



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 10:35 AM UTC

PDB ID : 2LK5 / pdb_00002lk5
BMRB ID : 17979
Title : Solution structure of the Zn(II) form of Desulforedoxin
Authors : Goodfellow, B.J.; Tavares, P.; Romao, M.J.; Czaja, C.; Rusnak, F.; Legall, J.; Moura, I.; Moura, J.J.G.
Deposited on : 2011-10-06

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : **FAILED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 27%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 29 models. Model 29 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:36, B:4-B:36 (67)	0.39	29

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 5, 6, 10, 11, 12, 13, 14, 16, 17, 21, 22, 23, 24, 25, 27, 28, 29
2	3, 4, 19, 20
3	2, 8, 9
4	15, 26
Single-model clusters	7; 18

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1016 atoms, of which 494 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Desulforedoxin.

Mol	Chain	Residues	Atoms						Trace
1	A	36	Total	C	H	N	O	S	0
			507	158	247	42	55	5	
1	B	36	Total	C	H	N	O	S	0
			507	158	247	42	55	5	

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

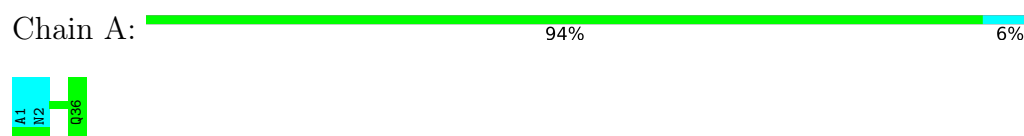
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1
2	B	1	Total	Zn
			1	1

4 Residue-property plots

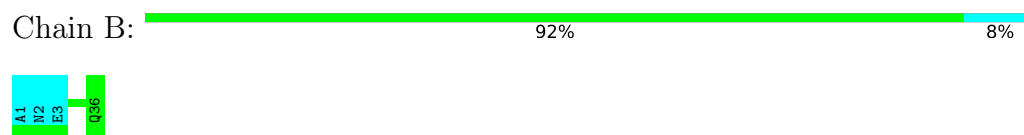
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Desulforedoxin



- Molecule 1: Desulforedoxin

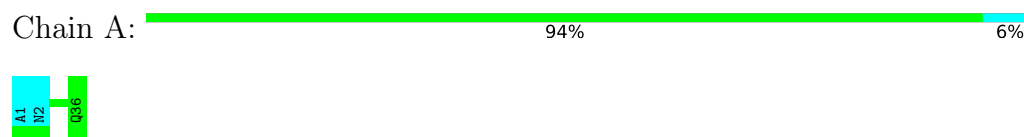


4.2 Scores per residue for each member of the ensemble

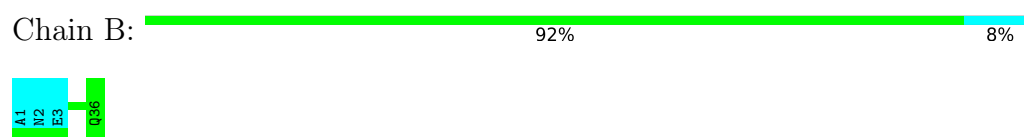
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Desulforedoxin

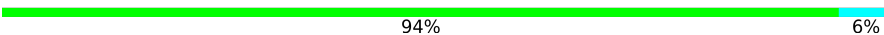


- Molecule 1: Desulforedoxin



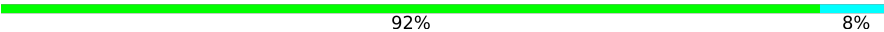
4.2.2 Score per residue for model 2

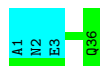
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



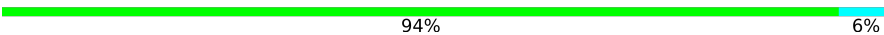
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



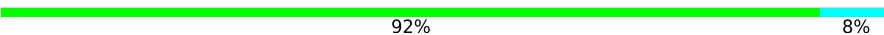
4.2.3 Score per residue for model 3

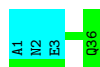
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



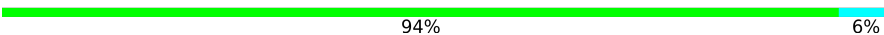
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



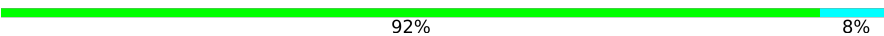
4.2.4 Score per residue for model 4

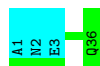
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



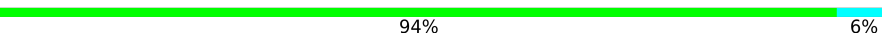
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.5 Score per residue for model 5

- Molecule 1: Desulforedoxin

Chain A:  94% 6%



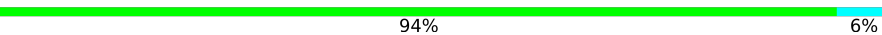
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.6 Score per residue for model 6

- Molecule 1: Desulforedoxin

Chain A:  94% 6%



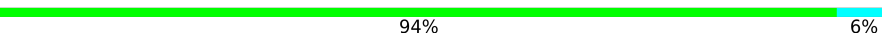
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



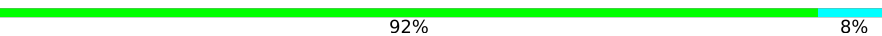
4.2.7 Score per residue for model 7

- Molecule 1: Desulforedoxin

Chain A:  94% 6%



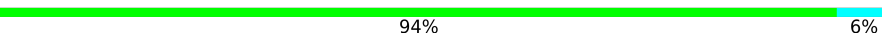
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.8 Score per residue for model 8

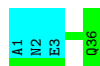
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



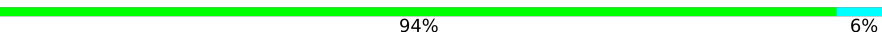
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.9 Score per residue for model 9

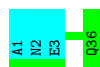
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



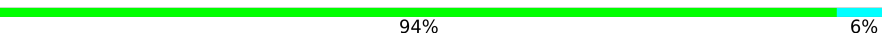
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



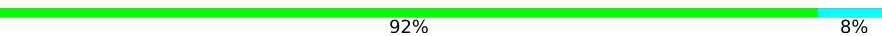
4.2.10 Score per residue for model 10

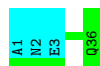
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



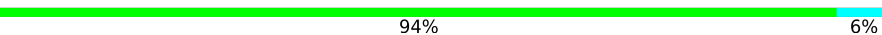
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.11 Score per residue for model 11

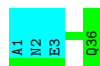
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



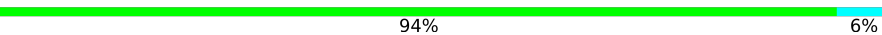
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.12 Score per residue for model 12

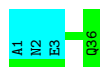
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



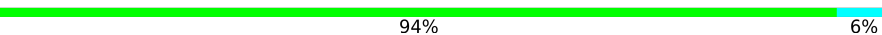
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



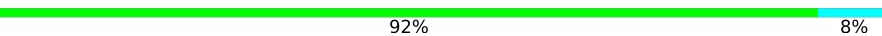
4.2.13 Score per residue for model 13

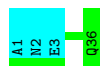
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



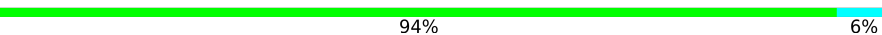
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.14 Score per residue for model 14

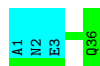
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



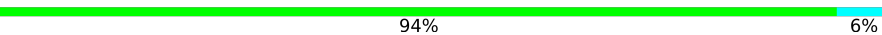
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.15 Score per residue for model 15

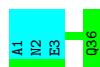
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



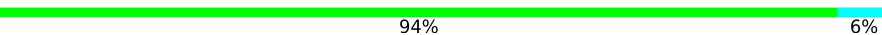
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



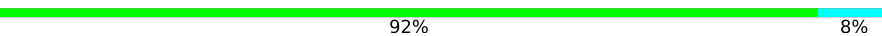
4.2.16 Score per residue for model 16

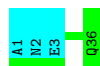
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



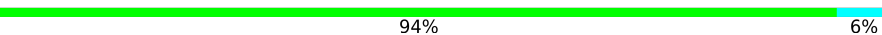
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.17 Score per residue for model 17

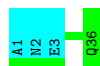
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



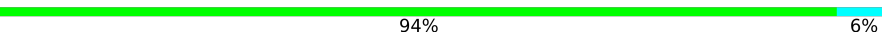
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.18 Score per residue for model 18

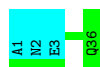
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



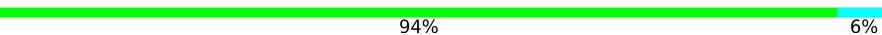
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



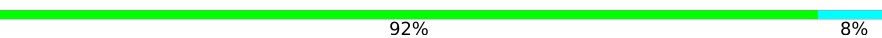
4.2.19 Score per residue for model 19

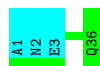
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



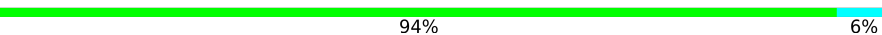
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.20 Score per residue for model 20

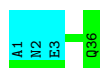
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



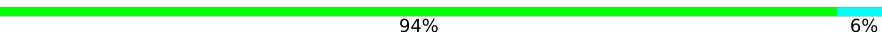
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.21 Score per residue for model 21

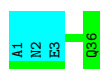
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



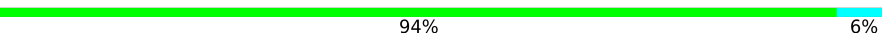
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



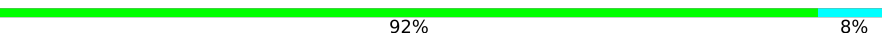
4.2.22 Score per residue for model 22

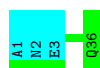
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



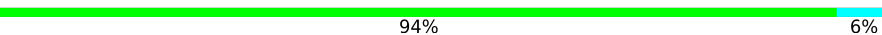
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.23 Score per residue for model 23

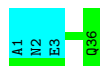
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



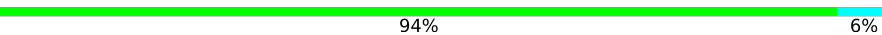
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.24 Score per residue for model 24

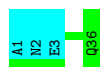
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



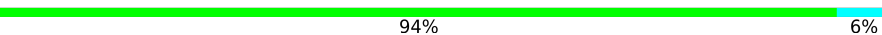
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



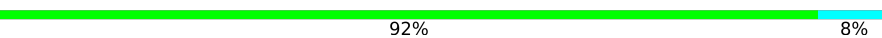
4.2.25 Score per residue for model 25

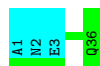
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



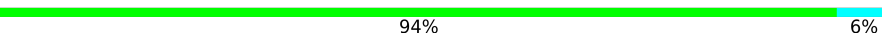
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.26 Score per residue for model 26

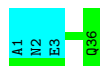
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



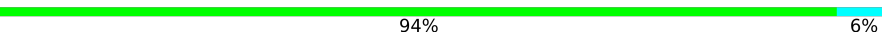
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



4.2.27 Score per residue for model 27

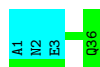
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



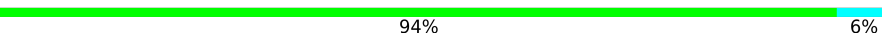
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



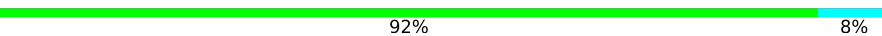
4.2.28 Score per residue for model 28

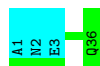
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



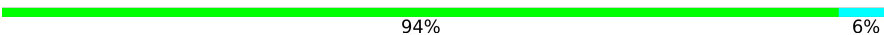
- Molecule 1: Desulforedoxin

Chain B:  92% 8%



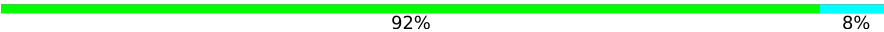
4.2.29 Score per residue for model 29 (medoid)

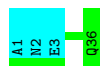
- Molecule 1: Desulforedoxin

Chain A:  94% 6%



- Molecule 1: Desulforedoxin

Chain B:  92% 8%



5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 29 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
DIANA	structure solution	2.8
DIANA	refinement	2.8

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	231
Number of shifts mapped to atoms	231
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	27%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

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

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 27% for the well-defined parts and 26% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	231
Number of shifts mapped to atoms	231
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

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 27%, i.e. 223 atoms were assigned a chemical shift out of a possible 822. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	74/347 (21%)	74/146 (51%)	0/134 (0%)	0/67 (0%)
Sidechain	147/457 (32%)	147/296 (50%)	0/151 (0%)	0/10 (0%)
Aromatic	2/18 (11%)	2/8 (25%)	0/10 (0%)	0/0 (—%)
Overall	223/822 (27%)	223/450 (50%)	0/295 (0%)	0/77 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 26%, i.e. 231 atoms were assigned a chemical shift out of a possible 876. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	77/372 (21%)	77/156 (49%)	0/144 (0%)	0/72 (0%)
Sidechain	152/486 (31%)	152/314 (48%)	0/160 (0%)	0/12 (0%)
Aromatic	2/18 (11%)	2/8 (25%)	0/10 (0%)	0/0 (—%)
Overall	231/876 (26%)	231/478 (48%)	0/314 (0%)	0/84 (0%)

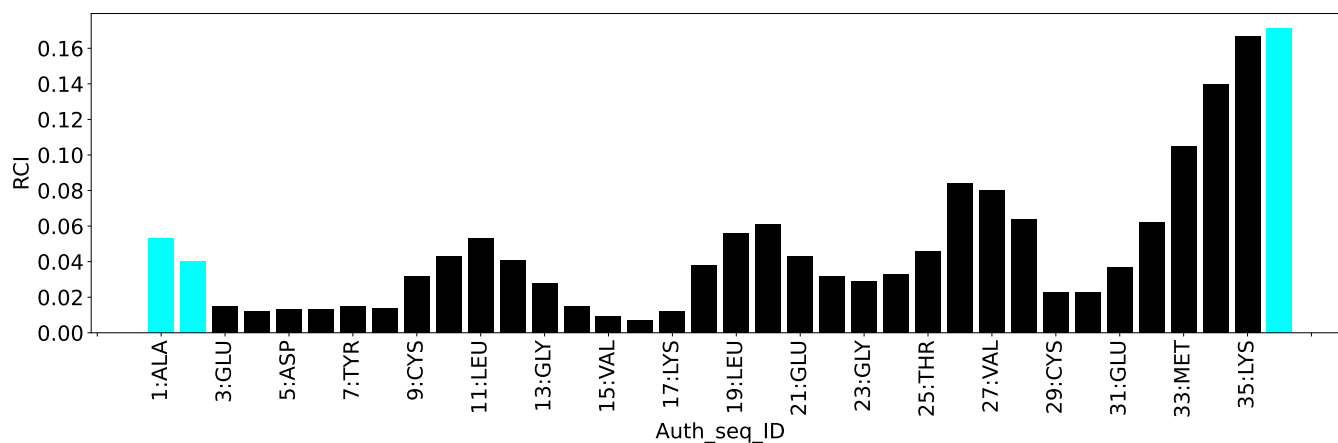
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	670
Intra-residue ($ i-j =0$)	138
Sequential ($ i-j =1$)	172
Medium range ($ i-j >1$ and $ i-j <5$)	70
Long range ($ i-j \geq 5$)	176
Inter-chain	26
Hydrogen bond restraints	60
Disulfide bond restraints	10
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	9.1
Number of long range restraints per residue ¹	2.9

