Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 03:07 PM EDT

PDB ID	:	2LK5
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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

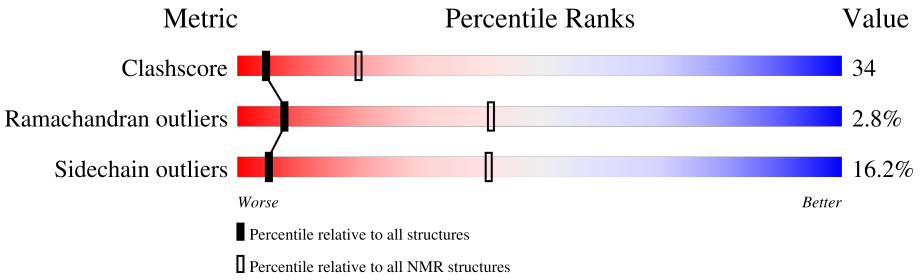
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 27%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	36	53% 36% 6% 6%
1	B	36	39% 44% 8% 8%

2 Ensemble composition and analysis (i)

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 (i)

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
			Total	C	H	N	O	S	
1	A	36	507	158	247	42	55	5	0
1	B	36	507	158	247	42	55	5	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

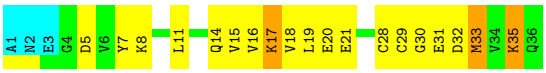
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for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

• Molecule 1: Desulforedoxin

Chain A: 53% 36% 6% 6%

• Molecule 1: Desulforedoxin

Chain B: 39% 44% 8% 8%



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

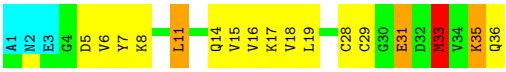
4.2.1 Score per residue for model 1

• Molecule 1: Desulforedoxin

Chain A: 47% 42% 6% 6%

• Molecule 1: Desulforedoxin

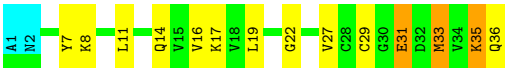
Chain B: 44% 36% 8% • 8%



4.2.2 Score per residue for model 2

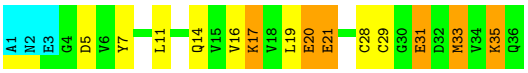
- Molecule 1: Desulforedoxin

Chain A: 56% 31% 8% 6%



- Molecule 1: Desulforedoxin

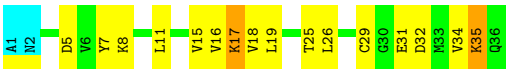
Chain B: 53% 22% 17% 8%



4.2.3 Score per residue for model 3

- Molecule 1: Desulforedoxin

Chain A: 50% 39% 6% 6%



- Molecule 1: Desulforedoxin

Chain B: 36% 42% 14% 8%

4.2.4 Score per residue for model 4

- Molecule 1: Desulforedoxin

Chain A: 67% 17% 11% 6%

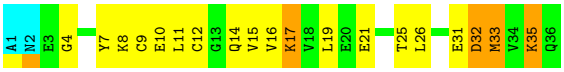
- Molecule 1: Desulforedoxin

Chain B: 31% 53% 8% 8%

4.2.5 Score per residue for model 5

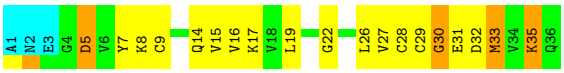
- Molecule 1: Desulforedoxin

Chain A: 42% 42% 11% 6%



- Molecule 1: Desulforedoxin

Chain B: 39% 42% 11% 8%



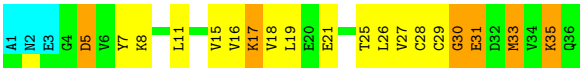
4.2.6 Score per residue for model 6

- Molecule 1: Desulforedoxin

Chain A: 53% 33% 8% 6%

- Molecule 1: Desulforedoxin

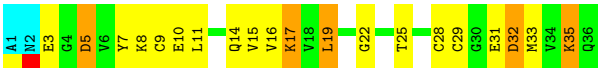
Chain B: 39% 36% 17% 8%



4.2.7 Score per residue for model 7

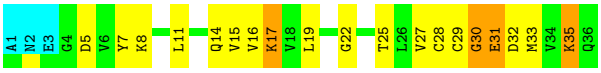
- Molecule 1: Desulforedoxin

Chain A: 39% 42% 14% 6%



- Molecule 1: Desulforedoxin

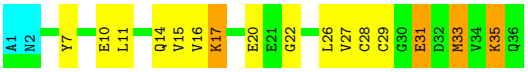
Chain B: 39% 42% 11% 8%



4.2.8 Score per residue for model 8

- Molecule 1: Desulforedoxin

Chain A: 50% 33% 11% 6%



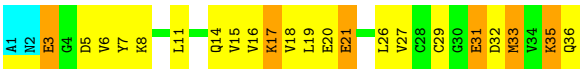
- Molecule 1: Desulforedoxin

Chain B: 44% 39% 8% 8%

4.2.9 Score per residue for model 9

- Molecule 1: Desulforedoxin

Chain A: 33% 44% 17% 6%



- Molecule 1: Desulforedoxin

Chain B: 33% 44% 14% 8%

4.2.10 Score per residue for model 10

- Molecule 1: Desulforedoxin

Chain A: 42% 42% 11% 6%

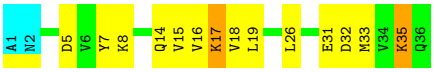
- Molecule 1: Desulforedoxin

Chain B: 39% 36% 17% 8%

4.2.11 Score per residue for model 11

- Molecule 1: Desulforedoxin

Chain A: 56% 33% 6% 6%



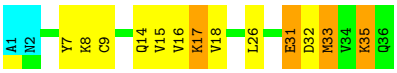
- Molecule 1: Desulforedoxin

Chain B: 17% 61% 14% 8%

4.2.12 Score per residue for model 12

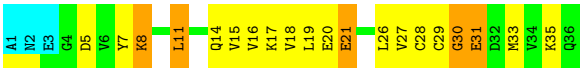
- Molecule 1: Desulforedoxin

Chain A: 58% 25% 11% 6%



- Molecule 1: Desulforedoxin

Chain B: 36% 42% 14% 8%



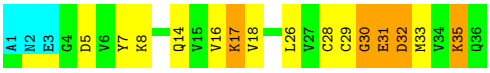
4.2.13 Score per residue for model 13

- Molecule 1: Desulforedoxin

Chain A: 56% 31% 8% 6%

- Molecule 1: Desulforedoxin

Chain B: 50% 28% 14% 8%



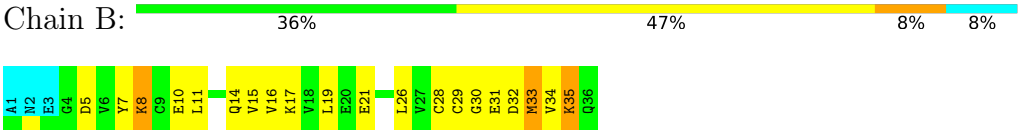
4.2.14 Score per residue for model 14

- Molecule 1: Desulforedoxin

Chain A:

- Molecule 1: Desulforedoxin

Chain B:



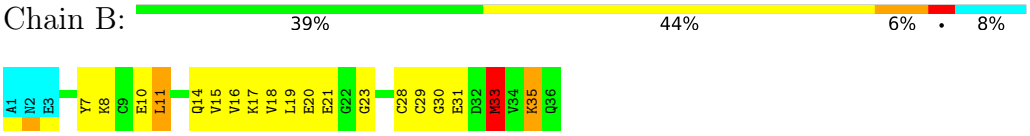
4.2.15 Score per residue for model 15

- Molecule 1: Desulforedoxin

Chain A:

- Molecule 1: Desulforedoxin

Chain B:



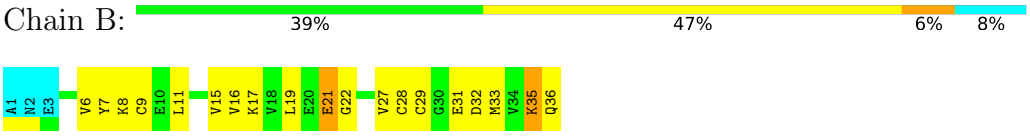
4.2.16 Score per residue for model 16

- Molecule 1: Desulforedoxin

Chain A:

- Molecule 1: Desulforedoxin

Chain B:



4.2.17 Score per residue for model 17

- Molecule 1: Desulforedoxin

Chain A: 61% 31% • 6%

A1 N2 Y7 K8 L11 V15 V16 K17 V18 L19 E20 E21 E31 D32 K35 Q36

- Molecule 1: Desulforedoxin

Chain B: 44% 33% 14% 8%

A1 N2 E3 G4 D5 V6 Y7 K8 C9 V15 V16 K17 V18 L19 G23 C28 C29 G30 E31 D32 M33 V34 K35 Q36

4.2.18 Score per residue for model 18

- Molecule 1: Desulforedoxin

Chain A: 67% 25% • 6%

A1 N2 Y7 C12 G13 Q14 V15 V16 K17 E21 L26 D32 M33 V34 K35 Q36

- Molecule 1: Desulforedoxin

Chain B: 31% 53% 8% 8%

A1 N2 E3 Y7 K8 Q14 V15 V16 K17 V18 L19 E20 E21 G22 G23 G24 T25 L26 V27 C28 C29 G30 E31 D32 M33 V34 K35 Q36

4.2.19 Score per residue for model 19

- Molecule 1: Desulforedoxin

Chain A: 58% 33% • 6%

A1 N2 Y7 K8 C9 E10 L11 V15 V16 K17 V18 L19 E20 E21 C29 G30 E31 D32 K35 Q36

- Molecule 1: Desulforedoxin

Chain B: 47% 31% 14% 8%

A1 N2 E3 G4 D5 V6 Y7 K8 C9 E10 L11 Q14 V15 V16 K17 V18 L19 C28 C29 G30 E31 D32 M33 V34 K35 Q36

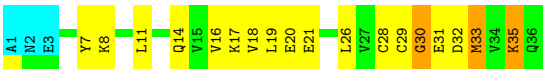
4.2.20 Score per residue for model 20

- Molecule 1: Desulforedoxin

Chain A: 56% 31% 8% 6%

- Molecule 1: Desulforedoxin

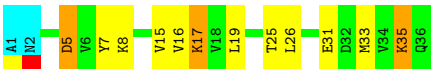
Chain B: 42% 42% 8% 8%



4.2.21 Score per residue for model 21

- Molecule 1: Desulforedoxin

Chain A: 61% 25% 8% 6%



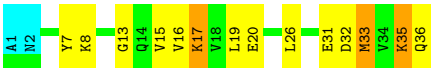
- Molecule 1: Desulforedoxin

Chain B: 36% 44% 11% 8%

4.2.22 Score per residue for model 22

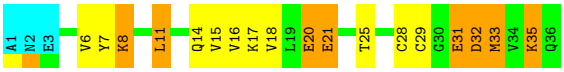
- Molecule 1: Desulforedoxin

Chain A: 56% 31% 8% 6%



- Molecule 1: Desulforedoxin

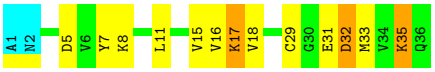
Chain B: 42% 28% 22% 8%



4.2.23 Score per residue for model 23

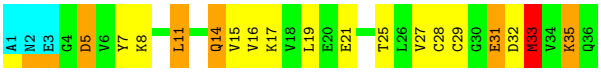
- Molecule 1: Desulforedoxin

Chain A: 58% 28% 8% 6%



- Molecule 1: Desulforedoxin

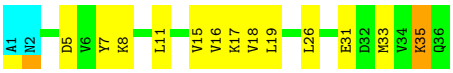
Chain B: 42% 33% 14% • 8%



4.2.24 Score per residue for model 24

- Molecule 1: Desulforedoxin

Chain A: 58% 33% • 6%



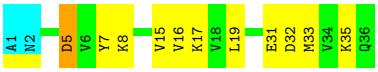
- Molecule 1: Desulforedoxin

Chain B: 44% 31% 14% • 8%

4.2.25 Score per residue for model 25

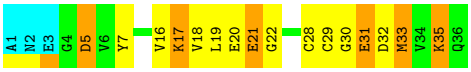
- Molecule 1: Desulforedoxin

Chain A: 64% 28% • 6%



- Molecule 1: Desulforedoxin

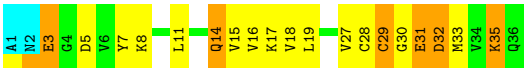
Chain B: 47% 28% 17% 8%



4.2.26 Score per residue for model 26

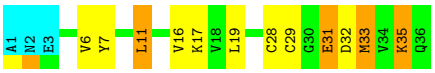
- Molecule 1: Desulforedoxin

Chain A: 42% 36% 17% 6%



- Molecule 1: Desulforedoxin

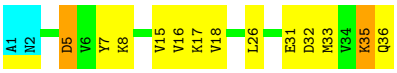
Chain B: 58% 22% 11% 8%



4.2.27 Score per residue for model 27

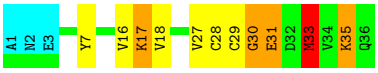
- Molecule 1: Desulforedoxin

Chain A: 58% 31% 6% 6%



- Molecule 1: Desulforedoxin

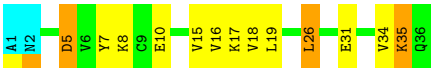
Chain B: 61% 17% 11% • 8%



4.2.28 Score per residue for model 28

- Molecule 1: Desulforedoxin

Chain A: 58% 28% 8% 6%



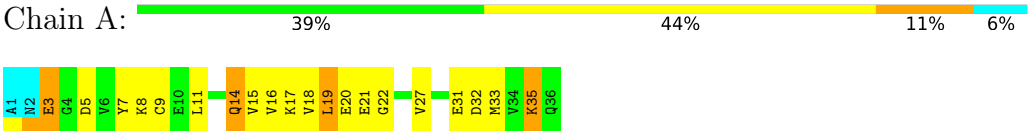
- Molecule 1: Desulforedoxin

Chain B: 44% 36% 8% • 8%

4.2.29 Score per residue for model 29 (medoid)

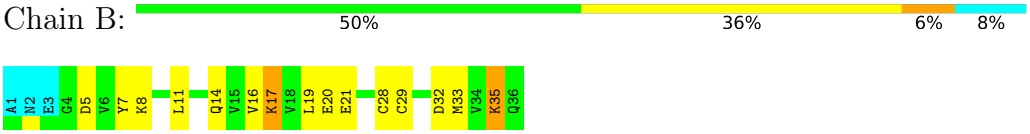
- Molecule 1: Desulforedoxin

Chain A:



- Molecule 1: Desulforedoxin

Chain B:



5 Refinement protocol and experimental data overview (i)

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)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	247	236	239	17±5
1	B	238	230	233	22±5
All	All	14123	13514	13688	940

