



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 06:53 PM UTC

PDB ID : 2MOW / pdb_00002mow
BMRB ID : 19954
Title : Structure of Nrd1p CID - Trf4p NIM complex
Authors : Kabzinski, T.; Stefl, R.; Kubicek, K.
Deposited on : 2014-05-06

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

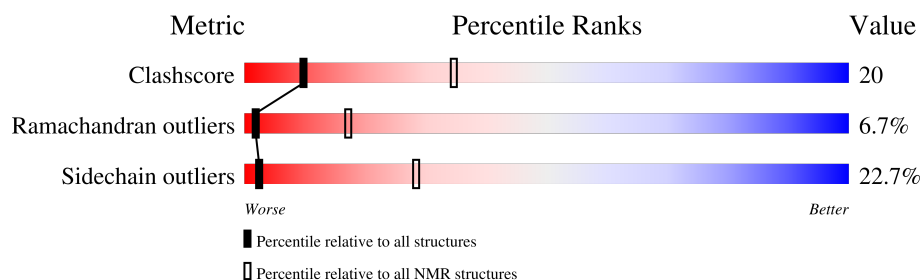
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 71%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	161	35% 39% 7% 19%
2	B	12	17% 8% 75%

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:6-A:20, A:24-A:85, A:91-A:134, A:144-A:152, B:1008-B:1010 (133)	0.56	8

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 3 clusters. No single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2722 atoms, of which 1339 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein NRD1.

Mol	Chain	Residues	Atoms						Trace
1	A	161	Total	C	H	N	O	S	0
			2549	801	1265	228	249	6	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	LEU	-	expression tag	UNP P53617
A	155	GLU	-	expression tag	UNP P53617
A	156	HIS	-	expression tag	UNP P53617
A	157	HIS	-	expression tag	UNP P53617
A	158	HIS	-	expression tag	UNP P53617
A	159	HIS	-	expression tag	UNP P53617
A	160	HIS	-	expression tag	UNP P53617
A	161	HIS	-	expression tag	UNP P53617

- Molecule 2 is a protein called Poly(A) RNA polymerase protein 2.

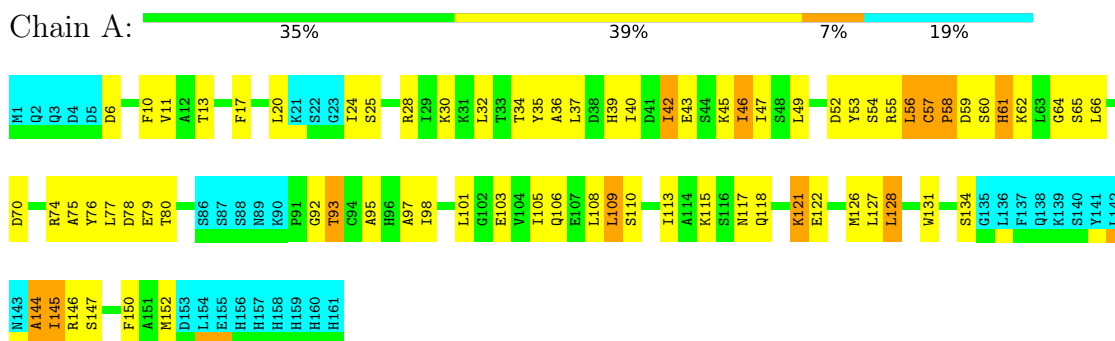
Mol	Chain	Residues	Atoms						Trace
2	B	12	Total	C	H	N	O		0
			173	60	74	13	26		

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: Protein NRD1



• Molecule 2: Poly(A) RNA polymerase protein 2

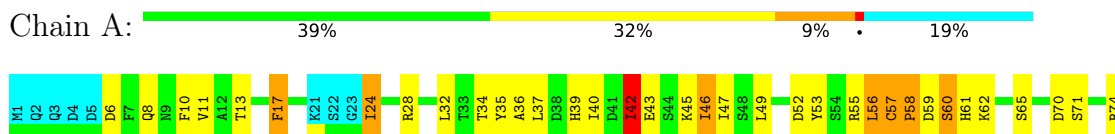


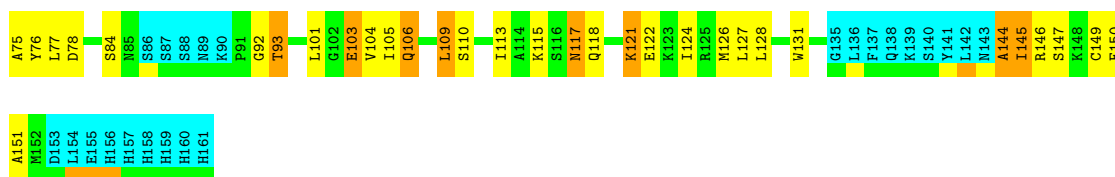
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Protein NRD1



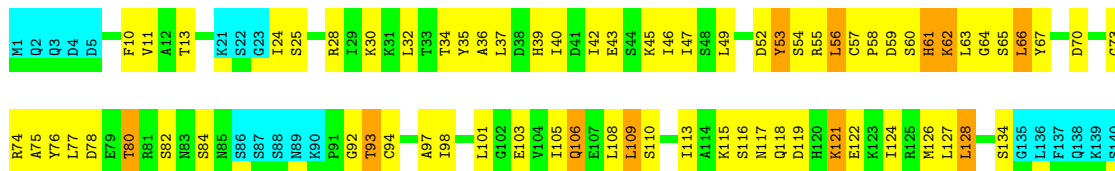


• Molecule 2: Poly(A) RNA polymerase protein 2



4.2.2 Score per residue for model 2

• Molecule 1: Protein NRD1

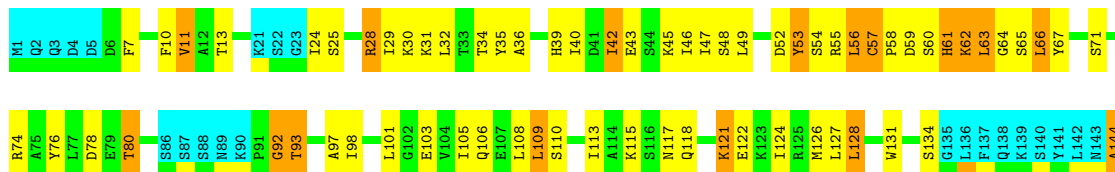


• Molecule 2: Poly(A) RNA polymerase protein 2



4.2.3 Score per residue for model 3

• Molecule 1: Protein NRD1



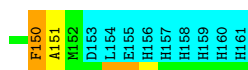


- Molecule 2: Poly(A) RNA polymerase protein 2

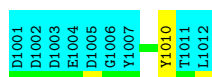


4.2.4 Score per residue for model 4

- Molecule 1: Protein NRD1

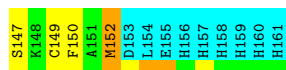
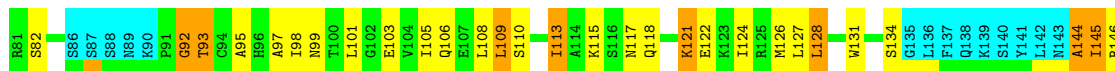


- Molecule 2: Poly(A) RNA polymerase protein 2



4.2.5 Score per residue for model 5

- Molecule 1: Protein NRD1

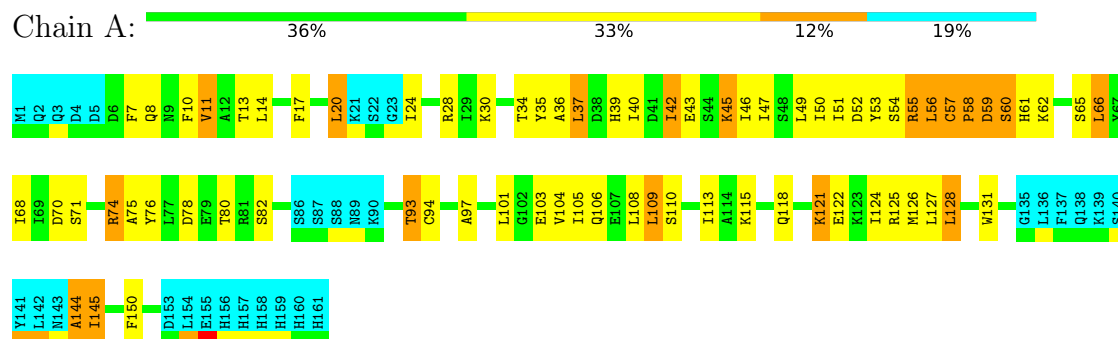


- Molecule 2: Poly(A) RNA polymerase protein 2



4.2.6 Score per residue for model 6

- Molecule 1: Protein NRD1

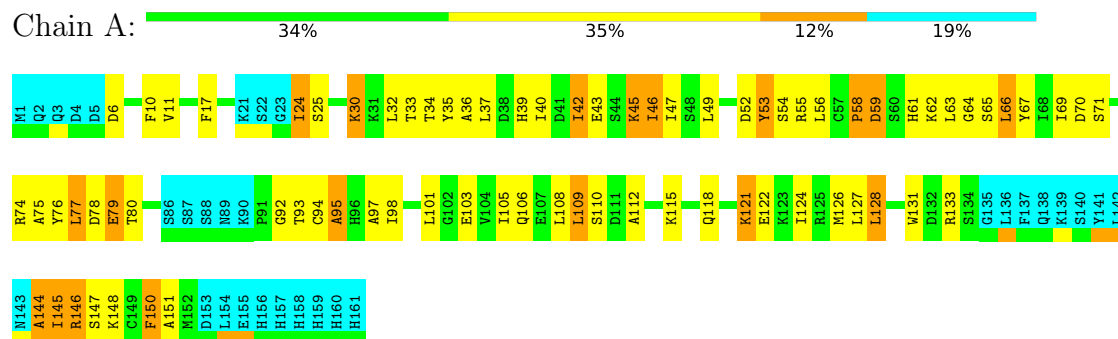


- Molecule 2: Poly(A) RNA polymerase protein 2



4.2.7 Score per residue for model 7

- Molecule 1: Protein NRD1

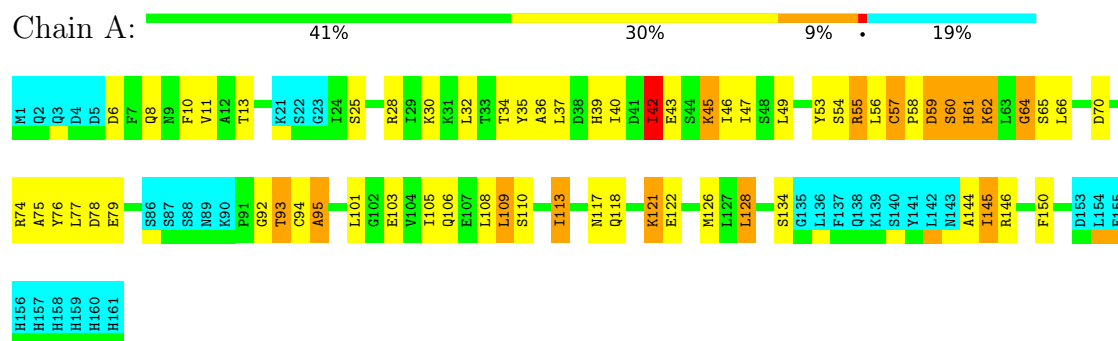


- Molecule 2: Poly(A) RNA polymerase protein 2



4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Protein NRD1

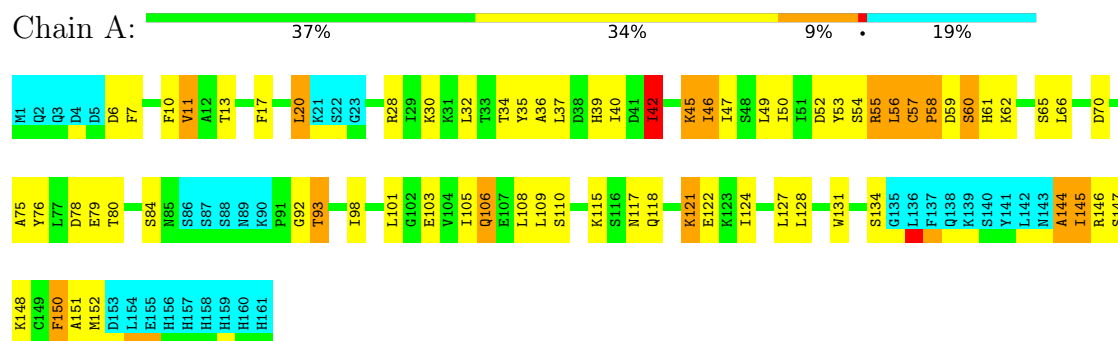


- Molecule 2: Poly(A) RNA polymerase protein 2



4.2.9 Score per residue for model 9

- Molecule 1: Protein NRD1

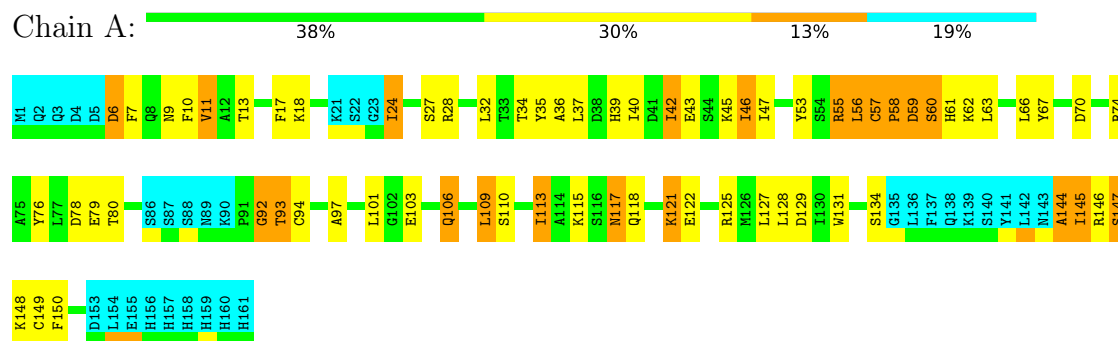


- Molecule 2: Poly(A) RNA polymerase protein 2



4.2.10 Score per residue for model 10

- Molecule 1: Protein NRD1

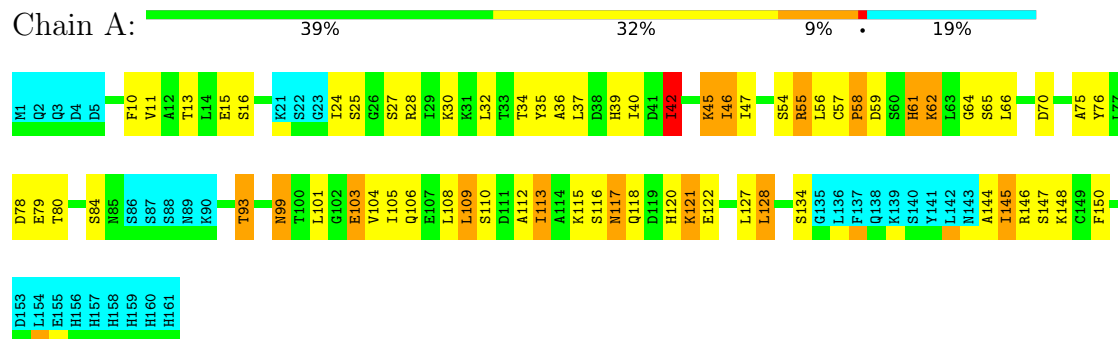


- Molecule 2: Poly(A) RNA polymerase protein 2



4.2.11 Score per residue for model 11

- Molecule 1: Protein NRD1

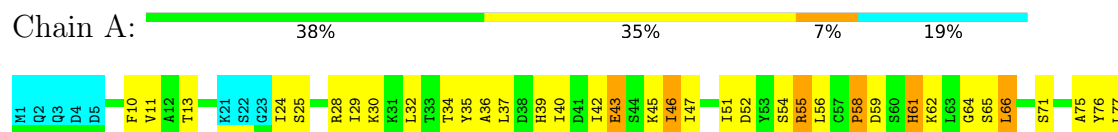


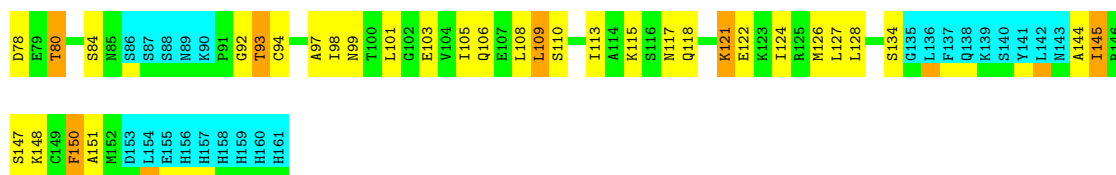
- Molecule 2: Poly(A) RNA polymerase protein 2



4.2.12 Score per residue for model 12

- Molecule 1: Protein NRD1



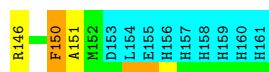
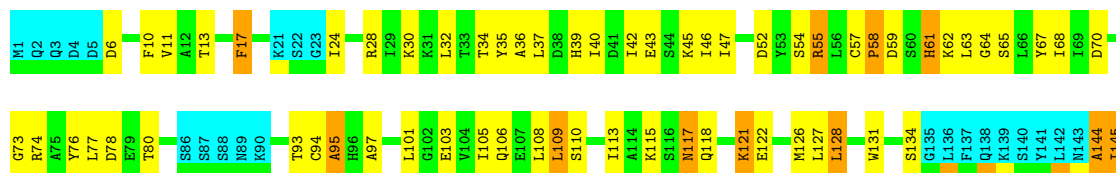