¹Long 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)	25.5	0.2
0.2-0.5 (Medium)	11.0	0.5
>0.5 (Large)	33.1	4.11

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 ⓘ

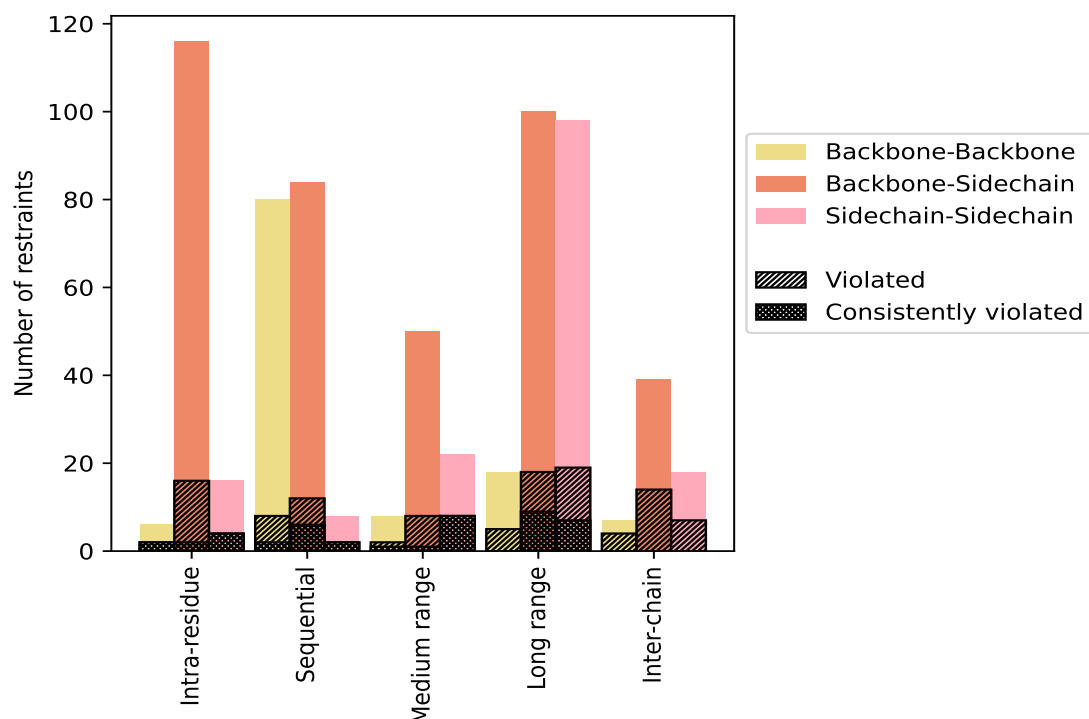
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	138	20.6	22	15.9	3.3	8	5.8	1.2
Backbone-Backbone	6	0.9	2	33.3	0.3	2	33.3	0.3
Backbone-Sidechain	116	17.3	16	13.8	2.4	2	1.7	0.3
Sidechain-Sidechain	16	2.4	4	25.0	0.6	4	25.0	0.6
Sequential (i-j =1)	172	25.7	22	12.8	3.3	10	5.8	1.5
Backbone-Backbone	80	11.9	8	10.0	1.2	2	2.5	0.3
Backbone-Sidechain	84	12.5	12	14.3	1.8	6	7.1	0.9
Sidechain-Sidechain	8	1.2	2	25.0	0.3	2	25.0	0.3
Medium range (i-j >1 & i-j <5)	70	10.4	17	24.3	2.5	10	14.3	1.5
Backbone-Backbone	8	1.2	2	25.0	0.3	1	12.5	0.1
Backbone-Sidechain	42	6.3	7	16.7	1.0	1	2.4	0.1
Sidechain-Sidechain	20	3.0	8	40.0	1.2	8	40.0	1.2
Long range (i-j ≥5)	176	26.3	32	18.2	4.8	16	9.1	2.4
Backbone-Backbone	18	2.7	5	27.8	0.7	0	0.0	0.0
Backbone-Sidechain	68	10.1	12	17.6	1.8	9	13.2	1.3
Sidechain-Sidechain	90	13.4	15	16.7	2.2	7	7.8	1.0
Inter-chain	26	3.9	5	19.2	0.7	0	0.0	0.0
Backbone-Backbone	7	1.0	4	57.1	0.6	0	0.0	0.0
Backbone-Sidechain	13	1.9	1	7.7	0.1	0	0.0	0.0
Sidechain-Sidechain	6	0.9	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	60	9.0	16	26.7	2.4	0	0.0	0.0
Disulfide bond	10	1.5	4	40.0	0.6	0	0.0	0.0
Total	670	100.0	129	19.3	19.3	44	6.6	6.6
Backbone-Backbone	119	17.8	21	17.6	3.1	5	4.2	0.7
Backbone-Sidechain	389	58.1	68	17.5	10.1	18	4.6	2.7
Sidechain-Sidechain	162	24.2	40	24.7	6.0	21	13.0	3.1

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	12	12	13	28	8	73	1.05	3.64	1.16	0.34
2	13	15	12	22	6	68	1.08	3.79	1.1	0.48
3	16	12	13	23	10	74	1.02	3.76	1.14	0.31
4	13	14	13	27	8	75	1.02	3.83	1.12	0.31
5	14	13	13	24	10	74	1.06	4.03	1.17	0.35
6	10	12	12	24	9	67	1.11	4.08	1.18	0.55
7	14	12	12	26	9	73	1.06	3.88	1.17	0.35
8	11	15	12	25	13	76	1.02	3.71	1.12	0.37
9	11	13	13	23	11	71	1.07	4.0	1.14	0.36
10	13	11	12	25	5	66	1.12	3.74	1.15	0.52

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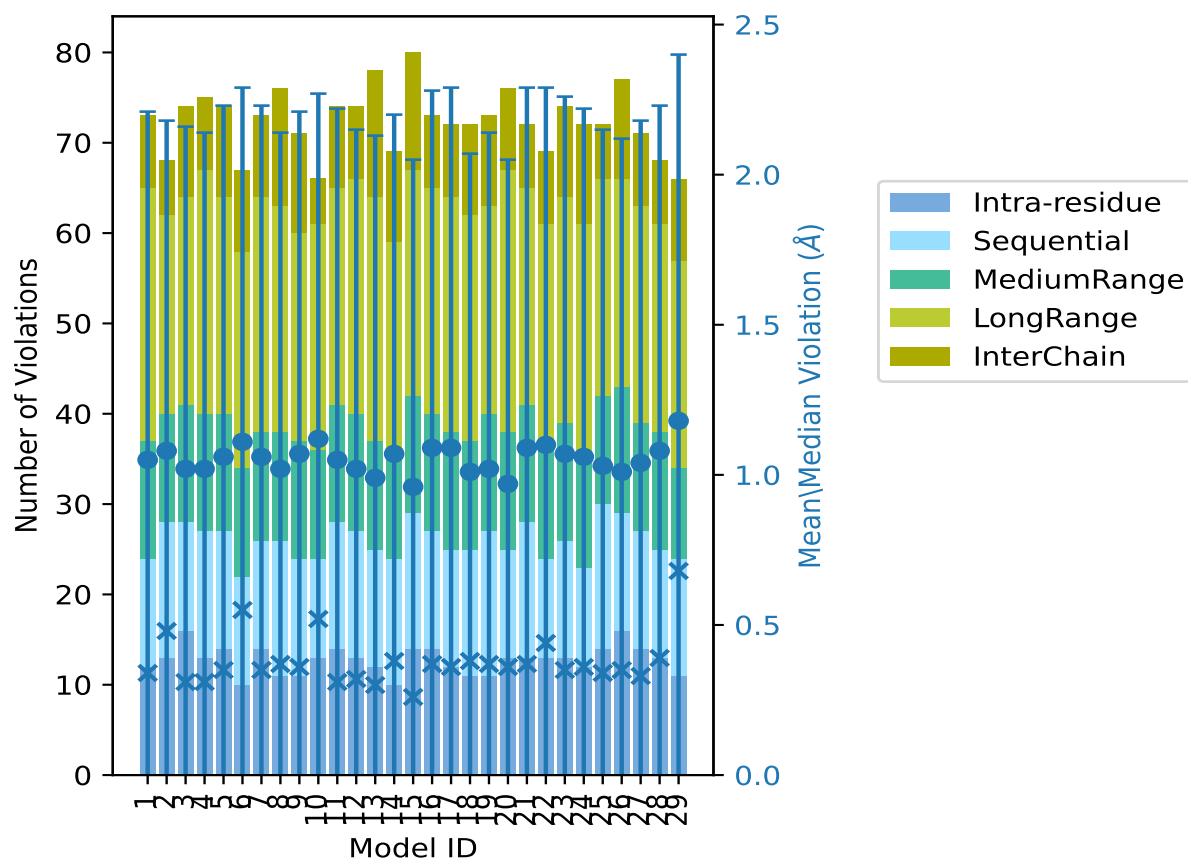
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	14	14	13	24	9	74	1.05	3.6	1.17	0.31
12	13	14	13	26	8	74	1.02	3.63	1.13	0.32
13	12	13	12	27	14	78	0.99	3.73	1.14	0.3
14	10	14	12	23	10	69	1.07	3.65	1.13	0.38
15	14	15	13	25	13	80	0.96	3.63	1.09	0.26
16	14	13	13	25	8	73	1.09	3.83	1.19	0.37
17	12	13	13	26	8	72	1.09	4.11	1.2	0.36
18	11	14	12	25	10	72	1.01	3.47	1.06	0.38
19	11	16	13	23	10	73	1.02	3.57	1.12	0.37
20	13	12	13	29	9	76	0.97	3.55	1.08	0.36
21	13	15	13	24	7	72	1.09	4.04	1.2	0.37
22	13	11	12	25	8	69	1.1	4.1	1.19	0.44
23	13	13	13	25	10	74	1.07	3.89	1.19	0.35
24	12	11	12	26	11	72	1.06	3.87	1.16	0.36
25	14	16	12	24	6	72	1.03	3.59	1.12	0.34
26	16	13	14	23	11	77	1.01	3.61	1.11	0.35
27	14	13	12	24	8	71	1.04	3.69	1.14	0.33
28	13	12	13	23	7	68	1.08	3.64	1.15	0.39
29	11	13	10	23	9	66	1.18	3.93	1.22	0.68

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 484(IR:116, SQ:150, MR:53, LR:144, IC:21) 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	%
4	2	2	4	1	13	1	3.4
0	1	1	0	1	3	2	6.9
0	1	1	1	0	3	3	10.3
0	0	0	0	0	0	4	13.8
1	1	0	2	0	4	5	17.2
1	1	0	0	0	2	6	20.7

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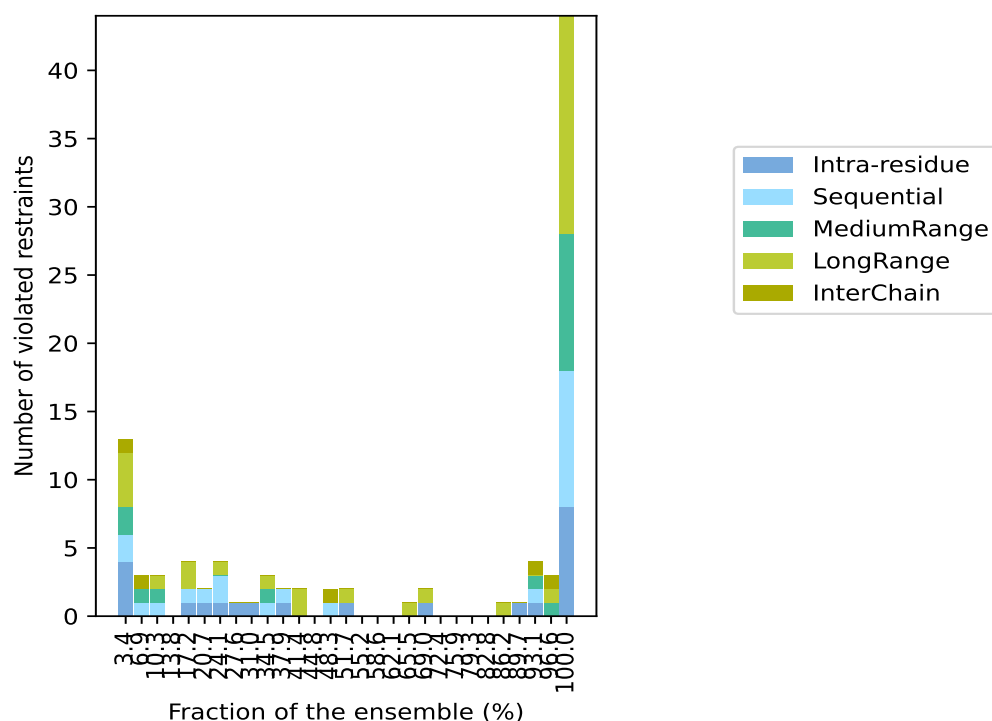
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	2	0	1	0	4	7	24.1
1	0	0	0	0	1	8	27.6
1	0	0	0	0	1	9	31.0
0	1	1	1	0	3	10	34.5
1	1	0	0	0	2	11	37.9
0	0	0	2	0	2	12	41.4
0	0	0	0	0	0	13	44.8
0	1	0	0	1	2	14	48.3
1	0	0	1	0	2	15	51.7
0	0	0	0	0	0	16	55.2
0	0	0	0	0	0	17	58.6
0	0	0	0	0	0	18	62.1
0	0	0	1	0	1	19	65.5
1	0	0	1	0	2	20	69.0
0	0	0	0	0	0	21	72.4
0	0	0	0	0	0	22	75.9
0	0	0	0	0	0	23	79.3
0	0	0	0	0	0	24	82.8
0	0	0	1	0	1	25	86.2
1	0	0	0	0	1	26	89.7
1	1	1	0	1	4	27	93.1
0	0	1	1	1	3	28	96.6
8	10	10	16	0	44	29	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