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:11:LEU:HD12	1:B:29:CYS:SG	0.93	2.03	3	9
1:B:16:VAL:HG22	1:B:33:MET:CE	0.92	1.94	24	4
1:A:27:VAL:HG13	1:A:31:GLU:O	0.88	1.67	26	7
1:A:10:GLU:O	1:A:11:LEU:HD23	0.85	1.69	8	1
1:B:16:VAL:HG22	1:B:33:MET:HE3	0.81	1.52	3	3
1:A:17:LYS:HZ1	1:A:19:LEU:HD12	0.81	1.33	7	1
1:B:8:LYS:CG	1:B:15:VAL:HG22	0.79	2.07	22	9
1:B:8:LYS:HB2	1:B:15:VAL:HG22	0.78	1.55	23	7
1:A:14:GLN:OE1	1:B:26:LEU:HD21	0.77	1.80	9	2
1:B:7:TYR:CD2	1:B:26:LEU:HD12	0.76	2.16	13	2
1:B:16:VAL:HG21	1:B:33:MET:CE	0.75	2.12	14	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LEU:HD11	1:A:31:GLU:HG3	0.74	1.58	8	1
1:B:8:LYS:HG2	1:B:15:VAL:HG22	0.74	1.57	22	1
1:A:16:VAL:HG21	1:A:33:MET:CE	0.73	2.12	10	10
1:A:11:LEU:HD11	1:A:31:GLU:OE1	0.72	1.84	6	6
1:A:11:LEU:HD22	1:A:31:GLU:OE1	0.72	1.85	7	1
1:A:7:TYR:CZ	1:A:35:LYS:HB3	0.71	2.21	24	16
1:B:11:LEU:HD23	1:B:29:CYS:SG	0.70	2.27	9	10
1:B:16:VAL:HG22	1:B:33:MET:SD	0.70	2.27	6	9
1:B:16:VAL:HG21	1:B:33:MET:HE1	0.69	1.62	14	6
1:A:14:GLN:HE22	1:B:26:LEU:HD21	0.69	1.48	18	1
1:A:26:LEU:HD21	1:B:14:GLN:NE2	0.68	2.04	22	8
1:B:8:LYS:HG3	1:B:15:VAL:HG22	0.67	1.66	21	9
1:A:26:LEU:HD21	1:B:14:GLN:OE1	0.66	1.89	5	2
1:A:11:LEU:HD23	1:A:29:CYS:CB	0.66	2.20	9	4
1:A:16:VAL:HG12	1:B:17:LYS:O	0.65	1.92	9	2
1:A:16:VAL:HG21	1:A:33:MET:HE1	0.64	1.68	11	6
1:A:11:LEU:HD23	1:A:29:CYS:SG	0.64	2.33	7	2
1:A:8:LYS:HG3	1:A:15:VAL:HG22	0.63	1.69	24	17
1:A:7:TYR:CE1	1:A:35:LYS:HB3	0.63	2.28	24	2
1:B:16:VAL:CG2	1:B:33:MET:CE	0.62	2.76	28	9
1:A:18:VAL:HA	1:B:16:VAL:HG12	0.62	1.71	12	14
1:B:11:LEU:HD11	1:B:31:GLU:HG3	0.62	1.71	26	4
1:A:15:VAL:HG21	1:B:20:GLU:OE2	0.60	1.96	8	1
1:B:10:GLU:HG3	1:B:34:VAL:HG21	0.60	1.73	11	2
1:B:4:GLY:H	1:B:17:LYS:NZ	0.59	1.95	17	1
1:B:8:LYS:HD3	1:B:9:CYS:O	0.58	1.98	24	1
1:A:19:LEU:O	1:A:19:LEU:HD13	0.58	1.99	15	3
1:B:8:LYS:CB	1:B:15:VAL:HG22	0.58	2.29	1	5
1:A:14:GLN:OE1	1:A:16:VAL:HG13	0.57	1.99	29	5
1:A:26:LEU:HB3	1:A:33:MET:HE2	0.57	1.75	27	2
1:A:17:LYS:O	1:B:16:VAL:HA	0.57	1.99	1	27
1:A:11:LEU:HD23	1:A:29:CYS:HB3	0.57	1.75	2	2
1:A:8:LYS:CG	1:A:15:VAL:HG22	0.57	2.30	9	9
1:A:11:LEU:HD12	1:A:29:CYS:SG	0.57	2.39	8	1
1:B:7:TYR:CE2	1:B:35:LYS:HB3	0.57	2.35	3	22
1:B:16:VAL:HG22	1:B:33:MET:HE1	0.57	1.73	24	2
1:B:5:ASP:O	1:B:18:VAL:HG23	0.56	1.99	25	2
1:A:19:LEU:HD12	1:A:20:GLU:OE1	0.56	2.01	6	1
1:A:31:GLU:CG	1:A:32:ASP:N	0.56	2.69	12	12
1:A:14:GLN:NE2	1:B:26:LEU:HD21	0.56	2.15	10	4
1:A:7:TYR:CE1	1:A:35:LYS:CB	0.56	2.89	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:VAL:HA	1:B:17:LYS:O	0.55	2.01	25	28
1:A:10:GLU:C	1:A:11:LEU:HD23	0.55	2.22	8	1
1:B:29:CYS:SG	1:B:29:CYS:O	0.55	2.64	9	22
1:B:7:TYR:CG	1:B:26:LEU:HD12	0.55	2.37	13	2
1:B:7:TYR:CE1	1:B:35:LYS:HB2	0.55	2.37	1	24
1:B:16:VAL:CG2	1:B:33:MET:HE1	0.55	2.32	24	4
1:B:25:THR:HG21	1:B:32:ASP:OD2	0.55	2.02	23	4
1:A:17:LYS:O	1:B:16:VAL:CB	0.55	2.55	3	23
1:A:26:LEU:CD2	1:B:14:GLN:OE1	0.55	2.55	3	2
1:A:25:THR:HG21	1:A:32:ASP:OD2	0.55	2.02	5	2
1:A:16:VAL:CG2	1:A:33:MET:CE	0.54	2.85	8	11
1:B:8:LYS:HA	1:B:14:GLN:O	0.54	2.01	19	9
1:B:7:TYR:CZ	1:B:35:LYS:CB	0.54	2.90	1	22
1:A:16:VAL:HG21	1:A:33:MET:HE3	0.54	1.79	2	2
1:B:6:VAL:HG12	1:B:36:GLN:HG3	0.53	1.79	21	5
1:A:27:VAL:HG22	1:A:32:ASP:OD1	0.53	2.02	26	1
1:B:19:LEU:HD13	1:B:19:LEU:O	0.53	2.04	15	1
1:A:11:LEU:HD23	1:A:29:CYS:HB2	0.53	1.81	10	1
1:A:16:VAL:CB	1:B:17:LYS:O	0.52	2.57	25	27
1:A:7:TYR:CE1	1:A:35:LYS:HB2	0.52	2.39	7	13
1:B:7:TYR:CZ	1:B:35:LYS:HB2	0.52	2.39	12	8
1:B:7:TYR:CE2	1:B:35:LYS:HB2	0.52	2.39	18	2
1:B:27:VAL:HG22	1:B:32:ASP:OD1	0.52	2.05	28	1
1:A:7:TYR:CZ	1:A:35:LYS:HB2	0.52	2.40	27	13
1:A:19:LEU:HD13	1:A:19:LEU:C	0.52	2.25	9	2
1:A:7:TYR:O	1:A:33:MET:CE	0.52	2.58	25	1
1:A:7:TYR:CZ	1:A:35:LYS:CB	0.51	2.93	7	11
1:B:17:LYS:HG2	1:B:18:VAL:N	0.51	2.19	22	1
1:A:11:LEU:HD12	1:A:29:CYS:HB2	0.51	1.82	3	2
1:A:16:VAL:HG22	1:A:33:MET:CE	0.51	2.35	24	2
1:B:7:TYR:CZ	1:B:35:LYS:HB3	0.51	2.41	6	24
1:A:14:GLN:OE1	1:A:16:VAL:CG1	0.51	2.59	20	6
1:A:16:VAL:HG12	1:B:18:VAL:HA	0.51	1.83	12	13
1:B:25:THR:CG2	1:B:32:ASP:OD1	0.51	2.59	18	4
1:A:7:TYR:O	1:A:33:MET:HE1	0.50	2.07	23	1
1:A:11:LEU:CD2	1:A:31:GLU:OE1	0.50	2.59	7	1
1:B:25:THR:HG23	1:B:32:ASP:OD1	0.50	2.06	9	2
1:B:28:CYS:O	1:B:29:CYS:SG	0.50	2.70	12	29
1:B:10:GLU:CG	1:B:34:VAL:HG21	0.50	2.36	11	2
1:A:11:LEU:CD1	1:A:31:GLU:OE1	0.50	2.59	14	2
1:A:7:TYR:CE2	1:A:35:LYS:HB2	0.50	2.41	25	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:27:VAL:HG13	1:B:31:GLU:O	0.50	2.05	6	4
1:B:25:THR:CG2	1:B:32:ASP:OD2	0.50	2.59	21	3
1:A:17:LYS:O	1:B:16:VAL:CA	0.50	2.60	1	14
1:A:18:VAL:HG12	1:A:18:VAL:O	0.49	2.07	6	2
1:A:15:VAL:CG2	1:B:20:GLU:OE2	0.49	2.60	8	1
1:A:16:VAL:HG22	1:A:33:MET:HE1	0.49	1.84	23	2
1:A:12:CYS:CB	1:B:23:GLY:HA2	0.49	2.37	18	1
1:A:16:VAL:CA	1:B:17:LYS:O	0.49	2.61	25	13
1:A:6:VAL:HG22	1:A:17:LYS:HG3	0.49	1.84	10	1
1:B:8:LYS:CG	1:B:9:CYS:N	0.48	2.75	5	4
1:A:17:LYS:HZ1	1:A:19:LEU:HD23	0.48	1.68	6	1
1:A:7:TYR:CE2	1:A:35:LYS:HB3	0.48	2.42	11	6
1:A:16:VAL:CG1	1:B:17:LYS:O	0.48	2.61	9	1
1:B:29:CYS:O	1:B:31:GLU:N	0.48	2.47	13	19
1:B:28:CYS:SG	1:B:33:MET:HG3	0.48	2.48	3	3
1:A:32:ASP:O	1:A:33:MET:C	0.48	2.52	23	6
1:A:7:TYR:CE1	1:A:35:LYS:HG3	0.48	2.44	20	1
1:A:8:LYS:HD2	1:A:15:VAL:HG22	0.48	1.85	28	3
1:A:19:LEU:C	1:A:19:LEU:HD13	0.47	2.29	6	1
1:A:28:CYS:O	1:A:29:CYS:C	0.47	2.51	7	3
1:B:21:GLU:CG	1:B:22:GLY:N	0.47	2.77	25	2
1:B:32:ASP:O	1:B:33:MET:C	0.47	2.52	5	8
1:A:19:LEU:HD13	1:A:19:LEU:O	0.47	2.10	6	1
1:B:14:GLN:OE1	1:B:16:VAL:CG1	0.47	2.62	21	1
1:A:35:LYS:CE	1:A:36:GLN:O	0.47	2.63	2	2
1:A:16:VAL:HG22	1:A:33:MET:HE3	0.47	1.86	24	1
1:B:27:VAL:CG1	1:B:28:CYS:N	0.46	2.77	16	6
1:B:16:VAL:CG2	1:B:33:MET:SD	0.46	3.02	6	3
1:B:16:VAL:HG21	1:B:33:MET:HE2	0.46	1.88	11	1
1:B:8:LYS:HB2	1:B:8:LYS:NZ	0.46	2.26	19	1
1:B:14:GLN:OE1	1:B:33:MET:SD	0.46	2.74	3	1
1:A:27:VAL:CG1	1:A:31:GLU:O	0.46	2.55	26	2
1:B:9:CYS:SG	1:B:31:GLU:OE1	0.46	2.74	17	1
1:B:20:GLU:OE1	1:B:21:GLU:N	0.46	2.49	11	2
1:A:14:GLN:OE1	1:B:22:GLY:N	0.46	2.49	5	4
1:B:29:CYS:O	1:B:29:CYS:SG	0.46	2.74	18	1
1:B:14:GLN:OE1	1:B:16:VAL:HG13	0.46	2.11	21	2
1:A:31:GLU:HG2	1:A:32:ASP:N	0.46	2.26	5	11
1:A:22:GLY:N	1:B:14:GLN:OE1	0.45	2.49	7	4
1:B:28:CYS:N	1:B:31:GLU:O	0.45	2.50	16	2
1:B:14:GLN:HG3	1:B:15:VAL:N	0.45	2.26	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:28:CYS:SG	1:B:33:MET:SD	0.45	3.14	2	5
1:B:18:VAL:HG12	1:B:18:VAL:O	0.45	2.11	4	1
1:A:26:LEU:CB	1:A:33:MET:HE2	0.45	2.42	27	1
1:A:29:CYS:O	1:A:30:GLY:C	0.45	2.54	26	1
1:B:17:LYS:HG3	1:B:18:VAL:N	0.44	2.26	10	5
1:A:16:VAL:HG22	1:A:33:MET:SD	0.44	2.52	26	1
1:A:12:CYS:SG	1:B:22:GLY:O	0.44	2.75	18	1
1:B:8:LYS:HD3	1:B:8:LYS:C	0.44	2.33	24	1
1:B:8:LYS:HG3	1:B:36:GLN:NE2	0.44	2.28	19	1
1:A:17:LYS:HG2	1:A:18:VAL:N	0.44	2.27	9	7
1:A:6:VAL:HG12	1:A:36:GLN:HG3	0.44	1.88	9	1
1:A:16:VAL:CG2	1:A:33:MET:HE1	0.44	2.42	25	2
1:A:16:VAL:HG11	1:B:26:LEU:HD21	0.44	1.88	20	1
1:A:26:LEU:CD2	1:B:14:GLN:NE2	0.44	2.79	1	2
1:A:35:LYS:NZ	1:A:36:GLN:O	0.44	2.49	1	1
1:B:11:LEU:HD11	1:B:31:GLU:CG	0.44	2.41	26	2
1:A:9:CYS:SG	1:A:31:GLU:OE1	0.44	2.76	12	1
1:A:4:GLY:HA2	1:A:17:LYS:CE	0.44	2.42	5	1
1:B:4:GLY:HA2	1:B:17:LYS:CE	0.44	2.43	11	2
1:B:8:LYS:CD	1:B:15:VAL:HG22	0.44	2.43	8	2
1:A:17:LYS:O	1:B:16:VAL:HG12	0.44	2.12	3	2
1:A:14:GLN:NE2	1:B:26:LEU:HD23	0.44	2.28	6	2
1:A:17:LYS:O	1:B:16:VAL:HB	0.43	2.12	3	4
1:B:29:CYS:C	1:B:31:GLU:N	0.43	2.71	9	13
1:A:20:GLU:O	1:A:21:GLU:O	0.43	2.36	9	1
1:A:8:LYS:HB2	1:A:15:VAL:HG22	0.43	1.90	19	1
1:A:9:CYS:O	1:A:31:GLU:OE1	0.43	2.35	13	3
1:A:7:TYR:CE2	1:A:35:LYS:HD3	0.43	2.48	3	1
1:A:7:TYR:HA	1:A:34:VAL:O	0.43	2.12	3	1
1:A:9:CYS:O	1:A:10:GLU:HB2	0.43	2.13	7	3
1:A:14:GLN:HG2	1:B:20:GLU:O	0.43	2.12	18	1
1:B:17:LYS:CG	1:B:18:VAL:N	0.43	2.80	3	5
1:A:14:GLN:HE22	1:B:26:LEU:HD23	0.43	1.73	6	1
1:A:10:GLU:HG3	1:A:34:VAL:CG2	0.43	2.44	1	1
1:A:16:VAL:CG2	1:A:33:MET:HE3	0.43	2.44	6	1
1:B:8:LYS:HG2	1:B:9:CYS:N	0.43	2.29	17	1
1:B:6:VAL:HG22	1:B:17:LYS:HG3	0.43	1.91	26	1
1:A:18:VAL:HG22	1:A:26:LEU:HD11	0.43	1.91	20	1
1:A:7:TYR:CZ	1:A:35:LYS:HD3	0.43	2.49	3	1
1:A:15:VAL:HG21	1:B:20:GLU:OE1	0.43	2.14	15	1
1:A:35:LYS:CD	1:A:36:GLN:O	0.42	2.66	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:GLU:HG3	1:A:32:ASP:N	0.42	2.29	12	1
1:B:8:LYS:HD3	1:B:9:CYS:N	0.42	2.29	19	2
1:A:19:LEU:HD22	1:B:15:VAL:HG11	0.42	1.91	14	1
1:A:14:GLN:NE2	1:B:26:LEU:CD2	0.42	2.83	6	1
1:B:29:CYS:O	1:B:30:GLY:C	0.42	2.58	8	17
1:A:9:CYS:O	1:A:31:GLU:OE2	0.42	2.36	7	2
1:B:7:TYR:HB3	1:B:33:MET:CE	0.42	2.44	3	2
1:A:15:VAL:CB	1:B:20:GLU:OE2	0.42	2.68	8	1
1:B:7:TYR:O	1:B:33:MET:SD	0.42	2.78	5	2
1:A:10:GLU:HG3	1:A:34:VAL:HG21	0.42	1.90	28	2
1:A:16:VAL:HB	1:B:17:LYS:O	0.42	2.14	12	2
1:A:8:LYS:CB	1:A:36:GLN:NE2	0.42	2.83	22	3
1:B:33:MET:HB3	1:B:33:MET:HE2	0.42	1.75	23	1
1:B:20:GLU:O	1:B:21:GLU:O	0.42	2.37	2	4
1:B:7:TYR:O	1:B:16:VAL:HG22	0.42	2.14	19	1
1:A:7:TYR:C	1:A:33:MET:CE	0.42	2.88	25	1
1:B:9:CYS:SG	1:B:31:GLU:OE2	0.42	2.78	19	2
1:A:15:VAL:HG12	1:B:19:LEU:CB	0.41	2.45	8	1
1:B:4:GLY:N	1:B:17:LYS:NZ	0.41	2.65	17	1
1:A:11:LEU:HB2	1:A:29:CYS:SG	0.41	2.54	26	1
1:A:16:VAL:HG21	1:A:33:MET:HE2	0.41	1.92	8	1
1:A:29:CYS:C	1:A:31:GLU:N	0.41	2.73	23	2
1:A:17:LYS:CG	1:A:18:VAL:N	0.41	2.83	29	1
1:A:8:LYS:HA	1:A:14:GLN:O	0.41	2.15	2	1
1:A:29:CYS:SG	1:A:29:CYS:O	0.41	2.79	7	1
1:A:13:GLY:O	1:B:20:GLU:CD	0.41	2.58	22	2
1:A:8:LYS:HE3	1:A:15:VAL:CG2	0.41	2.46	11	1
1:A:28:CYS:O	1:A:31:GLU:HB3	0.41	2.15	7	1
1:B:28:CYS:O	1:B:31:GLU:O	0.41	2.38	17	1
1:A:21:GLU:C	1:B:14:GLN:OE1	0.41	2.59	9	1
1:A:20:GLU:OE2	1:A:21:GLU:N	0.41	2.54	16	1
1:B:8:LYS:O	1:B:34:VAL:O	0.41	2.38	4	1
1:A:3:GLU:OE2	1:A:19:LEU:O	0.41	2.39	7	2
1:A:17:LYS:NZ	1:A:19:LEU:HD12	0.41	2.16	7	1
1:B:27:VAL:HG22	1:B:31:GLU:O	0.41	2.16	18	1
1:B:8:LYS:CG	1:B:36:GLN:OE1	0.41	2.69	24	1
1:B:20:GLU:O	1:B:21:GLU:C	0.40	2.59	12	1
1:A:8:LYS:CD	1:A:15:VAL:HG22	0.40	2.46	14	1
1:B:20:GLU:OE2	1:B:21:GLU:O	0.40	2.39	18	1
1:A:8:LYS:HB2	1:A:36:GLN:NE2	0.40	2.31	1	1
1:A:8:LYS:HD2	1:A:15:VAL:CG2	0.40	2.46	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:32:ASP:O	1:B:32:ASP:OD1	0.40	2.40	14	1
1:B:14:GLN:HG2	1:B:15:VAL:N	0.40	2.30	23	1
1:A:16:VAL:CG2	1:A:33:MET:SD	0.40	3.09	26	1
1:A:11:LEU:HG	1:A:12:CYS:N	0.40	2.31	5	1
1:A:8:LYS:CG	1:A:9:CYS:N	0.40	2.84	19	1
1:A:17:LYS:HB3	1:A:17:LYS:HZ2	0.40	1.75	23	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	33/36 (92%)	29±1 (87±4%)	4±1 (12±3%)	0±1 (1±2%)	16	63
1	B	32/36 (89%)	24±1 (77±3%)	6±1 (19±4%)	1±1 (4±3%)	5	29
All	All	1885/2088 (90%)	1538 (82%)	295 (16%)	52 (3%)	8	42

