42	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	43	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	44	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	45	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	46	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	47	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	48	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	49	0.43
(1,41)	1:A:25:ALA:H	1:A:25:ALA:HA	50	0.43
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	26	0.43
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	27	0.43
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	43	0.43
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	44	0.43
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	45	0.43
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	46	0.43
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	47	0.43
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	17	0.43
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	50	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	1	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	2	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	3	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	4	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	5	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	7	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	8	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	9	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	10	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	11	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	12	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	13	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	14	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	15	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	16	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	17	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	18	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	19	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	20	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	21	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	22	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	23	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	24	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	25	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	28	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	29	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	30	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	31	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	32	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	33	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	34	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	35	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	36	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	37	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	38	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	39	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	40	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	41	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	42	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	49	0.43
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	50	0.43
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	3	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	4	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	5	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	6	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	7	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	8	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	9	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	10	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	11	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	12	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	13	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	14	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	15	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	16	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	17	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	19	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	20	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	21	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	22	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	28	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	29	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	30	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	31	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	32	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	33	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	34	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	35	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	36	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	37	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	38	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	39	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	40	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	41	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	42	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	43	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	44	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	45	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	46	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	47	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	48	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	49	0.42
(1,73)	1:A:24:GLN:HA	1:A:25:ALA:H	50	0.42
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	20	0.42
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	48	0.42
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	6	0.42
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	26	0.42
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	27	0.42
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	43	0.42
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	44	0.42
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	45	0.42
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	46	0.42
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	47	0.42
(1,10)	1:A:36:ALA:H	1:A:36:ALA:HA	48	0.42
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	18	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	49	0.41
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	10	0.41
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	11	0.41
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	12	0.41
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	13	0.41
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	14	0.41
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	15	0.41
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	22	0.41
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	48	0.41
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	22	0.41
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	19	0.4
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	20	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	2	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	19	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	23	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	24	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	25	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	30	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	31	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	32	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	33	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	34	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	35	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	36	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	37	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	38	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	39	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	40	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	41	0.4
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	42	0.4
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	1	0.39
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	23	0.39
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	1	0.39
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	3	0.39
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	4	0.39
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	5	0.39
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	6	0.39
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	7	0.39
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	8	0.39
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	9	0.39
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	48	0.39
(1,130)	1:A:31:LYS:HA	1:A:35:GLU:H	21	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	49	0.38
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	2	0.37
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	18	0.37
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	24	0.37
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	25	0.37
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	26	0.37
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	27	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	2	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	3	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	4	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	5	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	6	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	7	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	8	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	10	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	11	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	12	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	13	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	14	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	15	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	16	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	17	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	18	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	19	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	21	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	24	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	25	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	26	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	27	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	28	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	30	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	31	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	32	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	33	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	34	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	35	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	36	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	37	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	38	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	39	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	41	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	42	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	43	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	45	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	46	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	47	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	48	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	49	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	50	0.37
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	1	0.37
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	3	0.37
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	4	0.37
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	5	0.37
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	6	0.37
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	7	0.37
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	8	0.37
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	9	0.37
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	9	0.36
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	20	0.36
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	22	0.36
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	29	0.36
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	40	0.36
(1,72)	1:A:23:GLU:HA	1:A:24:GLN:H	44	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	1	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	2	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	3	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	4	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	5	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	6	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	7	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	8	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	9	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	10	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	11	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	12	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	13	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	14	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	15	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	16	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	17	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	18	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	19	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	20	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	21	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	22	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	23	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	24	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	25	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	26	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	27	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	28	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	29	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	30	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	31	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	32	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	33	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	34	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	35	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	36	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	37	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	38	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	39	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	40	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	41	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	42	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	43	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	44	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	45	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	46	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	47	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	48	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	49	0.36
(1,209)	1:A:29:LEU:HA	1:A:29:LEU:HG	50	0.36
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	2	0.36
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	10	0.36
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	11	0.36
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	12	0.36
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	13	0.36
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	14	0.36
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	15	0.36
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	21	0.35
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	22	0.35
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	25	0.34
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	26	0.34
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	17	0.34
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	22	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	2	0.33
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	18	0.33
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	24	0.33