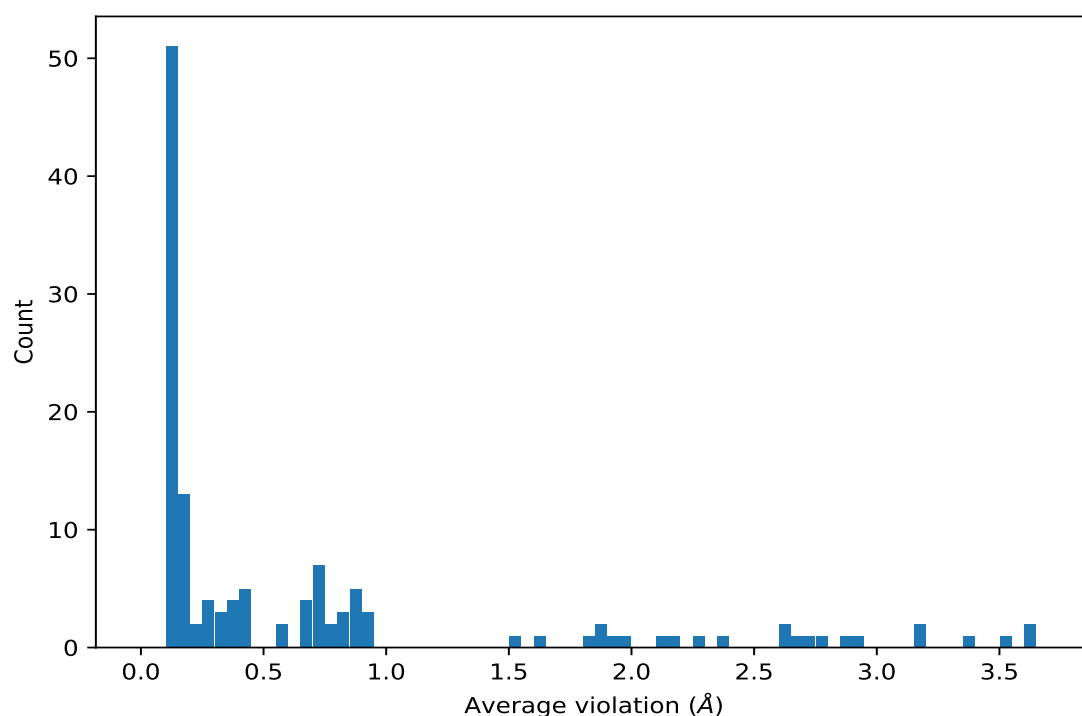
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	29	3.62	0.07	3.63
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	29	3.61	0.4	3.7
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	29	3.51	0.07	3.51
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	29	3.35	0.29	3.31
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	29	3.19	0.2	3.22
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	29	3.16	0.14	3.16
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	29	2.94	0.38	2.95
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	29	2.88	0.2	2.89
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	29	2.79	0.27	2.76
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	29	2.74	0.23	2.78
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	29	2.69	0.14	2.71
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	29	2.65	0.11	2.64
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	29	2.61	0.38	2.5
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	29	2.37	0.28	2.43
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	29	2.26	0.17	2.28
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	29	2.19	0.2	2.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	29	2.11	0.17	2.08
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	29	1.98	0.2	1.95
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	29	1.93	0.17	1.93
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	29	1.9	0.2	1.86
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	29	1.88	0.24	1.84
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	29	1.84	0.15	1.82
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	29	1.62	0.31	1.71
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	29	1.5	0.28	1.55
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	29	0.87	0.11	0.87
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	29	0.87	0.11	0.87
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	29	0.87	0.11	0.87
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	29	0.86	0.1	0.87
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	29	0.86	0.1	0.87
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	29	0.85	0.12	0.84
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	29	0.85	0.12	0.84
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	29	0.85	0.12	0.84
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	29	0.79	0.13	0.84
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	29	0.79	0.13	0.84
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	29	0.74	0.03	0.74
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	29	0.74	0.03	0.74
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	29	0.74	0.03	0.74
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	29	0.73	0.08	0.74
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	29	0.69	0.08	0.67
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	29	0.38	0.03	0.39
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	29	0.37	0.03	0.37
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	29	0.36	0.02	0.37
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	29	0.36	0.02	0.36
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	29	0.26	0.0	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	29	0.26	0.0	0.26
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	29	0.25	0.04	0.25
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	29	0.22	0.05	0.21
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	29	0.21	0.04	0.2
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	29	0.19	0.03	0.19
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	29	0.18	0.01	0.19
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	29	0.18	0.02	0.2
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	29	0.17	0.02	0.17
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	28	0.94	0.32	0.98
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	28	0.94	0.32	0.98
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	28	0.94	0.32	0.98
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	28	0.31	0.12	0.3
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	28	0.31	0.12	0.3
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	28	0.31	0.12	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	28	0.18	0.04	0.18
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	27	0.16	0.04	0.16
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	27	0.15	0.03	0.15
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	27	0.15	0.03	0.14
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	27	0.12	0.02	0.12
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	26	0.17	0.05	0.16
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	26	0.15	0.03	0.15
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	25	0.67	0.34	0.61
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	25	0.67	0.34	0.61
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	25	0.67	0.34	0.61
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	23	0.14	0.02	0.13
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	22	0.14	0.02	0.14
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	20	0.14	0.03	0.13
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	20	0.12	0.02	0.11
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	19	0.16	0.03	0.16
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	19	0.14	0.03	0.14
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	15	0.73	0.39	0.86
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	15	0.73	0.39	0.86
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	15	0.73	0.39	0.86
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	15	0.12	0.01	0.13
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	15	0.11	0.01	0.11
(3,24)	1:17:A:LYS:O	1:17:B:LYS:H	14	0.14	0.03	0.14
(2,138)	1:18:A:VAL:HA	1:16:B:VAL:HA	14	0.14	0.02	0.13
(5,6)	2:37:A:ZN:ZN	1:28:A:CYS:SG	14	0.12	0.01	0.12
(2,343)	1:16:B:VAL:HB	1:17:B:LYS:H	14	0.12	0.01	0.11
(4,10)	1:12:B:CYS:SG	1:29:B:CYS:SG	13	0.16	0.03	0.16
(3,26)	1:19:A:LEU:H	1:15:B:VAL:O	13	0.12	0.01	0.12
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE2	12	0.56	0.19	0.6
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE3	12	0.56	0.19	0.6
(3,52)	1:8:B:LYS:O	1:34:B:VAL:H	12	0.15	0.03	0.16
(2,265)	1:7:B:TYR:H	1:17:B:LYS:HA	12	0.14	0.04	0.13
(3,30)	1:20:A:GLU:O	1:15:B:VAL:H	12	0.14	0.03	0.12
(5,11)	2:37:B:ZN:ZN	1:12:B:CYS:CB	11	0.18	0.03	0.19
(2,320)	1:11:B:LEU:HA	1:11:B:LEU:HG	11	0.16	0.03	0.15
(2,210)	1:34:A:VAL:HB	1:35:A:LYS:H	11	0.13	0.03	0.13
(3,32)	1:26:A:LEU:O	1:33:A:MET:H	11	0.12	0.01	0.12
(2,38)	1:7:A:TYR:H	1:17:A:LYS:HA	10	0.14	0.03	0.12
(2,308)	1:9:B:CYS:SG	1:12:B:CYS:H	10	0.13	0.01	0.13
(2,421)	1:34:B:VAL:HB	1:35:B:LYS:H	10	0.12	0.01	0.12
(5,12)	2:37:B:ZN:ZN	1:12:B:CYS:SG	10	0.11	0.01	0.11
(2,207)	1:34:A:VAL:H	1:34:A:VAL:HB	9	0.14	0.02	0.14
(5,10)	2:37:B:ZN:ZN	1:12:B:CYS:CA	9	0.12	0.01	0.11