- Molecule 2: Poly(A) RNA polymerase protein 2

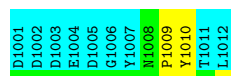


4.2.13 Score per residue for model 13

- Molecule 1: Protein NRD1



- Molecule 2: Poly(A) RNA polymerase protein 2



4.2.14 Score per residue for model 14

- Molecule 1: Protein NRD1



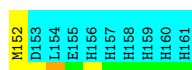


- Molecule 2: Poly(A) RNA polymerase protein 2



4.2.15 Score per residue for model 15

- Molecule 1: Protein NRD1

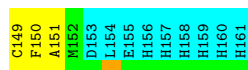


- Molecule 2: Poly(A) RNA polymerase protein 2



4.2.16 Score per residue for model 16

- Molecule 1: Protein NRD1

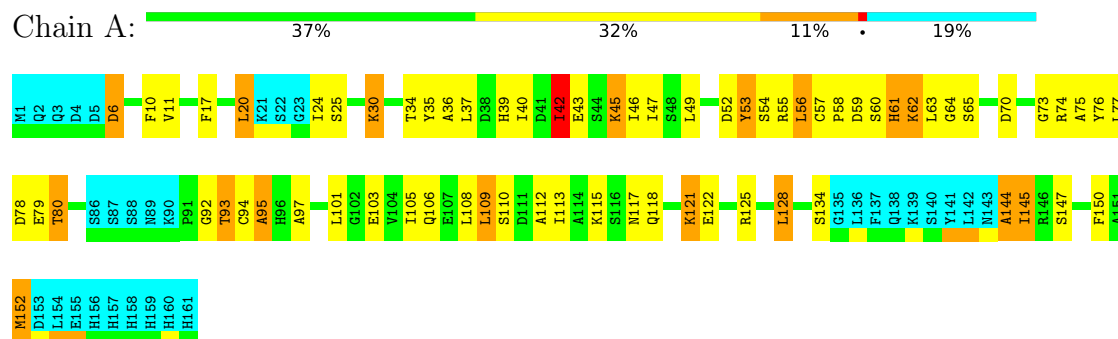


- Molecule 2: Poly(A) RNA polymerase protein 2



4.2.17 Score per residue for model 17

- Molecule 1: Protein NRD1

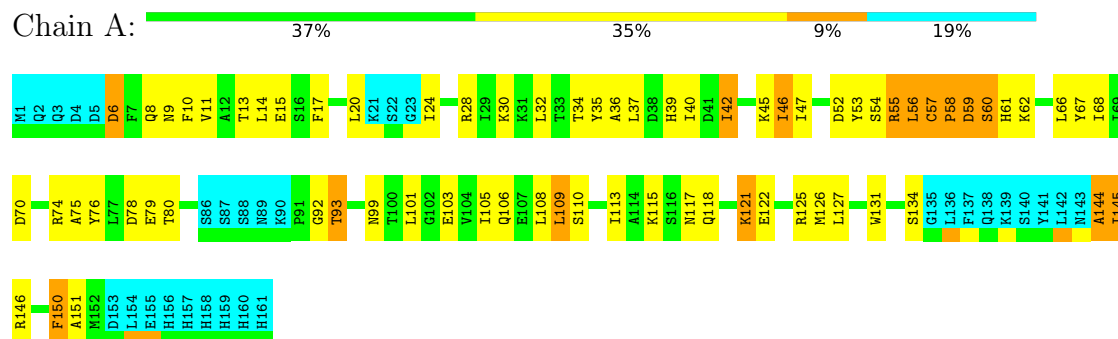


- Molecule 2: Poly(A) RNA polymerase protein 2



4.2.18 Score per residue for model 18

- Molecule 1: Protein NRD1

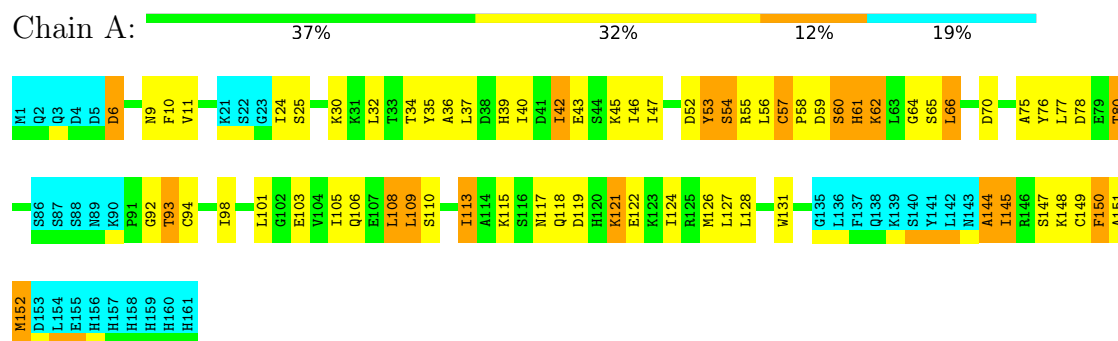


- Molecule 2: Poly(A) RNA polymerase protein 2



4.2.19 Score per residue for model 19

• Molecule 1: Protein NRD1

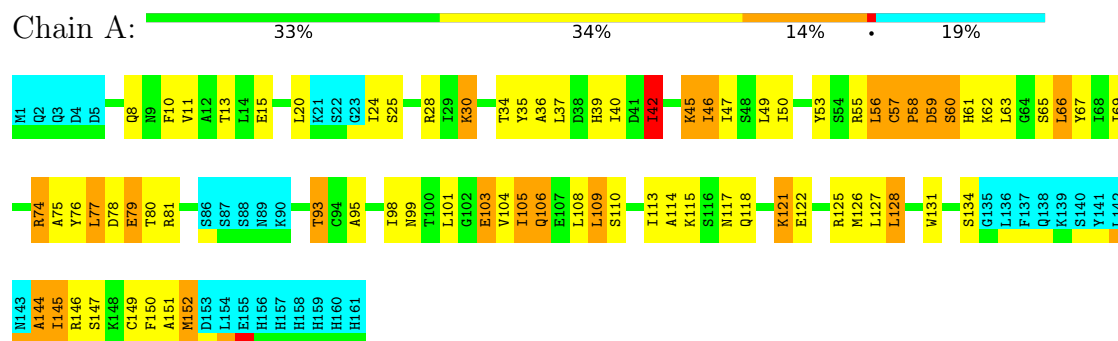


• Molecule 2: Poly(A) RNA polymerase protein 2



4.2.20 Score per residue for model 20

• Molecule 1: Protein NRD1



• Molecule 2: Poly(A) RNA polymerase protein 2



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CYANA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1475
Number of shifts mapped to atoms	1475
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1028	1039	1039	42±6
2	B	27	22	22	0±0
All	All	21100	21220	21220	832

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 20.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:LEU:HD11	1:A:145:ILE:HG21	0.85	1.46	12	6
1:A:17:PHE:O	1:A:20:LEU:HD22	0.84	1.71	9	3
1:A:109:LEU:HD22	1:A:128:LEU:HD11	0.83	1.50	9	2
1:A:47:ILE:HD12	1:A:101:LEU:HD11	0.82	1.47	20	20
1:A:109:LEU:HD13	1:A:145:ILE:HD12	0.82	1.49	12	12
1:A:20:LEU:C	1:A:20:LEU:HD23	0.75	2.06	6	3
1:A:150:PHE:CG	1:A:151:ALA:N	0.71	2.58	16	3
1:A:106:GLN:HA	1:A:144:ALA:HB2	0.71	1.61	9	2
1:A:105:ILE:HG13	1:A:109:LEU:HD12	0.70	1.64	18	18
1:A:10:PHE:CZ	1:A:46:ILE:HG23	0.69	2.22	13	20
1:A:37:LEU:HD21	1:A:75:ALA:HB1	0.68	1.66	7	10
1:A:63:LEU:HD12	1:A:67:TYR:CE2	0.67	2.25	3	1
1:A:105:ILE:CG1	1:A:109:LEU:HD12	0.66	2.20	13	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:HD23	1:A:20:LEU:O	0.66	1.91	6	3
1:A:150:PHE:CD1	1:A:151:ALA:N	0.66	2.64	20	3
1:A:66:LEU:HD22	1:A:127:LEU:HD23	0.65	1.69	2	5
1:A:66:LEU:CD2	1:A:127:LEU:HD23	0.65	2.22	19	4
1:A:62:LYS:O	1:A:66:LEU:HD12	0.65	1.91	3	8
1:A:128:LEU:HD11	1:A:145:ILE:HG13	0.64	1.70	4	6
1:A:37:LEU:HD11	1:A:75:ALA:CB	0.64	2.23	11	13
1:A:17:PHE:CD2	1:A:68:ILE:HD11	0.63	2.27	4	3
1:A:128:LEU:HD11	1:A:145:ILE:CB	0.63	2.24	8	6
1:A:127:LEU:HD12	2:B:1009:PRO:HG3	0.62	1.71	20	4
1:A:54:SER:OG	1:A:55:ARG:N	0.62	2.31	13	13
1:A:150:PHE:CE1	1:A:151:ALA:HB2	0.62	2.30	16	2
1:A:36:ALA:HB1	1:A:76:TYR:OH	0.61	1.95	3	18
1:A:109:LEU:HD13	1:A:145:ILE:CD1	0.61	2.26	13	8
1:A:53:TYR:HA	1:A:56:LEU:HD12	0.60	1.73	17	12
1:A:54:SER:O	1:A:61:HIS:CG	0.60	2.54	11	11
1:A:76:TYR:O	1:A:80:THR:HG22	0.60	1.96	16	18
1:A:57:CYS:HB2	1:A:61:HIS:CG	0.59	2.31	16	9
1:A:20:LEU:HD11	1:A:24:ILE:N	0.58	2.13	6	1
1:A:39:HIS:CB	1:A:42:ILE:HD11	0.58	2.28	8	16
1:A:53:TYR:CD1	1:A:53:TYR:C	0.58	2.81	16	15
1:A:54:SER:OG	1:A:108:LEU:HD22	0.58	1.99	6	9
1:A:37:LEU:HD11	1:A:75:ALA:HB1	0.58	1.75	12	8
1:A:40:ILE:CG2	1:A:93:THR:HG22	0.58	2.28	18	4
1:A:80:THR:HG21	1:A:98:ILE:HD12	0.57	1.76	12	6
1:A:17:PHE:CZ	1:A:24:ILE:HG23	0.57	2.34	10	3
1:A:42:ILE:HG22	1:A:45:LYS:CE	0.57	2.29	8	7
1:A:66:LEU:HD23	1:A:127:LEU:HD23	0.57	1.75	19	2
1:A:58:PRO:O	1:A:59:ASP:C	0.57	2.47	18	14
1:A:61:HIS:CG	1:A:62:LYS:N	0.57	2.73	5	11
1:A:77:LEU:HD22	1:A:98:ILE:HD13	0.57	1.77	7	2
1:A:40:ILE:O	1:A:40:ILE:HG22	0.57	1.99	8	15
1:A:30:LYS:O	1:A:34:THR:HG22	0.57	2.00	5	18
1:A:47:ILE:CD1	1:A:101:LEU:HD11	0.56	2.29	20	13
1:A:128:LEU:HD11	1:A:145:ILE:CG1	0.56	2.30	20	8
1:A:105:ILE:HA	1:A:108:LEU:HD12	0.56	1.76	11	4
1:A:109:LEU:CD1	1:A:128:LEU:HD21	0.56	2.30	9	2
1:A:128:LEU:HD11	1:A:145:ILE:HB	0.56	1.76	8	2
1:A:66:LEU:HD22	1:A:127:LEU:CD2	0.56	2.30	6	3
1:A:37:LEU:HD23	1:A:79:GLU:CD	0.55	2.26	17	1
1:A:128:LEU:HD11	1:A:145:ILE:HD12	0.55	1.79	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:HIS:HB2	1:A:42:ILE:HD11	0.55	1.77	15	11
1:A:150:PHE:O	1:A:151:ALA:C	0.55	2.49	19	6
1:A:118:GLN:O	1:A:121:LYS:HG3	0.54	2.03	6	20
1:A:40:ILE:HG22	1:A:93:THR:HG22	0.54	1.79	18	12
1:A:128:LEU:HD13	1:A:145:ILE:HG21	0.54	1.77	9	2
1:A:127:LEU:HD21	1:A:131:TRP:CZ2	0.54	2.37	10	11
1:A:47:ILE:HD12	1:A:101:LEU:CD1	0.53	2.34	8	18
1:A:43:GLU:HB2	1:A:97:ALA:HB2	0.53	1.81	14	12
1:A:6:ASP:O	1:A:9:ASN:ND2	0.53	2.42	10	3
1:A:59:ASP:O	1:A:60:SER:C	0.53	2.50	10	15
1:A:13:THR:HG23	1:A:28:ARG:HD3	0.52	1.82	18	1
1:A:61:HIS:O	1:A:62:LYS:C	0.52	2.52	14	9
1:A:24:ILE:HD11	1:A:63:LEU:HB3	0.52	1.80	3	1
1:A:39:HIS:HB3	1:A:42:ILE:HD11	0.52	1.82	7	4
1:A:109:LEU:HD13	1:A:128:LEU:HD21	0.52	1.82	10	2
1:A:24:ILE:HD11	1:A:63:LEU:HG	0.51	1.82	5	3
1:A:145:ILE:H	1:A:145:ILE:HD13	0.51	1.66	12	1
1:A:105:ILE:HG12	1:A:109:LEU:HD12	0.51	1.82	13	1
1:A:104:VAL:HG23	1:A:108:LEU:HD11	0.51	1.83	11	1
1:A:57:CYS:O	1:A:61:HIS:HB3	0.50	2.06	2	6
1:A:37:LEU:HD23	1:A:79:GLU:HG3	0.50	1.84	18	7
1:A:13:THR:HG21	1:A:28:ARG:O	0.50	2.07	12	17
1:A:145:ILE:O	1:A:146:ARG:C	0.50	2.55	9	12
1:A:93:THR:O	1:A:94:CYS:C	0.50	2.55	8	5
1:A:66:LEU:HD13	1:A:124:ILE:HG12	0.49	1.83	5	6
1:A:37:LEU:HD23	1:A:79:GLU:CG	0.49	2.37	11	7
1:A:117:ASN:O	1:A:118:GLN:C	0.49	2.55	13	5
1:A:61:HIS:CD2	1:A:61:HIS:C	0.49	2.90	8	3
1:A:109:LEU:O	1:A:110:SER:C	0.49	2.55	1	20
1:A:24:ILE:HD12	1:A:67:TYR:CD2	0.49	2.42	5	3
1:A:51:ILE:HD13	1:A:104:VAL:HG21	0.49	1.85	4	2
1:A:128:LEU:HD11	1:A:145:ILE:CG2	0.49	2.38	16	3
1:A:128:LEU:HD13	1:A:145:ILE:HD12	0.49	1.84	9	1
1:A:10:PHE:CD1	1:A:32:LEU:HD23	0.48	2.43	18	16
1:A:63:LEU:HD11	1:A:67:TYR:CZ	0.48	2.43	15	5
1:A:94:CYS:O	1:A:95:ALA:C	0.48	2.56	8	4
1:A:92:GLY:O	1:A:93:THR:HG23	0.48	2.09	2	7
1:A:77:LEU:HD12	1:A:81:ARG:CD	0.48	2.39	20	1
1:A:113:ILE:HG12	1:A:124:ILE:HG21	0.48	1.84	16	3
1:A:14:LEU:CD1	1:A:68:ILE:HD13	0.48	2.39	18	3
1:A:109:LEU:HD22	1:A:145:ILE:HG21	0.47	1.86	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:GLY:O	1:A:65:SER:C	0.47	2.58	2	11
1:A:66:LEU:CD1	1:A:124:ILE:HG23	0.47	2.40	9	1
1:A:7:PHE:CE2	1:A:11:VAL:HG23	0.46	2.45	10	4
1:A:10:PHE:CE2	1:A:49:LEU:HD23	0.46	2.45	7	12
1:A:128:LEU:HD21	1:A:145:ILE:HB	0.46	1.87	19	1
1:A:80:THR:HG21	1:A:98:ILE:CD1	0.46	2.40	15	2
1:A:20:LEU:C	1:A:20:LEU:CD2	0.46	2.78	6	3
1:A:66:LEU:HD12	1:A:124:ILE:HG12	0.46	1.86	9	1
1:A:94:CYS:O	1:A:97:ALA:HB3	0.46	2.11	17	4
1:A:53:TYR:O	1:A:56:LEU:HB2	0.46	2.11	18	1
1:A:40:ILE:O	1:A:40:ILE:CG2	0.45	2.65	8	1
1:A:69:ILE:HG23	1:A:101:LEU:HD22	0.45	1.88	20	1
1:A:57:CYS:CB	1:A:58:PRO:HD2	0.45	2.41	14	9
1:A:17:PHE:CE2	1:A:68:ILE:HD11	0.45	2.46	4	1
1:A:116:SER:HB2	1:A:120:HIS:CB	0.45	2.42	15	2
1:A:58:PRO:C	1:A:62:LYS:HG3	0.45	2.36	14	1
1:A:128:LEU:HD21	1:A:145:ILE:HG13	0.45	1.88	8	5
1:A:77:LEU:C	1:A:77:LEU:HD13	0.44	2.37	17	1
1:A:65:SER:O	1:A:66:LEU:C	0.44	2.61	19	4
1:A:147:SER:C	1:A:149:CYS:N	0.43	2.75	20	3
1:A:17:PHE:CE1	1:A:24:ILE:HD13	0.43	2.48	7	1
1:A:148:LYS:O	1:A:149:CYS:C	0.43	2.61	10	2
1:A:103:GLU:HG2	1:A:104:VAL:HG13	0.43	1.89	4	5
1:A:34:THR:HG23	1:A:35:TYR:N	0.43	2.29	20	20
1:A:117:ASN:O	1:A:121:LYS:N	0.43	2.48	13	4
1:A:109:LEU:O	1:A:112:ALA:HB3	0.43	2.14	11	1
1:A:65:SER:O	1:A:69:ILE:HD12	0.43	2.14	7	1
1:A:115:LYS:O	1:A:116:SER:C	0.42	2.61	2	1
1:A:17:PHE:O	1:A:20:LEU:CD2	0.42	2.58	9	1
1:A:61:HIS:O	1:A:65:SER:N	0.42	2.52	19	3
1:A:128:LEU:HD22	1:A:145:ILE:CD1	0.42	2.45	9	1
1:A:47:ILE:HA	1:A:50:ILE:HD11	0.42	1.92	9	5
1:A:37:LEU:HD11	1:A:75:ALA:HB3	0.42	1.91	11	2
1:A:29:ILE:HA	1:A:32:LEU:HD12	0.41	1.92	12	2
1:A:62:LYS:CD	1:A:112:ALA:HA	0.41	2.45	7	3
1:A:18:LYS:CB	1:A:61:HIS:CE1	0.41	3.04	10	1
1:A:149:CYS:HA	1:A:152:MET:HE3	0.41	1.90	5	1
1:A:147:SER:O	1:A:148:LYS:C	0.41	2.63	10	1
1:A:150:PHE:CD1	1:A:150:PHE:C	0.41	2.99	20	1
1:A:55:ARG:O	1:A:56:LEU:C	0.41	2.64	10	1
1:A:37:LEU:HA	1:A:40:ILE:HD11	0.41	1.92	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:VAL:HG12	1:A:12:ALA:N	0.41	2.32	14	1
1:A:47:ILE:HG22	1:A:51:ILE:CD1	0.40	2.46	12	1
1:A:40:ILE:HG22	1:A:40:ILE:O	0.40	2.16	17	2
1:A:99:ASN:OD1	1:A:99:ASN:C	0.40	2.63	11	1
1:A:33:THR:O	1:A:34:THR:C	0.40	2.64	7	1
1:A:113:ILE:CD1	1:A:150:PHE:CE1	0.40	3.05	20	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	130/161 (81%)	94±4 (72±3%)	27±4 (21±3%)	9±2 (7±1%)	2	16
2	B	3/12 (25%)	3±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	2660/3460 (77%)	1936 (73%)	545 (20%)	179 (7%)	2	17

All 23 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	58	PRO	20
1	A	144	ALA	20
1	A	56	LEU	18
1	A	150	PHE	17
1	A	134	SER	14
1	A	46	ILE	10
1	A	24	ILE	9
1	A	60	SER	9
1	A	92	GLY	9
1	A	147	SER	8
1	A	95	ALA	8
1	A	42	ILE	7
1	A	62	LYS	6
1	A	20	LEU	5
1	A	108	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	106	GLN	3
1	A	6	ASP	3
1	A	79	GLU	3
1	A	84	SER	2
1	A	133	ARG	1
1	A	64	GLY	1
1	A	109	LEU	1
1	A	85	ASN	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	116/145 (80%)	90±2 (77±2%)	26±2 (23±2%)	2	28
2	B	3/11 (27%)	2±0 (75±14%)	1±0 (25±14%)	2	25
All	All	2380/3120 (76%)	1840 (77%)	540 (23%)	2	28