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	30	GLY	18
1	B	21	GLU	11
1	B	33	MET	9
1	A	33	MET	6
1	A	3	GLU	3
1	A	21	GLU	2
1	B	23	GLY	2
1	A	29	CYS	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	28/29 (97%)	24±1 (87±4%)	4±1 (13±4%)	7 48
1	B	27/29 (93%)	22±2 (81±6%)	5±2 (19±6%)	4 35
All	All	1595/1682 (95%)	1336 (84%)	259 (16%)	5 41

All 26 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	35	LYS	27
1	A	35	LYS	26
1	B	19	LEU	25
1	A	17	LYS	19
1	B	31	GLU	19
1	A	19	LEU	18
1	B	33	MET	17
1	B	17	LYS	17
1	A	32	ASP	11
1	B	32	ASP	11
1	B	11	LEU	9
1	A	31	GLU	9
1	B	20	GLU	7
1	B	5	ASP	7
1	B	8	LYS	6
1	A	33	MET	5
1	A	20	GLU	5
1	A	5	ASP	5
1	A	25	THR	3
1	B	10	GLU	3
1	A	14	GLN	3
1	B	14	GLN	2
1	A	26	LEU	2
1	B	25	THR	1
1	A	10	GLU	1
1	B	6	VAL	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 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 (i)

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

Total number of shifts	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 (i)

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

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 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	^{1}H	^{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%)

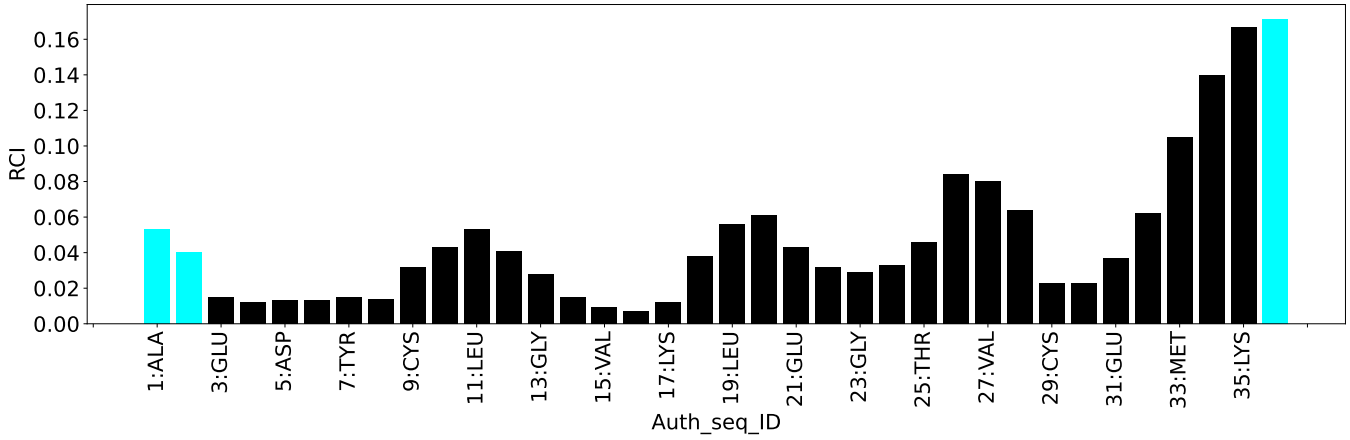
7.1.4 Statistically unusual chemical shifts (i)

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 (i)

8.1 Conformationally restricting restraints (i)

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)	170
Medium range (|i-j|>1 and |i-j|<5)	62
Long range (|i-j|≥5)	188
Inter-chain	26
Hydrogen bond restraints	60
Disulfide bond restraints	26
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	9.3
Number of long range restraints per residue[1]	3.2

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

8.2 Residual restraint violations (i)

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 (i)

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)	25.4	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 (i)

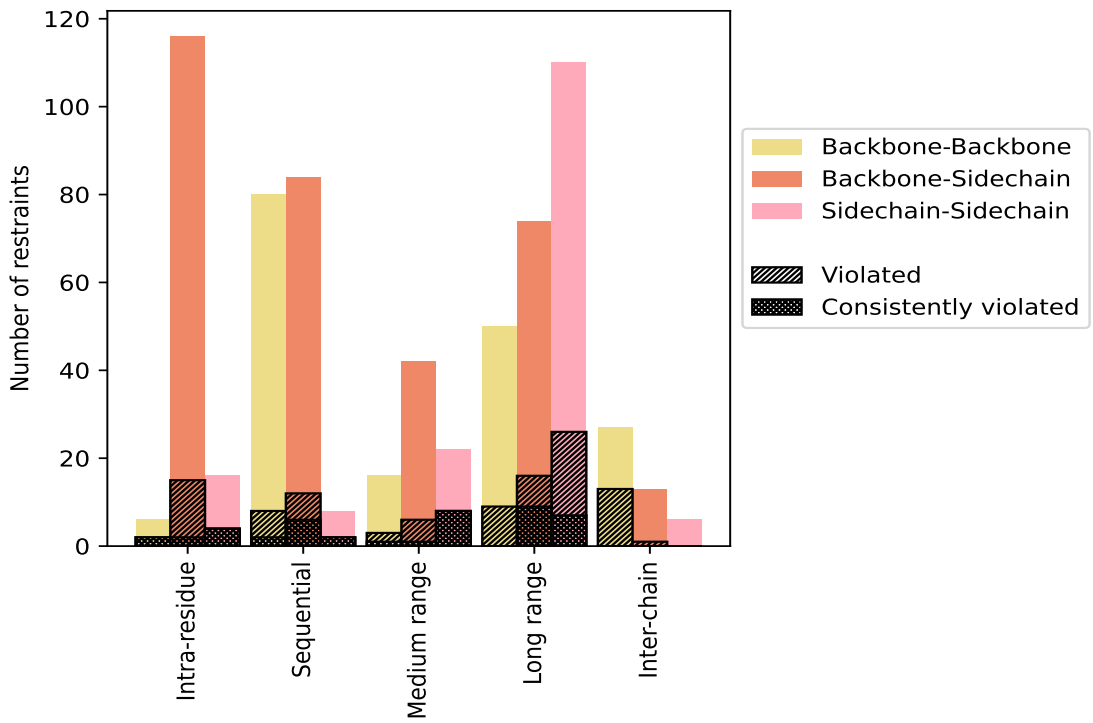
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	138	20.6	21	15.2	3.1	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	15	12.9	2.2	2	1.7	0.3
Sidechain-Sidechain	16	2.4	4	25.0	0.6	4	25.0	0.6
Sequential (|i-j|=1)	170	25.4	22	12.9	3.3	10	5.9	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	6	0.9	2	33.3	0.3	2	33.3	0.3
Medium range (|i-j|>1 & |i-j|<5)	62	9.3	13	21.0	1.9	10	16.1	1.5
Backbone-Backbone	8	1.2	2	25.0	0.3	1	12.5	0.1
Backbone-Sidechain	34	5.1	3	8.8	0.4	1	2.9	0.1
Sidechain-Sidechain	20	3.0	8	40.0	1.2	8	40.0	1.2
Long range (|i-j|≥5)	188	28.1	40	21.3	6.0	16	8.5	2.4
Backbone-Backbone	18	2.7	5	27.8	0.7	0	0.0	0.0
Backbone-Sidechain	74	11.0	16	21.6	2.4	9	12.2	1.3
Sidechain-Sidechain	96	14.3	19	19.8	2.8	7	7.3	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	14	23.3	2.1	0	0.0	0.0
Disulfide bond	26	3.9	10	38.5	1.5	0	0.0	0.0
Total	670	100.0	125	18.7	18.7	44	6.6	6.6
Backbone-Backbone	179	26.7	35	19.6	5.2	5	2.8	0.7
Backbone-Sidechain	329	49.1	50	15.2	7.5	18	5.5	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 disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	11	12	13	31	5	72	1.07	3.64	1.16	0.34
2	13	15	12	23	3	66	1.11	3.79	1.11	0.58
3	15	11	13	27	6	72	1.04	3.76	1.14	0.35
4	12	13	13	29	4	71	1.07	3.83	1.13	0.4
5	13	13	13	27	7	73	1.08	4.03	1.17	0.35
6	10	12	12	26	6	66	1.13	4.08	1.18	0.58
7	13	11	12	28	4	68	1.13	3.88	1.18	0.51
8	11	15	12	33	3	74	1.05	3.71	1.12	0.38
9	11	13	13	25	7	69	1.09	4.0	1.15	0.4
10	13	11	12	26	4	66	1.12	3.74	1.15	0.52
11	14	13	13	26	3	69	1.11	3.6	1.19	0.37

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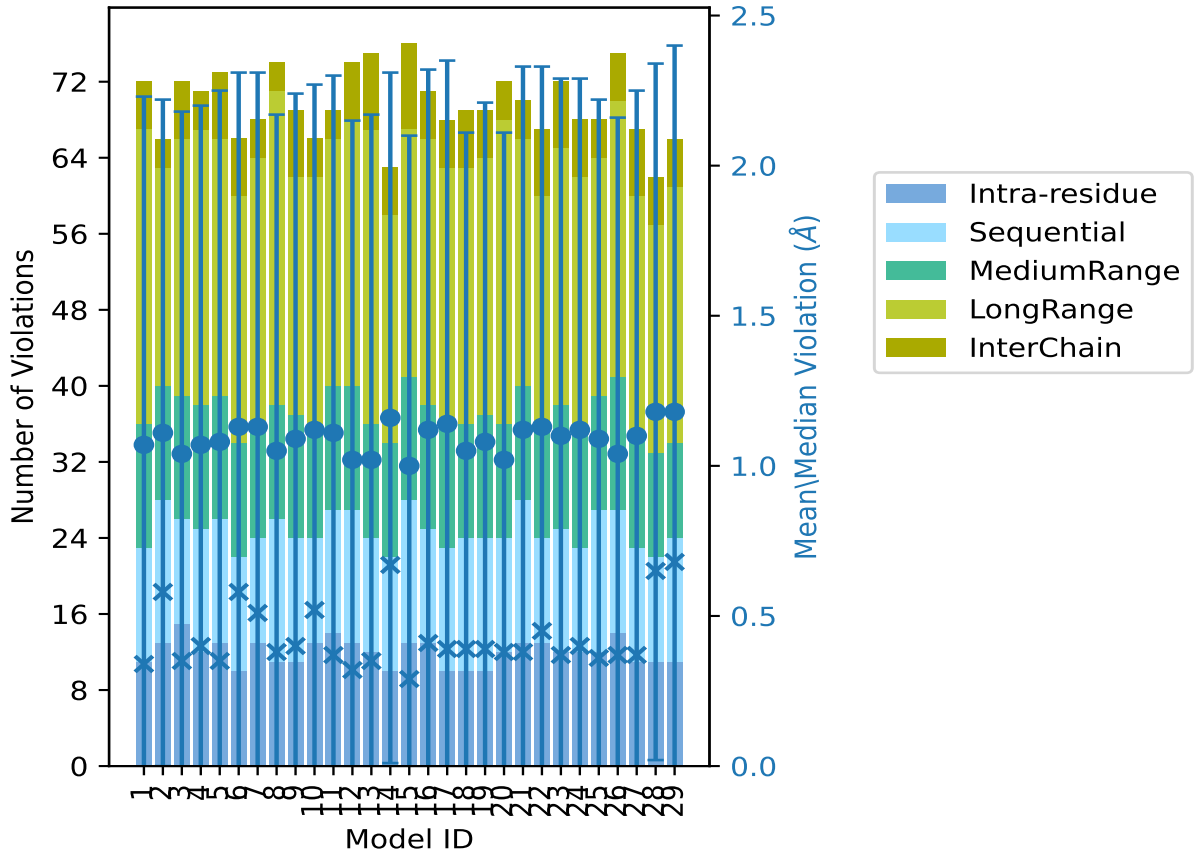
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	13	14	13	28	6	74	1.02	3.63	1.13	0.32
13	12	12	12	31	8	75	1.02	3.73	1.15	0.35
14	10	12	12	24	5	63	1.16	3.65	1.15	0.67
15	13	15	13	26	9	76	1.0	3.63	1.1	0.29
16	13	12	13	28	5	71	1.12	3.83	1.2	0.41
17	10	13	13	27	5	68	1.14	4.11	1.21	0.39
18	10	14	12	27	6	69	1.05	3.47	1.06	0.39
19	10	14	13	27	5	69	1.08	3.57	1.13	0.39
20	12	12	12	32	4	72	1.02	3.55	1.09	0.38
21	13	15	12	26	4	70	1.12	4.04	1.21	0.38
22	13	11	12	24	7	67	1.13	4.1	1.2	0.45
23	12	13	13	27	7	72	1.1	3.89	1.19	0.37
24	12	11	12	27	6	68	1.12	3.87	1.17	0.4
25	12	15	12	25	4	68	1.09	3.59	1.13	0.36
26	14	13	14	29	5	75	1.04	3.61	1.12	0.37
27	11	12	12	25	7	67	1.1	3.69	1.15	0.37
28	11	11	11	24	5	62	1.18	3.64	1.16	0.65
29	11	13	10	27	5	66	1.18	3.93	1.22	0.68

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

9.2.1 Bar graph : Distance Violation statistics for each model (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, 483(IR:117, SQ:148, MR:49, LR:148, 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]	%
3	2	0	5	1	11	1	3.4
0	1	1	2	1	5	2	6.9
0	2	0	1	0	3	3	10.3
2	1	0	3	0	6	4	13.8
1	0	0	2	0	3	5	17.2
0	1	0	0	0	1	6	20.7