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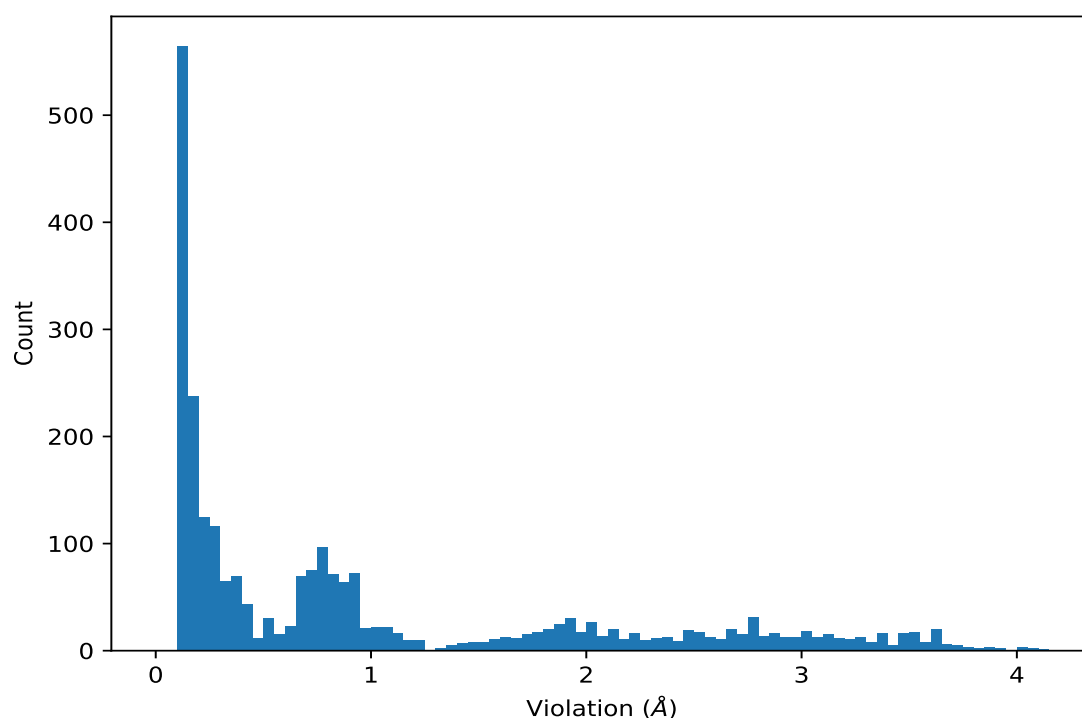
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,365)	1:20:B:GLU:H	1:20:B:GLU:HG3	8	0.12	0.02	0.11
(5,17)	2:37:B:ZN:ZN	1:29:B:CYS:CB	8	0.11	0.02	0.11
(2,393)	1:27:B:VAL:HB	1:28:B:CYS:H	7	0.13	0.01	0.13
(2,12)	1:4:A:GLY:HA3	1:5:A:ASP:H	7	0.13	0.01	0.13
(2,37)	1:7:A:TYR:H	1:16:A:VAL:H	7	0.13	0.02	0.12
(2,113)	1:15:A:VAL:H	1:15:A:VAL:HB	7	0.12	0.02	0.12
(5,16)	2:37:B:ZN:ZN	1:29:B:CYS:CA	7	0.11	0.01	0.11
(4,3)	1:9:A:CYS:SG	1:29:A:CYS:SG	6	0.12	0.02	0.12
(5,15)	2:37:B:ZN:ZN	1:28:B:CYS:SG	6	0.12	0.01	0.12
(2,147)	1:20:A:GLU:H	1:20:A:GLU:HG3	6	0.12	0.02	0.12
(3,36)	1:27:A:VAL:O	1:27:B:VAL:H	6	0.12	0.01	0.12
(3,18)	1:15:A:VAL:O	1:19:B:LEU:H	6	0.11	0.01	0.11
(2,124)	1:16:A:VAL:HB	1:17:A:LYS:H	6	0.11	0.01	0.11
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE1	5	0.4	0.17	0.37
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE2	5	0.4	0.17	0.37
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE3	5	0.4	0.17	0.37
(2,89)	1:11:A:LEU:H	1:11:A:LEU:HG	5	0.16	0.03	0.16
(2,239)	1:4:B:GLY:HA3	1:5:B:ASP:H	5	0.12	0.02	0.12
(2,69)	1:8:A:LYS:HA	1:33:A:MET:HB3	5	0.11	0.01	0.11
(4,5)	1:12:A:CYS:SG	1:29:A:CYS:SG	4	0.19	0.05	0.2
(1,98)	1:7:B:TYR:HE2	1:35:B:LYS:HE2	3	0.44	0.15	0.37
(1,98)	1:7:B:TYR:HE2	1:35:B:LYS:HE3	3	0.44	0.15	0.37
(3,14)	1:9:A:CYS:H	1:14:A:GLN:O	3	0.12	0.01	0.11
(2,348)	1:17:B:LYS:HA	1:18:B:VAL:H	3	0.11	0.0	0.11
(2,303)	1:9:B:CYS:HB2	1:13:B:GLY:H	3	0.11	0.01	0.11
(5,2)	2:37:A:ZN:ZN	1:12:A:CYS:CB	2	0.3	0.0	0.3
(5,7)	2:37:A:ZN:ZN	1:29:A:CYS:CA	2	0.15	0.02	0.15
(2,81)	1:9:A:CYS:SG	1:12:A:CYS:H	2	0.12	0.02	0.12
(2,129)	1:17:A:LYS:HA	1:18:A:VAL:H	2	0.12	0.01	0.12
(2,122)	1:16:A:VAL:HA	1:18:B:VAL:HA	2	0.11	0.0	0.11
(3,29)	1:20:A:GLU:O	1:15:B:VAL:N	2	0.11	0.0	0.11
(5,1)	2:37:A:ZN:ZN	1:12:A:CYS:CA	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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)
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	17	4.11
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	22	4.1
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	6	4.08
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	21	4.04
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	5	4.03
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	9	4.0
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	29	3.93
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	29	3.92
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	23	3.89
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	7	3.88
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	24	3.87
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	4	3.83
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	16	3.83
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	2	3.79
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	3	3.76
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	23	3.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	10	3.74
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	13	3.73
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	24	3.71
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	8	3.71
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	16	3.7
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	27	3.69
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	9	3.68
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	22	3.68
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	7	3.68
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	10	3.66
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	23	3.66
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	7	3.65
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	13	3.65
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	14	3.65
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	21	3.65
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	1	3.64
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	17	3.64
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	28	3.64
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	8	3.63
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	15	3.63
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	29	3.63
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	12	3.63
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	2	3.61
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	4	3.61
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	5	3.61
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	16	3.61
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	26	3.61
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	7	3.61
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	13	3.61
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	11	3.6
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	17	3.6
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	25	3.59
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	26	3.59
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	1	3.59
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	23	3.58
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	6	3.57
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	19	3.57
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	6	3.57
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	3	3.56
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	20	3.55
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	9	3.55
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	24	3.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	21	3.54
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	11	3.53
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	21	3.53
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	19	3.53
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	20	3.53
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	16	3.53
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	20	3.53
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	27	3.53
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	15	3.52
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	1	3.52
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	26	3.51
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	22	3.51
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	29	3.5
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	28	3.5
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	6	3.49
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	27	3.49
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	28	3.49
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	22	3.48
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	2	3.47
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	15	3.47
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	18	3.47
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	19	3.47
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	25	3.47
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	13	3.47
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	24	3.46
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	5	3.46
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	12	3.45
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	28	3.45
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	3	3.45
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	8	3.45
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	18	3.44
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	1	3.43
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	14	3.43
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	3	3.43
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	11	3.41
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	6	3.4
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	25	3.4
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	7	3.4
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	19	3.4
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	1	3.39
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	10	3.39
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	14	3.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	15	3.39
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	17	3.39
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	11	3.38
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	11	3.37
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	26	3.37
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	26	3.36
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	17	3.36
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	22	3.35
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	12	3.35
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	16	3.34
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	21	3.34
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	22	3.34
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	4	3.33
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	23	3.31
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	6	3.31
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	11	3.31
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	12	3.31
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	5	3.3
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	5	3.3
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	25	3.3
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	9	3.29
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	23	3.29
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	29	3.29
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	10	3.29
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	24	3.28
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	13	3.27
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	7	3.26
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	17	3.26
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	27	3.26
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	10	3.25
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	14	3.24
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	27	3.24
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	21	3.24
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	15	3.23
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	18	3.23
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	9	3.22
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	20	3.22
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	5	3.21
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	12	3.2
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	23	3.2
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	29	3.2
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	3	3.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	25	3.19
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	23	3.19
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	24	3.19
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	14	3.19
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	4	3.18
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	28	3.18
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	25	3.18
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	7	3.18
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	1	3.18
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	3	3.17
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	16	3.16
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	10	3.15
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	2	3.14
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	19	3.14
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	7	3.14
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	16	3.14
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	28	3.14
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	29	3.13
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	2	3.13
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	4	3.12
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	16	3.12
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	2	3.12
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	29	3.12
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	8	3.12
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	22	3.11
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	10	3.1
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	24	3.09
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	28	3.09
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	8	3.09
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	5	3.08
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	13	3.08
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	21	3.08
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	11	3.07
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	17	3.07
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	22	3.07
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	29	3.07
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	8	3.06
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	8	3.06
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	16	3.06
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	9	3.05
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	20	3.05
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	17	3.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	5	3.04
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	7	3.04
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	14	3.04
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	6	3.03
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	21	3.03
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	13	3.03
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	6	3.03
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	24	3.03
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	17	3.02
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	4	3.01
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	9	3.0
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	19	3.0
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	27	3.0
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	21	3.0
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	26	3.0
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	4	2.99
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	3	2.99
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	23	2.99
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	29	2.98
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	5	2.98
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	13	2.97
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	20	2.97
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	7	2.96
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	8	2.95
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	15	2.95
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	26	2.95
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	18	2.95
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	22	2.95
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	18	2.94
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	9	2.94
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	23	2.94
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	16	2.94
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	1	2.94
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	26	2.93
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	28	2.93
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	21	2.92
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	29	2.92
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	19	2.91
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	20	2.91
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	12	2.91
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	11	2.91
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	2	2.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	14	2.89
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	1	2.89
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	10	2.89
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	27	2.89
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	16	2.88
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	18	2.88
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	15	2.88
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	26	2.88
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	17	2.88
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	9	2.88
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	25	2.87
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	24	2.87
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	13	2.86
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	20	2.85
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	17	2.85
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	1	2.84
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	7	2.84
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	11	2.84
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	22	2.84
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	8	2.83
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	12	2.83
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	11	2.82
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	12	2.82
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	13	2.82
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	6	2.81
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	26	2.81
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	25	2.81
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	10	2.81
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	19	2.81
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	19	2.8
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	3	2.8
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	3	2.8
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	25	2.8
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	28	2.79
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	11	2.79
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	5	2.79
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	22	2.79
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	5	2.79
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	27	2.78
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	1	2.78
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	21	2.78
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	2	2.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	1	2.78
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	13	2.77
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	14	2.77
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	28	2.77
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	16	2.77
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	23	2.77
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	3	2.76
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	15	2.76
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	14	2.76
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	27	2.76
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	6	2.76
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	12	2.76
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	4	2.76
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	10	2.75
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	13	2.75
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	5	2.75
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	11	2.75
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	27	2.75
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	9	2.74
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	12	2.73
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	14	2.73
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	27	2.73
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	15	2.73
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	18	2.73
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	15	2.73
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	15	2.72
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	25	2.72
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	4	2.71
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	24	2.71
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	25	2.71
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	3	2.7
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	7	2.7
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	10	2.7
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	21	2.69
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	19	2.69
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	9	2.69
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	12	2.68
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	28	2.68
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	6	2.68
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	1	2.68
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	19	2.68
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	14	2.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	12	2.67
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	11	2.67
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	24	2.67
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	8	2.67
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	29	2.67
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	20	2.67
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	23	2.66
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	20	2.66
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	2	2.66
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	8	2.66
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	17	2.66
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	11	2.65
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	21	2.65
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	3	2.65
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	19	2.65
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	4	2.64
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	10	2.64
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	16	2.64
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	2	2.63
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	4	2.63
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	24	2.62
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	25	2.61
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	13	2.59
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	29	2.59
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	6	2.59
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	14	2.59
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	20	2.59
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	13	2.58
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	29	2.58
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	6	2.58
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	8	2.58
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	14	2.58
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	28	2.57
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	8	2.56
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	27	2.56
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	21	2.55
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	22	2.55
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	25	2.55
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	27	2.55
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	9	2.54
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	17	2.54
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	18	2.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	20	2.54
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	18	2.53
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	28	2.53
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	5	2.52
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	24	2.52
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	18	2.51
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	12	2.51
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	3	2.5
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	8	2.5
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	16	2.5
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	12	2.49
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	26	2.49
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	12	2.48
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	22	2.48
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	26	2.48
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	18	2.48
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	18	2.47
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	4	2.47
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	4	2.47
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	4	2.47
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	25	2.47
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	23	2.47
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	22	2.46
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	19	2.46
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	18	2.46
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	26	2.46
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	16	2.45
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	14	2.45
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	4	2.45
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	3	2.44
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	17	2.43
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	4	2.42
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	15	2.42
(2,254)	1:6:B:VAL:H	1:7:B:TYR:HD2	20	2.42
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	16	2.41
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	18	2.41
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	19	2.41
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	2	2.41
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	5	2.4
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	11	2.4
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	1	2.4
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	21	2.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	27	2.4
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	1	2.39
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	18	2.37
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	11	2.37
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	2	2.37
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	3	2.36
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	8	2.36
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	21	2.36
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	12	2.35
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	19	2.34
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	23	2.34
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	18	2.34
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	20	2.33
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	5	2.33
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	9	2.33
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	17	2.32
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	23	2.32
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	5	2.32
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	1	2.31
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	15	2.31
(2,27)	1:6:A:VAL:H	1:7:A:TYR:HD2	4	2.31
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	15	2.3
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	5	2.3
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	23	2.29
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	3	2.29
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	29	2.28
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	1	2.28
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	28	2.26
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	1	2.25
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	26	2.25
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	27	2.25
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	9	2.24
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	13	2.24
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	26	2.24
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	2	2.24
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	6	2.24
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	8	2.24
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	17	2.23
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	14	2.22
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	29	2.22
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	25	2.22
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	24	2.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	7	2.21
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	10	2.21
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	20	2.21
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	24	2.2
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	24	2.2
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	14	2.19
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	8	2.18
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	2	2.18
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	11	2.18
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	27	2.18
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	28	2.17
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	7	2.17
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	12	2.17
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	3	2.16
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	21	2.16
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	26	2.15
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	2	2.14
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	5	2.14
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	9	2.14
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	20	2.13