All 63 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	11	VAL	20
1	A	45	LYS	20
1	A	78	ASP	20
1	A	93	THR	20
1	A	103	GLU	20
1	A	106	GLN	20
1	A	121	LYS	20
1	A	122	GLU	20
1	A	145	ILE	20
1	A	109	LEU	18
1	A	115	LYS	17
1	A	42	ILE	15
1	A	52	ASP	15
1	A	55	ARG	15
1	A	57	CYS	15
1	A	126	MET	15

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Mol	Chain	Res	Type	Models (Total)
1	A	128	LEU	15
2	B	1010	TYR	15
1	A	117	ASN	14
1	A	70	ASP	13
1	A	25	SER	12
1	A	66	LEU	12
1	A	6	ASP	10
1	A	61	HIS	10
1	A	74	ARG	10
1	A	62	LYS	9
1	A	59	ASP	9
1	A	113	ILE	9
1	A	8	GLN	8
1	A	80	THR	8
1	A	65	SER	7
1	A	53	TYR	7
1	A	43	GLU	6
1	A	99	ASN	6
1	A	152	MET	5
1	A	30	LYS	5
1	A	125	ARG	5
1	A	71	SER	4
1	A	84	SER	4
1	A	15	GLU	4
1	A	77	LEU	4
1	A	148	LYS	4
1	A	82	SER	3
1	A	146	ARG	3
1	A	20	LEU	3
1	A	147	SER	3
1	A	17	PHE	2
1	A	119	ASP	2
1	A	31	LYS	2
1	A	83	ASN	2
1	A	60	SER	2
1	A	27	SER	2
1	A	28	ARG	1
1	A	48	SER	1
1	A	63	LEU	1
1	A	37	LEU	1
1	A	94	CYS	1
1	A	129	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	16	SER	1
1	A	24	ILE	1
1	A	81	ARG	1
1	A	54	SER	1
1	A	105	ILE	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 71% for the well-defined parts and 63% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1475
Number of shifts mapped to atoms	1475
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	147	1.80 ± 0.12	Should be checked
$^{13}\text{C}_\beta$	111	2.54 ± 0.14	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	146	0.33 ± 0.28	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 71%, i.e. 1309 atoms were assigned a chemical shift out of a possible 1832. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	512/664 (77%)	262/268 (98%)	126/266 (47%)	124/130 (95%)
Sidechain	782/1043 (75%)	562/679 (83%)	215/325 (66%)	5/39 (13%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	15/125 (12%)	15/62 (24%)	0/58 (0%)	0/5 (0%)
Overall	1309/1832 (71%)	839/1009 (83%)	341/649 (53%)	129/174 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 63%, i.e. 1475 atoms were assigned a chemical shift out of a possible 2340. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	599/867 (69%)	306/351 (87%)	147/346 (42%)	146/170 (86%)
Sidechain	861/1278 (67%)	628/826 (76%)	227/405 (56%)	6/47 (13%)
Aromatic	15/195 (8%)	15/99 (15%)	0/85 (0%)	0/11 (0%)
Overall	1475/2340 (63%)	949/1276 (74%)	374/836 (45%)	152/228 (67%)

7.1.4 Statistically unusual chemical shifts ⓘ

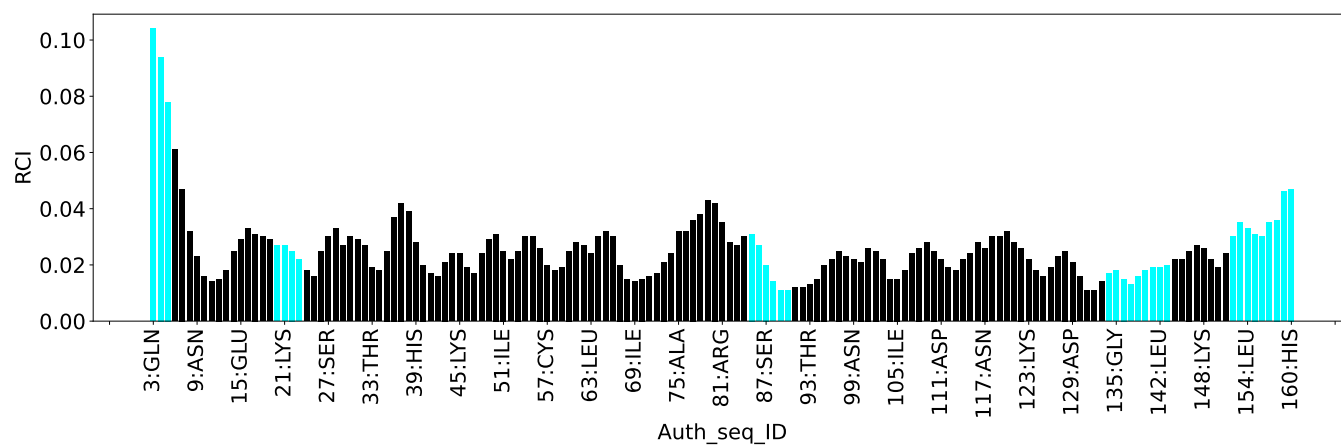
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	55	ARG	NE	110.24	76.53 – 92.65	15.9
1	A	81	ARG	NE	107.90	76.53 – 92.65	14.5
1	A	21	LYS	CE	47.66	37.57 – 46.21	6.7
1	A	139	LYS	CE	47.65	37.57 – 46.21	6.7
1	A	128	LEU	CD1	14.95	16.71 – 32.55	-6.1
1	A	10	PHE	HB2	1.18	1.20 – 4.80	-5.0

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2527
Intra-residue ($ i-j =0$)	548
Sequential ($ i-j =1$)	630
Medium range ($ i-j >1$ and $ i-j <5$)	684
Long range ($ i-j \geq 5$)	468
Inter-chain	34
Hydrogen bond restraints	163
Disulfide bond restraints	0
Total dihedral-angle restraints	222
Number of unmapped restraints	0
Number of restraints per residue	15.9
Number of long range restraints per residue ¹	2.7

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	75.3	0.2
0.2-0.5 (Medium)	39.1	0.5
>0.5 (Large)	5.1	4.83

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	37.5	9.98
10.0-20.0 (Medium)	2.6	16.93
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

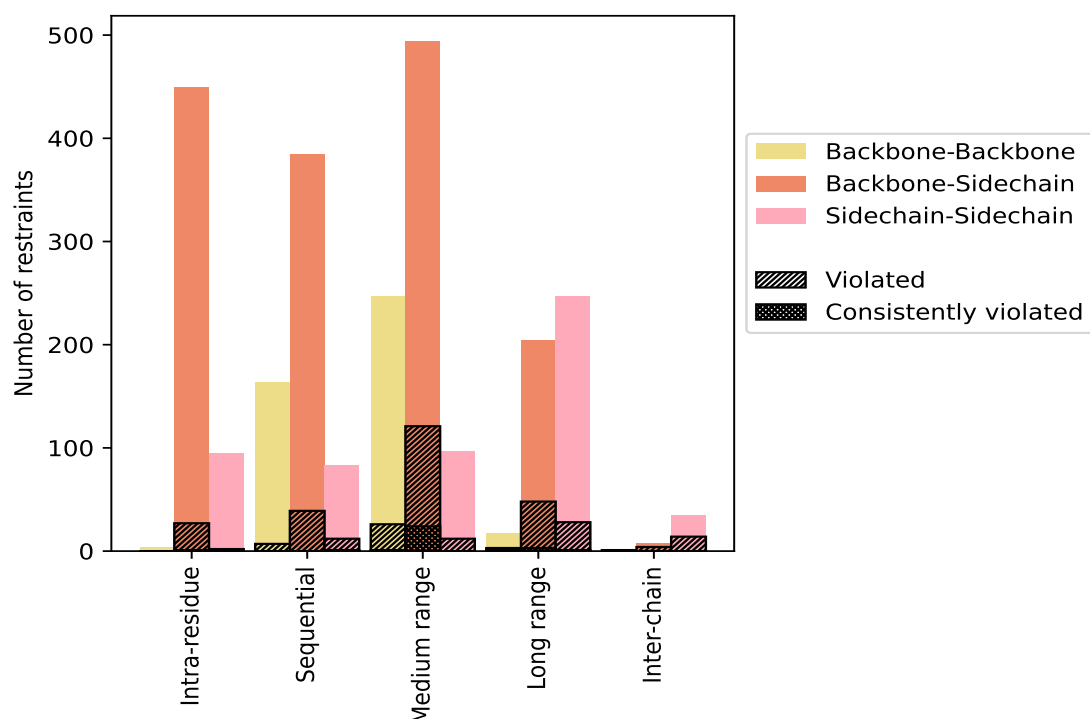
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	548	21.7	29	5.3	1.1	1	0.2	0.0
Backbone-Backbone	4	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	449	17.8	27	6.0	1.1	1	0.2	0.0
Sidechain-Sidechain	95	3.8	2	2.1	0.1	0	0.0	0.0
Sequential (i-j =1)	630	24.9	58	9.2	2.3	1	0.2	0.0
Backbone-Backbone	163	6.5	7	4.3	0.3	0	0.0	0.0
Backbone-Sidechain	384	15.2	39	10.2	1.5	0	0.0	0.0
Sidechain-Sidechain	83	3.3	12	14.5	0.5	1	1.2	0.0
Medium range (i-j >1 & i-j <5)	684	27.1	88	12.9	3.5	6	0.9	0.2
Backbone-Backbone	247	9.8	26	10.5	1.0	1	0.4	0.0
Backbone-Sidechain	340	13.5	50	14.7	2.0	5	1.5	0.2
Sidechain-Sidechain	97	3.8	12	12.4	0.5	0	0.0	0.0
Long range (i-j ≥5)	468	18.5	79	16.9	3.1	5	1.1	0.2
Backbone-Backbone	17	0.7	3	17.6	0.1	1	5.9	0.0
Backbone-Sidechain	204	8.1	48	23.5	1.9	3	1.5	0.1
Sidechain-Sidechain	247	9.8	28	11.3	1.1	1	0.4	0.0
Inter-chain	34	1.3	11	32.4	0.4	0	0.0	0.0
Backbone-Backbone	1	0.0	1	100.0	0.0	0	0.0	0.0
Backbone-Sidechain	6	0.2	3	50.0	0.1	0	0.0	0.0
Sidechain-Sidechain	27	1.1	7	25.9	0.3	0	0.0	0.0
Hydrogen bond	163	6.5	79	48.5	3.1	19	11.7	0.8
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2527	100.0	344	13.6	13.6	32	1.3	1.3
Backbone-Backbone	432	17.1	37	8.6	1.5	2	0.5	0.1
Backbone-Sidechain	1538	60.9	239	15.5	9.5	28	1.8	1.1
Sidechain-Sidechain	557	22.0	68	12.2	2.7	2	0.4	0.1

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	8	12	73	23	4	120	0.23	1.75	0.22	0.18
2	12	14	60	24	6	116	0.25	3.12	0.34	0.17
3	8	12	61	25	5	111	0.24	3.33	0.36	0.17
4	5	14	73	22	6	120	0.24	2.36	0.26	0.19
5	12	15	73	28	4	132	0.24	4.3	0.4	0.17
6	8	13	72	26	7	126	0.23	2.14	0.24	0.17
7	7	17	72	26	5	127	0.21	1.77	0.2	0.16
8	9	13	66	25	7	120	0.26	3.14	0.36	0.17
9	9	12	67	26	6	120	0.27	4.83	0.46	0.18
10	9	15	78	31	5	138	0.24	2.1	0.27	0.17

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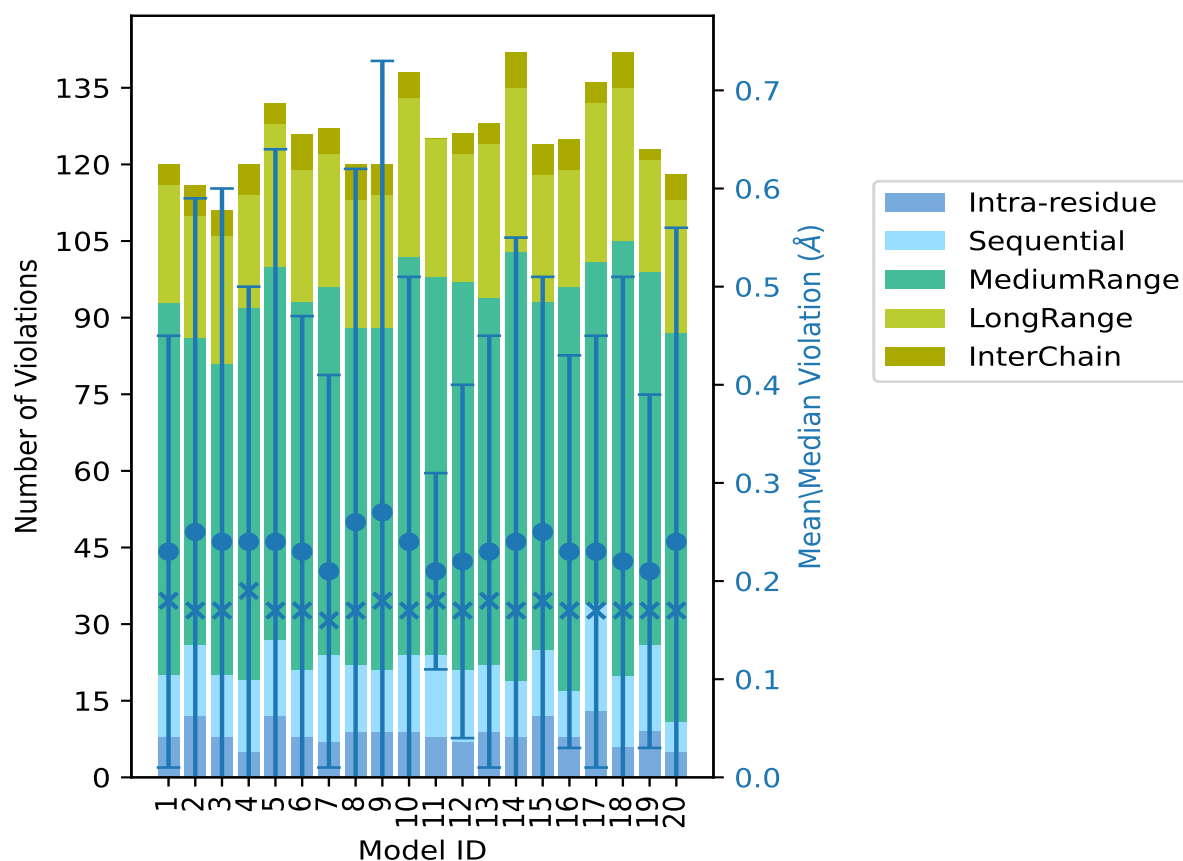
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	8	16	74	27	0	125	0.21	0.68	0.1	0.18
12	7	14	76	25	4	126	0.22	1.67	0.18	0.17
13	9	13	72	30	4	128	0.23	1.85	0.22	0.18
14	8	11	84	32	7	142	0.24	3.12	0.31	0.17
15	12	13	68	25	6	124	0.25	1.93	0.26	0.18
16	8	9	79	23	6	125	0.23	1.67	0.2	0.17
17	13	21	67	31	4	136	0.23	1.93	0.22	0.17
18	6	14	85	30	7	142	0.22	3.12	0.29	0.17
19	9	17	73	22	2	123	0.21	1.9	0.18	0.17
20	5	6	76	26	5	118	0.24	3.25	0.32	0.17

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

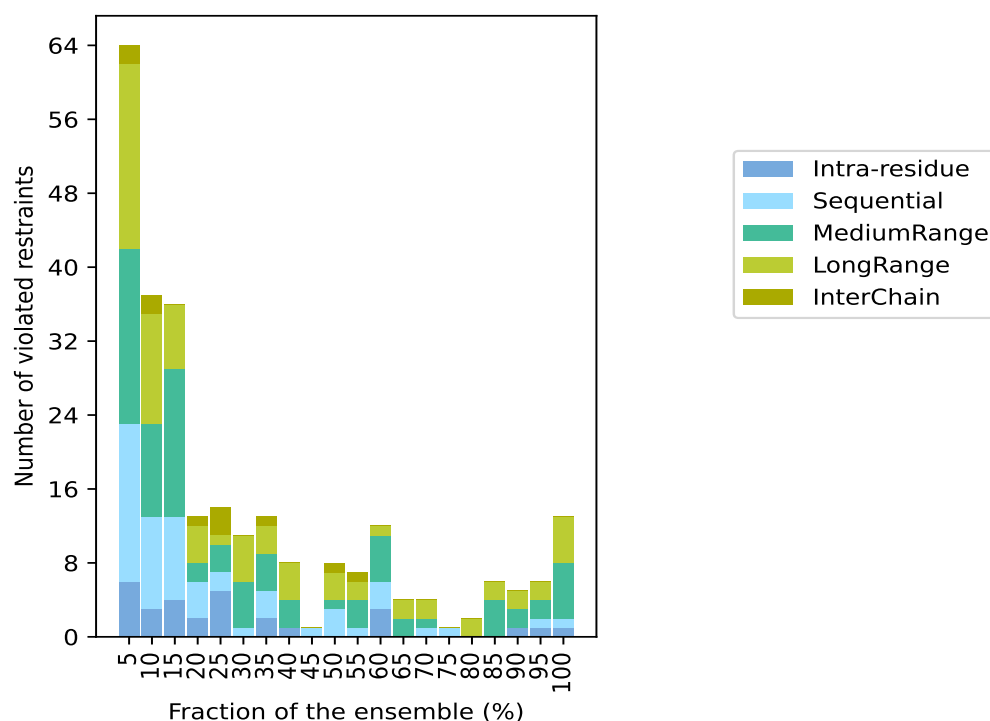
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2099(IR:519, SQ:572, MR:596, LR:389, IC:23) restraints are 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	%
6	17	19	20	2	64	1	5.0
3	10	10	12	2	37	2	10.0
4	9	16	7	0	36	3	15.0
2	4	2	4	1	13	4	20.0
5	2	3	1	3	14	5	25.0
0	1	5	5	0	11	6	30.0
2	3	4	3	1	13	7	35.0
1	0	3	4	0	8	8	40.0
0	1	0	0	0	1	9	45.0
0	3	1	3	1	8	10	50.0
0	1	3	2	1	7	11	55.0
3	3	5	1	0	12	12	60.0
0	0	2	2	0	4	13	65.0
0	1	1	2	0	4	14	70.0
0	1	0	0	0	1	15	75.0
0	0	0	2	0	2	16	80.0
0	0	4	2	0	6	17	85.0
1	0	2	2	0	5	18	90.0
1	1	2	2	0	6	19	95.0
1	1	6	5	0	13	20	100.0