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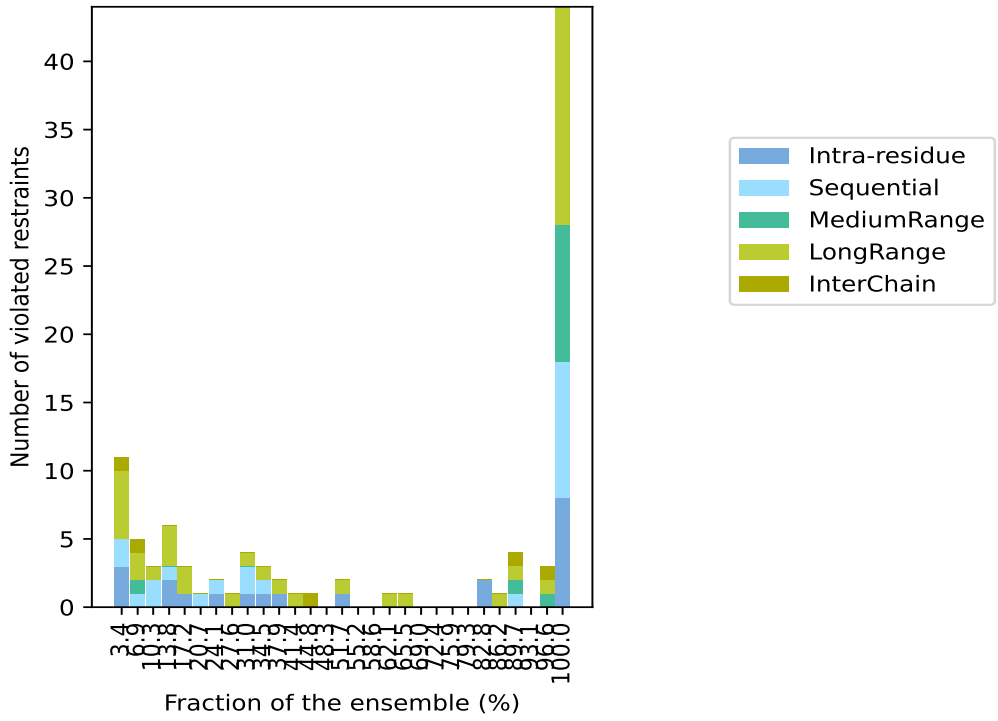
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	1	0	0	0	2	7	24.1
0	0	0	1	0	1	8	27.6
1	2	0	1	0	4	9	31.0
1	1	0	1	0	3	10	34.5
1	0	0	1	0	2	11	37.9
0	0	0	1	0	1	12	41.4
0	0	0	0	1	1	13	44.8
0	0	0	0	0	0	14	48.3
1	0	0	1	0	2	15	51.7
0	0	0	0	0	0	16	55.2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

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

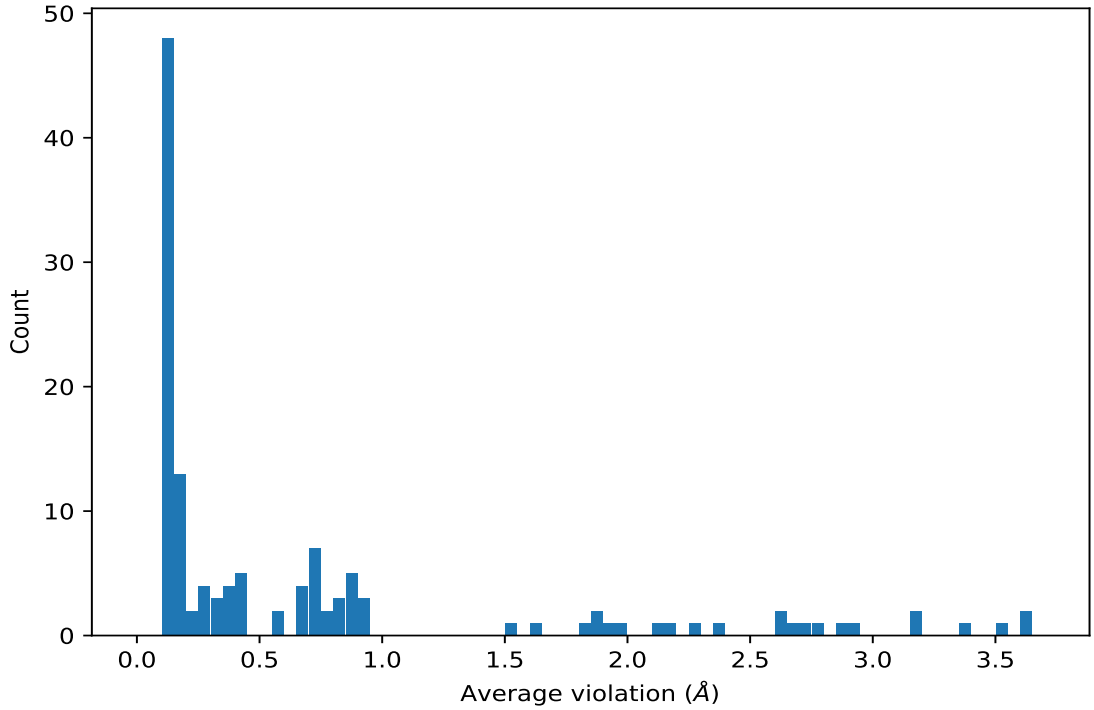
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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:B:6:VAL:HB	1:B:7:TYR:HD2	29	3.62	0.07	3.63
(2,245)	1:B:5:ASP:HB2	1:B:7:TYR:HE2	29	3.61	0.4	3.7
(2,30)	1:A:6:VAL:HB	1:A:7:TYR:HD2	29	3.51	0.07	3.51
(2,18)	1:A:5:ASP:HB2	1:A:7:TYR:HE2	29	3.35	0.29	3.31
(2,26)	1:A:6:VAL:H	1:A:7:TYR:HE2	29	3.19	0.2	3.22
(2,253)	1:B:6:VAL:H	1:B:7:TYR:HE2	29	3.16	0.14	3.16
(2,246)	1:B:5:ASP:HB2	1:B:7:TYR:HD2	29	2.94	0.38	2.95
(2,249)	1:B:5:ASP:HB3	1:B:7:TYR:HE2	29	2.88	0.2	2.89
(2,19)	1:A:5:ASP:HB2	1:A:7:TYR:HD2	29	2.79	0.27	2.76
(2,22)	1:A:5:ASP:HB3	1:A:7:TYR:HE2	29	2.74	0.23	2.78
(2,27)	1:A:6:VAL:H	1:A:7:TYR:HD2	29	2.69	0.14	2.71
(2,254)	1:B:6:VAL:H	1:B:7:TYR:HD2	29	2.65	0.11	2.64
(2,282)	1:B:7:TYR:HD1	1:B:34:VAL:H	29	2.61	0.38	2.5
(2,55)	1:A:7:TYR:HD1	1:A:34:VAL:H	29	2.37	0.28	2.43
(2,283)	1:B:7:TYR:HD1	1:B:34:VAL:HA	29	2.26	0.17	2.28
(2,280)	1:B:7:TYR:HD1	1:B:33: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:A:7:TYR:HD1	1:A:34:VAL:HA	29	2.11	0.17	2.08
(2,250)	1:B:5:ASP:HB3	1:B:7:TYR:HD2	29	1.98	0.2	1.95
(2,23)	1:A:5:ASP:HB3	1:A:7:TYR:HD2	29	1.93	0.17	1.93
(2,284)	1:B:7:TYR:HE1	1:B:35:LYS:H	29	1.9	0.2	1.86
(2,57)	1:A:7:TYR:HE1	1:A:35:LYS:H	29	1.88	0.24	1.84
(2,53)	1:A:7:TYR:HD1	1:A:33:MET:HB3	29	1.84	0.15	1.82
(2,279)	1:B:7:TYR:HD1	1:B:26:LEU:HG	29	1.62	0.31	1.71
(2,52)	1:A:7:TYR:HD1	1:A:26:LEU:HG	29	1.5	0.28	1.55
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG21	29	0.87	0.11	0.87
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG22	29	0.87	0.11	0.87
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG23	29	0.87	0.11	0.87
(1,83)	1:B:4:GLY:HA3	1:B:17:LYS:HB2	29	0.86	0.1	0.87
(1,83)	1:B:4:GLY:HA3	1:B:17:LYS:HB3	29	0.86	0.1	0.87
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG21	29	0.85	0.12	0.84
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG22	29	0.85	0.12	0.84
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG23	29	0.85	0.12	0.84
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB2	29	0.79	0.13	0.84
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB3	29	0.79	0.13	0.84
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	29	0.74	0.03	0.74
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	29	0.74	0.03	0.74
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	29	0.74	0.03	0.74
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	29	0.73	0.08	0.74
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	29	0.69	0.08	0.67
(2,263)	1:B:7:TYR:H	1:B:7:TYR:HD2	29	0.38	0.03	0.39
(2,36)	1:A:7:TYR:H	1:A:7:TYR:HD2	29	0.37	0.03	0.37
(2,43)	1:A:7:TYR:HB2	1:A:7:TYR:HE2	29	0.36	0.02	0.37
(2,270)	1:B:7:TYR:HB2	1:B:7:TYR:HE2	29	0.36	0.02	0.36
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	29	0.26	0.0	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	29	0.26	0.0	0.26
(2,135)	1:A:18:VAL:H	1:A:19:LEU:H	29	0.25	0.04	0.25
(2,296)	1:B:8:LYS:HA	1:B:33:MET:HB3	29	0.22	0.05	0.21
(2,402)	1:B:28:CYS:HB2	1:B:33:MET:HB2	29	0.21	0.04	0.2
(2,354)	1:B:18:VAL:H	1:B:19:LEU:H	29	0.19	0.03	0.19
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	29	0.18	0.01	0.19
(2,332)	1:B:14:GLN:H	1:B:14:GLN:HA	29	0.18	0.02	0.2
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	29	0.17	0.02	0.17
(2,228)	1:B:1:ALA:HB1	1:B:7:TYR:HE2	28	0.94	0.32	0.98
(2,228)	1:B:1:ALA:HB2	1:B:7:TYR:HE2	28	0.94	0.32	0.98
(2,228)	1:B:1:ALA:HB3	1:B:7:TYR:HE2	28	0.94	0.32	0.98
(2,184)	1:A:27:VAL:HG11	1:A:30:GLY:HA3	28	0.31	0.12	0.3
(2,184)	1:A:27:VAL:HG12	1:A:30:GLY:HA3	28	0.31	0.12	0.3
(2,184)	1:A:27:VAL:HG13	1:A:30: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:A:20:GLU:H	1:B:15:VAL:H	28	0.18	0.04	0.18
(5,14)	2:B:37:ZN:ZN	1:B:28:CYS:CB	26	0.17	0.05	0.16
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	26	0.16	0.04	0.16
(2,115)	1:A:15:VAL:H	1:B:20:GLU:H	26	0.15	0.03	0.16
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	26	0.15	0.03	0.14
(2,1)	1:A:1:ALA:HB1	1:A:7:TYR:HE2	25	0.67	0.34	0.61
(2,1)	1:A:1:ALA:HB2	1:A:7:TYR:HE2	25	0.67	0.34	0.61
(2,1)	1:A:1:ALA:HB3	1:A:7:TYR:HE2	25	0.67	0.34	0.61
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	24	0.15	0.02	0.15
(2,119)	1:A:16:VAL:HA	1:A:16:VAL:HB	24	0.12	0.02	0.12
(3,56)	1:B:26:LEU:O	1:B:33:MET:H	22	0.14	0.02	0.14
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	21	0.14	0.02	0.14
(2,391)	1:B:27:VAL:HA	1:B:33:MET:H	19	0.16	0.03	0.16
(2,264)	1:B:7:TYR:H	1:B:16:VAL:H	18	0.14	0.03	0.14
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	18	0.14	0.03	0.14
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE1	15	0.73	0.39	0.86
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE2	15	0.73	0.39	0.86
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE3	15	0.73	0.39	0.86
(2,336)	1:B:15:VAL:H	1:B:15:VAL:HB	15	0.13	0.02	0.13
(4,10)	1:B:12:CYS:SG	1:B:29:CYS:SG	13	0.16	0.03	0.16
(2,138)	1:A:18:VAL:HA	1:B:16:VAL:HA	13	0.14	0.02	0.13
(4,4)	1:A:12:CYS:SG	1:A:28:CYS:SG	13	0.13	0.01	0.13
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE2	12	0.56	0.19	0.6
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE3	12	0.56	0.19	0.6
(3,52)	1:B:8:LYS:O	1:B:34:VAL:H	12	0.15	0.03	0.16
(3,24)	1:A:17:LYS:O	1:B:17:LYS:H	12	0.14	0.02	0.14
(3,26)	1:A:19:LEU:H	1:B:15:VAL:O	12	0.12	0.01	0.12
(5,11)	2:B:37:ZN:ZN	1:B:12:CYS:CB	11	0.18	0.03	0.19
(2,320)	1:B:11:LEU:HA	1:B:11:LEU:HG	11	0.16	0.03	0.15
(3,30)	1:A:20:GLU:O	1:B:15:VAL:H	11	0.14	0.03	0.12
(5,6)	2:A:37:ZN:ZN	1:A:28:CYS:SG	11	0.12	0.01	0.13
(2,265)	1:B:7:TYR:H	1:B:17:LYS:HA	10	0.15	0.04	0.14
(2,308)	1:B:9:CYS:SG	1:B:12:CYS:H	10	0.13	0.01	0.13
(2,343)	1:B:16:VAL:HB	1:B:17:LYS:H	10	0.12	0.01	0.12
(3,32)	1:A:26:LEU:O	1:A:33:MET:H	10	0.12	0.01	0.12
(2,340)	1:B:16:VAL:HA	1:B:16:VAL:HB	10	0.12	0.01	0.12
(2,38)	1:A:7:TYR:H	1:A:17:LYS:HA	9	0.14	0.03	0.13
(2,207)	1:A:34:VAL:H	1:A:34:VAL:HB	9	0.14	0.02	0.14
(2,210)	1:A:34:VAL:HB	1:A:35:LYS:H	9	0.14	0.02	0.14
(2,421)	1:B:34:VAL:HB	1:B:35:LYS:H	9	0.12	0.01	0.12
(5,10)	2:B:37:ZN:ZN	1:B:12:CYS:CA	8	0.12	0.01	0.12
(2,12)	1:A:4:GLY:HA3	1:A:5:ASP:H	7	0.13	0.01	0.13