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	10	2.13
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	25	2.13
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	19	2.13
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	22	2.13
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	13	2.13
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	10	2.12
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	18	2.12
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	28	2.12
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	29	2.12
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	15	2.12
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	26	2.11
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	16	2.11
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	28	2.1
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	26	2.1
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	15	2.1
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	23	2.1
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	11	2.09
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	24	2.09
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	7	2.08
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	28	2.08
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	22	2.08
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	13	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	9	2.07
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	9	2.07
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	27	2.06
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	6	2.06
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	14	2.06
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	10	2.06
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	12	2.06
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	4	2.06
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	22	2.05
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	7	2.05
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	16	2.05
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	21	2.05
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	7	2.05
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	17	2.04
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	22	2.04
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	23	2.04
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	17	2.04
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	15	2.04
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	3	2.03
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	2	2.03
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	15	2.02
(2,282)	1:7:B:TYR:HD1	1:34:B:VAL:H	6	2.02
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	1	2.02
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	4	2.02
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	26	2.02
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	29	2.02
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	6	2.02
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	6	2.02
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	18	2.01
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	21	2.01
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	5	2.0
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	25	2.0
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	27	2.0
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	1	2.0
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	5	2.0
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	21	1.99
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	20	1.99
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	29	1.99
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	12	1.99
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	16	1.98
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	2	1.98
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	2	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	17	1.98
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	10	1.98
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	14	1.97
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	10	1.97
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	19	1.97
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	11	1.97
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	16	1.96
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	10	1.96
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	12	1.96
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	21	1.96
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	23	1.95
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	11	1.95
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	7	1.95
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	25	1.95
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	13	1.95
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	24	1.94
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	20	1.94
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	22	1.94
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	27	1.94
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	3	1.94
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	22	1.94
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	19	1.93
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	2	1.93
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	26	1.93
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	5	1.93
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	9	1.93
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	27	1.93
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	15	1.93
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	1	1.93
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	3	1.93
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	25	1.93
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	29	1.93
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	23	1.92
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	7	1.92
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	17	1.92
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	23	1.91
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	15	1.91
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	14	1.91
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	17	1.91
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	10	1.91
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	4	1.9
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	21	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,283)	1:7:B:TYR:HD1	1:34:B:VAL:HA	6	1.9
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	1	1.9
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	15	1.9
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	28	1.9
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	16	1.9
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	17	1.89
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	18	1.89
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	8	1.89
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	17	1.88
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	1	1.88
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	8	1.87
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	8	1.87
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	8	1.87
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	1	1.86
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	8	1.86
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	11	1.86
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	13	1.86
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	24	1.86
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	24	1.86
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	9	1.86
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	14	1.85
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	8	1.85
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	24	1.85
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	10	1.84
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	28	1.84
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	6	1.84
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	13	1.84
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	11	1.84
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	13	1.84
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	20	1.84
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	19	1.83
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	12	1.83
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	9	1.83
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	11	1.83
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	2	1.82
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	13	1.82
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	28	1.82
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	14	1.82
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	26	1.81
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	5	1.81
(2,55)	1:7:A:TYR:HD1	1:34:A:VAL:H	7	1.81
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	5	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	19	1.8
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	12	1.79
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	20	1.79
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	25	1.79
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	4	1.79
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	15	1.79
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	19	1.79
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	29	1.79
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	14	1.78
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	6	1.78
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	9	1.77
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	27	1.77
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	4	1.77
(2,56)	1:7:A:TYR:HD1	1:34:A:VAL:HA	3	1.77
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	16	1.77
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	27	1.77
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	23	1.76
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	21	1.75
(2,280)	1:7:B:TYR:HD1	1:33:B:MET:HB3	25	1.74
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	11	1.74
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	20	1.74
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	27	1.73
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	18	1.73
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	2	1.72
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	25	1.72
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	12	1.72
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	22	1.72
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	29	1.71
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	16	1.71
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	29	1.71
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	17	1.71
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	1	1.71
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	26	1.71
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	29	1.7
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	23	1.7
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	7	1.69
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	28	1.68
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	26	1.68
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	22	1.67
(2,250)	1:5:B:ASP:HB3	1:7:B:TYR:HD2	18	1.67
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	20	1.67
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	2	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	7	1.66
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	9	1.66
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	10	1.66
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	19	1.65
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	22	1.65
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	24	1.65
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	24	1.64
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	15	1.64
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	27	1.64
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	9	1.63
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	16	1.63
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	13	1.63
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	6	1.62
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	7	1.62
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	3	1.61
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	21	1.61
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	2	1.59
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	12	1.59
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	18	1.58
(2,57)	1:7:A:TYR:HE1	1:35:A:LYS:H	24	1.58
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	25	1.58
(2,284)	1:7:B:TYR:HE1	1:35:B:LYS:H	6	1.57
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	18	1.57
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	15	1.57
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	15	1.57
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	15	1.57
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	26	1.55
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	14	1.54
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	8	1.54
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	28	1.52
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	23	1.51
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	23	1.51
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	23	1.51
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	23	1.51
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	22	1.5
(2,53)	1:7:A:TYR:HD1	1:33:A:MET:HB3	3	1.49
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	14	1.47
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	9	1.47
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	9	1.47
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	9	1.47
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	19	1.46
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	19	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	19	1.46
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	10	1.45
(2,23)	1:5:A:ASP:HB3	1:7:A:TYR:HD2	4	1.45
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	19	1.44
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	15	1.43
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	4	1.41
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	4	1.41
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	4	1.41
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	19	1.39
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	17	1.37
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	17	1.37
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	17	1.37
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	5	1.35
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	7	1.34
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	28	1.33
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	7	1.24
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	7	1.24
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	7	1.24
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	25	1.24
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	24	1.24
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	24	1.24
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	24	1.24
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	4	1.21
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	9	1.21
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	10	1.21
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	29	1.19
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	29	1.19
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	29	1.19
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	18	1.19
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	15	1.17
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	15	1.17
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	15	1.17
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	16	1.16
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	16	1.16
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	16	1.16
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	22	1.15
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	22	1.15
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	22	1.15
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	2	1.14
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	2	1.14
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	2	1.14
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	26	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	26	1.11
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	26	1.11
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	10	1.11
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	10	1.11
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	10	1.11
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	20	1.1
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	9	1.1
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	9	1.1
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	9	1.1
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	13	1.09
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	13	1.09
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	13	1.09
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	14	1.08
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	14	1.08
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	14	1.08
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	2	1.08
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	13	1.07
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	13	1.07
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	13	1.07
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	25	1.07
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	25	1.07
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	25	1.07
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	17	1.06
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	17	1.06
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	17	1.06
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	18	1.05
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	18	1.05
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	18	1.05
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	6	1.05
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	6	1.05
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	6	1.05
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	21	1.03
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	21	1.03
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	21	1.03
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	5	1.03
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	5	1.03
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	5	1.03
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	3	1.03
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	3	1.03
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	3	1.03
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	25	1.03
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	25	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	26	1.01
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	26	1.01
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	26	1.01
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	7	1.01
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	7	1.01
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	7	1.01
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	11	1.0
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	11	1.0
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	11	1.0
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	8	1.0
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	8	1.0
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	19	0.99
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	19	0.99
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	19	0.99
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	20	0.99
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	20	0.99
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	20	0.99
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	21	0.97
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	21	0.97
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	21	0.97
(1,84)	1:4:B:GLY:HA3	1:17:B:LYS:HG2	6	0.97
(1,84)	1:4:B:GLY:HA3	1:17:B:LYS:HG3	6	0.97
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	5	0.97
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	5	0.97
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	15	0.96
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	15	0.96
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	15	0.96
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	4	0.96
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	11	0.96
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	11	0.96
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	10	0.96
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	10	0.96
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	29	0.95
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	29	0.95
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	29	0.95
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	2	0.94
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	2	0.94
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	2	0.94
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	5	0.94
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	5	0.94
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	5	0.94
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	20	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	20	0.94
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	20	0.94
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	26	0.94
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	26	0.94
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	26	0.94
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	5	0.94
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	5	0.94
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	17	0.94
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	17	0.94
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	20	0.94
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	20	0.94
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	19	0.93
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	19	0.93
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	19	0.93
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	2	0.93
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	2	0.93
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	2	0.93
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	2	0.92
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	2	0.92
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	2	0.92
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	25	0.92
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	25	0.92
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	25	0.92
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	28	0.92
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	28	0.92
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	28	0.92
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	16	0.92
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	16	0.92
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	16	0.92
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	9	0.92
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	9	0.92
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	27	0.92
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	27	0.92
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	4	0.91
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	4	0.91
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	4	0.91
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	23	0.91
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	23	0.91
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	23	0.91
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	28	0.91
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	28	0.91
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	28	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	16	0.91
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	16	0.91
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	16	0.91
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	16	0.91
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	4	0.9
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	4	0.9
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	4	0.9
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	18	0.9
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	10	0.9
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	10	0.9
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	10	0.9
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	21	0.9
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	21	0.9
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	21	0.9
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	15	0.9
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	15	0.9
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	23	0.9
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	23	0.9
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	26	0.9
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	26	0.9
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	6	0.89
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	6	0.89
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	6	0.89
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	22	0.89
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	22	0.89
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	22	0.89
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	26	0.89
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	26	0.89
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	26	0.89
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	23	0.89
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	23	0.89
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	23	0.89
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	3	0.89
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	21	0.89
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	21	0.89
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	28	0.89
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	28	0.89
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	24	0.88
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	24	0.88
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	24	0.88
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	14	0.88
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	14	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	4	0.88
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	4	0.88
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	11	0.88
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	11	0.88
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	20	0.88
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	20	0.88
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	3	0.87
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	3	0.87
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	3	0.87
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	13	0.87
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	13	0.87
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	13	0.87
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	15	0.87
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	15	0.87
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	15	0.87
(2,52)	1:7:A:TYR:HD1	1:26:A:LEU:HG	20	0.87
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	1	0.87
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	1	0.87
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	26	0.87
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	26	0.87
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	18	0.87
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	18	0.87
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	8	0.86
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	8	0.86
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	8	0.86
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	10	0.86
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	10	0.86
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	10	0.86
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	29	0.86
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	29	0.86
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	29	0.86
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	8	0.86
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	8	0.86
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	8	0.86
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	6	0.86
(2,279)	1:7:B:TYR:HD1	1:26:B:LEU:HG	13	0.86
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	13	0.86
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	13	0.86
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	22	0.86
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	22	0.86
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	23	0.86
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	23	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	12	0.85
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	2	0.85
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	19	0.85
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	19	0.85
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	19	0.85
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	19	0.85
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	19	0.85