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

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

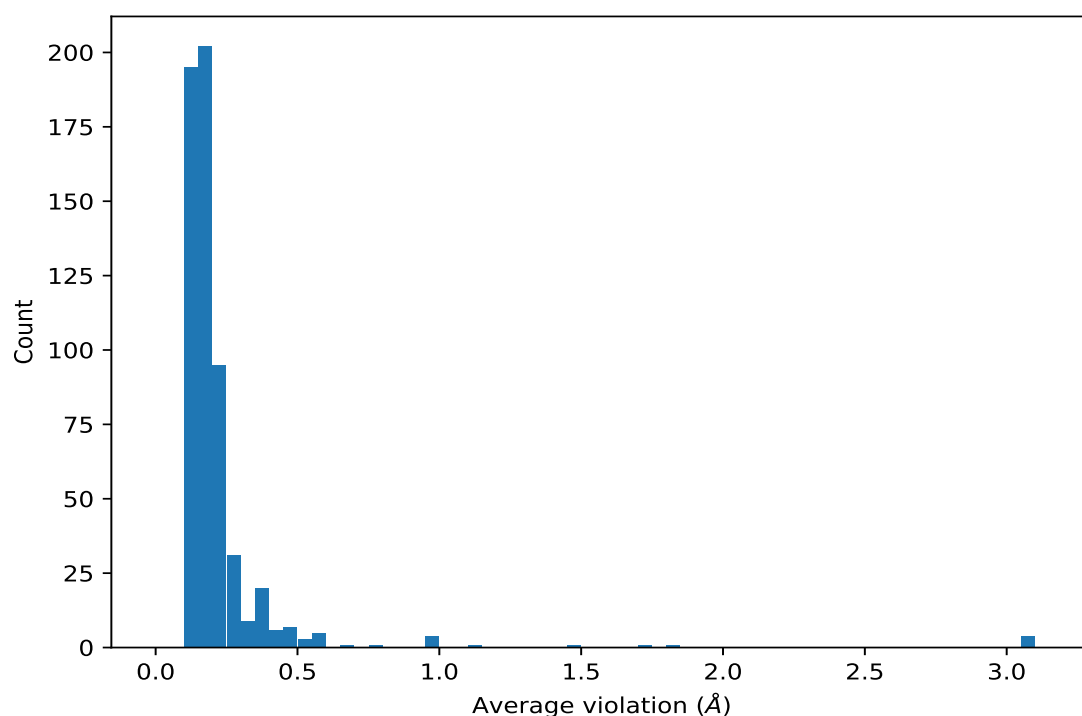
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	20	0.48	0.17	0.52
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	20	0.48	0.17	0.52
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	20	0.48	0.17	0.52
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	20	0.39	0.06	0.38
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	20	0.34	0.05	0.35
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	20	0.31	0.06	0.28
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	20	0.29	0.08	0.29
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	20	0.28	0.05	0.28
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	20	0.27	0.06	0.25
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	20	0.26	0.05	0.27
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	20	0.26	0.03	0.26
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	20	0.24	0.05	0.26
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	20	0.24	0.01	0.24
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	20	0.24	0.04	0.24
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	20	0.23	0.03	0.23
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	20	0.23	0.06	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	20	0.23	0.06	0.23
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	20	0.23	0.06	0.23
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	20	0.22	0.04	0.22
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	20	0.21	0.05	0.2
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	20	0.21	0.05	0.2
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	20	0.21	0.05	0.2
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	20	0.2	0.02	0.2
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	20	0.2	0.03	0.19
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	20	0.19	0.02	0.2
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	20	0.19	0.04	0.18
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	20	0.19	0.05	0.19
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	20	0.18	0.05	0.18
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	20	0.18	0.04	0.18
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	20	0.18	0.05	0.16
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	20	0.18	0.03	0.18
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	20	0.17	0.03	0.17
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	20	0.17	0.04	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	20	0.17	0.02	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	20	0.17	0.02	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	20	0.17	0.02	0.17
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	20	0.17	0.03	0.16
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	20	0.17	0.03	0.16
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	20	0.17	0.03	0.16
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	20	0.17	0.03	0.16
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	20	0.17	0.03	0.16
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	20	0.17	0.03	0.16
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	20	0.17	0.03	0.16
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	20	0.17	0.03	0.16
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	20	0.17	0.03	0.16
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	20	0.16	0.02	0.16
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	20	0.15	0.03	0.15
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	20	0.15	0.03	0.15
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	20	0.15	0.03	0.15
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	20	0.15	0.03	0.15
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	19	0.24	0.05	0.22
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	19	0.24	0.05	0.22
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	19	0.24	0.05	0.22
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	19	0.19	0.04	0.2
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	19	0.19	0.04	0.2
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	19	0.19	0.03	0.19
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	19	0.18	0.04	0.19
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	19	0.18	0.04	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	19	0.18	0.04	0.19
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	19	0.16	0.03	0.16
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	19	0.16	0.03	0.16
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	19	0.16	0.03	0.16
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	19	0.15	0.02	0.14
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	19	0.15	0.02	0.14
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	19	0.15	0.02	0.14
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	19	0.14	0.03	0.14
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	19	0.14	0.01	0.14
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	19	0.13	0.03	0.13
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	18	0.42	0.05	0.42
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	18	0.42	0.05	0.42
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	18	0.42	0.05	0.42
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	18	0.31	0.17	0.26
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	18	0.25	0.04	0.26
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	18	0.25	0.04	0.26
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	18	0.25	0.04	0.26
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	18	0.2	0.07	0.19
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	18	0.2	0.07	0.19
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	18	0.2	0.07	0.19
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	18	0.18	0.03	0.18
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	18	0.17	0.03	0.18
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	18	0.16	0.04	0.15
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	18	0.15	0.03	0.15
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	18	0.14	0.04	0.14
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	17	1.72	0.26	1.76
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	17	0.3	0.07	0.29
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	17	0.3	0.07	0.29
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	17	0.26	0.09	0.29
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	17	0.26	0.09	0.29
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	17	0.26	0.09	0.29
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	17	0.19	0.03	0.18
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	17	0.17	0.04	0.17
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	17	0.16	0.02	0.16
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	17	0.15	0.03	0.14
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	17	0.15	0.03	0.14
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	17	0.15	0.03	0.14
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	17	0.15	0.03	0.14
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	17	0.15	0.03	0.14
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	17	0.15	0.03	0.14
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	17	0.15	0.03	0.16
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	17	0.15	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	17	0.15	0.03	0.16
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	16	0.19	0.04	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	16	0.19	0.04	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	16	0.19	0.04	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	16	0.19	0.04	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	16	0.19	0.04	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	16	0.19	0.04	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	16	0.19	0.04	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	16	0.19	0.04	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	16	0.19	0.04	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	16	0.19	0.04	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	16	0.19	0.04	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	16	0.19	0.04	0.18
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	16	0.16	0.04	0.16
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	16	0.15	0.03	0.14
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	16	0.15	0.03	0.14
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	16	0.13	0.02	0.13
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	15	0.18	0.05	0.19
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	15	0.17	0.06	0.14
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	15	0.14	0.02	0.15
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	15	0.11	0.01	0.11
(2,1004)	1:149:A:CYS:HA	1:153:A:ASP:HA	14	0.2	0.09	0.18
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG2	14	0.19	0.13	0.13
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG3	14	0.19	0.13	0.13
(2,854)	1:109:A:LEU:HD21	1:128:A:LEU:HA	14	0.16	0.05	0.16
(2,854)	1:109:A:LEU:HD22	1:128:A:LEU:HA	14	0.16	0.05	0.16
(2,854)	1:109:A:LEU:HD23	1:128:A:LEU:HA	14	0.16	0.05	0.16
(2,599)	1:46:A:ILE:HG21	1:51:A:ILE:H	14	0.13	0.02	0.14
(2,599)	1:46:A:ILE:HG22	1:51:A:ILE:H	14	0.13	0.02	0.14
(2,599)	1:46:A:ILE:HG23	1:51:A:ILE:H	14	0.13	0.02	0.14
(1,64)	1:62:A:LYS:O	1:66:A:LEU:H	13	0.25	0.07	0.26
(2,1629)	1:142:A:LEU:H	1:146:A:ARG:HA	13	0.17	0.06	0.15
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG21	13	0.17	0.04	0.17
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG22	13	0.17	0.04	0.17
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG23	13	0.17	0.04	0.17
(2,128)	1:63:A:LEU:HD11	1:123:A:LYS:HA	13	0.17	0.05	0.16
(2,128)	1:63:A:LEU:HD12	1:123:A:LYS:HA	13	0.17	0.05	0.16
(2,128)	1:63:A:LEU:HD13	1:123:A:LYS:HA	13	0.17	0.05	0.16
(2,1216)	1:15:A:GLU:HB2	1:17:A:PHE:H	13	0.14	0.02	0.14
(2,1216)	1:15:A:GLU:HB3	1:17:A:PHE:H	13	0.14	0.02	0.14
(2,1634)	1:153:A:ASP:H	1:154:A:LEU:HB3	12	0.37	0.03	0.38
(2,1672)	1:115:A:LYS:HE2	1:116:A:SER:H	12	0.24	0.11	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1672)	1:115:A:LYS:HE3	1:116:A:SER:H	12	0.24	0.11	0.21
(2,1662)	1:54:A:SER:HB2	1:66:A:LEU:H	12	0.22	0.08	0.22
(2,1662)	1:54:A:SER:HB3	1:66:A:LEU:H	12	0.22	0.08	0.22
(2,369)	1:17:A:PHE:HA	1:20:A:LEU:HA	12	0.2	0.05	0.21
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD11	12	0.19	0.01	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD12	12	0.19	0.01	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD13	12	0.19	0.01	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD21	12	0.19	0.01	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD22	12	0.19	0.01	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD23	12	0.19	0.01	0.19
(2,1724)	1:154:A:LEU:H	1:154:A:LEU:HB3	12	0.18	0.03	0.16
(1,65)	1:63:A:LEU:O	1:67:A:TYR:N	12	0.16	0.03	0.15
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD21	12	0.15	0.04	0.14
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD22	12	0.15	0.04	0.14
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD23	12	0.15	0.04	0.14
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG2	12	0.14	0.03	0.15
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG3	12	0.14	0.03	0.15
(2,1533)	1:104:A:VAL:H	1:106:A:GLN:HG2	12	0.14	0.03	0.16
(2,1002)	1:154:A:LEU:H	1:154:A:LEU:HB2	12	0.13	0.01	0.13
(2,2009)	1:35:A:TYR:HD1	1:38:A:ASP:H	12	0.13	0.02	0.14
(2,2009)	1:35:A:TYR:HD2	1:38:A:ASP:H	12	0.13	0.02	0.14
(1,24)	1:28:A:ARG:O	1:32:A:LEU:H	12	0.13	0.02	0.13
(2,1541)	1:105:A:ILE:H	1:106:A:GLN:HB3	12	0.11	0.01	0.11
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB2	11	3.06	0.97	3.12
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB3	11	3.06	0.97	3.12
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB2	11	3.06	0.97	3.12
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB3	11	3.06	0.97	3.12
(1,58)	1:59:A:ASP:O	1:63:A:LEU:H	11	0.67	0.04	0.65
(1,57)	1:59:A:ASP:O	1:63:A:LEU:N	11	0.5	0.06	0.5
(2,1730)	1:155:A:GLU:H	1:156:A:HIS:H	11	0.3	0.13	0.23
(2,1693)	1:62:A:LYS:HD2	1:112:A:ALA:H	11	0.26	0.04	0.26
(2,1693)	1:62:A:LYS:HD3	1:112:A:ALA:H	11	0.26	0.04	0.26
(2,1242)	1:20:A:LEU:H	1:23:A:GLY:H	11	0.24	0.06	0.25
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD21	11	0.2	0.05	0.19
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD22	11	0.2	0.05	0.19
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD23	11	0.2	0.05	0.19
(2,568)	1:49:A:LEU:HG	1:53:A:TYR:HA	11	0.17	0.05	0.19
(1,63)	1:62:A:LYS:O	1:66:A:LEU:N	11	0.16	0.03	0.17
(2,1573)	1:113:A:ILE:H	1:115:A:LYS:H	11	0.16	0.04	0.17
(1,52)	1:50:A:ILE:O	1:54:A:SER:H	11	0.13	0.02	0.14
(2,15)	1:126:A:MET:HE3	2:1009:B:PRO:HG2	10	0.39	0.2	0.34
(2,15)	1:126:A:MET:HE2	2:1009:B:PRO:HG2	10	0.39	0.2	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,15)	1:126:A:MET:HE1	2:1009:B:PRO:HG2	10	0.39	0.2	0.34
(2,15)	1:126:A:MET:HE3	2:1009:B:PRO:HD2	10	0.39	0.2	0.34
(2,15)	1:126:A:MET:HE1	2:1009:B:PRO:HD2	10	0.39	0.2	0.34
(2,15)	1:126:A:MET:HE2	2:1009:B:PRO:HD2	10	0.39	0.2	0.34
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD11	10	0.29	0.08	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD12	10	0.29	0.08	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD13	10	0.29	0.08	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD21	10	0.29	0.08	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD22	10	0.29	0.08	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD23	10	0.29	0.08	0.3
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD11	10	0.18	0.05	0.19
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD12	10	0.18	0.05	0.19
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD13	10	0.18	0.05	0.19
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD11	10	0.18	0.05	0.19
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD12	10	0.18	0.05	0.19
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD13	10	0.18	0.05	0.19
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD11	10	0.18	0.05	0.19
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD12	10	0.18	0.05	0.19
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD13	10	0.18	0.05	0.19
(2,252)	1:153:A:ASP:HB3	1:154:A:LEU:HB3	10	0.18	0.07	0.14
(1,150)	1:148:A:LYS:O	1:152:A:MET:H	10	0.16	0.07	0.15
(2,230)	1:55:A:ARG:H	1:108:A:LEU:HB3	10	0.15	0.04	0.14
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG21	10	0.15	0.05	0.12
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG22	10	0.15	0.05	0.12
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG23	10	0.15	0.05	0.12
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG21	10	0.15	0.05	0.12
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG22	10	0.15	0.05	0.12
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG23	10	0.15	0.05	0.12
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG21	10	0.15	0.05	0.12
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG22	10	0.15	0.05	0.12
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG23	10	0.15	0.05	0.12
(1,14)	1:13:A:THR:O	1:17:A:PHE:H	10	0.15	0.03	0.14
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD2	10	0.15	0.02	0.15
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD3	10	0.15	0.02	0.15
(2,1942)	1:74:A:ARG:HD2	1:75:A:ALA:H	10	0.13	0.01	0.13
(2,1942)	1:74:A:ARG:HD3	1:75:A:ALA:H	10	0.13	0.01	0.13
(1,81)	1:71:A:SER:O	1:75:A:ALA:N	10	0.12	0.01	0.12
(1,34)	1:33:A:THR:O	1:37:A:LEU:H	10	0.12	0.01	0.12
(1,162)	2:1004:B:GLU:OE2	1:30:A:LYS:NZ	9	1.47	0.38	1.52
(1,60)	1:60:A:SER:O	1:64:A:GLY:H	9	0.35	0.04	0.34
(1,59)	1:60:A:SER:O	1:64:A:GLY:N	9	0.31	0.05	0.31
(2,2178)	1:55:A:ARG:HG2	1:56:A:LEU:H	9	0.19	0.01	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2178)	1:55:A:ARG:HG3	1:56:A:LEU:H	9	0.19	0.01	0.18
(1,68)	1:64:A:GLY:O	1:68:A:ILE:H	9	0.18	0.04	0.18
(1,92)	1:76:A:TYR:O	1:80:A:THR:H	9	0.14	0.02	0.14
(1,129)	1:122:A:GLU:O	1:126:A:MET:N	9	0.13	0.02	0.12
(1,43)	1:46:A:ILE:O	1:50:A:ILE:N	9	0.12	0.01	0.11
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD21	8	0.55	0.1	0.58
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD22	8	0.55	0.1	0.58
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD23	8	0.55	0.1	0.58
(2,876)	1:62:A:LYS:HD2	1:115:A:LYS:HA	8	0.3	0.09	0.3
(2,876)	1:62:A:LYS:HD3	1:115:A:LYS:HA	8	0.3	0.09	0.3
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB2	8	0.24	0.11	0.26
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB3	8	0.24	0.11	0.26
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB2	8	0.24	0.11	0.26
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB3	8	0.24	0.11	0.26
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB2	8	0.14	0.04	0.12
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB3	8	0.14	0.04	0.12
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB2	8	0.14	0.04	0.12
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB3	8	0.14	0.04	0.12
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB2	8	0.14	0.04	0.12
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB3	8	0.14	0.04	0.12
(2,1431)	1:63:A:LEU:HD11	1:66:A:LEU:H	8	0.14	0.03	0.15
(2,1431)	1:63:A:LEU:HD12	1:66:A:LEU:H	8	0.14	0.03	0.15
(2,1431)	1:63:A:LEU:HD13	1:66:A:LEU:H	8	0.14	0.03	0.15
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB2	8	0.14	0.03	0.13
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB3	8	0.14	0.03	0.13
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB2	8	0.14	0.03	0.13
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB3	8	0.14	0.03	0.13
(1,140)	1:127:A:LEU:O	1:131:A:TRP:H	8	0.13	0.02	0.12
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG12	8	0.12	0.02	0.11
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG13	8	0.12	0.02	0.11
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG12	8	0.12	0.02	0.11
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG13	8	0.12	0.02	0.11
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG12	8	0.12	0.02	0.11