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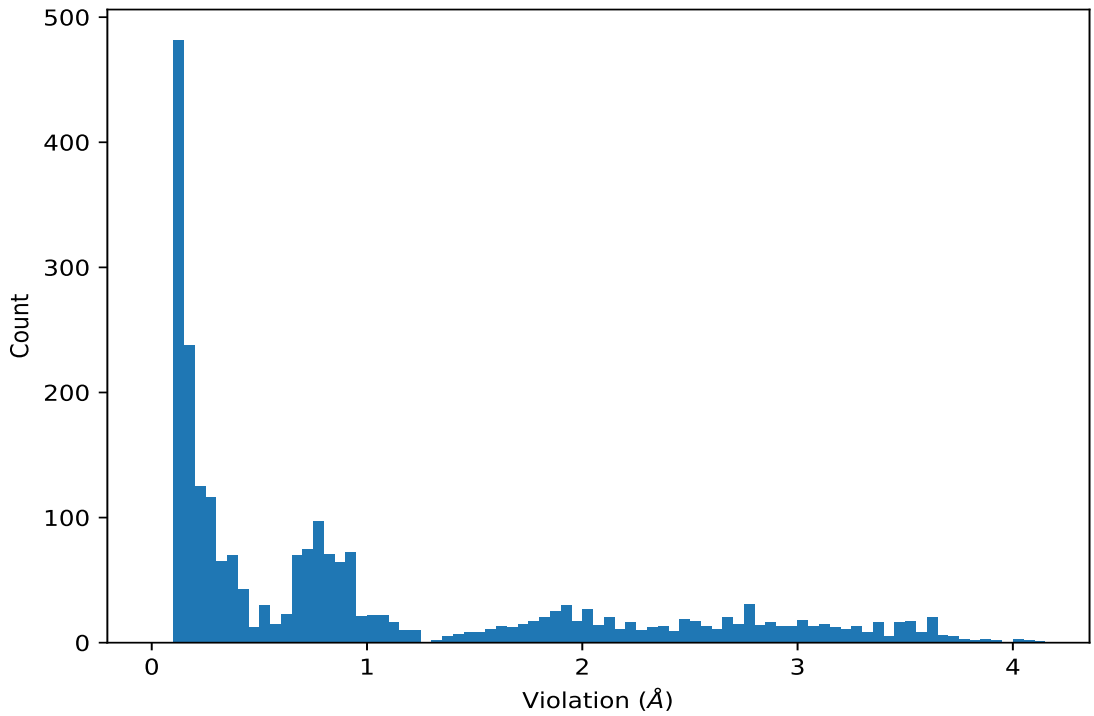
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,365)	1:B:20:GLU:H	1:B:20:GLU:HG3	7	0.12	0.02	0.11
(2,393)	1:B:27:VAL:HB	1:B:28:CYS:H	6	0.13	0.01	0.13
(4,3)	1:A:9:CYS:SG	1:A:29:CYS:SG	6	0.12	0.02	0.12
(5,15)	2:B:37:ZN:ZN	1:B:28:CYS:SG	6	0.12	0.01	0.12
(5,12)	2:B:37:ZN:ZN	1:B:12:CYS:SG	6	0.12	0.01	0.12
(2,54)	1:A:7:TYR:HD1	1:A:33:MET:HE1	5	0.4	0.17	0.37
(2,54)	1:A:7:TYR:HD1	1:A:33:MET:HE2	5	0.4	0.17	0.37
(2,54)	1:A:7:TYR:HD1	1:A:33:MET:HE3	5	0.4	0.17	0.37
(2,89)	1:A:11:LEU:H	1:A:11:LEU:HG	5	0.16	0.03	0.16
(2,37)	1:A:7:TYR:H	1:A:16:VAL:H	5	0.14	0.02	0.13
(3,36)	1:A:27:VAL:O	1:B:27:VAL:H	5	0.12	0.0	0.12
(4,5)	1:A:12:CYS:SG	1:A:29:CYS:SG	4	0.19	0.05	0.2
(2,113)	1:A:15:VAL:H	1:A:15:VAL:HB	4	0.14	0.02	0.14
(2,147)	1:A:20:GLU:H	1:A:20:GLU:HG3	4	0.13	0.02	0.13
(5,17)	2:B:37:ZN:ZN	1:B:29:CYS:CB	4	0.13	0.01	0.12
(2,239)	1:B:4:GLY:HA3	1:B:5:ASP:H	4	0.12	0.01	0.12
(3,18)	1:A:15:VAL:O	1:B:19:LEU:H	4	0.12	0.01	0.12
(5,16)	2:B:37:ZN:ZN	1:B:29:CYS:CA	4	0.12	0.01	0.12
(2,69)	1:A:8:LYS:HA	1:A:33:MET:HB3	4	0.12	0.01	0.12
(1,98)	1:B:7:TYR:HE2	1:B:35:LYS:HE2	3	0.44	0.15	0.37
(1,98)	1:B:7:TYR:HE2	1:B:35:LYS:HE3	3	0.44	0.15	0.37
(3,14)	1:A:9:CYS:H	1:A:14:GLN:O	3	0.12	0.01	0.11
(2,124)	1:A:16:VAL:HB	1:A:17:LYS:H	3	0.11	0.0	0.11
(2,348)	1:B:17:LYS:HA	1:B:18:VAL:H	3	0.11	0.0	0.11
(5,2)	2:A:37:ZN:ZN	1:A:12:CYS:CB	2	0.3	0.0	0.3
(5,7)	2:A:37:ZN:ZN	1:A:29:CYS:CA	2	0.15	0.02	0.15
(2,129)	1:A:17:LYS:HA	1:A:18:VAL:H	2	0.12	0.01	0.12
(2,303)	1:B:9:CYS:HB2	1:B:13:GLY:H	2	0.12	0.0	0.12
(2,122)	1:A:16:VAL:HA	1:B:18:VAL:HA	2	0.11	0.0	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,284)	1:B:7:TYR:HE1	1:B:35:LYS:H	21	1.9
(2,283)	1:B:7:TYR:HD1	1:B:34:VAL:HA	6	1.9
(2,279)	1:B:7:TYR:HD1	1:B:26:LEU:HG	1	1.9
(2,250)	1:B:5:ASP:HB3	1:B:7:TYR:HD2	15	1.9
(2,250)	1:B:5:ASP:HB3	1:B:7:TYR:HD2	28	1.9
(2,57)	1:A:7:TYR:HE1	1:A:35:LYS:H	18	1.89
(2,55)	1:A:7:TYR:HD1	1:A:34:VAL:H	8	1.89
(2,284)	1:B:7:TYR:HE1	1:B:35:LYS:H	17	1.89
(2,53)	1:A:7:TYR:HD1	1:A:33:MET:HB3	1	1.88
(2,279)	1:B:7:TYR:HD1	1:B:26:LEU:HG	17	1.88
(2,279)	1:B:7:TYR:HD1	1:B:26:LEU:HG	8	1.87
(2,250)	1:B:5:ASP:HB3	1:B:7:TYR:HD2	8	1.87
(2,23)	1:A:5:ASP:HB3	1:A:7:TYR:HD2	8	1.87
(2,56)	1:A:7:TYR:HD1	1:A:34:VAL:HA	24	1.86
(2,55)	1:A:7:TYR:HD1	1:A:34:VAL:H	9	1.86
(2,284)	1:B:7:TYR:HE1	1:B:35:LYS:H	1	1.86
(2,284)	1:B:7:TYR:HE1	1:B:35:LYS:H	8	1.86
(2,284)	1:B:7:TYR:HE1	1:B:35:LYS:H	11	1.86
(2,284)	1:B:7:TYR:HE1	1:B:35:LYS:H	13	1.86
(2,250)	1:B:5:ASP:HB3	1:B:7:TYR:HD2	24	1.86
(2,53)	1:A:7:TYR:HD1	1:A:33:MET:HB3	8	1.85
(2,53)	1:A:7:TYR:HD1	1:A:33:MET:HB3	24	1.85
(2,284)	1:B:7:TYR:HE1	1:B:35:LYS:H	14	1.85
(2,57)	1:A:7:TYR:HE1	1:A:35:LYS:H	11	1.84
(2,57)	1:A:7:TYR:HE1	1:A:35:LYS:H	13	1.84
(2,57)	1:A:7:TYR:HE1	1:A:35:LYS:H	20	1.84
(2,284)	1:B:7:TYR:HE1	1:B:35:LYS:H	10	1.84
(2,284)	1:B:7:TYR:HE1	1:B:35:LYS:H	28	1.84
(2,280)	1:B:7:TYR:HD1	1:B:33:MET:HB3	6	1.84
(2,250)	1:B:5:ASP:HB3	1:B:7:TYR:HD2	13	1.84
(2,57)	1:A:7:TYR:HE1	1:A:35:LYS:H	12	1.83
(2,56)	1:A:7:TYR:HD1	1:A:34:VAL:HA	9	1.83
(2,52)	1:A:7:TYR:HD1	1:A:26:LEU:HG	11	1.83
(2,250)	1:B:5:ASP:HB3	1:B:7:TYR:HD2	19	1.83
(2,53)	1:A:7:TYR:HD1	1:A:33:MET:HB3	2	1.82
(2,53)	1:A:7:TYR:HD1	1:A:33:MET:HB3	13	1.82
(2,53)	1:A:7:TYR:HD1	1:A:33:MET:HB3	28	1.82
(2,23)	1:A:5:ASP:HB3	1:A:7:TYR:HD2	14	1.82
(2,55)	1:A:7:TYR:HD1	1:A:34:VAL:H	7	1.81
(2,284)	1:B:7:TYR:HE1	1:B:35:LYS:H	26	1.81
(2,279)	1:B:7:TYR:HD1	1:B:26:LEU:HG	5	1.81
(2,53)	1:A:7:TYR:HD1	1:A:33:MET:HB3	5	1.8

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

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

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

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

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

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

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

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

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

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

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE2	16	0.78
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE3	16	0.78
(2,228)	1:B:1:ALA:HB1	1:B:7:TYR:HE2	8	0.78
(2,228)	1:B:1:ALA:HB2	1:B:7:TYR:HE2	8	0.78
(2,228)	1:B:1:ALA:HB3	1:B:7:TYR:HE2	8	0.78
(1,83)	1:B:4:GLY:HA3	1:B:17:LYS:HB2	10	0.78
(1,83)	1:B:4:GLY:HA3	1:B:17:LYS:HB3	10	0.78
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB2	6	0.78
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB3	6	0.78
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB2	25	0.78
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB3	25	0.78
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	10	0.77
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	20	0.77
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	3	0.77
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	3	0.77
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	3	0.77
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	4	0.77
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	4	0.77
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	4	0.77
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	15	0.77
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	15	0.77
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	15	0.77
(2,1)	1:A:1:ALA:HB1	1:A:7:TYR:HE2	1	0.77
(2,1)	1:A:1:ALA:HB2	1:A:7:TYR:HE2	1	0.77
(2,1)	1:A:1:ALA:HB3	1:A:7:TYR:HE2	1	0.77
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG21	12	0.76
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG22	12	0.76
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG23	12	0.76
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	5	0.76
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	24	0.76
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	25	0.76
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	1	0.76
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	1	0.76
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	1	0.76
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	21	0.76
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	21	0.76
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	21	0.76
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	23	0.76
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	23	0.76
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	23	0.76
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG21	9	0.76
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG22	9	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG23	9	0.76
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG21	14	0.76
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG22	14	0.76
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG23	14	0.76
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE1	12	0.76
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE2	12	0.76
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE3	12	0.76
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE2	18	0.76
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE3	18	0.76
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	6	0.75
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	5	0.75
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	5	0.75
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	5	0.75
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	8	0.75
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	8	0.75
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	8	0.75
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	13	0.75
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	13	0.75
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	13	0.75
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	17	0.75
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	17	0.75
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	17	0.75
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	24	0.75
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	24	0.75
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	24	0.75
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	26	0.75
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	26	0.75
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	26	0.75
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG21	1	0.75
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG22	1	0.75
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG23	1	0.75
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG21	7	0.75
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG22	7	0.75
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG23	7	0.75
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG21	16	0.75
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG22	16	0.75
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG23	16	0.75
(2,1)	1:A:1:ALA:HB1	1:A:7:TYR:HE2	13	0.75
(2,1)	1:A:1:ALA:HB2	1:A:7:TYR:HE2	13	0.75
(2,1)	1:A:1:ALA:HB3	1:A:7:TYR:HE2	13	0.75
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE2	10	0.75
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE3	10	0.75

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

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	20	0.72
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	22	0.72
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	22	0.72
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	22	0.72
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	28	0.72
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	28	0.72
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	28	0.72
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	16	0.72
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	17	0.72
(2,228)	1:B:1:ALA:HB1	1:B:7:TYR:HE2	18	0.72
(2,228)	1:B:1:ALA:HB2	1:B:7:TYR:HE2	18	0.72
(2,228)	1:B:1:ALA:HB3	1:B:7:TYR:HE2	18	0.72
(2,1)	1:A:1:ALA:HB1	1:A:7:TYR:HE2	29	0.72
(2,1)	1:A:1:ALA:HB2	1:A:7:TYR:HE2	29	0.72
(2,1)	1:A:1:ALA:HB3	1:A:7:TYR:HE2	29	0.72
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB2	21	0.72
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB3	21	0.72
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG21	7	0.71
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG22	7	0.71
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG23	7	0.71
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG21	28	0.71
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG22	28	0.71
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG23	28	0.71
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	9	0.71
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	9	0.71
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	9	0.71
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	27	0.71
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	27	0.71
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	27	0.71
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	8	0.71
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	13	0.71
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE2	14	0.71
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE3	14	0.71
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	18	0.7
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	18	0.7
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	18	0.7
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG21	5	0.7
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG22	5	0.7
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG23	5	0.7
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG21	12	0.7
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG22	12	0.7
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG23	12	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	4	0.7
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	11	0.7
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB2	15	0.7
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB3	15	0.7
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB2	19	0.7
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB3	19	0.7
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE2	20	0.7
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE3	20	0.7
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG21	27	0.69
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG22	27	0.69
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG23	27	0.69
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	22	0.69
(2,396)	1:B:27:VAL:HG11	1:B:30:GLY:HA3	2	0.69
(2,396)	1:B:27:VAL:HG12	1:B:30:GLY:HA3	2	0.69
(2,396)	1:B:27:VAL:HG13	1:B:30:GLY:HA3	2	0.69
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG21	17	0.69
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG22	17	0.69
(2,287)	1:B:7:TYR:HD2	1:B:18:VAL:HG23	17	0.69
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	21	0.69
(1,83)	1:B:4:GLY:HA3	1:B:17:LYS:HB2	22	0.69
(1,83)	1:B:4:GLY:HA3	1:B:17:LYS:HB3	22	0.69
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB2	27	0.69
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB3	27	0.69
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG21	6	0.68
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG22	6	0.68
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG23	6	0.68
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	1	0.68
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	13	0.68
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	28	0.68
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	29	0.68
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	22	0.68
(2,228)	1:B:1:ALA:HB1	1:B:7:TYR:HE2	9	0.68
(2,228)	1:B:1:ALA:HB2	1:B:7:TYR:HE2	9	0.68
(2,228)	1:B:1:ALA:HB3	1:B:7:TYR:HE2	9	0.68
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG21	24	0.67
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG22	24	0.67
(2,60)	1:A:7:TYR:HD2	1:A:18:VAL:HG23	24	0.67
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	9	0.67
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	16	0.67
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	9	0.67
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	14	0.67
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	25	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	29	0.67
(1,83)	1:B:4:GLY:HA3	1:B:17:LYS:HB2	18	0.67
(1,83)	1:B:4:GLY:HA3	1:B:17:LYS:HB3	18	0.67
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE2	26	0.67
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE3	26	0.67
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	11	0.66
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	12	0.66
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	23	0.66
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	24	0.66
(2,1)	1:A:1:ALA:HB1	1:A:7:TYR:HE2	8	0.66
(2,1)	1:A:1:ALA:HB2	1:A:7:TYR:HE2	8	0.66
(2,1)	1:A:1:ALA:HB3	1:A:7:TYR:HE2	8	0.66
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	10	0.65
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	15	0.65
(2,1)	1:A:1:ALA:HB1	1:A:7:TYR:HE2	16	0.65
(2,1)	1:A:1:ALA:HB2	1:A:7:TYR:HE2	16	0.65
(2,1)	1:A:1:ALA:HB3	1:A:7:TYR:HE2	16	0.65
(1,98)	1:B:7:TYR:HE2	1:B:35:LYS:HE2	20	0.65
(1,98)	1:B:7:TYR:HE2	1:B:35:LYS:HE3	20	0.65
(2,51)	1:A:7:TYR:HD1	1:A:8:LYS:H	17	0.64
(2,228)	1:B:1:ALA:HB1	1:B:7:TYR:HE2	1	0.64
(2,228)	1:B:1:ALA:HB2	1:B:7:TYR:HE2	1	0.64
(2,228)	1:B:1:ALA:HB3	1:B:7:TYR:HE2	1	0.64
(2,1)	1:A:1:ALA:HB1	1:A:7:TYR:HE2	27	0.64
(2,1)	1:A:1:ALA:HB2	1:A:7:TYR:HE2	27	0.64
(2,1)	1:A:1:ALA:HB3	1:A:7:TYR:HE2	27	0.64
(2,54)	1:A:7:TYR:HD1	1:A:33:MET:HE1	7	0.63
(2,54)	1:A:7:TYR:HD1	1:A:33:MET:HE2	7	0.63
(2,54)	1:A:7:TYR:HD1	1:A:33:MET:HE3	7	0.63
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	23	0.63
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	26	0.63
(2,228)	1:B:1:ALA:HB1	1:B:7:TYR:HE2	20	0.63
(2,228)	1:B:1:ALA:HB2	1:B:7:TYR:HE2	20	0.63
(2,228)	1:B:1:ALA:HB3	1:B:7:TYR:HE2	20	0.63
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	1	0.62
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	2	0.62
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	7	0.62
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	28	0.62
(2,278)	1:B:7:TYR:HD1	1:B:8:LYS:H	6	0.61
(2,1)	1:A:1:ALA:HB1	1:A:7:TYR:HE2	6	0.61
(2,1)	1:A:1:ALA:HB2	1:A:7:TYR:HE2	6	0.61
(2,1)	1:A:1:ALA:HB3	1:A:7:TYR:HE2	6	0.61