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	27	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	23	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	24	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	25	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	26	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	27	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	30	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	31	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	32	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	33	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	34	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	35	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	36	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	37	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	38	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	39	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	40	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	41	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	42	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	43	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	44	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	45	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	46	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	47	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	48	0.33
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	50	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	23	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	24	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	25	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	26	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	27	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	30	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	31	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	32	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	33	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	34	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	35	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	36	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	37	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	38	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	39	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	40	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	41	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	42	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	43	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	44	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	45	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	46	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	47	0.33
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	48	0.33
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	1	0.32
(1,82)	1:A:22:GLU:HA	1:A:26:LYS:H	23	0.32
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	16	0.32
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	50	0.32
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	16	0.31
(1,127)	1:A:31:LYS:HA	1:A:33:ASN:H	22	0.31
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	9	0.3
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	20	0.3
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	29	0.3
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	40	0.3
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	44	0.3
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	50	0.3
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	28	0.3
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	29	0.3
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	3	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	4	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	5	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	6	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	7	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	8	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	10	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	11	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	12	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	13	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	14	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	15	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	16	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	17	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	19	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	21	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	22	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	28	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	30	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	31	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	32	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	33	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	34	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	35	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	36	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	37	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	38	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	39	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	41	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	42	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	43	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	45	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	46	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	47	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	48	0.29
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	49	0.29
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	21	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	19	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	20	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	23	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	24	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	25	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	30	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	31	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	32	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	33	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	34	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	35	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	36	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	38	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	39	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	40	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	41	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	42	0.29
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	50	0.29
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	1	0.29
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	2	0.29
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	3	0.29
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	5	0.29
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	6	0.29
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	7	0.29
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	8	0.29
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	9	0.29
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	17	0.29
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	48	0.29
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	2	0.28
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	18	0.28
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	26	0.28
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	27	0.28
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	37	0.28
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	43	0.28
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	44	0.28
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	45	0.28
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	46	0.28
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	47	0.28
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	48	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	10	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	11	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	12	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	13	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	14	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	15	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	16	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	22	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	23	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	24	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	25	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	30	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	31	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	32	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	33	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	34	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	35	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	36	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	37	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	38	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	39	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	40	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	41	0.28
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	42	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	17	0.28
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	17	0.28
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	23	0.27
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	1	0.27
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	3	0.27
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	4	0.27
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	5	0.27
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	6	0.27
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	7	0.27
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	8	0.27
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	9	0.27
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	21	0.27
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	26	0.27
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	27	0.27
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	43	0.27
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	44	0.27
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	45	0.27
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	46	0.27
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	47	0.27
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	48	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	1	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	2	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	3	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	4	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	5	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	6	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	7	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	8	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	9	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	10	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	11	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	12	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	13	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	14	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	15	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	19	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	20	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	21	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	23	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	24	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	25	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	26	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	27	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	30	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	31	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	32	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	33	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	34	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	35	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	36	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	37	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	38	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	39	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	40	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	41	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	42	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	43	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	44	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	45	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	46	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	47	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	49	0.27
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	50	0.27
(1,88)	1:A:23:GLU:HA	1:A:27:THR:H	1	0.26
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	24	0.26
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	27	0.26
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	21	0.26
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	18	0.26
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	19	0.26
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	20	0.26
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	28	0.26
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	29	0.26
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	49	0.26
(1,142)	1:A:34:HIS:HA	1:A:36:ALA:H	50	0.26
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	16	0.26
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	17	0.26
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	18	0.26
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	28	0.26
(1,117)	1:A:29:LEU:HA	1:A:31:LYS:H	29	0.26
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	2	0.25
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	9	0.25
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	18	0.25
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	20	0.25
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	25	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	26	0.25
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	29	0.25
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	40	0.25
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	44	0.25
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	49	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	2	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	2	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	16	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	16	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	18	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	18	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	20	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	20	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	21	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	21	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	26	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	26	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	27	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	27	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	28	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	28	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	29	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	29	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	43	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	43	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	44	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	44	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	45	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	45	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	46	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	46	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	47	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	47	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	49	0.25
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	49	0.25