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG13	8	0.12	0.02	0.11
(2,1895)	1:67:A:TYR:H	1:70:A:ASP:HB2	8	0.12	0.01	0.12
(2,28)	2:1004:B:GLU:HB2	1:27:A:SER:H	7	0.58	0.39	0.48
(2,28)	2:1004:B:GLU:HB3	1:27:A:SER:H	7	0.58	0.39	0.48
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD11	7	0.42	0.03	0.4
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD12	7	0.42	0.03	0.4
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD13	7	0.42	0.03	0.4
(2,886)	1:113:A:ILE:HD11	1:151:A:ALA:H	7	0.35	0.25	0.19
(2,886)	1:113:A:ILE:HD12	1:151:A:ALA:H	7	0.35	0.25	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,886)	1:113:A:ILE:HD13	1:151:A:ALA:H	7	0.35	0.25	0.19
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB2	7	0.24	0.0	0.24
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB3	7	0.24	0.0	0.24
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB2	7	0.21	0.01	0.21
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB3	7	0.21	0.01	0.21
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG21	7	0.2	0.07	0.18
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG22	7	0.2	0.07	0.18
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG23	7	0.2	0.07	0.18
(2,1385)	1:52:A:ASP:H	1:53:A:TYR:HB2	7	0.17	0.04	0.17
(2,742)	1:76:A:TYR:HA	1:94:A:CYS:HA	7	0.17	0.04	0.19
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD11	7	0.16	0.03	0.15
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD12	7	0.16	0.03	0.15
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD13	7	0.16	0.03	0.15
(1,67)	1:64:A:GLY:O	1:68:A:ILE:N	7	0.15	0.03	0.16
(2,167)	1:63:A:LEU:HD11	1:67:A:TYR:HB2	7	0.14	0.04	0.13
(2,167)	1:63:A:LEU:HD12	1:67:A:TYR:HB2	7	0.14	0.04	0.13
(2,167)	1:63:A:LEU:HD13	1:67:A:TYR:HB2	7	0.14	0.04	0.13
(2,1727)	1:151:A:ALA:H	1:154:A:LEU:H	7	0.14	0.02	0.14
(2,1411)	1:59:A:ASP:H	1:61:A:HIS:H	7	0.13	0.01	0.13
(2,1840)	1:38:A:ASP:HA	1:40:A:ILE:H	7	0.12	0.01	0.12
(2,1494)	1:96:A:HIS:H	1:99:A:ASN:HD22	6	0.25	0.02	0.24
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD11	6	0.2	0.02	0.2
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD12	6	0.2	0.02	0.2
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD13	6	0.2	0.02	0.2
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD21	6	0.2	0.02	0.2
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD22	6	0.2	0.02	0.2
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD23	6	0.2	0.02	0.2
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD21	6	0.19	0.03	0.2
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD22	6	0.19	0.03	0.2
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD23	6	0.19	0.03	0.2
(2,397)	1:14:A:LEU:HD11	1:53:A:TYR:H	6	0.17	0.04	0.18
(2,397)	1:14:A:LEU:HD12	1:53:A:TYR:H	6	0.17	0.04	0.18
(2,397)	1:14:A:LEU:HD13	1:53:A:TYR:H	6	0.17	0.04	0.18
(2,2198)	1:59:A:ASP:HB2	1:61:A:HIS:H	6	0.16	0.01	0.16
(2,2198)	1:59:A:ASP:HB3	1:61:A:HIS:H	6	0.16	0.01	0.16
(2,190)	1:66:A:LEU:HD11	1:112:A:ALA:H	6	0.15	0.03	0.15
(2,190)	1:66:A:LEU:HD12	1:112:A:ALA:H	6	0.15	0.03	0.15
(2,190)	1:66:A:LEU:HD13	1:112:A:ALA:H	6	0.15	0.03	0.15
(2,1858)	1:148:A:LYS:HB2	1:150:A:PHE:H	6	0.15	0.02	0.14
(2,1858)	1:148:A:LYS:HB3	1:150:A:PHE:H	6	0.15	0.02	0.14
(2,1428)	1:53:A:TYR:HD1	1:65:A:SER:H	6	0.14	0.02	0.13
(2,1428)	1:53:A:TYR:HD2	1:65:A:SER:H	6	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1760)	1:37:A:LEU:HA	1:40:A:ILE:H	6	0.14	0.02	0.14
(1,144)	1:129:A:ASP:O	1:133:A:ARG:H	6	0.13	0.03	0.12
(2,301)	1:11:A:VAL:HG21	1:49:A:LEU:HB2	6	0.13	0.02	0.13
(2,301)	1:11:A:VAL:HG22	1:49:A:LEU:HB2	6	0.13	0.02	0.13
(2,301)	1:11:A:VAL:HG23	1:49:A:LEU:HB2	6	0.13	0.02	0.13
(2,1782)	1:69:A:ILE:HG21	1:74:A:ARG:H	6	0.12	0.02	0.12
(2,1782)	1:69:A:ILE:HG22	1:74:A:ARG:H	6	0.12	0.02	0.12
(2,1782)	1:69:A:ILE:HG23	1:74:A:ARG:H	6	0.12	0.02	0.12
(1,22)	1:27:A:SER:O	1:31:A:LYS:H	6	0.12	0.01	0.12
(1,132)	1:123:A:LYS:O	1:127:A:LEU:H	6	0.11	0.01	0.11
(1,154)	2:1009:B:PRO:HA	1:74:A:ARG:NH2	5	0.39	0.44	0.13
(2,1289)	1:37:A:LEU:H	1:37:A:LEU:HG	5	0.38	0.0	0.38
(3,7)	2:1004:B:GLU:HB2	1:30:A:LYS:HE2	5	0.29	0.16	0.26
(3,7)	2:1004:B:GLU:HB2	1:30:A:LYS:HE3	5	0.29	0.16	0.26
(3,7)	2:1004:B:GLU:HB3	1:30:A:LYS:HE2	5	0.29	0.16	0.26
(3,7)	2:1004:B:GLU:HB3	1:30:A:LYS:HE3	5	0.29	0.16	0.26
(2,27)	2:1001:B:ASP:HB2	1:21:A:LYS:HE2	5	0.25	0.09	0.28
(2,27)	2:1001:B:ASP:HB2	1:21:A:LYS:HE3	5	0.25	0.09	0.28
(2,27)	2:1001:B:ASP:HB3	1:21:A:LYS:HE2	5	0.25	0.09	0.28
(2,27)	2:1001:B:ASP:HB3	1:21:A:LYS:HE3	5	0.25	0.09	0.28
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD11	5	0.21	0.08	0.22
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD12	5	0.21	0.08	0.22
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD13	5	0.21	0.08	0.22
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG21	5	0.21	0.13	0.15
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG22	5	0.21	0.13	0.15
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG23	5	0.21	0.13	0.15
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG21	5	0.21	0.13	0.15
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG22	5	0.21	0.13	0.15
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG23	5	0.21	0.13	0.15
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG21	5	0.21	0.13	0.15
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG22	5	0.21	0.13	0.15
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG23	5	0.21	0.13	0.15
(2,2180)	1:55:A:ARG:HD2	1:56:A:LEU:HG	5	0.2	0.03	0.22
(2,2180)	1:55:A:ARG:HD3	1:56:A:LEU:HG	5	0.2	0.03	0.22
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD11	5	0.18	0.02	0.17
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD12	5	0.18	0.02	0.17
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD13	5	0.18	0.02	0.17
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD21	5	0.18	0.02	0.17
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD22	5	0.18	0.02	0.17
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD23	5	0.18	0.02	0.17
(2,2286)	1:122:A:GLU:H	1:122:A:GLU:HG2	5	0.17	0.06	0.2
(2,2286)	1:122:A:GLU:H	1:122:A:GLU:HG3	5	0.17	0.06	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD11	5	0.15	0.01	0.15
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD12	5	0.15	0.01	0.15
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD13	5	0.15	0.01	0.15
(1,128)	1:121:A:LYS:O	1:125:A:ARG:H	5	0.13	0.02	0.14
(2,169)	1:26:A:GLY:HA2	1:28:A:ARG:HB2	5	0.13	0.02	0.12
(2,203)	1:99:A:ASN:HB2	1:100:A:THR:H	5	0.12	0.01	0.13
(2,2100)	1:24:A:ILE:HB	1:64:A:GLY:HA2	5	0.12	0.02	0.11
(2,2100)	1:24:A:ILE:HB	1:64:A:GLY:HA3	5	0.12	0.02	0.11
(1,23)	1:28:A:ARG:O	1:32:A:LEU:N	5	0.11	0.01	0.11
(2,1630)	1:151:A:ALA:H	1:153:A:ASP:H	5	0.11	0.02	0.1
(2,1987)	1:111:A:ASP:H	1:111:A:ASP:HB3	5	0.1	0.0	0.1
(1,156)	2:1007:B:TYR:OH	1:70:A:ASP:OD2	4	1.82	0.07	1.81
(1,161)	2:1001:B:ASP:OD2	1:21:A:LYS:NZ	4	1.1	0.28	1.1
(2,26)	2:1003:B:ASP:HB2	1:25:A:SER:HB2	4	0.96	0.21	1.04
(2,26)	2:1003:B:ASP:HB2	1:25:A:SER:HB3	4	0.96	0.21	1.04
(2,26)	2:1003:B:ASP:HB3	1:25:A:SER:HB2	4	0.96	0.21	1.04
(2,26)	2:1003:B:ASP:HB3	1:25:A:SER:HB3	4	0.96	0.21	1.04
(2,1931)	1:141:A:TYR:H	1:142:A:LEU:H	4	0.26	0.07	0.26
(2,996)	1:152:A:MET:H	1:152:A:MET:HG3	4	0.23	0.01	0.22
(2,2181)	1:55:A:ARG:HD2	1:108:A:LEU:HD21	4	0.21	0.06	0.22
(2,2181)	1:55:A:ARG:HD2	1:108:A:LEU:HD22	4	0.21	0.06	0.22
(2,2181)	1:55:A:ARG:HD2	1:108:A:LEU:HD23	4	0.21	0.06	0.22
(2,2181)	1:55:A:ARG:HD3	1:108:A:LEU:HD21	4	0.21	0.06	0.22
(2,2181)	1:55:A:ARG:HD3	1:108:A:LEU:HD22	4	0.21	0.06	0.22
(2,2181)	1:55:A:ARG:HD3	1:108:A:LEU:HD23	4	0.21	0.06	0.22
(2,1060)	1:62:A:LYS:HG2	1:115:A:LYS:HE2	4	0.21	0.11	0.17
(2,1060)	1:62:A:LYS:HG2	1:115:A:LYS:HE3	4	0.21	0.11	0.17
(2,1060)	1:62:A:LYS:HG3	1:115:A:LYS:HE2	4	0.21	0.11	0.17
(2,1060)	1:62:A:LYS:HG3	1:115:A:LYS:HE3	4	0.21	0.11	0.17
(2,968)	1:109:A:LEU:HD11	1:128:A:LEU:HD21	4	0.16	0.08	0.12
(2,968)	1:109:A:LEU:HD11	1:128:A:LEU:HD22	4	0.16	0.08	0.12
(2,968)	1:109:A:LEU:HD11	1:128:A:LEU:HD23	4	0.16	0.08	0.12
(2,968)	1:109:A:LEU:HD12	1:128:A:LEU:HD21	4	0.16	0.08	0.12
(2,968)	1:109:A:LEU:HD12	1:128:A:LEU:HD22	4	0.16	0.08	0.12
(2,968)	1:109:A:LEU:HD12	1:128:A:LEU:HD23	4	0.16	0.08	0.12
(2,968)	1:109:A:LEU:HD13	1:128:A:LEU:HD21	4	0.16	0.08	0.12
(2,968)	1:109:A:LEU:HD13	1:128:A:LEU:HD22	4	0.16	0.08	0.12
(2,968)	1:109:A:LEU:HD13	1:128:A:LEU:HD23	4	0.16	0.08	0.12
(2,1105)	1:138:A:GLN:HA	1:139:A:LYS:HA	4	0.16	0.07	0.12
(1,158)	2:1008:B:ASN:O	2:1011:B:THR:N	4	0.15	0.03	0.14
(2,716)	1:77:A:LEU:H	1:77:A:LEU:HD11	4	0.14	0.03	0.12
(2,716)	1:77:A:LEU:H	1:77:A:LEU:HD12	4	0.14	0.03	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,716)	1:77:A:LEU:H	1:77:A:LEU:HD13	4	0.14	0.03	0.12
(2,1774)	1:39:A:HIS:HB2	1:41:A:ASP:H	4	0.12	0.01	0.13
(1,155)	2:1007:B:TYR:OH	1:74:A:ARG:NH2	4	0.12	0.01	0.12
(2,1192)	1:11:A:VAL:HG11	1:13:A:THR:H	4	0.11	0.0	0.11
(2,1192)	1:11:A:VAL:HG12	1:13:A:THR:H	4	0.11	0.0	0.11
(2,1192)	1:11:A:VAL:HG13	1:13:A:THR:H	4	0.11	0.0	0.11
(2,2328)	1:152:A:MET:HB2	1:153:A:ASP:HA	4	0.11	0.0	0.11
(2,2328)	1:152:A:MET:HB3	1:153:A:ASP:HA	4	0.11	0.0	0.11
(2,488)	1:40:A:ILE:HG21	1:41:A:ASP:H	4	0.11	0.01	0.1
(2,488)	1:40:A:ILE:HG22	1:41:A:ASP:H	4	0.11	0.01	0.1
(2,488)	1:40:A:ILE:HG23	1:41:A:ASP:H	4	0.11	0.01	0.1
(2,714)	1:76:A:TYR:HA	1:97:A:ALA:HB1	4	0.11	0.01	0.1
(2,714)	1:76:A:TYR:HA	1:97:A:ALA:HB2	4	0.11	0.01	0.1
(2,714)	1:76:A:TYR:HA	1:97:A:ALA:HB3	4	0.11	0.01	0.1
(2,1240)	1:20:A:LEU:H	1:20:A:LEU:HG	3	0.75	0.01	0.75
(2,2289)	1:122:A:GLU:HG2	1:123:A:LYS:H	3	0.48	0.01	0.49
(2,2289)	1:122:A:GLU:HG3	1:123:A:LYS:H	3	0.48	0.01	0.49
(2,1831)	1:120:A:HIS:H	1:122:A:GLU:HB3	3	0.47	0.02	0.47
(2,1219)	1:17:A:PHE:H	1:20:A:LEU:HD11	3	0.39	0.06	0.43
(2,1219)	1:17:A:PHE:H	1:20:A:LEU:HD12	3	0.39	0.06	0.43
(2,1219)	1:17:A:PHE:H	1:20:A:LEU:HD13	3	0.39	0.06	0.43
(2,2078)	1:8:A:GLN:H	1:9:A:ASN:HB2	3	0.37	0.02	0.37
(2,2078)	1:8:A:GLN:H	1:9:A:ASN:HB3	3	0.37	0.02	0.37
(2,1497)	1:122:A:GLU:H	1:122:A:GLU:HB3	3	0.35	0.01	0.35
(2,303)	1:8:A:GLN:HA	1:9:A:ASN:HD21	3	0.25	0.0	0.25
(2,30)	1:8:A:GLN:HG2	1:12:A:ALA:H	3	0.24	0.0	0.24
(2,30)	1:8:A:GLN:HG3	1:12:A:ALA:H	3	0.24	0.0	0.24
(2,197)	1:153:A:ASP:HA	1:155:A:GLU:HB2	3	0.24	0.05	0.24
(2,197)	1:153:A:ASP:HA	1:155:A:GLU:HB3	3	0.24	0.05	0.24
(2,2094)	1:20:A:LEU:HG	1:23:A:GLY:HA2	3	0.23	0.17	0.12
(2,2094)	1:20:A:LEU:HG	1:23:A:GLY:HA3	3	0.23	0.17	0.12
(2,1906)	1:23:A:GLY:H	1:24:A:ILE:HG12	3	0.21	0.05	0.22
(2,1906)	1:23:A:GLY:H	1:24:A:ILE:HG13	3	0.21	0.05	0.22
(2,31)	1:8:A:GLN:HG2	1:9:A:ASN:HD21	3	0.19	0.01	0.19
(2,31)	1:8:A:GLN:HG3	1:9:A:ASN:HD21	3	0.19	0.01	0.19
(2,2092)	1:20:A:LEU:HB2	1:23:A:GLY:H	3	0.19	0.05	0.16
(2,2092)	1:20:A:LEU:HB3	1:23:A:GLY:H	3	0.19	0.05	0.16
(2,1790)	1:142:A:LEU:H	1:142:A:LEU:HG	3	0.18	0.01	0.19
(2,322)	1:8:A:GLN:HA	1:11:A:VAL:HG11	3	0.17	0.0	0.17
(2,322)	1:8:A:GLN:HA	1:11:A:VAL:HG12	3	0.17	0.0	0.17
(2,322)	1:8:A:GLN:HA	1:11:A:VAL:HG13	3	0.17	0.0	0.17
(2,1876)	1:7:A:PHE:H	1:9:A:ASN:H	3	0.17	0.02	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,281)	1:128:A:LEU:HD11	1:129:A:ASP:H	3	0.14	0.05	0.11
(2,281)	1:128:A:LEU:HD12	1:129:A:ASP:H	3	0.14	0.05	0.11
(2,281)	1:128:A:LEU:HD13	1:129:A:ASP:H	3	0.14	0.05	0.11
(2,506)	1:40:A:ILE:HA	1:43:A:GLU:HG2	3	0.14	0.02	0.13
(2,506)	1:40:A:ILE:HA	1:43:A:GLU:HG3	3	0.14	0.02	0.13
(1,112)	1:107:A:GLU:O	1:111:A:ASP:H	3	0.13	0.0	0.13
(2,1063)	1:105:A:ILE:HG12	1:109:A:LEU:HG	3	0.13	0.02	0.12
(1,143)	1:129:A:ASP:O	1:133:A:ARG:N	3	0.13	0.03	0.11
(2,1019)	1:105:A:ILE:HD11	1:108:A:LEU:HB3	3	0.13	0.02	0.14
(2,1019)	1:105:A:ILE:HD12	1:108:A:LEU:HB3	3	0.13	0.02	0.14
(2,1019)	1:105:A:ILE:HD13	1:108:A:LEU:HB3	3	0.13	0.02	0.14
(2,1927)	1:50:A:ILE:HA	1:53:A:TYR:H	3	0.13	0.01	0.13
(2,2343)	1:102:A:GLY:H	1:137:A:PHE:HD1	3	0.13	0.03	0.11
(2,2343)	1:102:A:GLY:H	1:137:A:PHE:HD2	3	0.13	0.03	0.11
(2,2354)	1:102:A:GLY:H	1:137:A:PHE:HD1	3	0.13	0.03	0.11
(2,2354)	1:102:A:GLY:H	1:137:A:PHE:HD2	3	0.13	0.03	0.11
(2,2010)	1:122:A:GLU:H	1:123:A:LYS:H	3	0.13	0.01	0.12
(2,166)	1:69:A:ILE:HB	1:108:A:LEU:HD11	3	0.12	0.0	0.12
(2,166)	1:69:A:ILE:HB	1:108:A:LEU:HD12	3	0.12	0.0	0.12
(2,166)	1:69:A:ILE:HB	1:108:A:LEU:HD13	3	0.12	0.0	0.12
(2,298)	1:11:A:VAL:HG21	1:15:A:GLU:H	3	0.12	0.02	0.12
(2,298)	1:11:A:VAL:HG22	1:15:A:GLU:H	3	0.12	0.02	0.12
(2,298)	1:11:A:VAL:HG23	1:15:A:GLU:H	3	0.12	0.02	0.12
(2,962)	1:126:A:MET:HB3	1:126:A:MET:HE1	3	0.12	0.02	0.12
(2,962)	1:126:A:MET:HB3	1:126:A:MET:HE2	3	0.12	0.02	0.12
(2,962)	1:126:A:MET:HB3	1:126:A:MET:HE3	3	0.12	0.02	0.12
(2,1157)	1:9:A:ASN:H	1:35:A:TYR:HE1	3	0.12	0.01	0.12
(2,1157)	1:9:A:ASN:H	1:35:A:TYR:HE2	3	0.12	0.01	0.12
(1,88)	1:74:A:ARG:O	1:78:A:ASP:H	3	0.12	0.01	0.11
(2,933)	1:124:A:ILE:HG21	1:128:A:LEU:HD11	3	0.12	0.01	0.11
(2,933)	1:124:A:ILE:HG21	1:128:A:LEU:HD12	3	0.12	0.01	0.11
(2,933)	1:124:A:ILE:HG21	1:128:A:LEU:HD13	3	0.12	0.01	0.11
(2,933)	1:124:A:ILE:HG22	1:128:A:LEU:HD11	3	0.12	0.01	0.11
(2,933)	1:124:A:ILE:HG22	1:128:A:LEU:HD12	3	0.12	0.01	0.11
(2,933)	1:124:A:ILE:HG22	1:128:A:LEU:HD13	3	0.12	0.01	0.11
(2,933)	1:124:A:ILE:HG23	1:128:A:LEU:HD11	3	0.12	0.01	0.11
(2,933)	1:124:A:ILE:HG23	1:128:A:LEU:HD12	3	0.12	0.01	0.11
(2,933)	1:124:A:ILE:HG23	1:128:A:LEU:HD13	3	0.12	0.01	0.11
(2,942)	1:66:A:LEU:HD11	1:109:A:LEU:HD21	3	0.11	0.01	0.11
(2,942)	1:66:A:LEU:HD11	1:109:A:LEU:HD22	3	0.11	0.01	0.11
(2,942)	1:66:A:LEU:HD11	1:109:A:LEU:HD23	3	0.11	0.01	0.11
(2,942)	1:66:A:LEU:HD12	1:109:A:LEU:HD21	3	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,942)	1:66:A:LEU:HD12	1:109:A:LEU:HD22	3	0.11	0.01	0.11
(2,942)	1:66:A:LEU:HD12	1:109:A:LEU:HD23	3	0.11	0.01	0.11
(2,942)	1:66:A:LEU:HD13	1:109:A:LEU:HD21	3	0.11	0.01	0.11
(2,942)	1:66:A:LEU:HD13	1:109:A:LEU:HD22	3	0.11	0.01	0.11
(2,942)	1:66:A:LEU:HD13	1:109:A:LEU:HD23	3	0.11	0.01	0.11
(2,756)	1:80:A:THR:HG21	1:95:A:ALA:H	3	0.11	0.0	0.11
(2,756)	1:80:A:THR:HG22	1:95:A:ALA:H	3	0.11	0.0	0.11
(2,756)	1:80:A:THR:HG23	1:95:A:ALA:H	3	0.11	0.0	0.11
(2,807)	1:104:A:VAL:HA	1:107:A:GLU:HB3	3	0.11	0.01	0.1
(2,1009)	1:154:A:LEU:HA	1:155:A:GLU:H	3	0.11	0.0	0.11
(1,127)	1:121:A:LYS:O	1:125:A:ARG:N	3	0.11	0.01	0.1
(2,491)	1:40:A:ILE:HG21	1:41:A:ASP:HA	3	0.11	0.0	0.11
(2,491)	1:40:A:ILE:HG22	1:41:A:ASP:HA	3	0.11	0.0	0.11
(2,491)	1:40:A:ILE:HG23	1:41:A:ASP:HA	3	0.11	0.0	0.11
(1,96)	1:78:A:ASP:O	1:82:A:SER:H	3	0.1	0.0	0.1
(2,98)	1:24:A:ILE:HB	1:67:A:TYR:HE1	3	0.1	0.0	0.1
(2,98)	1:24:A:ILE:HB	1:67:A:TYR:HE2	3	0.1	0.0	0.1
(2,901)	1:126:A:MET:HA	1:129:A:ASP:HA	3	0.1	0.0	0.1
(2,24)	2:1005:B:ASP:HA	1:26:A:GLY:H	2	0.54	0.07	0.54
(2,16)	2:1009:B:PRO:HA	1:74:A:ARG:HE	2	0.52	0.31	0.52
(2,297)	1:6:A:ASP:HA	1:7:A:PHE:HB2	2	0.48	0.01	0.48
(2,1977)	1:110:A:SER:H	1:145:A:ILE:HG21	2	0.24	0.05	0.24
(2,1977)	1:110:A:SER:H	1:145:A:ILE:HG22	2	0.24	0.05	0.24
(2,1977)	1:110:A:SER:H	1:145:A:ILE:HG23	2	0.24	0.05	0.24
(2,1628)	1:148:A:LYS:HB2	1:149:A:CYS:H	2	0.23	0.01	0.23
(2,1628)	1:148:A:LYS:HB3	1:149:A:CYS:H	2	0.23	0.01	0.23
(2,982)	1:128:A:LEU:HD11	1:145:A:ILE:HB	2	0.22	0.06	0.22
(2,982)	1:128:A:LEU:HD12	1:145:A:ILE:HB	2	0.22	0.06	0.22
(2,982)	1:128:A:LEU:HD13	1:145:A:ILE:HB	2	0.22	0.06	0.22
(2,961)	1:123:A:LYS:HA	1:126:A:MET:HB3	2	0.22	0.02	0.22
(3,5)	2:1007:B:TYR:O	1:67:A:TYR:HE1	2	0.22	0.1	0.22
(2,381)	1:24:A:ILE:H	1:24:A:ILE:HD11	2	0.21	0.04	0.21
(2,381)	1:24:A:ILE:H	1:24:A:ILE:HD12	2	0.21	0.04	0.21
(2,381)	1:24:A:ILE:H	1:24:A:ILE:HD13	2	0.21	0.04	0.21
(2,2093)	1:20:A:LEU:HB2	1:24:A:ILE:H	2	0.21	0.01	0.21
(2,2093)	1:20:A:LEU:HB3	1:24:A:ILE:H	2	0.21	0.01	0.21
(1,149)	1:148:A:LYS:O	1:152:A:MET:N	2	0.2	0.08	0.2
(2,1133)	1:141:A:TYR:H	1:142:A:LEU:HD11	2	0.19	0.08	0.19
(2,1133)	1:141:A:TYR:H	1:142:A:LEU:HD12	2	0.19	0.08	0.19
(2,1133)	1:141:A:TYR:H	1:142:A:LEU:HD13	2	0.19	0.08	0.19
(2,2101)	1:24:A:ILE:HG12	1:64:A:GLY:HA2	2	0.19	0.01	0.19
(2,2101)	1:24:A:ILE:HG12	1:64:A:GLY:HA3	2	0.19	0.01	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2101)	1:24:A:ILE:HG13	1:64:A:GLY:HA2	2	0.19	0.01	0.19
(2,2101)	1:24:A:ILE:HG13	1:64:A:GLY:HA3	2	0.19	0.01	0.19
(2,106)	1:23:A:GLY:H	1:24:A:ILE:HA	2	0.18	0.01	0.18
(2,295)	1:6:A:ASP:HA	1:7:A:PHE:HA	2	0.18	0.0	0.18
(2,1902)	1:62:A:LYS:HD2	1:115:A:LYS:H	2	0.16	0.06	0.16
(2,1902)	1:62:A:LYS:HD3	1:115:A:LYS:H	2	0.16	0.06	0.16
(2,2341)	1:105:A:ILE:HD11	1:137:A:PHE:HD1	2	0.16	0.04	0.16
(2,2341)	1:105:A:ILE:HD11	1:137:A:PHE:HD2	2	0.16	0.04	0.16
(2,2341)	1:105:A:ILE:HD12	1:137:A:PHE:HD1	2	0.16	0.04	0.16
(2,2341)	1:105:A:ILE:HD12	1:137:A:PHE:HD2	2	0.16	0.04	0.16
(2,2341)	1:105:A:ILE:HD13	1:137:A:PHE:HD1	2	0.16	0.04	0.16
(2,2341)	1:105:A:ILE:HD13	1:137:A:PHE:HD2	2	0.16	0.04	0.16
(2,2352)	1:105:A:ILE:HD11	1:137:A:PHE:HD1	2	0.16	0.04	0.16
(2,2352)	1:105:A:ILE:HD11	1:137:A:PHE:HD2	2	0.16	0.04	0.16
(2,2352)	1:105:A:ILE:HD12	1:137:A:PHE:HD1	2	0.16	0.04	0.16
(2,2352)	1:105:A:ILE:HD12	1:137:A:PHE:HD2	2	0.16	0.04	0.16
(2,2352)	1:105:A:ILE:HD13	1:137:A:PHE:HD1	2	0.16	0.04	0.16
(2,2352)	1:105:A:ILE:HD13	1:137:A:PHE:HD2	2	0.16	0.04	0.16
(2,2206)	1:62:A:LYS:HD2	1:111:A:ASP:HB2	2	0.15	0.01	0.15
(2,2206)	1:62:A:LYS:HD2	1:111:A:ASP:HB3	2	0.15	0.01	0.15
(2,2206)	1:62:A:LYS:HD3	1:111:A:ASP:HB2	2	0.15	0.01	0.15
(2,2206)	1:62:A:LYS:HD3	1:111:A:ASP:HB3	2	0.15	0.01	0.15
(2,1158)	1:5:A:ASP:HA	1:9:A:ASN:H	2	0.15	0.0	0.15
(2,875)	1:113:A:ILE:HB	1:114:A:ALA:HB1	2	0.14	0.03	0.14
(2,875)	1:113:A:ILE:HB	1:114:A:ALA:HB2	2	0.14	0.03	0.14
(2,875)	1:113:A:ILE:HB	1:114:A:ALA:HB3	2	0.14	0.03	0.14
(1,157)	2:1008:B:ASN:OD1	2:1010:B:TYR:N	2	0.14	0.02	0.14
(2,1418)	1:58:A:PRO:HA	1:62:A:LYS:H	2	0.13	0.02	0.13
(1,153)	2:1009:B:PRO:O	1:74:A:ARG:HE	2	0.12	0.01	0.12
(2,387)	1:24:A:ILE:HD11	1:64:A:GLY:HA3	2	0.12	0.01	0.12
(2,387)	1:24:A:ILE:HD12	1:64:A:GLY:HA3	2	0.12	0.01	0.12
(2,387)	1:24:A:ILE:HD13	1:64:A:GLY:HA3	2	0.12	0.01	0.12
(2,744)	1:93:A:THR:HG21	1:94:A:CYS:HA	2	0.12	0.02	0.12
(2,744)	1:93:A:THR:HG22	1:94:A:CYS:HA	2	0.12	0.02	0.12
(2,744)	1:93:A:THR:HG23	1:94:A:CYS:HA	2	0.12	0.02	0.12
(2,1042)	1:63:A:LEU:HA	1:124:A:ILE:HG12	2	0.12	0.01	0.12
(2,1042)	1:63:A:LEU:HA	1:124:A:ILE:HG13	2	0.12	0.01	0.12
(2,1153)	1:14:A:LEU:HG	1:15:A:GLU:H	2	0.12	0.01	0.12
(2,334)	1:11:A:VAL:HA	1:14:A:LEU:HA	2	0.12	0.01	0.12
(2,613)	1:47:A:ILE:HG21	1:97:A:ALA:HB1	2	0.12	0.0	0.12
(2,613)	1:47:A:ILE:HG21	1:97:A:ALA:HB2	2	0.12	0.0	0.12
(2,613)	1:47:A:ILE:HG21	1:97:A:ALA:HB3	2	0.12	0.0	0.12