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	8	0.85
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	8	0.85
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	27	0.84
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	27	0.84
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	27	0.84
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	4	0.84
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	4	0.84
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	4	0.84
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	3	0.84
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	3	0.84
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	3	0.84
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	7	0.84
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	7	0.84
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	29	0.84
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	29	0.84
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	2	0.84
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	2	0.84
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	3	0.84
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	3	0.84
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	7	0.84
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	7	0.84
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	29	0.84
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	29	0.84
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	24	0.83
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	24	0.83
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	24	0.83
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	14	0.83
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	26	0.83
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	2	0.83
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	2	0.83
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	12	0.83
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	12	0.83
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	9	0.83
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	9	0.83
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	24	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	24	0.83
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	20	0.82
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	29	0.82
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	29	0.82
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	29	0.82
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	18	0.82
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	18	0.82
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	18	0.82
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	3	0.82
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	18	0.82
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	28	0.82
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	28	0.82
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	19	0.81
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	25	0.81
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	25	0.81
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	25	0.81
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	27	0.81
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	24	0.81
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	24	0.81
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE2	5	0.81
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE3	5	0.81
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	14	0.81
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	14	0.81
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	17	0.8
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	17	0.8
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	17	0.8
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	8	0.8
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	3	0.8
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	3	0.8
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	11	0.79
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	11	0.79
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	11	0.79
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	12	0.78
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	12	0.78
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	12	0.78
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	16	0.78
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	16	0.78
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	16	0.78
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	8	0.78
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	8	0.78
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	8	0.78
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	1	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	1	0.78
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	1	0.78
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	22	0.78
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	22	0.78
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	22	0.78
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	10	0.78
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	10	0.78
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	6	0.78
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	6	0.78
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	25	0.78
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	25	0.78
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	3	0.77
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	3	0.77
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	3	0.77
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	4	0.77
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	4	0.77
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	4	0.77
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	15	0.77
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	15	0.77
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	15	0.77
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	10	0.77
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	20	0.77
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	1	0.77
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	1	0.77
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	1	0.77
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	1	0.76
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	1	0.76
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	1	0.76
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	21	0.76
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	21	0.76
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	21	0.76
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	23	0.76
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	23	0.76
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	23	0.76
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	9	0.76
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	9	0.76
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	9	0.76
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	14	0.76
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	14	0.76
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	14	0.76
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	12	0.76
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	12	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	12	0.76
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	12	0.76
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	12	0.76
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	12	0.76
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	5	0.76
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	24	0.76
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	25	0.76
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE2	18	0.76
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE3	18	0.76
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	5	0.75
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	5	0.75
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	5	0.75
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	8	0.75
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	8	0.75
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	8	0.75
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	13	0.75
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	13	0.75
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	13	0.75
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	17	0.75
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	17	0.75
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	17	0.75
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	24	0.75
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	24	0.75
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	24	0.75
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	26	0.75
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	26	0.75
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	26	0.75
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	1	0.75
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	1	0.75
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	1	0.75
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	7	0.75
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	7	0.75
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	7	0.75
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	16	0.75
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	16	0.75
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	16	0.75
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	6	0.75
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	13	0.75
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	13	0.75
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	13	0.75
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE2	10	0.75
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE3	10	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	6	0.74
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	6	0.74
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	6	0.74
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	7	0.74
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	7	0.74
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	7	0.74
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	10	0.74
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	10	0.74
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	10	0.74
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	11	0.74
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	11	0.74
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	11	0.74
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	16	0.74
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	16	0.74
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	16	0.74
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	25	0.74
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	25	0.74
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	25	0.74
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	5	0.74
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	19	0.74
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	19	0.73
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	19	0.73
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	19	0.73
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	29	0.73
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	29	0.73
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	29	0.73
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	14	0.73
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	14	0.73
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	14	0.73
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	15	0.73
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	4	0.73
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	4	0.73
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	1	0.73
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	1	0.73
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	20	0.72
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	20	0.72
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	20	0.72
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	22	0.72
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	22	0.72
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	22	0.72
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	28	0.72
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	28	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	28	0.72
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	16	0.72
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	17	0.72
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	18	0.72
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	18	0.72
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	18	0.72
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	8	0.72
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	8	0.72
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	8	0.72
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	11	0.72
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	11	0.72
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	11	0.72
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	29	0.72
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	29	0.72
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	29	0.72
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	21	0.72
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	21	0.72
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	9	0.71
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	9	0.71
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	9	0.71
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	27	0.71
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	27	0.71
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	27	0.71
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	8	0.71
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	13	0.71
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	7	0.71
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	7	0.71
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	7	0.71
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	28	0.71
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	28	0.71
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	28	0.71
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE2	14	0.71
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE3	14	0.71
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	18	0.7
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	18	0.7
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	18	0.7
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	5	0.7
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	5	0.7
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	5	0.7
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	12	0.7
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	12	0.7
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	12	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	4	0.7
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	11	0.7
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE2	20	0.7
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE3	20	0.7
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	15	0.7
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	15	0.7
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	19	0.7
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	19	0.7
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	2	0.69
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	2	0.69
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	2	0.69
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG21	17	0.69
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG22	17	0.69
(2,287)	1:7:B:TYR:HD2	1:18:B:VAL:HG23	17	0.69
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	21	0.69
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	27	0.69
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	27	0.69
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	27	0.69
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	22	0.69
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	22	0.69
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	22	0.69
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	27	0.69
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	27	0.69
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	22	0.68
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	9	0.68
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	9	0.68
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	9	0.68
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	6	0.68
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	6	0.68
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	6	0.68
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	1	0.68
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	13	0.68
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	28	0.68
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	29	0.68
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	9	0.67
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	14	0.67
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	25	0.67
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	29	0.67
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG21	24	0.67
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG22	24	0.67
(2,60)	1:7:A:TYR:HD2	1:18:A:VAL:HG23	24	0.67
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	9	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	16	0.67
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	18	0.67
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	18	0.67
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE2	26	0.67
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE3	26	0.67
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	24	0.66
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	11	0.66
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	12	0.66
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	23	0.66
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	8	0.66
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	8	0.66
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	8	0.66
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	10	0.65
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	15	0.65
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	16	0.65
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	16	0.65
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	16	0.65
(1,98)	1:7:B:TYR:HE2	1:35:B:LYS:HE2	20	0.65
(1,98)	1:7:B:TYR:HE2	1:35:B:LYS:HE3	20	0.65
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	1	0.64
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	1	0.64
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	1	0.64
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	17	0.64
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	27	0.64
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	27	0.64
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	27	0.64
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	23	0.63
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	26	0.63
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	20	0.63
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	20	0.63
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	20	0.63
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE1	7	0.63
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE2	7	0.63
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE3	7	0.63
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	1	0.62
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	2	0.62
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	7	0.62
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	28	0.62
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	6	0.61
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	6	0.61
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	6	0.61
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	6	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,396)	1:27:B:VAL:HG11	1:30:B:GLY:HA3	14	0.6
(2,396)	1:27:B:VAL:HG12	1:30:B:GLY:HA3	14	0.6
(2,396)	1:27:B:VAL:HG13	1:30:B:GLY:HA3	14	0.6
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	21	0.6
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	11	0.6
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	11	0.6
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	11	0.6
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	27	0.58
(2,51)	1:7:A:TYR:HD1	1:8:A:LYS:H	7	0.58
(2,278)	1:7:B:TYR:HD1	1:8:B:LYS:H	3	0.56
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	22	0.55
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	22	0.55
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	22	0.55
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB2	6	0.55
(1,83)	1:4:B:GLY:HA3	1:17:B:LYS:HB3	6	0.55
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	23	0.54
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	23	0.54
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	23	0.54
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE2	2	0.54
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE3	2	0.54
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE1	28	0.53
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE2	28	0.53
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE3	28	0.53
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	20	0.52
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	20	0.52
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	20	0.52
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	23	0.52
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	23	0.52
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	23	0.52
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	26	0.51
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	26	0.51
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	26	0.51
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	17	0.51
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	17	0.51
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	9	0.5
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	9	0.5
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	9	0.5
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	26	0.5
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	26	0.5
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	26	0.5
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	25	0.5
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	25	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	25	0.5
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE2	8	0.5
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE3	8	0.5
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	12	0.49
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	12	0.49
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	12	0.49
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	3	0.48
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	3	0.48
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	3	0.48
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	13	0.46
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	13	0.46
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	22	0.45
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	13	0.45
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	13	0.45
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	13	0.45
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	27	0.44
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	27	0.44
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	27	0.44
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	7	0.44
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	7	0.44
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	7	0.44
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	22	0.44
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE2	4	0.43
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE3	4	0.43
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	2	0.42
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	2	0.42
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	2	0.42
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	4	0.42
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	16	0.42
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	29	0.42
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	11	0.41
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	16	0.41
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	19	0.41
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	21	0.41
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	2	0.41
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	2	0.41
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	2	0.41
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	24	0.41
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB2	12	0.41
(1,7)	1:4:A:GLY:HA3	1:17:A:LYS:HB3	12	0.41
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	5	0.4
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	9	0.4
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	14	0.4
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	17	0.4
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	26	0.4
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	29	0.4
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	3	0.4
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	3	0.4
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	3	0.4
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	8	0.4
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	8	0.4
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	8	0.4
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	4	0.4
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	28	0.4
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	18	0.4
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	18	0.4
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	18	0.4
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	23	0.39
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	18	0.39
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	7	0.39
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	13	0.39
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	3	0.39
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	3	0.39
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	19	0.39
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	21	0.39
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	23	0.39
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	5	0.38
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	12	0.38
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	19	0.38
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	20	0.38
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	1	0.38
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	2	0.38
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	6	0.38
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	28	0.38
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	2	0.38
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	14	0.38
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	18	0.38
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	24	0.38
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	10	0.38
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	13	0.38
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	14	0.38
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	15	0.38
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	17	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	21	0.38
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	21	0.38
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	21	0.38
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	4	0.37
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	8	0.37
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	11	0.37
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	16	0.37
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	17	0.37
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	21	0.37
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	29	0.37
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	10	0.37
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	15	0.37
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	20	0.37
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	24	0.37
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	21	0.37
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	21	0.37
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	21	0.37
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE1	16	0.37
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE2	16	0.37
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE3	16	0.37
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	5	0.37
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	8	0.37
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	10	0.37
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	15	0.37
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	19	0.37
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	20	0.37
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	22	0.37
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	26	0.37
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	27	0.37
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	18	0.37
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	25	0.37
(1,98)	1:7:B:TYR:HE2	1:35:B:LYS:HE2	18	0.37
(1,98)	1:7:B:TYR:HE2	1:35:B:LYS:HE3	18	0.37
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	9	0.36
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	13	0.36
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	22	0.36