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	3	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	4	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	5	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	6	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	7	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	8	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	11	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	12	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	13	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	14	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	15	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	16	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	17	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	19	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	21	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	22	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	28	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	30	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	31	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	32	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	33	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	34	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	35	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	36	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	37	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	38	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	39	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	41	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	42	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	43	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	45	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	46	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	47	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	48	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	49	0.24
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	50	0.24
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	28	0.24
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	29	0.24
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	17	0.24
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	49	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	1	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	1	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	3	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	3	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	4	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	4	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	5	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	6	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	6	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	7	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	7	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	8	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	8	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	9	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	9	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	10	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	10	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	11	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	11	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	12	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	12	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	13	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	13	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	14	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	14	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	15	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	15	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	19	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	19	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	23	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	23	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	24	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	24	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	25	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	25	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	30	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	30	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	31	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	31	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	32	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	32	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	33	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	33	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	34	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	34	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	35	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	35	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	36	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	36	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	37	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	37	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	38	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	38	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	39	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	39	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	40	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	40	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	41	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	41	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	42	0.24
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	42	0.24
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	10	0.23
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	11	0.23
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	12	0.23
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	13	0.23
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	14	0.23
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	15	0.23
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	18	0.23
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	19	0.23
(1,151)	1:A:35:GLU:HA	1:A:39:LEU:H	20	0.23
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	1	0.21
(1,85)	1:A:23:GLU:HA	1:A:25:ALA:H	23	0.21
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	17	0.21
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	17	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	1	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	2	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	4	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	5	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	6	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	7	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	8	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	10	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	11	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	12	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	13	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	14	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	15	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	16	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	17	0.21
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	22	0.21
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	50	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	50	0.21
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	22	0.2
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	3	0.2
(1,159)	1:A:37:GLU:HA	1:A:40:PHE:H	9	0.2
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	50	0.19
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	22	0.18
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	22	0.18
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	48	0.18
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	48	0.18
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	16	0.18
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	16	0.17
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	18	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	3	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	3	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	4	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	4	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	5	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	5	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	6	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	6	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	7	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	7	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	8	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	8	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	9	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	9	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	10	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	10	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	11	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	11	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	12	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	12	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	13	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	13	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	14	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	14	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	15	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	15	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	16	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	16	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	17	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	19	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	19	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	20	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	20	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	21	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	21	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	28	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	28	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	29	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	29	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	30	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	30	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	31	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	31	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	32	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	32	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	33	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	33	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	34	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	34	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	35	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	35	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	36	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	36	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	37	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	37	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	38	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	38	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	39	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	39	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	40	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	40	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	41	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	41	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	42	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	42	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	43	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	43	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	44	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	44	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	45	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	45	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	46	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	46	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	47	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	47	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	49	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	49	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	50	0.17
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	50	0.17
(1,207)	1:A:39:LEU:H	1:A:39:LEU:HG	49	0.17
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	18	0.17
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	21	0.17
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	28	0.17
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	29	0.17
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	28	0.16
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	29	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	1	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	2	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	3	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	4	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	5	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	6	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	7	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	8	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	9	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	10	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	11	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	12	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	13	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	14	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	15	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	20	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	26	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	27	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	33	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	36	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	40	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	41	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	43	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	44	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	45	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	46	0.16
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	47	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	26	0.15
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	27	0.15
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	43	0.15
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	44	0.15
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	45	0.15
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	46	0.15
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	47	0.15
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	19	0.15
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	23	0.15
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	24	0.15
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	25	0.15
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	30	0.15
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	31	0.15
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	32	0.15
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	34	0.15
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	35	0.15
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	37	0.15
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	38	0.15
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	39	0.15
(1,133)	1:A:32:PHE:H	1:A:34:HIS:H	42	0.15
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	50	0.15
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB2	22	0.15