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

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:A:1:ALA:HB3	1:A:7:TYR:HE2	25	0.5
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE2	8	0.5
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE3	8	0.5
(2,184)	1:A:27:VAL:HG11	1:A:30:GLY:HA3	12	0.49
(2,184)	1:A:27:VAL:HG12	1:A:30:GLY:HA3	12	0.49
(2,184)	1:A:27:VAL:HG13	1:A:30:GLY:HA3	12	0.49
(2,228)	1:B:1:ALA:HB1	1:B:7:TYR:HE2	3	0.48
(2,228)	1:B:1:ALA:HB2	1:B:7:TYR:HE2	3	0.48
(2,228)	1:B:1:ALA:HB3	1:B:7:TYR:HE2	3	0.48
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB2	13	0.46
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB3	13	0.46
(2,263)	1:B:7:TYR:H	1:B:7:TYR:HD2	22	0.45
(2,228)	1:B:1:ALA:HB1	1:B:7:TYR:HE2	13	0.45
(2,228)	1:B:1:ALA:HB2	1:B:7:TYR:HE2	13	0.45
(2,228)	1:B:1:ALA:HB3	1:B:7:TYR:HE2	13	0.45
(2,36)	1:A:7:TYR:H	1:A:7:TYR:HD2	22	0.44
(2,228)	1:B:1:ALA:HB1	1:B:7:TYR:HE2	27	0.44
(2,228)	1:B:1:ALA:HB2	1:B:7:TYR:HE2	27	0.44
(2,228)	1:B:1:ALA:HB3	1:B:7:TYR:HE2	27	0.44
(2,184)	1:A:27:VAL:HG11	1:A:30:GLY:HA3	7	0.44
(2,184)	1:A:27:VAL:HG12	1:A:30:GLY:HA3	7	0.44
(2,184)	1:A:27:VAL:HG13	1:A:30:GLY:HA3	7	0.44
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE2	4	0.43
(1,22)	1:A:7:TYR:HE2	1:A:35:LYS:HE3	4	0.43
(2,36)	1:A:7:TYR:H	1:A:7:TYR:HD2	16	0.42
(2,36)	1:A:7:TYR:H	1:A:7:TYR:HD2	29	0.42
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE1	2	0.42
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE2	2	0.42
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE3	2	0.42
(2,263)	1:B:7:TYR:H	1:B:7:TYR:HD2	4	0.42
(2,36)	1:A:7:TYR:H	1:A:7:TYR:HD2	24	0.41
(2,263)	1:B:7:TYR:H	1:B:7:TYR:HD2	11	0.41
(2,263)	1:B:7:TYR:H	1:B:7:TYR:HD2	16	0.41
(2,263)	1:B:7:TYR:H	1:B:7:TYR:HD2	19	0.41
(2,263)	1:B:7:TYR:H	1:B:7:TYR:HD2	21	0.41
(2,184)	1:A:27:VAL:HG11	1:A:30:GLY:HA3	2	0.41
(2,184)	1:A:27:VAL:HG12	1:A:30:GLY:HA3	2	0.41
(2,184)	1:A:27:VAL:HG13	1:A:30:GLY:HA3	2	0.41
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB2	12	0.41
(1,7)	1:A:4:GLY:HA3	1:A:17:LYS:HB3	12	0.41
(2,43)	1:A:7:TYR:HB2	1:A:7:TYR:HE2	4	0.4
(2,36)	1:A:7:TYR:H	1:A:7:TYR:HD2	28	0.4

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

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

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,270)	1:B:7:TYR:HB2	1:B:7:TYR:HE2	13	0.36
(2,270)	1:B:7:TYR:HB2	1:B:7:TYR:HE2	22	0.36
(2,43)	1:A:7:TYR:HB2	1:A:7:TYR:HE2	1	0.35
(2,43)	1:A:7:TYR:HB2	1:A:7:TYR:HE2	9	0.35
(2,43)	1:A:7:TYR:HB2	1:A:7:TYR:HE2	13	0.35
(2,43)	1:A:7:TYR:HB2	1:A:7:TYR:HE2	23	0.35
(2,36)	1:A:7:TYR:H	1:A:7:TYR:HD2	1	0.35
(2,36)	1:A:7:TYR:H	1:A:7:TYR:HD2	2	0.35
(2,36)	1:A:7:TYR:H	1:A:7:TYR:HD2	5	0.35
(2,36)	1:A:7:TYR:H	1:A:7:TYR:HD2	7	0.35
(2,36)	1:A:7:TYR:H	1:A:7:TYR:HD2	9	0.35
(2,36)	1:A:7:TYR:H	1:A:7:TYR:HD2	11	0.35
(2,36)	1:A:7:TYR:H	1:A:7:TYR:HD2	12	0.35
(2,36)	1:A:7:TYR:H	1:A:7:TYR:HD2	27	0.35
(2,270)	1:B:7:TYR:HB2	1:B:7:TYR:HE2	7	0.35
(2,270)	1:B:7:TYR:HB2	1:B:7:TYR:HE2	10	0.35
(2,270)	1:B:7:TYR:HB2	1:B:7:TYR:HE2	14	0.35
(2,270)	1:B:7:TYR:HB2	1:B:7:TYR:HE2	25	0.35
(2,270)	1:B:7:TYR:HB2	1:B:7:TYR:HE2	26	0.35
(2,263)	1:B:7:TYR:H	1:B:7:TYR:HD2	23	0.35
(2,184)	1:A:27:VAL:HG11	1:A:30:GLY:HA3	5	0.35
(2,184)	1:A:27:VAL:HG12	1:A:30:GLY:HA3	5	0.35
(2,184)	1:A:27:VAL:HG13	1:A:30:GLY:HA3	5	0.35
(2,43)	1:A:7:TYR:HB2	1:A:7:TYR:HE2	11	0.34
(2,43)	1:A:7:TYR:HB2	1:A:7:TYR:HE2	12	0.34
(2,43)	1:A:7:TYR:HB2	1:A:7:TYR:HE2	17	0.34
(2,43)	1:A:7:TYR:HB2	1:A:7:TYR:HE2	21	0.34
(2,270)	1:B:7:TYR:HB2	1:B:7:TYR:HE2	1	0.34
(2,270)	1:B:7:TYR:HB2	1:B:7:TYR:HE2	2	0.34
(2,270)	1:B:7:TYR:HB2	1:B:7:TYR:HE2	6	0.34
(2,270)	1:B:7:TYR:HB2	1:B:7:TYR:HE2	15	0.34
(2,270)	1:B:7:TYR:HB2	1:B:7:TYR:HE2	23	0.34
(2,270)	1:B:7:TYR:HB2	1:B:7:TYR:HE2	24	0.34
(2,270)	1:B:7:TYR:HB2	1:B:7:TYR:HE2	28	0.34
(2,263)	1:B:7:TYR:H	1:B:7:TYR:HD2	18	0.34
(2,263)	1:B:7:TYR:H	1:B:7:TYR:HD2	25	0.34
(2,184)	1:A:27:VAL:HG11	1:A:30:GLY:HA3	20	0.34
(2,184)	1:A:27:VAL:HG12	1:A:30:GLY:HA3	20	0.34
(2,184)	1:A:27:VAL:HG13	1:A:30:GLY:HA3	20	0.34
(2,43)	1:A:7:TYR:HB2	1:A:7:TYR:HE2	7	0.33
(2,402)	1:B:28:CYS:HB2	1:B:33:MET:HB2	5	0.33
(2,36)	1:A:7:TYR:H	1:A:7:TYR:HD2	26	0.33

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

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:A:27:VAL:HG11	1:A:30:GLY:HA3	10	0.28
(2,184)	1:A:27:VAL:HG12	1:A:30:GLY:HA3	10	0.28
(2,184)	1:A:27:VAL:HG13	1:A:30:GLY:HA3	10	0.28
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	1	0.28
(2,135)	1:A:18:VAL:H	1:A:19:LEU:H	3	0.28
(2,135)	1:A:18:VAL:H	1:A:19:LEU:H	5	0.28
(2,135)	1:A:18:VAL:H	1:A:19:LEU:H	12	0.28
(2,135)	1:A:18:VAL:H	1:A:19:LEU:H	15	0.28
(2,135)	1:A:18:VAL:H	1:A:19:LEU:H	28	0.28
(2,1)	1:A:1:ALA:HB1	1:A:7:TYR:HE2	5	0.28
(2,1)	1:A:1:ALA:HB2	1:A:7:TYR:HE2	5	0.28
(2,1)	1:A:1:ALA:HB3	1:A:7:TYR:HE2	5	0.28
(2,402)	1:B:28:CYS:HB2	1:B:33:MET:HB2	4	0.27
(2,402)	1:B:28:CYS:HB2	1:B:33:MET:HB2	16	0.27
(2,402)	1:B:28:CYS:HB2	1:B:33:MET:HB2	17	0.27
(2,296)	1:B:8:LYS:HA	1:B:33:MET:HB3	21	0.27
(2,184)	1:A:27:VAL:HG11	1:A:30:GLY:HA3	25	0.27
(2,184)	1:A:27:VAL:HG12	1:A:30:GLY:HA3	25	0.27
(2,184)	1:A:27:VAL:HG13	1:A:30:GLY:HA3	25	0.27
(2,184)	1:A:27:VAL:HG11	1:A:30:GLY:HA3	28	0.27
(2,184)	1:A:27:VAL:HG12	1:A:30:GLY:HA3	28	0.27
(2,184)	1:A:27:VAL:HG13	1:A:30:GLY:HA3	28	0.27
(2,135)	1:A:18:VAL:H	1:A:19:LEU:H	11	0.27
(2,135)	1:A:18:VAL:H	1:A:19:LEU:H	13	0.27
(4,5)	1:A:12:CYS:SG	1:A:29:CYS:SG	8	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	1	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	2	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	5	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	6	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	7	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	8	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	9	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	10	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	11	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	12	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	13	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	14	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	15	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	16	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	17	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	18	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	19	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	20	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	21	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	22	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	23	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	24	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	25	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	26	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	27	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	28	0.26
(2,47)	1:A:7:TYR:HB3	1:A:7:TYR:HD1	29	0.26
(2,296)	1:B:8:LYS:HA	1:B:33:MET:HB3	12	0.26
(2,296)	1:B:8:LYS:HA	1:B:33:MET:HB3	26	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	1	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	2	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	3	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	4	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	5	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	6	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	7	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	8	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	9	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	10	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	11	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	12	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	13	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	14	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	15	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	16	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	17	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	18	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	19	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	20	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	21	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	22	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	23	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	24	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	25	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	26	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	27	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	28	0.26
(2,274)	1:B:7:TYR:HB3	1:B:7:TYR:HD1	29	0.26
(2,184)	1:A:27:VAL:HG11	1:A:30:GLY:HA3	4	0.26

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

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

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

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,296)	1:B:8:LYS:HA	1:B:33:MET:HB3	16	0.2
(2,296)	1:B:8:LYS:HA	1:B:33:MET:HB3	20	0.2
(2,265)	1:B:7:TYR:H	1:B:17:LYS:HA	8	0.2
(2,265)	1:B:7:TYR:H	1:B:17:LYS:HA	24	0.2
(2,264)	1:B:7:TYR:H	1:B:16:VAL:H	8	0.2
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	4	0.2
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	10	0.2
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	21	0.2
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	1	0.2
(2,115)	1:A:15:VAL:H	1:B:20:GLU:H	13	0.2
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	3	0.2
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	4	0.2
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	7	0.2
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	19	0.2
(5,14)	2:B:37:ZN:ZN	1:B:28:CYS:CB	25	0.19
(5,11)	2:B:37:ZN:ZN	1:B:12:CYS:CB	4	0.19
(5,11)	2:B:37:ZN:ZN	1:B:12:CYS:CB	16	0.19
(4,5)	1:A:12:CYS:SG	1:A:29:CYS:SG	7	0.19
(4,10)	1:B:12:CYS:SG	1:B:29:CYS:SG	26	0.19
(3,56)	1:B:26:LEU:O	1:B:33:MET:H	24	0.19
(3,52)	1:B:8:LYS:O	1:B:34:VAL:H	17	0.19
(2,402)	1:B:28:CYS:HB2	1:B:33:MET:HB2	10	0.19
(2,402)	1:B:28:CYS:HB2	1:B:33:MET:HB2	21	0.19
(2,402)	1:B:28:CYS:HB2	1:B:33:MET:HB2	27	0.19
(2,38)	1:A:7:TYR:H	1:A:17:LYS:HA	23	0.19
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	18	0.19
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	20	0.19
(2,354)	1:B:18:VAL:H	1:B:19:LEU:H	5	0.19
(2,354)	1:B:18:VAL:H	1:B:19:LEU:H	8	0.19
(2,354)	1:B:18:VAL:H	1:B:19:LEU:H	16	0.19
(2,354)	1:B:18:VAL:H	1:B:19:LEU:H	18	0.19
(2,332)	1:B:14:GLN:H	1:B:14:GLN:HA	8	0.19
(2,320)	1:B:11:LEU:HA	1:B:11:LEU:HG	15	0.19
(2,296)	1:B:8:LYS:HA	1:B:33:MET:HB3	4	0.19
(2,296)	1:B:8:LYS:HA	1:B:33:MET:HB3	9	0.19
(2,296)	1:B:8:LYS:HA	1:B:33:MET:HB3	22	0.19
(2,296)	1:B:8:LYS:HA	1:B:33:MET:HB3	25	0.19
(2,264)	1:B:7:TYR:H	1:B:16:VAL:H	11	0.19
(2,184)	1:A:27:VAL:HG11	1:A:30:GLY:HA3	11	0.19
(2,184)	1:A:27:VAL:HG12	1:A:30:GLY:HA3	11	0.19
(2,184)	1:A:27:VAL:HG13	1:A:30:GLY:HA3	11	0.19
(2,184)	1:A:27:VAL:HG11	1:A:30:GLY:HA3	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:A:27:VAL:HG12	1:A:30:GLY:HA3	14	0.19
(2,184)	1:A:27:VAL:HG13	1:A:30:GLY:HA3	14	0.19
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	9	0.19
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	26	0.19
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	8	0.19
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	12	0.19
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	7	0.19
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	9	0.19
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	11	0.19
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	26	0.19
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	27	0.19
(2,135)	1:A:18:VAL:H	1:A:19:LEU:H	10	0.19
(2,135)	1:A:18:VAL:H	1:A:19:LEU:H	19	0.19
(2,135)	1:A:18:VAL:H	1:A:19:LEU:H	29	0.19
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	5	0.19
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	9	0.19
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	10	0.19
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	11	0.19
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	12	0.19
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	14	0.19
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	15	0.19
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	16	0.19
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	17	0.19
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	21	0.19
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	22	0.19
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	27	0.19
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	28	0.19
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	29	0.19
(2,1)	1:A:1:ALA:HB1	1:A:7:TYR:HE2	4	0.19
(2,1)	1:A:1:ALA:HB2	1:A:7:TYR:HE2	4	0.19
(2,1)	1:A:1:ALA:HB3	1:A:7:TYR:HE2	4	0.19
(5,14)	2:B:37:ZN:ZN	1:B:28:CYS:CB	2	0.18
(5,14)	2:B:37:ZN:ZN	1:B:28:CYS:CB	11	0.18
(5,11)	2:B:37:ZN:ZN	1:B:12:CYS:CB	17	0.18
(4,10)	1:B:12:CYS:SG	1:B:29:CYS:SG	16	0.18
(3,56)	1:B:26:LEU:O	1:B:33:MET:H	18	0.18
(3,52)	1:B:8:LYS:O	1:B:34:VAL:H	4	0.18
(3,52)	1:B:8:LYS:O	1:B:34:VAL:H	13	0.18
(3,24)	1:A:17:LYS:O	1:B:17:LYS:H	3	0.18
(3,24)	1:A:17:LYS:O	1:B:17:LYS:H	19	0.18
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	9	0.18
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	22	0.18