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	6	0.36
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	16	0.36
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	25	0.36
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	28	0.36
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	29	0.36
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	8	0.36
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	20	0.36
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	7	0.35
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	10	0.35
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	14	0.35
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	25	0.35
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	26	0.35
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	23	0.35
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	5	0.35
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	5	0.35
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	5	0.35
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	1	0.35
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	9	0.35
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	13	0.35
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	23	0.35
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	1	0.35
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	2	0.35
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	5	0.35
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	7	0.35
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	9	0.35
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	11	0.35
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	12	0.35
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	27	0.35
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	1	0.34
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	2	0.34
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	6	0.34
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	15	0.34
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	23	0.34
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	24	0.34
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	28	0.34
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	18	0.34
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	25	0.34
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	20	0.34
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	20	0.34
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	20	0.34
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	11	0.34
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	12	0.34
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	17	0.34
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	21	0.34
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	5	0.33
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	9	0.33
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	9	0.33
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	12	0.33
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	27	0.33
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	23	0.33
(2,43)	1:7:A:TYR:HB2	1:7:A:TYR:HE2	7	0.33
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	26	0.33
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	7	0.33
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	7	0.33
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	7	0.33
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	27	0.32
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	1	0.32
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	1	0.32
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	1	0.32
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	13	0.32
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	13	0.32
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	13	0.32
(2,270)	1:7:B:TYR:HB2	1:7:B:TYR:HE2	3	0.31
(2,263)	1:7:B:TYR:H	1:7:B:TYR:HD2	3	0.31
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	1	0.31
(2,103)	1:12:A:CYS:HB3	1:23:B:GLY:H	18	0.31
(2,36)	1:7:A:TYR:H	1:7:A:TYR:HD2	4	0.31
(1,98)	1:7:B:TYR:HE2	1:35:B:LYS:HE2	12	0.31
(1,98)	1:7:B:TYR:HE2	1:35:B:LYS:HE3	12	0.31
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE2	25	0.31
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE3	25	0.31
(5,2)	2:37:A:ZN:ZN	1:12:A:CYS:CB	8	0.3
(5,2)	2:37:A:ZN:ZN	1:12:A:CYS:CB	26	0.3
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	15	0.3
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	15	0.3
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	15	0.3
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	27	0.3
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	27	0.3
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	27	0.3
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE1	3	0.3
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE2	3	0.3
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE3	3	0.3
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE2	1	0.3
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE3	1	0.3
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	7	0.29
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	21	0.29
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	24	0.29
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	10	0.28
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	10	0.28
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	10	0.28
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	1	0.28
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	3	0.28
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	5	0.28
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	12	0.28
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	15	0.28
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	28	0.28
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	5	0.28
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	5	0.28
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	5	0.28
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	4	0.27
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	16	0.27
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	17	0.27
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	21	0.27
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	25	0.27
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	25	0.27
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	25	0.27
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	28	0.27
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	28	0.27
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	28	0.27
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	11	0.27
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	13	0.27
(4,5)	1:12:A:CYS:SG	1:29:A:CYS:SG	8	0.26
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	12	0.26
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	26	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	1	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	2	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	3	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	4	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	5	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	6	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	7	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	8	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	9	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	10	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	11	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	12	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	13	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	14	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	16	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	17	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	18	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	19	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	20	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	21	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	22	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	23	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	24	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	25	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	26	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	27	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	28	0.26
(2,274)	1:7:B:TYR:HB3	1:7:B:TYR:HD1	29	0.26
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	4	0.26
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	4	0.26
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	4	0.26
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	27	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	1	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	2	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	5	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	6	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	7	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	8	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	9	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	10	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	11	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	12	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	13	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	14	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	15	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	16	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	17	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	18	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	19	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	20	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	21	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	22	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	23	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	24	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	25	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	26	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	27	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	28	0.26
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	29	0.26
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	1	0.25
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	15	0.25
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	15	0.25
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	18	0.25
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	16	0.25
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	17	0.25
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	18	0.25
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	26	0.25
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	3	0.25
(2,47)	1:7:A:TYR:HB3	1:7:A:TYR:HD1	4	0.25
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE2	6	0.25
(1,22)	1:7:A:TYR:HE2	1:35:A:LYS:HE3	6	0.25
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	14	0.24
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	19	0.24
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	18	0.24
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	23	0.24
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	3	0.24
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	20	0.24
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	26	0.24
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	17	0.24
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	19	0.24
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	19	0.24
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	19	0.24
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	8	0.24
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	23	0.24
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	6	0.24
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	6	0.24
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	20	0.24
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	25	0.24
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	29	0.23
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	23	0.23
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	3	0.23
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	4	0.23
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	15	0.23
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	1	0.23
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	3	0.23
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	5	0.23
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	7	0.23
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	24	0.23
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	24	0.23
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	24	0.23
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	2	0.23
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	23	0.23
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	28	0.23
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	22	0.23
(5,11)	2:37:B:ZN:ZN	1:12:B:CYS:CB	5	0.22
(5,11)	2:37:B:ZN:ZN	1:12:B:CYS:CB	23	0.22
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	26	0.22
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	27	0.22
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	22	0.22
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	22	0.22
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	2	0.22
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	29	0.22
(2,228)	1:1:B:ALA:HB1	1:7:B:TYR:HE2	12	0.22
(2,228)	1:1:B:ALA:HB2	1:7:B:TYR:HE2	12	0.22
(2,228)	1:1:B:ALA:HB3	1:7:B:TYR:HE2	12	0.22
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	10	0.22
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	4	0.22
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	9	0.22
(2,89)	1:11:A:LEU:H	1:11:A:LEU:HG	5	0.22
(1,2)	1:1:A:ALA:HB1	1:7:A:TYR:HD2	15	0.22
(1,2)	1:1:A:ALA:HB2	1:7:A:TYR:HD2	15	0.22
(1,2)	1:1:A:ALA:HB3	1:7:A:TYR:HD2	15	0.22
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	8	0.21
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	13	0.21
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	20	0.21
(5,11)	2:37:B:ZN:ZN	1:12:B:CYS:CB	1	0.21
(4,10)	1:12:B:CYS:SG	1:29:B:CYS:SG	17	0.21
(3,30)	1:20:A:GLU:O	1:15:B:VAL:H	9	0.21
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	9	0.21
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	19	0.21
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	12	0.21
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	1	0.21
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	12	0.21
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	23	0.21
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	6	0.21
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	25	0.21
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	27	0.21
(2,320)	1:11:B:LEU:HA	1:11:B:LEU:HG	22	0.21
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	27	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,265)	1:7:B:TYR:H	1:17:B:LYS:HA	13	0.21
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	12	0.21
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	3	0.21
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	5	0.21
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	11	0.21
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	24	0.21
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	5	0.21
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	22	0.21
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	12	0.21
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	18	0.21
(5,11)	2:37:B:ZN:ZN	1:12:B:CYS:CB	26	0.2
(4,5)	1:12:A:CYS:SG	1:29:A:CYS:SG	26	0.2
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	13	0.2
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	2	0.2
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	8	0.2
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	13	0.2
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	14	0.2
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	24	0.2
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	29	0.2
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	3	0.2
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	15	0.2
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	17	0.2
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	24	0.2
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	13	0.2
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	19	0.2
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	21	0.2
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	24	0.2
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	27	0.2
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	2	0.2
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	7	0.2
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	10	0.2
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	11	0.2
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	13	0.2
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	14	0.2
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	18	0.2
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	19	0.2
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	20	0.2
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	24	0.2
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	28	0.2
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	29	0.2
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	8	0.2
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	16	0.2
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	20	0.2
(2,265)	1:7:B:TYR:H	1:17:B:LYS:HA	8	0.2
(2,265)	1:7:B:TYR:H	1:17:B:LYS:HA	24	0.2
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	8	0.2
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	4	0.2
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	10	0.2
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	21	0.2
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	1	0.2
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	13	0.2
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	3	0.2
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	4	0.2
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	7	0.2
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	19	0.2
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	25	0.19
(5,11)	2:37:B:ZN:ZN	1:12:B:CYS:CB	4	0.19
(5,11)	2:37:B:ZN:ZN	1:12:B:CYS:CB	16	0.19
(4,10)	1:12:B:CYS:SG	1:29:B:CYS:SG	26	0.19
(4,5)	1:12:A:CYS:SG	1:29:A:CYS:SG	7	0.19
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	24	0.19
(3,52)	1:8:B:LYS:O	1:34:B:VAL:H	17	0.19
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	10	0.19
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	21	0.19
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	27	0.19
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	18	0.19
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	20	0.19
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	5	0.19
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	8	0.19
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	16	0.19
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	18	0.19
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	8	0.19
(2,320)	1:11:B:LEU:HA	1:11:B:LEU:HG	15	0.19
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	4	0.19
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	9	0.19
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	22	0.19
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	25	0.19
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	11	0.19
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	11	0.19
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	11	0.19
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	11	0.19
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	14	0.19
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	14	0.19
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	9	0.19
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	26	0.19
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	8	0.19
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	12	0.19
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	7	0.19
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	9	0.19
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	11	0.19
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	26	0.19
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	27	0.19
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	10	0.19
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	19	0.19
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	29	0.19
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	5	0.19
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	9	0.19
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	10	0.19
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	11	0.19
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	12	0.19
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	14	0.19
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	15	0.19
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	16	0.19
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	17	0.19
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	21	0.19
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	22	0.19
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	27	0.19
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	28	0.19
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	29	0.19
(2,38)	1:7:A:TYR:H	1:17:A:LYS:HA	23	0.19
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	4	0.19
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	4	0.19
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	4	0.19
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	2	0.18
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	11	0.18
(5,11)	2:37:B:ZN:ZN	1:12:B:CYS:CB	17	0.18
(4,10)	1:12:B:CYS:SG	1:29:B:CYS:SG	16	0.18
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	18	0.18
(3,52)	1:8:B:LYS:O	1:34:B:VAL:H	4	0.18
(3,52)	1:8:B:LYS:O	1:34:B:VAL:H	13	0.18
(3,24)	1:17:A:LYS:O	1:17:B:LYS:H	3	0.18
(3,24)	1:17:A:LYS:O	1:17:B:LYS:H	19	0.18
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	9	0.18
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	22	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	25	0.18
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	11	0.18
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	12	0.18
(2,365)	1:20:B:GLU:H	1:20:B:GLU:HG3	10	0.18
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	3	0.18
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	6	0.18
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	9	0.18
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	28	0.18
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	24	0.18
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	9	0.18
(2,320)	1:11:B:LEU:HA	1:11:B:LEU:HG	3	0.18
(2,320)	1:11:B:LEU:HA	1:11:B:LEU:HG	21	0.18
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	6	0.18
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	14	0.18
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	19	0.18
(2,210)	1:34:A:VAL:HB	1:35:A:LYS:H	1	0.18
(2,207)	1:34:A:VAL:H	1:34:A:VAL:HB	8	0.18
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	4	0.18
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	5	0.18
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	15	0.18
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	15	0.18
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	16	0.18
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	17	0.18
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	25	0.18
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	17	0.18
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	21	0.18
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	28	0.18
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	8	0.18
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	9	0.18
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	20	0.18
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	1	0.18
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	6	0.18
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	13	0.18
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	20	0.18
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	23	0.18
(2,89)	1:11:A:LEU:H	1:11:A:LEU:HG	2	0.18
(2,38)	1:7:A:TYR:H	1:17:A:LYS:HA	9	0.18
(2,1)	1:1:A:ALA:HB1	1:7:A:TYR:HE2	12	0.18
(2,1)	1:1:A:ALA:HB2	1:7:A:TYR:HE2	12	0.18
(2,1)	1:1:A:ALA:HB3	1:7:A:TYR:HE2	12	0.18
(4,10)	1:12:B:CYS:SG	1:29:B:CYS:SG	5	0.17
(4,10)	1:12:B:CYS:SG	1:29:B:CYS:SG	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	1	0.17
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	13	0.17
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	23	0.17
(3,52)	1:8:B:LYS:O	1:34:B:VAL:H	16	0.17
(3,30)	1:20:A:GLU:O	1:15:B:VAL:H	13	0.17
(3,24)	1:17:A:LYS:O	1:17:B:LYS:H	22	0.17
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	12	0.17
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	16	0.17
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	23	0.17
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	15	0.17
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	7	0.17
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	12	0.17
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	28	0.17
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	20	0.17
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	22	0.17
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	28	0.17
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	2	0.17
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	7	0.17
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	10	0.17
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	14	0.17
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	17	0.17
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	29	0.17
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	21	0.17
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	22	0.17
(2,320)	1:11:B:LEU:HA	1:11:B:LEU:HG	12	0.17
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	24	0.17
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	28	0.17
(2,207)	1:34:A:VAL:H	1:34:A:VAL:HB	4	0.17
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	6	0.17
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	6	0.17
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	6	0.17
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	22	0.17
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	22	0.17
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	22	0.17
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	1	0.17
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	25	0.17
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	7	0.17
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	14	0.17
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	22	0.17
(2,138)	1:18:A:VAL:HA	1:16:B:VAL:HA	12	0.17
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	4	0.17
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	10	0.17
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	13	0.17
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	16	0.17
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	23	0.17
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	24	0.17
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	14	0.17
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	3	0.17
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	19	0.17
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	21	0.17
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	18	0.17
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	24	0.17
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	25	0.17
(2,37)	1:7:A:TYR:H	1:16:A:VAL:H	18	0.17
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	5	0.16
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	7	0.16
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	27	0.16
(5,11)	2:37:B:ZN:ZN	1:12:B:CYS:CB	15	0.16
(5,7)	2:37:A:ZN:ZN	1:29:A:CYS:CA	26	0.16
(4,10)	1:12:B:CYS:SG	1:29:B:CYS:SG	4	0.16
(4,10)	1:12:B:CYS:SG	1:29:B:CYS:SG	23	0.16
(4,3)	1:9:A:CYS:SG	1:29:A:CYS:SG	18	0.16
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	15	0.16
(3,52)	1:8:B:LYS:O	1:34:B:VAL:H	5	0.16
(3,52)	1:8:B:LYS:O	1:34:B:VAL:H	14	0.16
(3,30)	1:20:A:GLU:O	1:15:B:VAL:H	7	0.16
(3,24)	1:17:A:LYS:O	1:17:B:LYS:H	18	0.16
(3,24)	1:17:A:LYS:O	1:17:B:LYS:H	21	0.16
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	7	0.16
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	23	0.16
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	27	0.16
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	1	0.16
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	10	0.16
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	18	0.16
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	24	0.16
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	26	0.16
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	27	0.16
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	2	0.16
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	7	0.16
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	1	0.16
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	4	0.16
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	22	0.16
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	26	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	8	0.16
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	12	0.16
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	13	0.16
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	26	0.16
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	7	0.16
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	11	0.16
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	25	0.16
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	3	0.16
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	3	0.16
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	15	0.16
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	23	0.16
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	26	0.16