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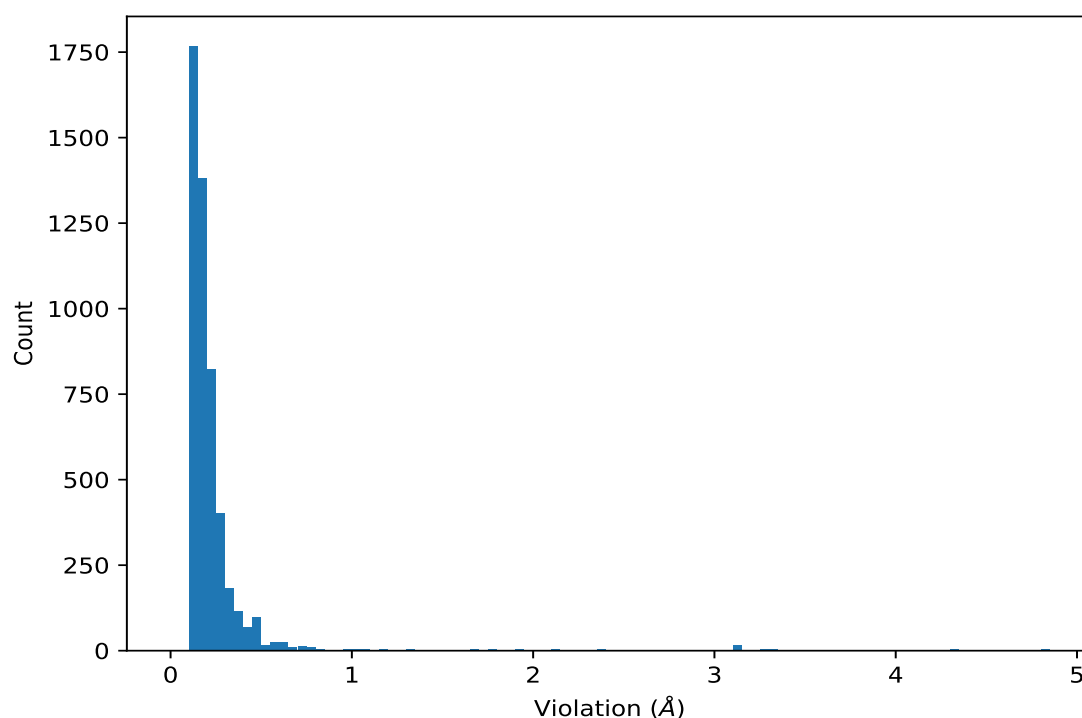
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,613)	1:47:A:ILE:HG22	1:97:A:ALA:HB1	2	0.12	0.0	0.12
(2,613)	1:47:A:ILE:HG22	1:97:A:ALA:HB2	2	0.12	0.0	0.12
(2,613)	1:47:A:ILE:HG22	1:97:A:ALA:HB3	2	0.12	0.0	0.12
(2,613)	1:47:A:ILE:HG23	1:97:A:ALA:HB1	2	0.12	0.0	0.12
(2,613)	1:47:A:ILE:HG23	1:97:A:ALA:HB2	2	0.12	0.0	0.12
(2,613)	1:47:A:ILE:HG23	1:97:A:ALA:HB3	2	0.12	0.0	0.12
(2,1130)	1:117:A:ASN:HA	1:117:A:ASN:HD21	2	0.12	0.0	0.12
(2,187)	1:104:A:VAL:HG11	1:105:A:ILE:H	2	0.11	0.01	0.11
(2,187)	1:104:A:VAL:HG12	1:105:A:ILE:H	2	0.11	0.01	0.11
(2,187)	1:104:A:VAL:HG13	1:105:A:ILE:H	2	0.11	0.01	0.11
(2,1577)	1:115:A:LYS:H	1:115:A:LYS:HB3	2	0.11	0.01	0.11
(2,2137)	1:39:A:HIS:HB2	1:42:A:ILE:H	2	0.11	0.0	0.11
(2,2137)	1:39:A:HIS:HB3	1:42:A:ILE:H	2	0.11	0.0	0.11
(2,2237)	1:94:A:CYS:HB2	1:95:A:ALA:HA	2	0.11	0.0	0.11
(2,2237)	1:94:A:CYS:HB3	1:95:A:ALA:HA	2	0.11	0.0	0.11
(1,134)	1:124:A:ILE:O	1:128:A:LEU:H	2	0.11	0.0	0.11
(2,157)	1:118:A:GLN:HA	1:121:A:LYS:HD2	2	0.11	0.0	0.11
(2,735)	1:80:A:THR:HG21	1:94:A:CYS:HA	2	0.11	0.0	0.11
(2,735)	1:80:A:THR:HG22	1:94:A:CYS:HA	2	0.11	0.0	0.11
(2,735)	1:80:A:THR:HG23	1:94:A:CYS:HA	2	0.11	0.0	0.11
(2,1062)	1:43:A:GLU:HA	1:47:A:ILE:HG12	2	0.11	0.0	0.11
(2,1143)	1:7:A:PHE:H	1:10:A:PHE:HB3	2	0.11	0.0	0.11
(2,1645)	1:43:A:GLU:H	1:93:A:THR:H	2	0.11	0.0	0.11
(2,2287)	1:122:A:GLU:HA	1:125:A:ARG:HD2	2	0.11	0.0	0.11
(2,2287)	1:122:A:GLU:HA	1:125:A:ARG:HD3	2	0.11	0.0	0.11