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

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,56)	1:B:26:LEU:O	1:B:33:MET:H	1	0.17
(3,56)	1:B:26:LEU:O	1:B:33:MET:H	13	0.17
(3,56)	1:B:26:LEU:O	1:B:33:MET:H	23	0.17
(3,52)	1:B:8:LYS:O	1:B:34:VAL:H	16	0.17
(3,30)	1:A:20:GLU:O	1:B:15:VAL:H	13	0.17
(3,24)	1:A:17:LYS:O	1:B:17:LYS:H	22	0.17
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	12	0.17
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	16	0.17
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	23	0.17
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	15	0.17
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	7	0.17
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	12	0.17
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	28	0.17
(2,402)	1:B:28:CYS:HB2	1:B:33:MET:HB2	20	0.17
(2,402)	1:B:28:CYS:HB2	1:B:33:MET:HB2	22	0.17
(2,402)	1:B:28:CYS:HB2	1:B:33:MET:HB2	28	0.17
(2,391)	1:B:27:VAL:HA	1:B:33:MET:H	2	0.17
(2,391)	1:B:27:VAL:HA	1:B:33:MET:H	7	0.17
(2,37)	1:A:7:TYR:H	1:A:16:VAL:H	18	0.17
(2,354)	1:B:18:VAL:H	1:B:19:LEU:H	10	0.17
(2,354)	1:B:18:VAL:H	1:B:19:LEU:H	14	0.17
(2,354)	1:B:18:VAL:H	1:B:19:LEU:H	17	0.17
(2,354)	1:B:18:VAL:H	1:B:19:LEU:H	29	0.17
(2,332)	1:B:14:GLN:H	1:B:14:GLN:HA	21	0.17
(2,332)	1:B:14:GLN:H	1:B:14:GLN:HA	22	0.17
(2,320)	1:B:11:LEU:HA	1:B:11:LEU:HG	12	0.17
(2,296)	1:B:8:LYS:HA	1:B:33:MET:HB3	24	0.17
(2,296)	1:B:8:LYS:HA	1:B:33:MET:HB3	28	0.17
(2,207)	1:A:34:VAL:H	1:A:34:VAL:HB	4	0.17
(2,184)	1:A:27:VAL:HG11	1:A:30:GLY:HA3	6	0.17
(2,184)	1:A:27:VAL:HG12	1:A:30:GLY:HA3	6	0.17
(2,184)	1:A:27:VAL:HG13	1:A:30:GLY:HA3	6	0.17
(2,184)	1:A:27:VAL:HG11	1:A:30:GLY:HA3	22	0.17
(2,184)	1:A:27:VAL:HG12	1:A:30:GLY:HA3	22	0.17
(2,184)	1:A:27:VAL:HG13	1:A:30:GLY:HA3	22	0.17
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	1	0.17
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	25	0.17
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	7	0.17
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	14	0.17
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	22	0.17
(2,138)	1:A:18:VAL:HA	1:B:16:VAL:HA	12	0.17
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	6	0.17
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	10	0.17
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	13	0.17
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	16	0.17
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	23	0.17
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	24	0.17
(2,135)	1:A:18:VAL:H	1:A:19:LEU:H	14	0.17
(2,115)	1:A:15:VAL:H	1:B:20:GLU:H	3	0.17
(2,115)	1:A:15:VAL:H	1:B:20:GLU:H	19	0.17
(2,115)	1:A:15:VAL:H	1:B:20:GLU:H	21	0.17
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	18	0.17
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	24	0.17
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	25	0.17
(5,7)	2:A:37:ZN:ZN	1:A:29:CYS:CA	26	0.16
(5,14)	2:B:37:ZN:ZN	1:B:28:CYS:CB	5	0.16
(5,14)	2:B:37:ZN:ZN	1:B:28:CYS:CB	7	0.16
(5,14)	2:B:37:ZN:ZN	1:B:28:CYS:CB	27	0.16
(5,11)	2:B:37:ZN:ZN	1:B:12:CYS:CB	15	0.16
(4,3)	1:A:9:CYS:SG	1:A:29:CYS:SG	18	0.16
(4,10)	1:B:12:CYS:SG	1:B:29:CYS:SG	4	0.16
(4,10)	1:B:12:CYS:SG	1:B:29:CYS:SG	23	0.16
(3,56)	1:B:26:LEU:O	1:B:33:MET:H	15	0.16
(3,52)	1:B:8:LYS:O	1:B:34:VAL:H	5	0.16
(3,52)	1:B:8:LYS:O	1:B:34:VAL:H	14	0.16
(3,30)	1:A:20:GLU:O	1:B:15:VAL:H	7	0.16
(3,24)	1:A:17:LYS:O	1:B:17:LYS:H	18	0.16
(3,24)	1:A:17:LYS:O	1:B:17:LYS:H	21	0.16
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	7	0.16
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	23	0.16
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	27	0.16
(2,89)	1:A:11:LEU:H	1:A:11:LEU:HG	20	0.16
(2,54)	1:A:7:TYR:HD1	1:A:33:MET:HE1	18	0.16
(2,54)	1:A:7:TYR:HD1	1:A:33:MET:HE2	18	0.16
(2,54)	1:A:7:TYR:HD1	1:A:33:MET:HE3	18	0.16
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	1	0.16
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	10	0.16
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	18	0.16
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	24	0.16
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	26	0.16
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	27	0.16
(2,402)	1:B:28:CYS:HB2	1:B:33:MET:HB2	2	0.16
(2,402)	1:B:28:CYS:HB2	1:B:33:MET:HB2	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,391)	1:B:27:VAL:HA	1:B:33:MET:H	1	0.16
(2,391)	1:B:27:VAL:HA	1:B:33:MET:H	4	0.16
(2,391)	1:B:27:VAL:HA	1:B:33:MET:H	22	0.16
(2,391)	1:B:27:VAL:HA	1:B:33:MET:H	26	0.16
(2,38)	1:A:7:TYR:H	1:A:17:LYS:HA	5	0.16
(2,38)	1:A:7:TYR:H	1:A:17:LYS:HA	20	0.16
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	8	0.16
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	12	0.16
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	13	0.16
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	26	0.16
(2,354)	1:B:18:VAL:H	1:B:19:LEU:H	7	0.16
(2,354)	1:B:18:VAL:H	1:B:19:LEU:H	11	0.16
(2,354)	1:B:18:VAL:H	1:B:19:LEU:H	25	0.16
(2,336)	1:B:15:VAL:H	1:B:15:VAL:HB	3	0.16
(2,332)	1:B:14:GLN:H	1:B:14:GLN:HA	3	0.16
(2,332)	1:B:14:GLN:H	1:B:14:GLN:HA	15	0.16
(2,332)	1:B:14:GLN:H	1:B:14:GLN:HA	23	0.16
(2,332)	1:B:14:GLN:H	1:B:14:GLN:HA	26	0.16
(2,210)	1:A:34:VAL:HB	1:A:35:LYS:H	13	0.16
(2,210)	1:A:34:VAL:HB	1:A:35:LYS:H	25	0.16
(2,207)	1:A:34:VAL:H	1:A:34:VAL:HB	2	0.16
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	17	0.16
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	28	0.16
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	9	0.16
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	18	0.16
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	27	0.16
(2,147)	1:A:20:GLU:H	1:A:20:GLU:HG3	13	0.16
(2,138)	1:A:18:VAL:HA	1:B:16:VAL:HA	23	0.16
(2,138)	1:A:18:VAL:HA	1:B:16:VAL:HA	24	0.16
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	12	0.16
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	20	0.16
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	25	0.16
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	29	0.16
(2,115)	1:A:15:VAL:H	1:B:20:GLU:H	1	0.16
(2,115)	1:A:15:VAL:H	1:B:20:GLU:H	4	0.16
(2,115)	1:A:15:VAL:H	1:B:20:GLU:H	10	0.16
(2,115)	1:A:15:VAL:H	1:B:20:GLU:H	24	0.16
(2,115)	1:A:15:VAL:H	1:B:20:GLU:H	25	0.16
(2,113)	1:A:15:VAL:H	1:A:15:VAL:HB	22	0.16
(2,110)	1:A:14:GLN:H	1:A:14:GLN:HE21	25	0.16
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	2	0.16
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	8	0.16

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

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

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	18	0.14
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	24	0.14
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	27	0.14
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	28	0.14
(3,18)	1:A:15:VAL:O	1:B:19:LEU:H	20	0.14
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	3	0.14
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	13	0.14
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	25	0.14
(3,14)	1:A:9:CYS:H	1:A:14:GLN:O	27	0.14
(2,81)	1:A:9:CYS:SG	1:A:12:CYS:H	26	0.14
(2,421)	1:B:34:VAL:HB	1:B:35:LYS:H	8	0.14
(2,421)	1:B:34:VAL:HB	1:B:35:LYS:H	12	0.14
(2,421)	1:B:34:VAL:HB	1:B:35:LYS:H	29	0.14
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	14	0.14
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	29	0.14
(2,402)	1:B:28:CYS:HB2	1:B:33:MET:HB2	25	0.14
(2,393)	1:B:27:VAL:HB	1:B:28:CYS:H	27	0.14
(2,37)	1:A:7:TYR:H	1:A:16:VAL:H	15	0.14
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	2	0.14
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	4	0.14
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	9	0.14
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	19	0.14
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	23	0.14
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	24	0.14
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	25	0.14
(2,343)	1:B:16:VAL:HB	1:B:17:LYS:H	21	0.14
(2,343)	1:B:16:VAL:HB	1:B:17:LYS:H	29	0.14
(2,336)	1:B:15:VAL:H	1:B:15:VAL:HB	12	0.14
(2,332)	1:B:14:GLN:H	1:B:14:GLN:HA	17	0.14
(2,320)	1:B:11:LEU:HA	1:B:11:LEU:HG	1	0.14
(2,320)	1:B:11:LEU:HA	1:B:11:LEU:HG	4	0.14
(2,320)	1:B:11:LEU:HA	1:B:11:LEU:HG	16	0.14
(2,308)	1:B:9:CYS:SG	1:B:12:CYS:H	4	0.14
(2,308)	1:B:9:CYS:SG	1:B:12:CYS:H	26	0.14
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE1	20	0.14
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE2	20	0.14
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE3	20	0.14
(2,265)	1:B:7:TYR:H	1:B:17:LYS:HA	3	0.14
(2,264)	1:B:7:TYR:H	1:B:16:VAL:H	12	0.14
(2,264)	1:B:7:TYR:H	1:B:16:VAL:H	29	0.14
(2,210)	1:A:34:VAL:HB	1:A:35:LYS:H	5	0.14
(2,207)	1:A:34:VAL:H	1:A:34:VAL:HB	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,207)	1:A:34:VAL:H	1:A:34:VAL:HB	9	0.14
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	14	0.14
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	19	0.14
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	20	0.14
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	29	0.14
(2,147)	1:A:20:GLU:H	1:A:20:GLU:HG3	26	0.14
(2,138)	1:A:18:VAL:HA	1:B:16:VAL:HA	3	0.14
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	18	0.14
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	19	0.14
(2,135)	1:A:18:VAL:H	1:A:19:LEU:H	2	0.14
(2,119)	1:A:16:VAL:HA	1:A:16:VAL:HB	11	0.14
(2,119)	1:A:16:VAL:HA	1:A:16:VAL:HB	20	0.14
(1,79)	1:B:1:ALA:HB1	1:B:7:TYR:HD2	23	0.14
(1,79)	1:B:1:ALA:HB2	1:B:7:TYR:HD2	23	0.14
(1,79)	1:B:1:ALA:HB3	1:B:7:TYR:HD2	23	0.14
(5,7)	2:A:37:ZN:ZN	1:A:29:CYS:CA	8	0.13
(5,6)	2:A:37:ZN:ZN	1:A:28:CYS:SG	5	0.13
(5,6)	2:A:37:ZN:ZN	1:A:28:CYS:SG	8	0.13
(5,6)	2:A:37:ZN:ZN	1:A:28:CYS:SG	18	0.13
(5,6)	2:A:37:ZN:ZN	1:A:28:CYS:SG	19	0.13
(5,6)	2:A:37:ZN:ZN	1:A:28:CYS:SG	26	0.13
(5,17)	2:B:37:ZN:ZN	1:B:29:CYS:CB	8	0.13
(5,15)	2:B:37:ZN:ZN	1:B:28:CYS:SG	4	0.13
(5,14)	2:B:37:ZN:ZN	1:B:28:CYS:CB	22	0.13
(5,14)	2:B:37:ZN:ZN	1:B:28:CYS:CB	23	0.13
(5,14)	2:B:37:ZN:ZN	1:B:28:CYS:CB	28	0.13
(5,12)	2:B:37:ZN:ZN	1:B:12:CYS:SG	11	0.13
(5,12)	2:B:37:ZN:ZN	1:B:12:CYS:SG	19	0.13
(5,11)	2:B:37:ZN:ZN	1:B:12:CYS:CB	3	0.13
(4,4)	1:A:12:CYS:SG	1:A:28:CYS:SG	16	0.13
(4,4)	1:A:12:CYS:SG	1:A:28:CYS:SG	17	0.13
(4,4)	1:A:12:CYS:SG	1:A:28:CYS:SG	21	0.13
(4,4)	1:A:12:CYS:SG	1:A:28:CYS:SG	28	0.13
(4,3)	1:A:9:CYS:SG	1:A:29:CYS:SG	5	0.13
(3,56)	1:B:26:LEU:O	1:B:33:MET:H	3	0.13
(3,56)	1:B:26:LEU:O	1:B:33:MET:H	4	0.13
(3,56)	1:B:26:LEU:O	1:B:33:MET:H	5	0.13
(3,56)	1:B:26:LEU:O	1:B:33:MET:H	6	0.13
(3,56)	1:B:26:LEU:O	1:B:33:MET:H	7	0.13
(3,56)	1:B:26:LEU:O	1:B:33:MET:H	17	0.13
(3,52)	1:B:8:LYS:O	1:B:34:VAL:H	11	0.13
(3,32)	1:A:26:LEU:O	1:A:33:MET:H	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:A:26:LEU:O	1:A:33:MET:H	22	0.13
(3,26)	1:A:19:LEU:H	1:B:15:VAL:O	5	0.13
(3,26)	1:A:19:LEU:H	1:B:15:VAL:O	9	0.13
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	26	0.13
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	29	0.13
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	6	0.13
(3,15)	1:A:15:VAL:N	1:B:20:GLU:O	22	0.13
(2,89)	1:A:11:LEU:H	1:A:11:LEU:HG	7	0.13
(2,89)	1:A:11:LEU:H	1:A:11:LEU:HG	10	0.13
(2,69)	1:A:8:LYS:HA	1:A:33:MET:HB3	7	0.13
(2,421)	1:B:34:VAL:HB	1:B:35:LYS:H	23	0.13
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	20	0.13
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	22	0.13
(2,393)	1:B:27:VAL:HB	1:B:28:CYS:H	2	0.13
(2,393)	1:B:27:VAL:HB	1:B:28:CYS:H	6	0.13
(2,391)	1:B:27:VAL:HA	1:B:33:MET:H	10	0.13
(2,391)	1:B:27:VAL:HA	1:B:33:MET:H	14	0.13
(2,391)	1:B:27:VAL:HA	1:B:33:MET:H	16	0.13
(2,38)	1:A:7:TYR:H	1:A:17:LYS:HA	10	0.13
(2,37)	1:A:7:TYR:H	1:A:16:VAL:H	19	0.13
(2,365)	1:B:20:GLU:H	1:B:20:GLU:HG3	22	0.13
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	14	0.13
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	17	0.13
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	27	0.13
(2,343)	1:B:16:VAL:HB	1:B:17:LYS:H	9	0.13
(2,343)	1:B:16:VAL:HB	1:B:17:LYS:H	26	0.13
(2,340)	1:B:16:VAL:HA	1:B:16:VAL:HB	8	0.13
(2,340)	1:B:16:VAL:HA	1:B:16:VAL:HB	10	0.13
(2,340)	1:B:16:VAL:HA	1:B:16:VAL:HB	11	0.13
(2,336)	1:B:15:VAL:H	1:B:15:VAL:HB	21	0.13
(2,336)	1:B:15:VAL:H	1:B:15:VAL:HB	29	0.13
(2,332)	1:B:14:GLN:H	1:B:14:GLN:HA	4	0.13
(2,320)	1:B:11:LEU:HA	1:B:11:LEU:HG	5	0.13
(2,320)	1:B:11:LEU:HA	1:B:11:LEU:HG	23	0.13
(2,308)	1:B:9:CYS:SG	1:B:12:CYS:H	3	0.13
(2,308)	1:B:9:CYS:SG	1:B:12:CYS:H	12	0.13
(2,308)	1:B:9:CYS:SG	1:B:12:CYS:H	15	0.13
(2,308)	1:B:9:CYS:SG	1:B:12:CYS:H	16	0.13
(2,308)	1:B:9:CYS:SG	1:B:12:CYS:H	17	0.13
(2,265)	1:B:7:TYR:H	1:B:17:LYS:HA	15	0.13
(2,265)	1:B:7:TYR:H	1:B:17:LYS:HA	21	0.13
(2,264)	1:B:7:TYR:H	1:B:16:VAL:H	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,264)	1:B:7:TYR:H	1:B:16:VAL:H	14	0.13
(2,264)	1:B:7:TYR:H	1:B:16:VAL:H	20	0.13
(2,264)	1:B:7:TYR:H	1:B:16:VAL:H	21	0.13
(2,210)	1:A:34:VAL:HB	1:A:35:LYS:H	12	0.13
(2,210)	1:A:34:VAL:HB	1:A:35:LYS:H	21	0.13
(2,207)	1:A:34:VAL:H	1:A:34:VAL:HB	15	0.13
(2,207)	1:A:34:VAL:H	1:A:34:VAL:HB	20	0.13
(2,188)	1:A:28:CYS:H	1:A:33:MET:HB2	20	0.13
(2,184)	1:A:27:VAL:HG11	1:A:30:GLY:HA3	16	0.13
(2,184)	1:A:27:VAL:HG12	1:A:30:GLY:HA3	16	0.13
(2,184)	1:A:27:VAL:HG13	1:A:30:GLY:HA3	16	0.13
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	19	0.13
(2,138)	1:A:18:VAL:HA	1:B:16:VAL:HA	5	0.13
(2,138)	1:A:18:VAL:HA	1:B:16:VAL:HA	6	0.13
(2,138)	1:A:18:VAL:HA	1:B:16:VAL:HA	15	0.13
(2,138)	1:A:18:VAL:HA	1:B:16:VAL:HA	28	0.13
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	22	0.13
(2,129)	1:A:17:LYS:HA	1:A:18:VAL:H	21	0.13
(2,12)	1:A:4:GLY:HA3	1:A:5:ASP:H	4	0.13
(2,12)	1:A:4:GLY:HA3	1:A:5:ASP:H	15	0.13
(2,12)	1:A:4:GLY:HA3	1:A:5:ASP:H	20	0.13
(2,115)	1:A:15:VAL:H	1:B:20:GLU:H	6	0.13
(2,108)	1:A:14:GLN:H	1:A:14:GLN:HA	26	0.13
(5,6)	2:A:37:ZN:ZN	1:A:28:CYS:SG	20	0.12
(5,17)	2:B:37:ZN:ZN	1:B:29:CYS:CB	11	0.12
(5,16)	2:B:37:ZN:ZN	1:B:29:CYS:CA	8	0.12
(5,15)	2:B:37:ZN:ZN	1:B:28:CYS:SG	12	0.12
(5,15)	2:B:37:ZN:ZN	1:B:28:CYS:SG	16	0.12
(5,15)	2:B:37:ZN:ZN	1:B:28:CYS:SG	21	0.12
(5,15)	2:B:37:ZN:ZN	1:B:28:CYS:SG	26	0.12
(5,14)	2:B:37:ZN:ZN	1:B:28:CYS:CB	15	0.12
(5,14)	2:B:37:ZN:ZN	1:B:28:CYS:CB	16	0.12
(5,14)	2:B:37:ZN:ZN	1:B:28:CYS:CB	17	0.12
(5,14)	2:B:37:ZN:ZN	1:B:28:CYS:CB	26	0.12
(5,12)	2:B:37:ZN:ZN	1:B:12:CYS:SG	29	0.12
(5,10)	2:B:37:ZN:ZN	1:B:12:CYS:CA	8	0.12
(5,10)	2:B:37:ZN:ZN	1:B:12:CYS:CA	14	0.12
(5,10)	2:B:37:ZN:ZN	1:B:12:CYS:CA	20	0.12
(4,5)	1:A:12:CYS:SG	1:A:29:CYS:SG	20	0.12
(4,4)	1:A:12:CYS:SG	1:A:28:CYS:SG	13	0.12
(4,4)	1:A:12:CYS:SG	1:A:28:CYS:SG	24	0.12
(4,4)	1:A:12:CYS:SG	1:A:28:CYS:SG	27	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,3)	1:A:9:CYS:SG	1:A:29:CYS:SG	10	0.12
(4,3)	1:A:9:CYS:SG	1:A:29:CYS:SG	20	0.12
(4,10)	1:B:12:CYS:SG	1:B:29:CYS:SG	24	0.12
(3,56)	1:B:26:LEU:O	1:B:33:MET:H	25	0.12
(3,52)	1:B:8:LYS:O	1:B:34:VAL:H	29	0.12
(3,36)	1:A:27:VAL:O	1:B:27:VAL:H	13	0.12
(3,36)	1:A:27:VAL:O	1:B:27:VAL:H	23	0.12
(3,36)	1:A:27:VAL:O	1:B:27:VAL:H	24	0.12
(3,36)	1:A:27:VAL:O	1:B:27:VAL:H	28	0.12
(3,32)	1:A:26:LEU:O	1:A:33:MET:H	12	0.12
(3,32)	1:A:26:LEU:O	1:A:33:MET:H	19	0.12
(3,30)	1:A:20:GLU:O	1:B:15:VAL:H	8	0.12
(3,30)	1:A:20:GLU:O	1:B:15:VAL:H	15	0.12
(3,30)	1:A:20:GLU:O	1:B:15:VAL:H	16	0.12
(3,30)	1:A:20:GLU:O	1:B:15:VAL:H	17	0.12
(3,30)	1:A:20:GLU:O	1:B:15:VAL:H	29	0.12
(3,26)	1:A:19:LEU:H	1:B:15:VAL:O	1	0.12
(3,26)	1:A:19:LEU:H	1:B:15:VAL:O	12	0.12
(3,26)	1:A:19:LEU:H	1:B:15:VAL:O	15	0.12
(3,26)	1:A:19:LEU:H	1:B:15:VAL:O	17	0.12
(3,26)	1:A:19:LEU:H	1:B:15:VAL:O	23	0.12
(3,24)	1:A:17:LYS:O	1:B:17:LYS:H	14	0.12
(3,24)	1:A:17:LYS:O	1:B:17:LYS:H	29	0.12
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	3	0.12
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	5	0.12
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	6	0.12
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	9	0.12
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	15	0.12
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	19	0.12
(3,18)	1:A:15:VAL:O	1:B:19:LEU:H	19	0.12
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	12	0.12
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	16	0.12
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	26	0.12
(2,69)	1:A:8:LYS:HA	1:A:33:MET:HB3	1	0.12
(2,421)	1:B:34:VAL:HB	1:B:35:LYS:H	9	0.12
(2,421)	1:B:34:VAL:HB	1:B:35:LYS:H	11	0.12
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	11	0.12
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	13	0.12
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	16	0.12
(2,418)	1:B:34:VAL:H	1:B:34:VAL:HB	19	0.12
(2,402)	1:B:28:CYS:HB2	1:B:33:MET:HB2	6	0.12
(2,393)	1:B:27:VAL:HB	1:B:28:CYS:H	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:B:27:VAL:HB	1:B:28:CYS:H	26	0.12
(2,38)	1:A:7:TYR:H	1:A:17:LYS:HA	12	0.12
(2,38)	1:A:7:TYR:H	1:A:17:LYS:HA	28	0.12
(2,371)	1:B:21:GLU:HA	1:B:22:GLY:H	22	0.12
(2,37)	1:A:7:TYR:H	1:A:16:VAL:H	1	0.12
(2,37)	1:A:7:TYR:H	1:A:16:VAL:H	2	0.12
(2,365)	1:B:20:GLU:H	1:B:20:GLU:HG3	11	0.12
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	5	0.12
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	15	0.12
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	21	0.12
(2,343)	1:B:16:VAL:HB	1:B:17:LYS:H	17	0.12
(2,343)	1:B:16:VAL:HB	1:B:17:LYS:H	25	0.12
(2,340)	1:B:16:VAL:HA	1:B:16:VAL:HB	3	0.12
(2,340)	1:B:16:VAL:HA	1:B:16:VAL:HB	4	0.12
(2,340)	1:B:16:VAL:HA	1:B:16:VAL:HB	16	0.12
(2,340)	1:B:16:VAL:HA	1:B:16:VAL:HB	23	0.12
(2,334)	1:B:14:GLN:H	1:B:14:GLN:HE21	28	0.12
(2,308)	1:B:9:CYS:SG	1:B:12:CYS:H	23	0.12
(2,303)	1:B:9:CYS:HB2	1:B:13:GLY:H	19	0.12
(2,296)	1:B:8:LYS:HA	1:B:33:MET:HB3	13	0.12
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE1	27	0.12
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE2	27	0.12
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE3	27	0.12
(2,265)	1:B:7:TYR:H	1:B:17:LYS:HA	23	0.12
(2,264)	1:B:7:TYR:H	1:B:16:VAL:H	6	0.12
(2,264)	1:B:7:TYR:H	1:B:16:VAL:H	10	0.12
(2,264)	1:B:7:TYR:H	1:B:16:VAL:H	13	0.12
(2,239)	1:B:4:GLY:HA3	1:B:5:ASP:H	15	0.12
(2,239)	1:B:4:GLY:HA3	1:B:5:ASP:H	25	0.12
(2,207)	1:A:34:VAL:H	1:A:34:VAL:HB	3	0.12
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	6	0.12
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	7	0.12
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	11	0.12
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	24	0.12
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	29	0.12
(2,147)	1:A:20:GLU:H	1:A:20:GLU:HG3	7	0.12
(2,138)	1:A:18:VAL:HA	1:B:16:VAL:HA	13	0.12
(2,137)	1:A:18:VAL:HA	1:A:20:GLU:H	2	0.12
(2,124)	1:A:16:VAL:HB	1:A:17:LYS:H	8	0.12
(2,12)	1:A:4:GLY:HA3	1:A:5:ASP:H	18	0.12
(2,119)	1:A:16:VAL:HA	1:A:16:VAL:HB	1	0.12
(2,119)	1:A:16:VAL:HA	1:A:16:VAL:HB	2	0.12