(2,210)	1:34:A:VAL:HB	1:35:A:LYS:H	13	0.16
(2,210)	1:34:A:VAL:HB	1:35:A:LYS:H	25	0.16
(2,207)	1:34:A:VAL:H	1:34:A:VAL:HB	2	0.16
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	17	0.16
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	28	0.16
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	9	0.16
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	18	0.16
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	27	0.16
(2,147)	1:20:A:GLU:H	1:20:A:GLU:HG3	13	0.16
(2,138)	1:18:A:VAL:HA	1:16:B:VAL:HA	23	0.16
(2,138)	1:18:A:VAL:HA	1:16:B:VAL:HA	24	0.16
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	12	0.16
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	20	0.16
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	25	0.16
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	29	0.16
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	1	0.16
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	4	0.16
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	10	0.16
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	24	0.16
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	25	0.16
(2,113)	1:15:A:VAL:H	1:15:A:VAL:HB	22	0.16
(2,110)	1:14:A:GLN:H	1:14:A:GLN:HE21	25	0.16
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	2	0.16
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	8	0.16
(2,89)	1:11:A:LEU:H	1:11:A:LEU:HG	20	0.16
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE1	18	0.16
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE2	18	0.16
(2,54)	1:7:A:TYR:HD1	1:33:A:MET:HE3	18	0.16
(2,38)	1:7:A:TYR:H	1:17:A:LYS:HA	5	0.16
(2,38)	1:7:A:TYR:H	1:17:A:LYS:HA	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,17)	2:37:B:ZN:ZN	1:29:B:CYS:CB	13	0.15
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	18	0.15
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	24	0.15
(5,11)	2:37:B:ZN:ZN	1:12:B:CYS:CB	12	0.15
(5,11)	2:37:B:ZN:ZN	1:12:B:CYS:CB	21	0.15
(4,10)	1:12:B:CYS:SG	1:29:B:CYS:SG	1	0.15
(4,10)	1:12:B:CYS:SG	1:29:B:CYS:SG	12	0.15
(4,10)	1:12:B:CYS:SG	1:29:B:CYS:SG	21	0.15
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	10	0.15
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	16	0.15
(3,52)	1:8:B:LYS:O	1:34:B:VAL:H	8	0.15
(3,40)	1:28:A:CYS:O	1:31:A:GLU:H	7	0.15
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	1	0.15
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	20	0.15
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	2	0.15
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	3	0.15
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	6	0.15
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	15	0.15
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	21	0.15
(2,393)	1:27:B:VAL:HB	1:28:B:CYS:H	12	0.15
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	6	0.15
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	23	0.15
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	1	0.15
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	10	0.15
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	11	0.15
(2,354)	1:18:B:VAL:H	1:19:B:LEU:H	2	0.15
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	7	0.15
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	13	0.15
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	15	0.15
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	1	0.15
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	5	0.15
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	12	0.15
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	16	0.15
(2,320)	1:11:B:LEU:HA	1:11:B:LEU:HG	26	0.15
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	19	0.15
(2,265)	1:7:B:TYR:H	1:17:B:LYS:HA	10	0.15
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	1	0.15
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	9	0.15
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	24	0.15
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	28	0.15
(2,239)	1:4:B:GLY:HA3	1:5:B:ASP:H	18	0.15
(2,210)	1:34:A:VAL:HB	1:35:A:LYS:H	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	17	0.15
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	17	0.15
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	17	0.15
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	18	0.15
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	18	0.15
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	18	0.15
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	16	0.15
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	21	0.15
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	13	0.15
(2,138)	1:18:A:VAL:HA	1:16:B:VAL:HA	1	0.15
(2,138)	1:18:A:VAL:HA	1:16:B:VAL:HA	11	0.15
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	3	0.15
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	8	0.15
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	14	0.15
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	15	0.15
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	9	0.15
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	11	0.15
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	17	0.15
(2,113)	1:15:A:VAL:H	1:15:A:VAL:HB	16	0.15
(2,12)	1:4:A:GLY:HA3	1:5:A:ASP:H	2	0.15
(5,16)	2:37:B:ZN:ZN	1:29:B:CYS:CA	24	0.14
(5,15)	2:37:B:ZN:ZN	1:28:B:CYS:SG	1	0.14
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	6	0.14
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	10	0.14
(5,10)	2:37:B:ZN:ZN	1:12:B:CYS:CA	19	0.14
(5,6)	2:37:A:ZN:ZN	1:28:A:CYS:SG	3	0.14
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	6	0.14
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	14	0.14
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	25	0.14
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	29	0.14
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	8	0.14
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	11	0.14
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	28	0.14
(3,52)	1:8:B:LYS:O	1:34:B:VAL:H	9	0.14
(3,32)	1:26:A:LEU:O	1:33:A:MET:H	20	0.14
(3,32)	1:26:A:LEU:O	1:33:A:MET:H	27	0.14
(3,30)	1:20:A:GLU:O	1:15:B:VAL:H	26	0.14
(3,30)	1:20:A:GLU:O	1:15:B:VAL:H	27	0.14
(3,24)	1:17:A:LYS:O	1:17:B:LYS:H	4	0.14
(3,24)	1:17:A:LYS:O	1:17:B:LYS:H	13	0.14
(3,24)	1:17:A:LYS:O	1:17:B:LYS:H	25	0.14
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	18	0.14
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	24	0.14
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	27	0.14
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	28	0.14
(3,18)	1:15:A:VAL:O	1:19:B:LEU:H	20	0.14
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	3	0.14
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	13	0.14
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	25	0.14
(3,14)	1:9:A:CYS:H	1:14:A:GLN:O	27	0.14
(2,421)	1:34:B:VAL:HB	1:35:B:LYS:H	8	0.14
(2,421)	1:34:B:VAL:HB	1:35:B:LYS:H	12	0.14
(2,421)	1:34:B:VAL:HB	1:35:B:LYS:H	29	0.14
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	14	0.14
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	29	0.14
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	25	0.14
(2,393)	1:27:B:VAL:HB	1:28:B:CYS:H	27	0.14
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	2	0.14
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	4	0.14
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	9	0.14
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	19	0.14
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	23	0.14
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	24	0.14
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	25	0.14
(2,343)	1:16:B:VAL:HB	1:17:B:LYS:H	21	0.14
(2,343)	1:16:B:VAL:HB	1:17:B:LYS:H	29	0.14
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	12	0.14
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	17	0.14
(2,320)	1:11:B:LEU:HA	1:11:B:LEU:HG	1	0.14
(2,320)	1:11:B:LEU:HA	1:11:B:LEU:HG	4	0.14
(2,320)	1:11:B:LEU:HA	1:11:B:LEU:HG	16	0.14
(2,308)	1:9:B:CYS:SG	1:12:B:CYS:H	4	0.14
(2,308)	1:9:B:CYS:SG	1:12:B:CYS:H	26	0.14
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	20	0.14
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	20	0.14
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	20	0.14
(2,265)	1:7:B:TYR:H	1:17:B:LYS:HA	3	0.14
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	12	0.14
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	29	0.14
(2,210)	1:34:A:VAL:HB	1:35:A:LYS:H	5	0.14
(2,207)	1:34:A:VAL:H	1:34:A:VAL:HB	7	0.14
(2,207)	1:34:A:VAL:H	1:34:A:VAL:HB	9	0.14
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	19	0.14
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	20	0.14
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	29	0.14
(2,147)	1:20:A:GLU:H	1:20:A:GLU:HG3	26	0.14
(2,138)	1:18:A:VAL:HA	1:16:B:VAL:HA	3	0.14
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	18	0.14
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	19	0.14
(2,135)	1:18:A:VAL:H	1:19:A:LEU:H	2	0.14
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	11	0.14
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	20	0.14
(2,81)	1:9:A:CYS:SG	1:12:A:CYS:H	26	0.14
(2,37)	1:7:A:TYR:H	1:16:A:VAL:H	15	0.14
(1,79)	1:1:B:ALA:HB1	1:7:B:TYR:HD2	23	0.14
(1,79)	1:1:B:ALA:HB2	1:7:B:TYR:HD2	23	0.14
(1,79)	1:1:B:ALA:HB3	1:7:B:TYR:HD2	23	0.14
(5,17)	2:37:B:ZN:ZN	1:29:B:CYS:CB	8	0.13
(5,15)	2:37:B:ZN:ZN	1:28:B:CYS:SG	4	0.13
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	22	0.13
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	23	0.13
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	28	0.13
(5,12)	2:37:B:ZN:ZN	1:12:B:CYS:SG	11	0.13
(5,12)	2:37:B:ZN:ZN	1:12:B:CYS:SG	19	0.13
(5,11)	2:37:B:ZN:ZN	1:12:B:CYS:CB	3	0.13
(5,7)	2:37:A:ZN:ZN	1:29:A:CYS:CA	8	0.13
(5,6)	2:37:A:ZN:ZN	1:28:A:CYS:SG	5	0.13
(5,6)	2:37:A:ZN:ZN	1:28:A:CYS:SG	8	0.13
(5,6)	2:37:A:ZN:ZN	1:28:A:CYS:SG	18	0.13
(5,6)	2:37:A:ZN:ZN	1:28:A:CYS:SG	19	0.13
(5,6)	2:37:A:ZN:ZN	1:28:A:CYS:SG	26	0.13
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	16	0.13
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	17	0.13
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	21	0.13
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	28	0.13
(4,3)	1:9:A:CYS:SG	1:29:A:CYS:SG	5	0.13
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	3	0.13
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	4	0.13
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	5	0.13
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	6	0.13
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	7	0.13
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	17	0.13
(3,52)	1:8:B:LYS:O	1:34:B:VAL:H	11	0.13
(3,32)	1:26:A:LEU:O	1:33:A:MET:H	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:26:A:LEU:O	1:33:A:MET:H	22	0.13
(3,26)	1:19:A:LEU:H	1:15:B:VAL:O	5	0.13
(3,26)	1:19:A:LEU:H	1:15:B:VAL:O	9	0.13
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	26	0.13
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	29	0.13
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	6	0.13
(3,15)	1:15:A:VAL:N	1:20:B:GLU:O	22	0.13
(2,421)	1:34:B:VAL:HB	1:35:B:LYS:H	23	0.13
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	20	0.13
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	22	0.13
(2,393)	1:27:B:VAL:HB	1:28:B:CYS:H	2	0.13
(2,393)	1:27:B:VAL:HB	1:28:B:CYS:H	6	0.13
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	10	0.13
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	14	0.13
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	16	0.13
(2,365)	1:20:B:GLU:H	1:20:B:GLU:HG3	22	0.13
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	14	0.13
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	17	0.13
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	27	0.13
(2,343)	1:16:B:VAL:HB	1:17:B:LYS:H	9	0.13
(2,343)	1:16:B:VAL:HB	1:17:B:LYS:H	26	0.13
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	8	0.13
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	10	0.13
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	11	0.13
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	21	0.13
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	29	0.13
(2,332)	1:14:B:GLN:H	1:14:B:GLN:HA	4	0.13
(2,320)	1:11:B:LEU:HA	1:11:B:LEU:HG	5	0.13
(2,320)	1:11:B:LEU:HA	1:11:B:LEU:HG	23	0.13
(2,308)	1:9:B:CYS:SG	1:12:B:CYS:H	3	0.13
(2,308)	1:9:B:CYS:SG	1:12:B:CYS:H	12	0.13
(2,308)	1:9:B:CYS:SG	1:12:B:CYS:H	15	0.13
(2,308)	1:9:B:CYS:SG	1:12:B:CYS:H	16	0.13
(2,308)	1:9:B:CYS:SG	1:12:B:CYS:H	17	0.13
(2,265)	1:7:B:TYR:H	1:17:B:LYS:HA	15	0.13
(2,265)	1:7:B:TYR:H	1:17:B:LYS:HA	21	0.13
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	4	0.13
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	14	0.13
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	20	0.13
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	21	0.13
(2,210)	1:34:A:VAL:HB	1:35:A:LYS:H	12	0.13
(2,210)	1:34:A:VAL:HB	1:35:A:LYS:H	21	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,207)	1:34:A:VAL:H	1:34:A:VAL:HB	15	0.13
(2,207)	1:34:A:VAL:H	1:34:A:VAL:HB	20	0.13
(2,188)	1:28:A:CYS:H	1:33:A:MET:HB2	20	0.13
(2,184)	1:27:A:VAL:HG11	1:30:A:GLY:HA3	16	0.13
(2,184)	1:27:A:VAL:HG12	1:30:A:GLY:HA3	16	0.13
(2,184)	1:27:A:VAL:HG13	1:30:A:GLY:HA3	16	0.13
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	19	0.13
(2,138)	1:18:A:VAL:HA	1:16:B:VAL:HA	5	0.13
(2,138)	1:18:A:VAL:HA	1:16:B:VAL:HA	6	0.13
(2,138)	1:18:A:VAL:HA	1:16:B:VAL:HA	15	0.13
(2,138)	1:18:A:VAL:HA	1:16:B:VAL:HA	28	0.13
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	22	0.13
(2,129)	1:17:A:LYS:HA	1:18:A:VAL:H	21	0.13
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	6	0.13
(2,108)	1:14:A:GLN:H	1:14:A:GLN:HA	26	0.13
(2,89)	1:11:A:LEU:H	1:11:A:LEU:HG	7	0.13
(2,89)	1:11:A:LEU:H	1:11:A:LEU:HG	10	0.13
(2,69)	1:8:A:LYS:HA	1:33:A:MET:HB3	7	0.13
(2,38)	1:7:A:TYR:H	1:17:A:LYS:HA	10	0.13
(2,37)	1:7:A:TYR:H	1:16:A:VAL:H	19	0.13
(2,12)	1:4:A:GLY:HA3	1:5:A:ASP:H	4	0.13
(2,12)	1:4:A:GLY:HA3	1:5:A:ASP:H	15	0.13
(2,12)	1:4:A:GLY:HA3	1:5:A:ASP:H	20	0.13
(5,17)	2:37:B:ZN:ZN	1:29:B:CYS:CB	11	0.12
(5,16)	2:37:B:ZN:ZN	1:29:B:CYS:CA	8	0.12
(5,15)	2:37:B:ZN:ZN	1:28:B:CYS:SG	12	0.12
(5,15)	2:37:B:ZN:ZN	1:28:B:CYS:SG	16	0.12
(5,15)	2:37:B:ZN:ZN	1:28:B:CYS:SG	21	0.12
(5,15)	2:37:B:ZN:ZN	1:28:B:CYS:SG	26	0.12
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	15	0.12
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	16	0.12
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	17	0.12
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	26	0.12
(5,12)	2:37:B:ZN:ZN	1:12:B:CYS:SG	29	0.12
(5,10)	2:37:B:ZN:ZN	1:12:B:CYS:CA	8	0.12
(5,10)	2:37:B:ZN:ZN	1:12:B:CYS:CA	14	0.12
(5,10)	2:37:B:ZN:ZN	1:12:B:CYS:CA	20	0.12
(5,6)	2:37:A:ZN:ZN	1:28:A:CYS:SG	20	0.12
(4,10)	1:12:B:CYS:SG	1:29:B:CYS:SG	24	0.12
(4,5)	1:12:A:CYS:SG	1:29:A:CYS:SG	20	0.12
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	13	0.12
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	24	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	27	0.12
(4,3)	1:9:A:CYS:SG	1:29:A:CYS:SG	10	0.12
(4,3)	1:9:A:CYS:SG	1:29:A:CYS:SG	20	0.12
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	25	0.12
(3,52)	1:8:B:LYS:O	1:34:B:VAL:H	29	0.12
(3,36)	1:27:A:VAL:O	1:27:B:VAL:H	13	0.12
(3,36)	1:27:A:VAL:O	1:27:B:VAL:H	23	0.12
(3,36)	1:27:A:VAL:O	1:27:B:VAL:H	24	0.12
(3,36)	1:27:A:VAL:O	1:27:B:VAL:H	28	0.12
(3,32)	1:26:A:LEU:O	1:33:A:MET:H	12	0.12
(3,32)	1:26:A:LEU:O	1:33:A:MET:H	19	0.12
(3,30)	1:20:A:GLU:O	1:15:B:VAL:H	8	0.12
(3,30)	1:20:A:GLU:O	1:15:B:VAL:H	15	0.12
(3,30)	1:20:A:GLU:O	1:15:B:VAL:H	16	0.12
(3,30)	1:20:A:GLU:O	1:15:B:VAL:H	17	0.12
(3,30)	1:20:A:GLU:O	1:15:B:VAL:H	29	0.12
(3,26)	1:19:A:LEU:H	1:15:B:VAL:O	1	0.12
(3,26)	1:19:A:LEU:H	1:15:B:VAL:O	12	0.12
(3,26)	1:19:A:LEU:H	1:15:B:VAL:O	15	0.12
(3,26)	1:19:A:LEU:H	1:15:B:VAL:O	17	0.12
(3,26)	1:19:A:LEU:H	1:15:B:VAL:O	23	0.12
(3,24)	1:17:A:LYS:O	1:17:B:LYS:H	14	0.12
(3,24)	1:17:A:LYS:O	1:17:B:LYS:H	29	0.12
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	3	0.12
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	5	0.12
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	6	0.12
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	9	0.12
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	15	0.12
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	19	0.12
(3,18)	1:15:A:VAL:O	1:19:B:LEU:H	19	0.12
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	12	0.12
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	16	0.12
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	26	0.12
(2,421)	1:34:B:VAL:HB	1:35:B:LYS:H	9	0.12
(2,421)	1:34:B:VAL:HB	1:35:B:LYS:H	11	0.12
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	11	0.12
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	13	0.12
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	16	0.12
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	19	0.12
(2,402)	1:28:B:CYS:HB2	1:33:B:MET:HB2	6	0.12
(2,393)	1:27:B:VAL:HB	1:28:B:CYS:H	15	0.12
(2,393)	1:27:B:VAL:HB	1:28:B:CYS:H	26	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,371)	1:21:B:GLU:HA	1:22:B:GLY:H	22	0.12
(2,365)	1:20:B:GLU:H	1:20:B:GLU:HG3	11	0.12
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	5	0.12
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	15	0.12
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	21	0.12
(2,343)	1:16:B:VAL:HB	1:17:B:LYS:H	17	0.12
(2,343)	1:16:B:VAL:HB	1:17:B:LYS:H	25	0.12
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	3	0.12
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	4	0.12
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	16	0.12
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	23	0.12
(2,334)	1:14:B:GLN:H	1:14:B:GLN:HE21	28	0.12
(2,308)	1:9:B:CYS:SG	1:12:B:CYS:H	23	0.12
(2,303)	1:9:B:CYS:HB2	1:13:B:GLY:H	19	0.12
(2,296)	1:8:B:LYS:HA	1:33:B:MET:HB3	13	0.12
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	27	0.12
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	27	0.12
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	27	0.12
(2,265)	1:7:B:TYR:H	1:17:B:LYS:HA	23	0.12
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	6	0.12
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	10	0.12
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	13	0.12
(2,240)	1:5:B:ASP:H	1:5:B:ASP:HB2	25	0.12
(2,240)	1:5:B:ASP:H	1:5:B:ASP:HB3	25	0.12
(2,239)	1:4:B:GLY:HA3	1:5:B:ASP:H	15	0.12
(2,239)	1:4:B:GLY:HA3	1:5:B:ASP:H	25	0.12
(2,207)	1:34:A:VAL:H	1:34:A:VAL:HB	3	0.12
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	6	0.12
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	7	0.12
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	11	0.12
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	24	0.12
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	29	0.12
(2,147)	1:20:A:GLU:H	1:20:A:GLU:HG3	7	0.12
(2,138)	1:18:A:VAL:HA	1:16:B:VAL:HA	13	0.12
(2,137)	1:18:A:VAL:HA	1:20:A:GLU:H	2	0.12
(2,124)	1:16:A:VAL:HB	1:17:A:LYS:H	8	0.12
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	1	0.12
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	2	0.12
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	4	0.12
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	6	0.12
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	8	0.12
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	18	0.12
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	21	0.12
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	25	0.12
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	26	0.12
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	29	0.12
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	2	0.12
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	15	0.12
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	16	0.12
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	27	0.12
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	28	0.12
(2,113)	1:15:A:VAL:H	1:15:A:VAL:HB	12	0.12
(2,113)	1:15:A:VAL:H	1:15:A:VAL:HB	28	0.12
(2,69)	1:8:A:LYS:HA	1:33:A:MET:HB3	1	0.12
(2,38)	1:7:A:TYR:H	1:17:A:LYS:HA	12	0.12
(2,38)	1:7:A:TYR:H	1:17:A:LYS:HA	28	0.12
(2,37)	1:7:A:TYR:H	1:16:A:VAL:H	1	0.12
(2,37)	1:7:A:TYR:H	1:16:A:VAL:H	2	0.12
(2,12)	1:4:A:GLY:HA3	1:5:A:ASP:H	18	0.12
(5,17)	2:37:B:ZN:ZN	1:29:B:CYS:CB	29	0.11
(5,16)	2:37:B:ZN:ZN	1:29:B:CYS:CA	3	0.11
(5,16)	2:37:B:ZN:ZN	1:29:B:CYS:CA	13	0.11
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	3	0.11
(5,14)	2:37:B:ZN:ZN	1:28:B:CYS:CB	4	0.11
(5,12)	2:37:B:ZN:ZN	1:12:B:CYS:SG	6	0.11
(5,12)	2:37:B:ZN:ZN	1:12:B:CYS:SG	8	0.11
(5,12)	2:37:B:ZN:ZN	1:12:B:CYS:SG	9	0.11
(5,10)	2:37:B:ZN:ZN	1:12:B:CYS:CA	11	0.11
(5,10)	2:37:B:ZN:ZN	1:12:B:CYS:CA	13	0.11
(5,10)	2:37:B:ZN:ZN	1:12:B:CYS:CA	25	0.11
(5,10)	2:37:B:ZN:ZN	1:12:B:CYS:CA	29	0.11
(5,6)	2:37:A:ZN:ZN	1:28:A:CYS:SG	1	0.11
(5,6)	2:37:A:ZN:ZN	1:28:A:CYS:SG	17	0.11
(5,6)	2:37:A:ZN:ZN	1:28:A:CYS:SG	23	0.11
(5,6)	2:37:A:ZN:ZN	1:28:A:CYS:SG	24	0.11
(5,1)	2:37:A:ZN:ZN	1:12:A:CYS:CA	7	0.11
(4,10)	1:12:B:CYS:SG	1:29:B:CYS:SG	3	0.11
(4,10)	1:12:B:CYS:SG	1:29:B:CYS:SG	22	0.11
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	1	0.11
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	10	0.11
(4,3)	1:9:A:CYS:SG	1:29:A:CYS:SG	13	0.11
(4,3)	1:9:A:CYS:SG	1:29:A:CYS:SG	19	0.11
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	21	0.11
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	22	0.11
(3,56)	1:26:B:LEU:O	1:33:B:MET:H	29	0.11
(3,52)	1:8:B:LYS:O	1:34:B:VAL:H	19	0.11
(3,52)	1:8:B:LYS:O	1:34:B:VAL:H	20	0.11
(3,36)	1:27:A:VAL:O	1:27:B:VAL:H	5	0.11
(3,32)	1:26:A:LEU:O	1:33:A:MET:H	1	0.11
(3,32)	1:26:A:LEU:O	1:33:A:MET:H	4	0.11
(3,32)	1:26:A:LEU:O	1:33:A:MET:H	11	0.11
(3,32)	1:26:A:LEU:O	1:33:A:MET:H	25	0.11
(3,30)	1:20:A:GLU:O	1:15:B:VAL:H	6	0.11
(3,29)	1:20:A:GLU:O	1:15:B:VAL:N	9	0.11
(3,26)	1:19:A:LEU:H	1:15:B:VAL:O	4	0.11
(3,26)	1:19:A:LEU:H	1:15:B:VAL:O	22	0.11
(3,26)	1:19:A:LEU:H	1:15:B:VAL:O	24	0.11
(3,26)	1:19:A:LEU:H	1:15:B:VAL:O	27	0.11
(3,26)	1:19:A:LEU:H	1:15:B:VAL:O	29	0.11
(3,24)	1:17:A:LYS:O	1:17:B:LYS:H	10	0.11
(3,24)	1:17:A:LYS:O	1:17:B:LYS:H	26	0.11
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	14	0.11
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	21	0.11
(3,18)	1:15:A:VAL:O	1:19:B:LEU:H	15	0.11
(3,18)	1:15:A:VAL:O	1:19:B:LEU:H	22	0.11
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	5	0.11
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	10	0.11
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	14	0.11
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	18	0.11
(3,14)	1:9:A:CYS:H	1:14:A:GLN:O	1	0.11
(3,14)	1:9:A:CYS:H	1:14:A:GLN:O	17	0.11
(2,421)	1:34:B:VAL:HB	1:35:B:LYS:H	17	0.11
(2,421)	1:34:B:VAL:HB	1:35:B:LYS:H	19	0.11
(2,421)	1:34:B:VAL:HB	1:35:B:LYS:H	25	0.11
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	20	0.11
(2,391)	1:27:B:VAL:HA	1:33:B:MET:H	28	0.11
(2,365)	1:20:B:GLU:H	1:20:B:GLU:HG3	3	0.11
(2,365)	1:20:B:GLU:H	1:20:B:GLU:HG3	5	0.11
(2,365)	1:20:B:GLU:H	1:20:B:GLU:HG3	13	0.11
(2,365)	1:20:B:GLU:H	1:20:B:GLU:HG3	26	0.11
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	6	0.11
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	16	0.11
(2,348)	1:17:B:LYS:HA	1:18:B:VAL:H	2	0.11
(2,348)	1:17:B:LYS:HA	1:18:B:VAL:H	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,348)	1:17:B:LYS:HA	1:18:B:VAL:H	19	0.11
(2,343)	1:16:B:VAL:HB	1:17:B:LYS:H	5	0.11
(2,343)	1:16:B:VAL:HB	1:17:B:LYS:H	11	0.11
(2,343)	1:16:B:VAL:HB	1:17:B:LYS:H	16	0.11
(2,343)	1:16:B:VAL:HB	1:17:B:LYS:H	18	0.11
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	2	0.11
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	17	0.11
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	21	0.11
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	5	0.11
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	9	0.11
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	11	0.11
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	16	0.11
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	22	0.11
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	25	0.11
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	27	0.11
(2,316)	1:11:B:LEU:H	1:11:B:LEU:HG	24	0.11
(2,308)	1:9:B:CYS:SG	1:12:B:CYS:H	1	0.11
(2,308)	1:9:B:CYS:SG	1:12:B:CYS:H	5	0.11
(2,303)	1:9:B:CYS:HB2	1:13:B:GLY:H	11	0.11
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE1	22	0.11
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE2	22	0.11
(2,281)	1:7:B:TYR:HD1	1:33:B:MET:HE3	22	0.11
(2,265)	1:7:B:TYR:H	1:17:B:LYS:HA	7	0.11
(2,265)	1:7:B:TYR:H	1:17:B:LYS:HA	18	0.11
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	7	0.11
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	25	0.11
(2,239)	1:4:B:GLY:HA3	1:5:B:ASP:H	4	0.11
(2,210)	1:34:A:VAL:HB	1:35:A:LYS:H	14	0.11
(2,210)	1:34:A:VAL:HB	1:35:A:LYS:H	23	0.11
(2,207)	1:34:A:VAL:H	1:34:A:VAL:HB	26	0.11
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	18	0.11
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	20	0.11
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	27	0.11
(2,149)	1:20:A:GLU:H	1:15:B:VAL:H	2	0.11
(2,147)	1:20:A:GLU:H	1:20:A:GLU:HG3	11	0.11
(2,138)	1:18:A:VAL:HA	1:16:B:VAL:HA	7	0.11
(2,138)	1:18:A:VAL:HA	1:16:B:VAL:HA	27	0.11
(2,129)	1:17:A:LYS:HA	1:18:A:VAL:H	2	0.11
(2,124)	1:16:A:VAL:HB	1:17:A:LYS:H	3	0.11
(2,124)	1:16:A:VAL:HB	1:17:A:LYS:H	21	0.11
(2,122)	1:16:A:VAL:HA	1:18:B:VAL:HA	15	0.11
(2,122)	1:16:A:VAL:HA	1:18:B:VAL:HA	23	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	3	0.11
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	5	0.11
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	10	0.11
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	12	0.11
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	15	0.11
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	17	0.11
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	19	0.11
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	23	0.11
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	24	0.11
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	27	0.11
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	5	0.11
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	8	0.11
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	14	0.11
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	26	0.11
(2,80)	1:9:A:CYS:SG	1:12:A:CYS:N	9	0.11
(2,69)	1:8:A:LYS:HA	1:33:A:MET:HB3	12	0.11
(2,69)	1:8:A:LYS:HA	1:33:A:MET:HB3	27	0.11
(2,38)	1:7:A:TYR:H	1:17:A:LYS:HA	13	0.11
(2,38)	1:7:A:TYR:H	1:17:A:LYS:HA	21	0.11
(2,25)	1:6:A:VAL:H	1:7:A:TYR:HA	15	0.11
(2,12)	1:4:A:GLY:HA3	1:5:A:ASP:H	13	0.11
(2,12)	1:4:A:GLY:HA3	1:5:A:ASP:H	19	0.11
(5,17)	2:37:B:ZN:ZN	1:29:B:CYS:CB	9	0.1
(5,17)	2:37:B:ZN:ZN	1:29:B:CYS:CB	14	0.1
(5,17)	2:37:B:ZN:ZN	1:29:B:CYS:CB	20	0.1
(5,17)	2:37:B:ZN:ZN	1:29:B:CYS:CB	24	0.1
(5,16)	2:37:B:ZN:ZN	1:29:B:CYS:CA	7	0.1
(5,16)	2:37:B:ZN:ZN	1:29:B:CYS:CA	15	0.1
(5,16)	2:37:B:ZN:ZN	1:29:B:CYS:CA	28	0.1
(5,12)	2:37:B:ZN:ZN	1:12:B:CYS:SG	7	0.1
(5,12)	2:37:B:ZN:ZN	1:12:B:CYS:SG	13	0.1
(5,12)	2:37:B:ZN:ZN	1:12:B:CYS:SG	14	0.1
(5,12)	2:37:B:ZN:ZN	1:12:B:CYS:SG	18	0.1
(5,10)	2:37:B:ZN:ZN	1:12:B:CYS:CA	9	0.1
(5,6)	2:37:A:ZN:ZN	1:28:A:CYS:SG	2	0.1
(5,6)	2:37:A:ZN:ZN	1:28:A:CYS:SG	6	0.1
(5,6)	2:37:A:ZN:ZN	1:28:A:CYS:SG	15	0.1
(5,1)	2:37:A:ZN:ZN	1:12:A:CYS:CA	8	0.1
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	11	0.1
(4,4)	1:12:A:CYS:SG	1:28:A:CYS:SG	23	0.1
(3,54)	1:9:B:CYS:H	1:14:B:GLN:O	22	0.1
(3,36)	1:27:A:VAL:O	1:27:B:VAL:H	21	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:26:A:LEU:O	1:33:A:MET:H	24	0.1
(3,30)	1:20:A:GLU:O	1:15:B:VAL:H	19	0.1
(3,29)	1:20:A:GLU:O	1:15:B:VAL:N	13	0.1
(3,26)	1:19:A:LEU:H	1:15:B:VAL:O	14	0.1
(3,24)	1:17:A:LYS:O	1:17:B:LYS:H	8	0.1
(3,24)	1:17:A:LYS:O	1:17:B:LYS:H	20	0.1
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	2	0.1
(3,22)	1:17:A:LYS:H	1:17:B:LYS:O	11	0.1
(3,18)	1:15:A:VAL:O	1:19:B:LEU:H	4	0.1
(3,18)	1:15:A:VAL:O	1:19:B:LEU:H	11	0.1
(3,16)	1:15:A:VAL:H	1:20:B:GLU:O	24	0.1
(3,4)	1:6:A:VAL:O	1:36:A:GLN:H	24	0.1
(2,421)	1:34:B:VAL:HB	1:35:B:LYS:H	4	0.1
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	4	0.1
(2,418)	1:34:B:VAL:H	1:34:B:VAL:HB	17	0.1
(2,393)	1:27:B:VAL:HB	1:28:B:CYS:H	25	0.1
(2,365)	1:20:B:GLU:H	1:20:B:GLU:HG3	23	0.1
(2,356)	1:18:B:VAL:HA	1:20:B:GLU:H	28	0.1
(2,343)	1:16:B:VAL:HB	1:17:B:LYS:H	7	0.1
(2,343)	1:16:B:VAL:HB	1:17:B:LYS:H	13	0.1
(2,343)	1:16:B:VAL:HB	1:17:B:LYS:H	14	0.1
(2,343)	1:16:B:VAL:HB	1:17:B:LYS:H	19	0.1
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	1	0.1
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	5	0.1
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	25	0.1
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	27	0.1
(2,340)	1:16:B:VAL:HA	1:16:B:VAL:HB	28	0.1
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	17	0.1
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	18	0.1
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	19	0.1
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	20	0.1
(2,336)	1:15:B:VAL:H	1:15:B:VAL:HB	26	0.1
(2,303)	1:9:B:CYS:HB2	1:13:B:GLY:H	28	0.1
(2,265)	1:7:B:TYR:H	1:17:B:LYS:HA	17	0.1
(2,265)	1:7:B:TYR:H	1:17:B:LYS:HA	25	0.1
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	15	0.1
(2,264)	1:7:B:TYR:H	1:16:B:VAL:H	17	0.1
(2,239)	1:4:B:GLY:HA3	1:5:B:ASP:H	28	0.1
(2,210)	1:34:A:VAL:HB	1:35:A:LYS:H	11	0.1
(2,210)	1:34:A:VAL:HB	1:35:A:LYS:H	27	0.1
(2,181)	1:27:A:VAL:HB	1:28:A:CYS:H	3	0.1
(2,147)	1:20:A:GLU:H	1:20:A:GLU:HG3	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,147)	1:20:A:GLU:H	1:20:A:GLU:HG3	27	0.1
(2,138)	1:18:A:VAL:HA	1:16:B:VAL:HA	18	0.1
(2,124)	1:16:A:VAL:HB	1:17:A:LYS:H	14	0.1
(2,124)	1:16:A:VAL:HB	1:17:A:LYS:H	16	0.1
(2,124)	1:16:A:VAL:HB	1:17:A:LYS:H	19	0.1
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	7	0.1
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	16	0.1
(2,119)	1:16:A:VAL:HA	1:16:A:VAL:HB	28	0.1
(2,115)	1:15:A:VAL:H	1:20:B:GLU:H	7	0.1
(2,113)	1:15:A:VAL:H	1:15:A:VAL:HB	3	0.1
(2,113)	1:15:A:VAL:H	1:15:A:VAL:HB	26	0.1
(2,113)	1:15:A:VAL:H	1:15:A:VAL:HB	27	0.1
(2,81)	1:9:A:CYS:SG	1:12:A:CYS:H	20	0.1
(2,76)	1:9:A:CYS:HB2	1:13:A:GLY:H	21	0.1
(2,69)	1:8:A:LYS:HA	1:33:A:MET:HB3	14	0.1
(2,38)	1:7:A:TYR:H	1:17:A:LYS:HA	11	0.1
(2,37)	1:7:A:TYR:H	1:16:A:VAL:H	4	0.1
(2,37)	1:7:A:TYR:H	1:16:A:VAL:H	22	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found