¹Number of violated models, ²Standard 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)
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB2	9	4.83
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB3	9	4.83
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB2	9	4.83
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB3	9	4.83
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB2	5	4.3
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB3	5	4.3
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB2	5	4.3
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB3	5	4.3
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB2	3	3.33
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB3	3	3.33
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB2	3	3.33
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB3	3	3.33
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB2	20	3.25
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB3	20	3.25
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB2	20	3.25
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB3	20	3.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB2	8	3.14
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB3	8	3.14
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB2	8	3.14
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB3	8	3.14
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB2	2	3.12
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB3	2	3.12
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB2	2	3.12
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB3	2	3.12
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB2	14	3.12
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB3	14	3.12
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB2	14	3.12
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB3	14	3.12
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB2	18	3.12
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB3	18	3.12
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB2	18	3.12
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB3	18	3.12
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB2	4	2.36
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB3	4	2.36
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB2	4	2.36
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB3	4	2.36
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB2	6	2.14
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB3	6	2.14
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB2	6	2.14
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB3	6	2.14
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	10	2.1
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	3	2.05
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	8	2.03
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	17	1.93
(1,156)	2:1007:B:TYR:OH	1:70:A:ASP:OD2	15	1.93
(1,162)	2:1004:B:GLU:OE2	1:30:A:LYS:NZ	10	1.91
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	19	1.9
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	5	1.88
(1,162)	2:1004:B:GLU:OE2	1:30:A:LYS:NZ	13	1.85
(1,156)	2:1007:B:TYR:OH	1:70:A:ASP:OD2	8	1.84
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	4	1.81
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	7	1.77
(1,156)	2:1007:B:TYR:OH	1:70:A:ASP:OD2	2	1.77
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	13	1.76
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	1	1.75
(1,156)	2:1007:B:TYR:OH	1:70:A:ASP:OD2	10	1.75
(1,162)	2:1004:B:GLU:OE2	1:30:A:LYS:NZ	15	1.7
(1,162)	2:1004:B:GLU:OE2	1:30:A:LYS:NZ	1	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	12	1.67
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	16	1.67
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	14	1.61
(1,162)	2:1004:B:GLU:OE2	1:30:A:LYS:NZ	9	1.52
(1,162)	2:1004:B:GLU:OE2	1:30:A:LYS:NZ	18	1.5
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	15	1.47
(1,161)	2:1001:B:ASP:OD2	1:21:A:LYS:NZ	14	1.44
(1,162)	2:1004:B:GLU:OE2	1:30:A:LYS:NZ	2	1.41
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	20	1.39
(2,28)	2:1004:B:GLU:HB2	1:27:A:SER:H	17	1.34
(2,28)	2:1004:B:GLU:HB3	1:27:A:SER:H	17	1.34
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	9	1.32
(1,161)	2:1001:B:ASP:OD2	1:21:A:LYS:NZ	16	1.29
(1,154)	2:1009:B:PRO:HA	1:74:A:ARG:NH2	7	1.25
(1,159)	2:1005:B:ASP:OD2	1:25:A:SER:OG	6	1.16
(2,26)	2:1003:B:ASP:HB2	1:25:A:SER:HB2	6	1.15
(2,26)	2:1003:B:ASP:HB2	1:25:A:SER:HB3	6	1.15
(2,26)	2:1003:B:ASP:HB3	1:25:A:SER:HB2	6	1.15
(2,26)	2:1003:B:ASP:HB3	1:25:A:SER:HB3	6	1.15
(2,26)	2:1003:B:ASP:HB2	1:25:A:SER:HB2	18	1.08
(2,26)	2:1003:B:ASP:HB2	1:25:A:SER:HB3	18	1.08
(2,26)	2:1003:B:ASP:HB3	1:25:A:SER:HB2	18	1.08
(2,26)	2:1003:B:ASP:HB3	1:25:A:SER:HB3	18	1.08
(2,26)	2:1003:B:ASP:HB2	1:25:A:SER:HB2	9	1.0
(2,26)	2:1003:B:ASP:HB2	1:25:A:SER:HB3	9	1.0
(2,26)	2:1003:B:ASP:HB3	1:25:A:SER:HB2	9	1.0
(2,26)	2:1003:B:ASP:HB3	1:25:A:SER:HB3	9	1.0
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB2	17	0.99
(3,2)	1:23:A:GLY:HA2	2:1001:B:ASP:HB3	17	0.99
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB2	17	0.99
(3,2)	1:23:A:GLY:HA3	2:1001:B:ASP:HB3	17	0.99
(1,161)	2:1001:B:ASP:OD2	1:21:A:LYS:NZ	15	0.92
(1,162)	2:1004:B:GLU:OE2	1:30:A:LYS:NZ	4	0.84
(2,16)	2:1009:B:PRO:HA	1:74:A:ARG:HE	7	0.83
(2,28)	2:1004:B:GLU:HB2	1:27:A:SER:H	20	0.82
(2,28)	2:1004:B:GLU:HB3	1:27:A:SER:H	20	0.82
(1,162)	2:1004:B:GLU:OE2	1:30:A:LYS:NZ	6	0.8
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	1	0.78
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	1	0.78
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	1	0.78
(1,58)	1:59:A:ASP:O	1:63:A:LEU:H	7	0.77
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	16	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	16	0.76
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	16	0.76
(2,1240)	1:20:A:LEU:H	1:20:A:LEU:HG	6	0.76
(2,1240)	1:20:A:LEU:H	1:20:A:LEU:HG	17	0.75
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	20	0.74
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	20	0.74
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	20	0.74
(2,1240)	1:20:A:LEU:H	1:20:A:LEU:HG	9	0.74
(1,161)	2:1001:B:ASP:OD2	1:21:A:LYS:NZ	12	0.74
(2,28)	2:1004:B:GLU:HB2	1:27:A:SER:H	16	0.73
(2,28)	2:1004:B:GLU:HB3	1:27:A:SER:H	16	0.73
(1,58)	1:59:A:ASP:O	1:63:A:LEU:H	12	0.72
(2,15)	1:126:A:MET:HE2	2:1009:B:PRO:HD2	10	0.71
(2,886)	1:113:A:ILE:HD11	1:151:A:ALA:H	20	0.7
(2,886)	1:113:A:ILE:HD12	1:151:A:ALA:H	20	0.7
(2,886)	1:113:A:ILE:HD13	1:151:A:ALA:H	20	0.7
(1,58)	1:59:A:ASP:O	1:63:A:LEU:H	11	0.68
(1,58)	1:59:A:ASP:O	1:63:A:LEU:H	15	0.68
(1,58)	1:59:A:ASP:O	1:63:A:LEU:H	17	0.68
(2,15)	1:126:A:MET:HE2	2:1009:B:PRO:HG2	2	0.67
(2,1914)	1:22:A:SER:H	1:24:A:ILE:H	14	0.66
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD21	5	0.65
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD22	5	0.65
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD23	5	0.65
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	16	0.65
(1,58)	1:59:A:ASP:O	1:63:A:LEU:H	8	0.65
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD21	13	0.64
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD22	13	0.64
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD23	13	0.64
(1,58)	1:59:A:ASP:O	1:63:A:LEU:H	3	0.64
(1,58)	1:59:A:ASP:O	1:63:A:LEU:H	13	0.64
(1,58)	1:59:A:ASP:O	1:63:A:LEU:H	5	0.63
(1,58)	1:59:A:ASP:O	1:63:A:LEU:H	2	0.62
(1,58)	1:59:A:ASP:O	1:63:A:LEU:H	19	0.62
(1,57)	1:59:A:ASP:O	1:63:A:LEU:N	7	0.62
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD21	3	0.61
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD22	3	0.61
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD23	3	0.61
(2,886)	1:113:A:ILE:HD11	1:151:A:ALA:H	16	0.61
(2,886)	1:113:A:ILE:HD12	1:151:A:ALA:H	16	0.61
(2,886)	1:113:A:ILE:HD13	1:151:A:ALA:H	16	0.61
(2,26)	2:1003:B:ASP:HB2	1:25:A:SER:HB2	14	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,26)	2:1003:B:ASP:HB2	1:25:A:SER:HB3	14	0.61
(2,26)	2:1003:B:ASP:HB3	1:25:A:SER:HB2	14	0.61
(2,26)	2:1003:B:ASP:HB3	1:25:A:SER:HB3	14	0.61
(2,24)	2:1005:B:ASP:HA	1:26:A:GLY:H	3	0.61
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD21	8	0.6
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD22	8	0.6
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD23	8	0.6
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	14	0.6
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	14	0.6
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	14	0.6
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	8	0.59
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	8	0.59
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	8	0.59
(1,57)	1:59:A:ASP:O	1:63:A:LEU:N	12	0.58
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD21	9	0.57
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD22	9	0.57
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD23	9	0.57
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	3	0.57
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	3	0.57
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	3	0.57
(2,886)	1:113:A:ILE:HD11	1:151:A:ALA:H	1	0.57
(2,886)	1:113:A:ILE:HD12	1:151:A:ALA:H	1	0.57
(2,886)	1:113:A:ILE:HD13	1:151:A:ALA:H	1	0.57
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	12	0.57
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	6	0.56
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	6	0.56
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	6	0.56
(2,15)	1:126:A:MET:HE1	2:1009:B:PRO:HD2	8	0.56
(1,57)	1:59:A:ASP:O	1:63:A:LEU:N	11	0.56
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	17	0.55
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	17	0.55
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	17	0.55
(2,224)	1:43:A:GLU:HG2	1:44:A:SER:HB3	8	0.55
(2,224)	1:43:A:GLU:HG3	1:44:A:SER:HB3	8	0.55
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	2	0.54
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	2	0.54
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	2	0.54
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD21	2	0.53
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD22	2	0.53
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD23	2	0.53
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	11	0.52
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	11	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	11	0.52
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	15	0.52
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	15	0.52
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	15	0.52
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	15	0.52
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	14	0.52
(1,57)	1:59:A:ASP:O	1:63:A:LEU:N	5	0.51
(1,57)	1:59:A:ASP:O	1:63:A:LEU:N	13	0.5
(1,57)	1:59:A:ASP:O	1:63:A:LEU:N	15	0.5
(3,7)	2:1004:B:GLU:HB2	1:30:A:LYS:HE2	17	0.49
(3,7)	2:1004:B:GLU:HB2	1:30:A:LYS:HE3	17	0.49
(3,7)	2:1004:B:GLU:HB3	1:30:A:LYS:HE2	17	0.49
(3,7)	2:1004:B:GLU:HB3	1:30:A:LYS:HE3	17	0.49
(2,2289)	1:122:A:GLU:HG2	1:123:A:LYS:H	12	0.49
(2,2289)	1:122:A:GLU:HG3	1:123:A:LYS:H	12	0.49
(2,2289)	1:122:A:GLU:HG2	1:123:A:LYS:H	15	0.49
(2,2289)	1:122:A:GLU:HG3	1:123:A:LYS:H	15	0.49
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	5	0.49
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	5	0.49
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	5	0.49
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	16	0.49
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	16	0.49
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	16	0.49
(2,1831)	1:120:A:HIS:H	1:122:A:GLU:HB3	12	0.49
(2,1730)	1:155:A:GLU:H	1:156:A:HIS:H	8	0.49
(2,876)	1:62:A:LYS:HD2	1:115:A:LYS:HA	14	0.49
(2,876)	1:62:A:LYS:HD3	1:115:A:LYS:HA	14	0.49
(2,297)	1:6:A:ASP:HA	1:7:A:PHE:HB2	11	0.49
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	4	0.49
(2,28)	2:1004:B:GLU:HB2	1:27:A:SER:H	14	0.48
(2,28)	2:1004:B:GLU:HB3	1:27:A:SER:H	14	0.48
(2,15)	1:126:A:MET:HE1	2:1009:B:PRO:HG2	4	0.48
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	10	0.48
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	2	0.47
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	2	0.47
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	2	0.47
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	6	0.47
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	6	0.47
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	6	0.47
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	12	0.47
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	12	0.47
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	12	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1831)	1:120:A:HIS:H	1:122:A:GLU:HB3	17	0.47
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	10	0.47
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	10	0.47
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	10	0.47
(2,1730)	1:155:A:GLU:H	1:156:A:HIS:H	6	0.47
(2,1730)	1:155:A:GLU:H	1:156:A:HIS:H	14	0.47
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	19	0.47
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	19	0.47
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	19	0.47
(2,297)	1:6:A:ASP:HA	1:7:A:PHE:HB2	4	0.47
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	13	0.47
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	18	0.47
(2,24)	2:1005:B:ASP:HA	1:26:A:GLY:H	8	0.47
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG21	3	0.47
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG22	3	0.47
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG23	3	0.47
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG21	3	0.47
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG22	3	0.47
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG23	3	0.47
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG21	3	0.47
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG22	3	0.47
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG23	3	0.47
(1,57)	1:59:A:ASP:O	1:63:A:LEU:N	17	0.47
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD11	20	0.46
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD12	20	0.46
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD13	20	0.46
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD21	20	0.46
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD22	20	0.46
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD23	20	0.46
(2,2289)	1:122:A:GLU:HG2	1:123:A:LYS:H	17	0.46
(2,2289)	1:122:A:GLU:HG3	1:123:A:LYS:H	17	0.46
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG2	15	0.46
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG3	15	0.46
(2,2094)	1:20:A:LEU:HG	1:23:A:GLY:HA2	14	0.46
(2,2094)	1:20:A:LEU:HG	1:23:A:GLY:HA3	14	0.46
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD11	9	0.46
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD12	9	0.46
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD13	9	0.46
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD21	11	0.46
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD22	11	0.46
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD23	11	0.46
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	5	0.46
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	5	0.46
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	6	0.46
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	6	0.46
(3,7)	2:1004:B:GLU:HB2	1:30:A:LYS:HE2	16	0.45
(3,7)	2:1004:B:GLU:HB2	1:30:A:LYS:HE3	16	0.45
(3,7)	2:1004:B:GLU:HB3	1:30:A:LYS:HE2	16	0.45
(3,7)	2:1004:B:GLU:HB3	1:30:A:LYS:HE3	16	0.45
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD11	19	0.45
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD12	19	0.45
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD13	19	0.45
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	7	0.45
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	7	0.45
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	7	0.45
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	8	0.45
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	8	0.45
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	8	0.45
(2,1831)	1:120:A:HIS:H	1:122:A:GLU:HB3	15	0.45
(2,1730)	1:155:A:GLU:H	1:156:A:HIS:H	16	0.45
(1,57)	1:59:A:ASP:O	1:63:A:LEU:N	3	0.45
(1,57)	1:59:A:ASP:O	1:63:A:LEU:N	8	0.45
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	11	0.45
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	1	0.44
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	1	0.44
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	1	0.44
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	9	0.44
(2,1672)	1:115:A:LYS:HE2	1:116:A:SER:H	1	0.44
(2,1672)	1:115:A:LYS:HE3	1:116:A:SER:H	1	0.44
(1,57)	1:59:A:ASP:O	1:63:A:LEU:N	19	0.44
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	7	0.44
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG2	17	0.43
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG3	17	0.43
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB2	14	0.43
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB3	14	0.43
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB2	14	0.43
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB3	14	0.43
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD11	7	0.43
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD12	7	0.43
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD13	7	0.43
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	19	0.43
(2,1219)	1:17:A:PHE:H	1:20:A:LEU:HD11	9	0.43
(2,1219)	1:17:A:PHE:H	1:20:A:LEU:HD12	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1219)	1:17:A:PHE:H	1:20:A:LEU:HD13	9	0.43
(2,1219)	1:17:A:PHE:H	1:20:A:LEU:HD11	17	0.43
(2,1219)	1:17:A:PHE:H	1:20:A:LEU:HD12	17	0.43
(2,1219)	1:17:A:PHE:H	1:20:A:LEU:HD13	17	0.43
(2,1004)	1:149:A:CYS:HA	1:153:A:ASP:HA	19	0.43
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	12	0.43
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	19	0.43
(2,2349)	1:136:A:LEU:HG	1:137:A:PHE:HE1	11	0.42
(2,2349)	1:136:A:LEU:HG	1:137:A:PHE:HE2	11	0.42
(2,2338)	1:136:A:LEU:HG	1:137:A:PHE:HE1	11	0.42
(2,2338)	1:136:A:LEU:HG	1:137:A:PHE:HE2	11	0.42
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG2	12	0.42
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG3	12	0.42
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	11	0.42
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	11	0.42
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	11	0.42
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	19	0.42
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	19	0.42
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	19	0.42
(2,1634)	1:153:A:ASP:H	1:154:A:LEU:HB3	1	0.42
(2,1634)	1:153:A:ASP:H	1:154:A:LEU:HB3	5	0.42
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	10	0.42
(1,57)	1:59:A:ASP:O	1:63:A:LEU:N	2	0.42
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	6	0.42
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	3	0.41
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	3	0.41
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	3	0.41
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	14	0.41
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	14	0.41
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	14	0.41
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	9	0.41
(1,60)	1:60:A:SER:O	1:64:A:GLY:H	14	0.41
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	16	0.41
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	14	0.41
(2,2078)	1:8:A:GLN:H	1:9:A:ASN:HB2	19	0.4
(2,2078)	1:8:A:GLN:H	1:9:A:ASN:HB3	19	0.4
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD11	4	0.4
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD12	4	0.4
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD13	4	0.4
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD11	12	0.4
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD12	12	0.4
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD13	12	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	18	0.4
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	18	0.4
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	18	0.4
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	20	0.4
(1,60)	1:60:A:SER:O	1:64:A:GLY:H	10	0.4
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	3	0.4
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	5	0.4
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	2	0.4
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD11	13	0.39
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD12	13	0.39
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD13	13	0.39
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	20	0.39
(2,1672)	1:115:A:LYS:HE2	1:116:A:SER:H	4	0.39
(2,1672)	1:115:A:LYS:HE3	1:116:A:SER:H	4	0.39
(2,1289)	1:37:A:LEU:H	1:37:A:LEU:HG	5	0.39
(2,1289)	1:37:A:LEU:H	1:37:A:LEU:HG	14	0.39
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	18	0.39
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	18	0.39
(2,1060)	1:62:A:LYS:HG2	1:115:A:LYS:HE2	10	0.39
(2,1060)	1:62:A:LYS:HG2	1:115:A:LYS:HE3	10	0.39
(2,1060)	1:62:A:LYS:HG3	1:115:A:LYS:HE2	10	0.39
(2,1060)	1:62:A:LYS:HG3	1:115:A:LYS:HE3	10	0.39
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	10	0.39
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	10	0.39
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	10	0.39
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	10	0.39
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	8	0.39
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	18	0.39
(2,2147)	1:43:A:GLU:HB2	1:94:A:CYS:H	8	0.38
(2,2147)	1:43:A:GLU:HB3	1:94:A:CYS:H	8	0.38
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD11	18	0.38
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD12	18	0.38
(2,1993)	1:154:A:LEU:H	1:154:A:LEU:HD13	18	0.38
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	15	0.38
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	15	0.38
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	15	0.38
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	17	0.38
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	17	0.38
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	17	0.38
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	4	0.38
(2,1634)	1:153:A:ASP:H	1:154:A:LEU:HB3	6	0.38
(2,1634)	1:153:A:ASP:H	1:154:A:LEU:HB3	10	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1634)	1:153:A:ASP:H	1:154:A:LEU:HB3	11	0.38
(2,1634)	1:153:A:ASP:H	1:154:A:LEU:HB3	17	0.38
(2,1289)	1:37:A:LEU:H	1:37:A:LEU:HG	4	0.38
(2,1289)	1:37:A:LEU:H	1:37:A:LEU:HG	13	0.38
(2,1289)	1:37:A:LEU:H	1:37:A:LEU:HG	15	0.38
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	9	0.38
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	9	0.38
(2,15)	1:126:A:MET:HE3	2:1009:B:PRO:HG2	1	0.38
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	1	0.38
(1,59)	1:60:A:SER:O	1:64:A:GLY:N	14	0.38
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	2	0.38
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	8	0.38
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	17	0.38
(2,2078)	1:8:A:GLN:H	1:9:A:ASN:HB2	10	0.37
(2,2078)	1:8:A:GLN:H	1:9:A:ASN:HB3	10	0.37
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	13	0.37
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	13	0.37
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	13	0.37
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	7	0.37
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	7	0.37
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	7	0.37
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	19	0.37
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	19	0.37
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	19	0.37
(2,1662)	1:54:A:SER:HB2	1:66:A:LEU:H	19	0.37
(2,1662)	1:54:A:SER:HB3	1:66:A:LEU:H	19	0.37
(2,1634)	1:153:A:ASP:H	1:154:A:LEU:HB3	2	0.37
(2,1634)	1:153:A:ASP:H	1:154:A:LEU:HB3	8	0.37
(2,27)	2:1001:B:ASP:HB2	1:21:A:LYS:HE2	15	0.37
(2,27)	2:1001:B:ASP:HB2	1:21:A:LYS:HE3	15	0.37
(2,27)	2:1001:B:ASP:HB3	1:21:A:LYS:HE2	15	0.37
(2,27)	2:1001:B:ASP:HB3	1:21:A:LYS:HE3	15	0.37
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	13	0.37
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	16	0.37
(1,59)	1:60:A:SER:O	1:64:A:GLY:N	10	0.37
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	9	0.37
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	13	0.37
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	17	0.37
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	5	0.37
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	12	0.37
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	18	0.36
(2,1672)	1:115:A:LYS:HE2	1:116:A:SER:H	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1672)	1:115:A:LYS:HE3	1:116:A:SER:H	9	0.36
(2,1634)	1:153:A:ASP:H	1:154:A:LEU:HB3	3	0.36
(2,1497)	1:122:A:GLU:H	1:122:A:GLU:HB3	12	0.36
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	14	0.36
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	14	0.36
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	10	0.36
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	10	0.36
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	10	0.36
(2,89)	1:15:A:GLU:HB2	1:16:A:SER:HB3	11	0.36
(2,89)	1:15:A:GLU:HB3	1:16:A:SER:HB3	11	0.36
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	11	0.36
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	9	0.36
(1,60)	1:60:A:SER:O	1:64:A:GLY:H	9	0.36
(1,60)	1:60:A:SER:O	1:64:A:GLY:H	16	0.36
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	6	0.36
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	10	0.36
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	4	0.36
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	10	0.36
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	15	0.35
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	15	0.35