(1,119)	1:A:29:LEU:HA	1:A:32:PHE:HB3	22	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	3	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	4	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	5	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	6	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	7	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	8	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	9	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	10	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	11	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	12	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	13	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	14	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	15	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	16	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	17	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	19	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	20	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	21	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	22	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	28	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	29	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	30	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	31	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	32	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	33	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	34	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	35	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	36	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	37	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	38	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	39	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	40	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	41	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	42	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	43	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	44	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	45	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	46	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	47	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	48	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	49	0.15
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	50	0.15
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	20	0.14
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	21	0.14
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	2	0.14
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	2	0.14
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	18	0.14
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	18	0.14
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	24	0.14
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	24	0.14
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	25	0.14
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	25	0.14
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	26	0.14
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	26	0.14
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	27	0.14
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	27	0.14
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	25	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	23	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	24	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	25	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	26	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	27	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	30	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	31	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	32	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	33	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	34	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	35	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	36	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	37	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	38	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	39	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	40	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	41	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	42	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	43	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	44	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	45	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	46	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	47	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	48	0.14
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	50	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	3	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	4	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	5	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	6	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	7	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	8	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	10	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	11	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	12	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	13	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	14	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	15	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	16	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	17	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	19	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	21	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	22	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	28	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	30	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	31	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	32	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	33	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	34	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	35	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	36	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	37	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	38	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	39	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	41	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	42	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	43	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	45	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	46	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	47	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	48	0.14
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	49	0.14
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	1	0.14
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	2	0.14
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	18	0.14
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	23	0.14
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	24	0.14
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	25	0.14
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	26	0.14
(1,101)	1:A:26:LYS:HA	1:A:28:PHE:H	27	0.14
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	2	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	3	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	4	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	5	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	6	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	7	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	8	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	9	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	10	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	11	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	12	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	13	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	14	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	15	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	19	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	23	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	24	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	25	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	30	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	32	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	33	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	34	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	35	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	36	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	37	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	38	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	39	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	40	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	41	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	1	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	2	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	3	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	4	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	5	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	6	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	7	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	8	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	9	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	10	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	11	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	12	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	13	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	14	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	15	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	16	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	17	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	18	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	19	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	20	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	21	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	22	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	23	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	24	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	26	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	27	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	28	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	29	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	30	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	31	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	32	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	33	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	34	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	35	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	36	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	37	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	38	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	39	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	40	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	41	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	42	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	43	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	44	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	45	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	46	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	47	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	48	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	49	0.13
(1,179)	1:A:29:LEU:H	1:A:29:LEU:HG	50	0.13
(1,170)	1:A:39:LEU:HA	1:A:41:TYR:H	49	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	23	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	24	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	25	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	26	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	27	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	30	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	31	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	32	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	33	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	34	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	35	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	36	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	37	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	38	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	39	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	40	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	41	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	42	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	43	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	44	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	45	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	46	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	47	0.13
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	48	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	50	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	1	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	2	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	3	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	4	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	5	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	6	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	7	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	8	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	9	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	10	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	11	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	12	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	13	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	14	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	15	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	19	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	23	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	24	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	25	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	30	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	31	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	32	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	33	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	34	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	35	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	36	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	37	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	38	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	39	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	40	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	41	0.13
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	42	0.13
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	9	0.13
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	20	0.13
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	29	0.13
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	40	0.13
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	44	0.13
(1,102)	1:A:26:LYS:H	1:A:28:PHE:H	50	0.13
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	1	0.12
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	31	0.12
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	42	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	1	0.12
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	1	0.12
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE1	23	0.12
(1,230)	1:A:28:PHE:H	1:A:28:PHE:HE2	23	0.12
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	16	0.12
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	18	0.12
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	20	0.12
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	21	0.12
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	26	0.12
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	27	0.12
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	28	0.12
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	29	0.12
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	43	0.12
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	44	0.12
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	45	0.12
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	46	0.12
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	47	0.12
(1,36)	1:A:32:PHE:HA	1:A:32:PHE:HB2	22	0.11
(1,36)	1:A:32:PHE:HA	1:A:32:PHE:HB3	22	0.11
(1,36)	1:A:32:PHE:HA	1:A:32:PHE:HB2	48	0.11
(1,36)	1:A:32:PHE:HA	1:A:32:PHE:HB3	48	0.11
(1,232)	1:A:34:HIS:H	1:A:34:HIS:HD1	22	0.11
(1,162)	1:A:40:PHE:HA	1:A:40:PHE:HB2	49	0.11
(1,128)	1:A:31:LYS:H	1:A:33:ASN:H	49	0.11

10 Dihedral-angle violation analysis (i)

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