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

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,56)	1:B:26:LEU:O	1:B:33:MET:H	29	0.11
(3,52)	1:B:8:LYS:O	1:B:34:VAL:H	19	0.11
(3,52)	1:B:8:LYS:O	1:B:34:VAL:H	20	0.11
(3,36)	1:A:27:VAL:O	1:B:27:VAL:H	5	0.11
(3,32)	1:A:26:LEU:O	1:A:33:MET:H	1	0.11
(3,32)	1:A:26:LEU:O	1:A:33:MET:H	4	0.11
(3,32)	1:A:26:LEU:O	1:A:33:MET:H	11	0.11
(3,32)	1:A:26:LEU:O	1:A:33:MET:H	25	0.11
(3,30)	1:A:20:GLU:O	1:B:15:VAL:H	6	0.11
(3,29)	1:A:20:GLU:O	1:B:15:VAL:N	9	0.11
(3,26)	1:A:19:LEU:H	1:B:15:VAL:O	4	0.11
(3,26)	1:A:19:LEU:H	1:B:15:VAL:O	22	0.11
(3,26)	1:A:19:LEU:H	1:B:15:VAL:O	24	0.11
(3,26)	1:A:19:LEU:H	1:B:15:VAL:O	27	0.11
(3,26)	1:A:19:LEU:H	1:B:15:VAL:O	29	0.11
(3,24)	1:A:17:LYS:O	1:B:17:LYS:H	10	0.11
(3,24)	1:A:17:LYS:O	1:B:17:LYS:H	26	0.11
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	14	0.11
(3,22)	1:A:17:LYS:H	1:B:17:LYS:O	21	0.11
(3,18)	1:A:15:VAL:O	1:B:19:LEU:H	15	0.11
(3,18)	1:A:15:VAL:O	1:B:19:LEU:H	22	0.11
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	5	0.11
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	10	0.11
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	14	0.11
(3,16)	1:A:15:VAL:H	1:B:20:GLU:O	18	0.11
(3,14)	1:A:9:CYS:H	1:A:14:GLN:O	1	0.11
(3,14)	1:A:9:CYS:H	1:A:14:GLN:O	17	0.11
(2,80)	1:A:9:CYS:SG	1:A:12:CYS:N	9	0.11
(2,69)	1:A:8:LYS:HA	1:A:33:MET:HB3	12	0.11
(2,69)	1:A:8:LYS:HA	1:A:33:MET:HB3	27	0.11
(2,421)	1:B:34:VAL:HB	1:B:35:LYS:H	17	0.11
(2,421)	1:B:34:VAL:HB	1:B:35:LYS:H	19	0.11
(2,421)	1:B:34:VAL:HB	1:B:35:LYS:H	25	0.11
(2,391)	1:B:27:VAL:HA	1:B:33:MET:H	20	0.11
(2,391)	1:B:27:VAL:HA	1:B:33:MET:H	28	0.11
(2,38)	1:A:7:TYR:H	1:A:17:LYS:HA	13	0.11
(2,38)	1:A:7:TYR:H	1:A:17:LYS:HA	21	0.11
(2,365)	1:B:20:GLU:H	1:B:20:GLU:HG3	3	0.11
(2,365)	1:B:20:GLU:H	1:B:20:GLU:HG3	5	0.11
(2,365)	1:B:20:GLU:H	1:B:20:GLU:HG3	13	0.11
(2,365)	1:B:20:GLU:H	1:B:20:GLU:HG3	26	0.11
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,356)	1:B:18:VAL:HA	1:B:20:GLU:H	16	0.11
(2,348)	1:B:17:LYS:HA	1:B:18:VAL:H	2	0.11
(2,348)	1:B:17:LYS:HA	1:B:18:VAL:H	8	0.11
(2,348)	1:B:17:LYS:HA	1:B:18:VAL:H	19	0.11
(2,343)	1:B:16:VAL:HB	1:B:17:LYS:H	5	0.11
(2,343)	1:B:16:VAL:HB	1:B:17:LYS:H	11	0.11
(2,343)	1:B:16:VAL:HB	1:B:17:LYS:H	16	0.11
(2,343)	1:B:16:VAL:HB	1:B:17:LYS:H	18	0.11
(2,340)	1:B:16:VAL:HA	1:B:16:VAL:HB	2	0.11
(2,340)	1:B:16:VAL:HA	1:B:16:VAL:HB	17	0.11
(2,340)	1:B:16:VAL:HA	1:B:16:VAL:HB	21	0.11
(2,336)	1:B:15:VAL:H	1:B:15:VAL:HB	5	0.11
(2,336)	1:B:15:VAL:H	1:B:15:VAL:HB	9	0.11
(2,336)	1:B:15:VAL:H	1:B:15:VAL:HB	11	0.11
(2,336)	1:B:15:VAL:H	1:B:15:VAL:HB	16	0.11
(2,336)	1:B:15:VAL:H	1:B:15:VAL:HB	22	0.11
(2,336)	1:B:15:VAL:H	1:B:15:VAL:HB	25	0.11
(2,336)	1:B:15:VAL:H	1:B:15:VAL:HB	27	0.11
(2,316)	1:B:11:LEU:H	1:B:11:LEU:HG	24	0.11
(2,308)	1:B:9:CYS:SG	1:B:12:CYS:H	1	0.11
(2,308)	1:B:9:CYS:SG	1:B:12:CYS:H	5	0.11
(2,303)	1:B:9:CYS:HB2	1:B:13:GLY:H	11	0.11
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE1	22	0.11
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE2	22	0.11
(2,281)	1:B:7:TYR:HD1	1:B:33:MET:HE3	22	0.11
(2,265)	1:B:7:TYR:H	1:B:17:LYS:HA	7	0.11
(2,265)	1:B:7:TYR:H	1:B:17:LYS:HA	18	0.11
(2,264)	1:B:7:TYR:H	1:B:16:VAL:H	7	0.11
(2,264)	1:B:7:TYR:H	1:B:16:VAL:H	25	0.11
(2,25)	1:A:6:VAL:H	1:A:7:TYR:HA	15	0.11
(2,239)	1:B:4:GLY:HA3	1:B:5:ASP:H	4	0.11
(2,210)	1:A:34:VAL:HB	1:A:35:LYS:H	14	0.11
(2,210)	1:A:34:VAL:HB	1:A:35:LYS:H	23	0.11
(2,207)	1:A:34:VAL:H	1:A:34:VAL:HB	26	0.11
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	18	0.11
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	20	0.11
(2,181)	1:A:27:VAL:HB	1:A:28:CYS:H	27	0.11
(2,149)	1:A:20:GLU:H	1:B:15:VAL:H	2	0.11
(2,147)	1:A:20:GLU:H	1:A:20:GLU:HG3	11	0.11
(2,138)	1:A:18:VAL:HA	1:B:16:VAL:HA	7	0.11
(2,138)	1:A:18:VAL:HA	1:B:16:VAL:HA	27	0.11
(2,129)	1:A:17:LYS:HA	1:A:18:VAL:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,124)	1:A:16:VAL:HB	1:A:17:LYS:H	3	0.11
(2,124)	1:A:16:VAL:HB	1:A:17:LYS:H	21	0.11
(2,122)	1:A:16:VAL:HA	1:B:18:VAL:HA	15	0.11
(2,122)	1:A:16:VAL:HA	1:B:18:VAL:HA	23	0.11
(2,12)	1:A:4:GLY:HA3	1:A:5:ASP:H	13	0.11
(2,12)	1:A:4:GLY:HA3	1:A:5:ASP:H	19	0.11
(2,119)	1:A:16:VAL:HA	1:A:16:VAL:HB	3	0.11
(2,119)	1:A:16:VAL:HA	1:A:16:VAL:HB	5	0.11
(2,119)	1:A:16:VAL:HA	1:A:16:VAL:HB	10	0.11
(2,119)	1:A:16:VAL:HA	1:A:16:VAL:HB	12	0.11
(2,119)	1:A:16:VAL:HA	1:A:16:VAL:HB	15	0.11
(2,119)	1:A:16:VAL:HA	1:A:16:VAL:HB	17	0.11
(2,119)	1:A:16:VAL:HA	1:A:16:VAL:HB	19	0.11
(2,119)	1:A:16:VAL:HA	1:A:16:VAL:HB	23	0.11
(2,119)	1:A:16:VAL:HA	1:A:16:VAL:HB	24	0.11
(2,119)	1:A:16:VAL:HA	1:A:16:VAL:HB	27	0.11
(2,115)	1:A:15:VAL:H	1:B:20:GLU:H	5	0.11
(2,115)	1:A:15:VAL:H	1:B:20:GLU:H	8	0.11
(2,115)	1:A:15:VAL:H	1:B:20:GLU:H	14	0.11
(2,115)	1:A:15:VAL:H	1:B:20:GLU:H	26	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found