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	15	0.35
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	19	0.35
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	19	0.35
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	19	0.35
(2,1931)	1:141:A:TYR:H	1:142:A:LEU:H	6	0.35
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD11	11	0.35
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD12	11	0.35
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD13	11	0.35
(2,1693)	1:62:A:LYS:HD2	1:112:A:ALA:H	5	0.35
(2,1693)	1:62:A:LYS:HD3	1:112:A:ALA:H	5	0.35
(2,1634)	1:153:A:ASP:H	1:154:A:LEU:HB3	14	0.35
(2,1634)	1:153:A:ASP:H	1:154:A:LEU:HB3	16	0.35
(2,1497)	1:122:A:GLU:H	1:122:A:GLU:HB3	17	0.35
(2,1242)	1:20:A:LEU:H	1:23:A:GLY:H	11	0.35
(2,876)	1:62:A:LYS:HD2	1:115:A:LYS:HA	16	0.35
(2,876)	1:62:A:LYS:HD3	1:115:A:LYS:HA	16	0.35
(1,154)	2:1009:B:PRO:HA	1:74:A:ARG:NH2	18	0.35
(1,150)	1:148:A:LYS:O	1:152:A:MET:H	19	0.35
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	11	0.35
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	20	0.35
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB2	5	0.34
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB3	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB2	5	0.34
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB3	5	0.34
(2,2078)	1:8:A:GLN:H	1:9:A:ASN:HB2	18	0.34
(2,2078)	1:8:A:GLN:H	1:9:A:ASN:HB3	18	0.34
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	13	0.34
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	12	0.34
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	12	0.34
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	9	0.34
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	9	0.34
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	9	0.34
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	3	0.34
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	1	0.34
(1,60)	1:60:A:SER:O	1:64:A:GLY:H	1	0.34
(1,60)	1:60:A:SER:O	1:64:A:GLY:H	4	0.34
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	4	0.34
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	15	0.34
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	7	0.34
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	9	0.34
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	13	0.34
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	4	0.33
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	4	0.33
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	4	0.33
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD21	16	0.33
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD22	16	0.33
(2,1949)	1:142:A:LEU:H	1:142:A:LEU:HD23	16	0.33
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	1	0.33
(2,1693)	1:62:A:LYS:HD2	1:112:A:ALA:H	15	0.33
(2,1693)	1:62:A:LYS:HD3	1:112:A:ALA:H	15	0.33
(2,1662)	1:54:A:SER:HB2	1:66:A:LEU:H	3	0.33
(2,1662)	1:54:A:SER:HB3	1:66:A:LEU:H	3	0.33
(2,1629)	1:142:A:LEU:H	1:146:A:ARG:HA	1	0.33
(2,1497)	1:122:A:GLU:H	1:122:A:GLU:HB3	15	0.33
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	10	0.33
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	10	0.33
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	18	0.33
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	18	0.33
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	18	0.33
(2,1013)	1:106:A:GLN:HB3	1:144:A:ALA:HA	10	0.33
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	13	0.33
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	16	0.33
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	20	0.33
(1,64)	1:62:A:LYS:O	1:66:A:LEU:H	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:60:A:SER:O	1:64:A:GLY:H	20	0.33
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	5	0.33
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	16	0.33
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	6	0.33
(3,5)	2:1007:B:TYR:O	1:67:A:TYR:HE1	15	0.32
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD11	4	0.32
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD12	4	0.32
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD13	4	0.32
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD21	4	0.32
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD22	4	0.32
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD23	4	0.32
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD11	7	0.32
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD12	7	0.32
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD13	7	0.32
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD21	7	0.32
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD22	7	0.32
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD23	7	0.32
(2,2142)	1:40:A:ILE:HD11	1:43:A:GLU:HB2	8	0.32
(2,2142)	1:40:A:ILE:HD11	1:43:A:GLU:HB3	8	0.32
(2,2142)	1:40:A:ILE:HD12	1:43:A:GLU:HB2	8	0.32
(2,2142)	1:40:A:ILE:HD12	1:43:A:GLU:HB3	8	0.32
(2,2142)	1:40:A:ILE:HD13	1:43:A:GLU:HB2	8	0.32
(2,2142)	1:40:A:ILE:HD13	1:43:A:GLU:HB3	8	0.32
(2,1957)	1:128:A:LEU:HD11	1:145:A:ILE:H	20	0.32
(2,1957)	1:128:A:LEU:HD12	1:145:A:ILE:H	20	0.32
(2,1957)	1:128:A:LEU:HD13	1:145:A:ILE:H	20	0.32
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	17	0.32
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	6	0.32
(2,1634)	1:153:A:ASP:H	1:154:A:LEU:HB3	15	0.32
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	13	0.32
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	13	0.32
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	13	0.32
(2,1004)	1:149:A:CYS:HA	1:153:A:ASP:HA	1	0.32
(2,1004)	1:149:A:CYS:HA	1:153:A:ASP:HA	16	0.32
(2,876)	1:62:A:LYS:HD2	1:115:A:LYS:HA	6	0.32
(2,876)	1:62:A:LYS:HD3	1:115:A:LYS:HA	6	0.32
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	20	0.32
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	20	0.32
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	20	0.32
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	1	0.32
(2,137)	1:128:A:LEU:HA	1:128:A:LEU:HD21	19	0.32
(2,137)	1:128:A:LEU:HA	1:128:A:LEU:HD22	19	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:128:A:LEU:HA	1:128:A:LEU:HD23	19	0.32
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	11	0.32
(1,59)	1:60:A:SER:O	1:64:A:GLY:N	9	0.32
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	19	0.32
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	10	0.32
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	1	0.32
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	2	0.32
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD11	13	0.31
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD12	13	0.31
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD13	13	0.31
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD21	13	0.31
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD22	13	0.31
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD23	13	0.31
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	2	0.31
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	5	0.31
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	16	0.31
(2,1672)	1:115:A:LYS:HE2	1:116:A:SER:H	8	0.31
(2,1672)	1:115:A:LYS:HE3	1:116:A:SER:H	8	0.31
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	5	0.31
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	5	0.31
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	12	0.31
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	12	0.31
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	12	0.31
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG21	9	0.31
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG22	9	0.31
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG23	9	0.31
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	11	0.31
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	11	0.31
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	11	0.31
(2,28)	2:1004:B:GLU:HB2	1:27:A:SER:H	9	0.31
(2,28)	2:1004:B:GLU:HB3	1:27:A:SER:H	9	0.31
(2,27)	2:1001:B:ASP:HB2	1:21:A:LYS:HE2	18	0.31
(2,27)	2:1001:B:ASP:HB2	1:21:A:LYS:HE3	18	0.31
(2,27)	2:1001:B:ASP:HB3	1:21:A:LYS:HE2	18	0.31
(2,27)	2:1001:B:ASP:HB3	1:21:A:LYS:HE3	18	0.31
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	1	0.31
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	13	0.31
(1,64)	1:62:A:LYS:O	1:66:A:LEU:H	15	0.31
(1,64)	1:62:A:LYS:O	1:66:A:LEU:H	17	0.31
(1,64)	1:62:A:LYS:O	1:66:A:LEU:H	19	0.31
(1,60)	1:60:A:SER:O	1:64:A:GLY:H	6	0.31
(1,59)	1:60:A:SER:O	1:64:A:GLY:N	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:60:A:SER:O	1:64:A:GLY:N	16	0.31
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	18	0.31
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	3	0.31
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	11	0.31
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	14	0.31
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	18	0.31
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD11	1	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD12	1	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD13	1	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD21	1	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD22	1	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD23	1	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD11	12	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD12	12	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD13	12	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD21	12	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD22	12	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD23	12	0.3
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	11	0.3
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	11	0.3
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	11	0.3
(2,1931)	1:141:A:TYR:H	1:142:A:LEU:H	19	0.3
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	5	0.3
(2,1242)	1:20:A:LEU:H	1:23:A:GLY:H	13	0.3
(2,1219)	1:17:A:PHE:H	1:20:A:LEU:HD11	6	0.3
(2,1219)	1:17:A:PHE:H	1:20:A:LEU:HD12	6	0.3
(2,1219)	1:17:A:PHE:H	1:20:A:LEU:HD13	6	0.3
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	4	0.3
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	4	0.3
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	7	0.3
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	7	0.3
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	7	0.3
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	17	0.3
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	17	0.3
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	17	0.3
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	16	0.3
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	16	0.3
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	16	0.3
(2,968)	1:109:A:LEU:HD11	1:128:A:LEU:HD21	19	0.3
(2,968)	1:109:A:LEU:HD11	1:128:A:LEU:HD22	19	0.3
(2,968)	1:109:A:LEU:HD11	1:128:A:LEU:HD23	19	0.3
(2,968)	1:109:A:LEU:HD12	1:128:A:LEU:HD21	19	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,968)	1:109:A:LEU:HD12	1:128:A:LEU:HD22	19	0.3
(2,968)	1:109:A:LEU:HD12	1:128:A:LEU:HD23	19	0.3
(2,968)	1:109:A:LEU:HD13	1:128:A:LEU:HD21	19	0.3
(2,968)	1:109:A:LEU:HD13	1:128:A:LEU:HD22	19	0.3
(2,968)	1:109:A:LEU:HD13	1:128:A:LEU:HD23	19	0.3
(2,876)	1:62:A:LYS:HD2	1:115:A:LYS:HA	20	0.3
(2,876)	1:62:A:LYS:HD3	1:115:A:LYS:HA	20	0.3
(2,197)	1:153:A:ASP:HA	1:155:A:GLU:HB2	16	0.3
(2,197)	1:153:A:ASP:HA	1:155:A:GLU:HB3	16	0.3
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	11	0.3
(1,64)	1:62:A:LYS:O	1:66:A:LEU:H	8	0.3
(1,59)	1:60:A:SER:O	1:64:A:GLY:N	4	0.3
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	20	0.3
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	12	0.3
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD11	18	0.29
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD12	18	0.29
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD13	18	0.29
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD21	18	0.29
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD22	18	0.29
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD23	18	0.29
(2,2317)	1:150:A:PHE:HB2	1:152:A:MET:H	20	0.29
(2,2317)	1:150:A:PHE:HB3	1:152:A:MET:H	20	0.29
(2,1977)	1:110:A:SER:H	1:145:A:ILE:HG21	10	0.29
(2,1977)	1:110:A:SER:H	1:145:A:ILE:HG22	10	0.29
(2,1977)	1:110:A:SER:H	1:145:A:ILE:HG23	10	0.29
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	15	0.29
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	15	0.29
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	15	0.29
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	17	0.29
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	17	0.29
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	17	0.29
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	20	0.29
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	20	0.29
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	20	0.29
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	15	0.29
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	3	0.29
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	14	0.29
(2,1629)	1:142:A:LEU:H	1:146:A:ARG:HA	13	0.29
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	6	0.29
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	6	0.29
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	6	0.29
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	20	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	20	0.29
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	4	0.29
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	4	0.29
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	4	0.29
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	11	0.29
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	11	0.29
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	11	0.29
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD11	16	0.29
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD12	16	0.29
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD13	16	0.29
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD11	16	0.29
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD12	16	0.29
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD13	16	0.29
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD11	16	0.29
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD12	16	0.29
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD13	16	0.29
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	13	0.29
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	13	0.29
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	13	0.29
(2,876)	1:62:A:LYS:HD2	1:115:A:LYS:HA	1	0.29
(2,876)	1:62:A:LYS:HD3	1:115:A:LYS:HA	1	0.29
(2,15)	1:126:A:MET:HE3	2:1009:B:PRO:HD2	5	0.29
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	2	0.29
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	3	0.29
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	11	0.29
(1,64)	1:62:A:LYS:O	1:66:A:LEU:H	3	0.29
(1,60)	1:60:A:SER:O	1:64:A:GLY:H	18	0.29
(1,59)	1:60:A:SER:O	1:64:A:GLY:N	20	0.29
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	8	0.29
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	16	0.29
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	13	0.29
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	5	0.29
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	8	0.29
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	10	0.29
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	12	0.29
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	17	0.29
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB2	12	0.28
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB3	12	0.28
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB2	12	0.28
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB3	12	0.28
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB2	13	0.28
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB3	13	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB2	13	0.28
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB3	13	0.28
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD21	5	0.28
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD22	5	0.28
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD23	5	0.28
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD21	13	0.28
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD22	13	0.28
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD23	13	0.28
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	11	0.28
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	9	0.28
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	9	0.28
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	9	0.28
(2,1693)	1:62:A:LYS:HD2	1:112:A:ALA:H	12	0.28
(2,1693)	1:62:A:LYS:HD3	1:112:A:ALA:H	12	0.28
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	15	0.28
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	2	0.28
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	2	0.28
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	2	0.28
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	20	0.28
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	20	0.28
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	20	0.28
(2,1494)	1:96:A:HIS:H	1:99:A:ASN:HD22	12	0.28
(2,1242)	1:20:A:LEU:H	1:23:A:GLY:H	7	0.28
(2,1242)	1:20:A:LEU:H	1:23:A:GLY:H	12	0.28
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	1	0.28
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	1	0.28
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	13	0.28
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	13	0.28
(2,982)	1:128:A:LEU:HD11	1:145:A:ILE:HB	10	0.28
(2,982)	1:128:A:LEU:HD12	1:145:A:ILE:HB	10	0.28
(2,982)	1:128:A:LEU:HD13	1:145:A:ILE:HB	10	0.28
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG21	10	0.28
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG22	10	0.28
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG23	10	0.28
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	1	0.28
(2,369)	1:17:A:PHE:HA	1:20:A:LEU:HA	12	0.28
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	14	0.28
(2,252)	1:153:A:ASP:HB3	1:154:A:LEU:HB3	4	0.28
(2,252)	1:153:A:ASP:HB3	1:154:A:LEU:HB3	13	0.28
(2,252)	1:153:A:ASP:HB3	1:154:A:LEU:HB3	18	0.28
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	8	0.28
(2,28)	2:1004:B:GLU:HB2	1:27:A:SER:H	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,28)	2:1004:B:GLU:HB3	1:27:A:SER:H	4	0.28
(2,27)	2:1001:B:ASP:HB2	1:21:A:LYS:HE2	6	0.28
(2,27)	2:1001:B:ASP:HB2	1:21:A:LYS:HE3	6	0.28
(2,27)	2:1001:B:ASP:HB3	1:21:A:LYS:HE2	6	0.28
(2,27)	2:1001:B:ASP:HB3	1:21:A:LYS:HE3	6	0.28
(2,15)	1:126:A:MET:HE1	2:1009:B:PRO:HG2	19	0.28
(1,149)	1:148:A:LYS:O	1:152:A:MET:N	19	0.28
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	4	0.28
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	5	0.28
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	14	0.28
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	15	0.28
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	10	0.28
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	11	0.28
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	15	0.28
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	2	0.28
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	10	0.28
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	18	0.28
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	9	0.28
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	10	0.28
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	9	0.28
(1,54)	1:51:A:ILE:O	1:55:A:ARG:H	1	0.28
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	2	0.28
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	5	0.28
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	6	0.28
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	9	0.28
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	4	0.28
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	14	0.28
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	4	0.28
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	20	0.28
(2,2181)	1:55:A:ARG:HD2	1:108:A:LEU:HD21	15	0.27
(2,2181)	1:55:A:ARG:HD2	1:108:A:LEU:HD22	15	0.27
(2,2181)	1:55:A:ARG:HD2	1:108:A:LEU:HD23	15	0.27
(2,2181)	1:55:A:ARG:HD3	1:108:A:LEU:HD21	15	0.27
(2,2181)	1:55:A:ARG:HD3	1:108:A:LEU:HD22	15	0.27
(2,2181)	1:55:A:ARG:HD3	1:108:A:LEU:HD23	15	0.27
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	13	0.27
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	13	0.27
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	13	0.27
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	19	0.27
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	19	0.27
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	19	0.27
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	20	0.27
(2,1906)	1:23:A:GLY:H	1:24:A:ILE:HG12	9	0.27
(2,1906)	1:23:A:GLY:H	1:24:A:ILE:HG13	9	0.27
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	4	0.27
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	4	0.27
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	4	0.27
(2,1693)	1:62:A:LYS:HD2	1:112:A:ALA:H	10	0.27
(2,1693)	1:62:A:LYS:HD3	1:112:A:ALA:H	10	0.27
(2,1662)	1:54:A:SER:HB2	1:66:A:LEU:H	2	0.27
(2,1662)	1:54:A:SER:HB3	1:66:A:LEU:H	2	0.27
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	9	0.27
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	12	0.27
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	4	0.27
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	1	0.27
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	1	0.27
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	1	0.27
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	13	0.27
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	13	0.27
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	13	0.27
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	15	0.27
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	15	0.27
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	15	0.27
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	17	0.27
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	17	0.27
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	17	0.27
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	19	0.27
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	19	0.27
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	19	0.27
(2,1494)	1:96:A:HIS:H	1:99:A:ASN:HD22	5	0.27
(2,1133)	1:141:A:TYR:H	1:142:A:LEU:HD11	16	0.27
(2,1133)	1:141:A:TYR:H	1:142:A:LEU:HD12	16	0.27
(2,1133)	1:141:A:TYR:H	1:142:A:LEU:HD13	16	0.27
(2,1105)	1:138:A:GLN:HA	1:139:A:LYS:HA	13	0.27
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	2	0.27
(2,854)	1:109:A:LEU:HD21	1:128:A:LEU:HA	3	0.27
(2,854)	1:109:A:LEU:HD22	1:128:A:LEU:HA	3	0.27
(2,854)	1:109:A:LEU:HD23	1:128:A:LEU:HA	3	0.27
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	3	0.27
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	3	0.27
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	3	0.27
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	6	0.27
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	3	0.27
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	12	0.27
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	18	0.27
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	20	0.27
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	4	0.27
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	6	0.27
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	16	0.27
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	14	0.27
(1,59)	1:60:A:SER:O	1:64:A:GLY:N	6	0.27
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	17	0.27
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	9	0.27
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	5	0.27
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	3	0.27
(3,7)	2:1004:B:GLU:HB2	1:30:A:LYS:HE2	3	0.26
(3,7)	2:1004:B:GLU:HB2	1:30:A:LYS:HE3	3	0.26
(3,7)	2:1004:B:GLU:HB3	1:30:A:LYS:HE2	3	0.26
(3,7)	2:1004:B:GLU:HB3	1:30:A:LYS:HE3	3	0.26
(3,3)	2:1009:B:PRO:HB2	1:74:A:ARG:NH2	7	0.26
(3,3)	2:1009:B:PRO:HB3	1:74:A:ARG:NH2	7	0.26
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	11	0.26
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	11	0.26
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	11	0.26
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	11	0.26
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	11	0.26
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	11	0.26
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	11	0.26
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	11	0.26
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	11	0.26
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	11	0.26
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	11	0.26
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	11	0.26
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	14	0.26
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	14	0.26
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	14	0.26
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	14	0.26
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	14	0.26
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	14	0.26
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	14	0.26
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	14	0.26
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	14	0.26
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	14	0.26
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	14	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	14	0.26
(2,2181)	1:55:A:ARG:HD2	1:108:A:LEU:HD21	13	0.26
(2,2181)	1:55:A:ARG:HD2	1:108:A:LEU:HD22	13	0.26
(2,2181)	1:55:A:ARG:HD2	1:108:A:LEU:HD23	13	0.26
(2,2181)	1:55:A:ARG:HD3	1:108:A:LEU:HD21	13	0.26
(2,2181)	1:55:A:ARG:HD3	1:108:A:LEU:HD22	13	0.26
(2,2181)	1:55:A:ARG:HD3	1:108:A:LEU:HD23	13	0.26
(2,2092)	1:20:A:LEU:HB2	1:23:A:GLY:H	9	0.26
(2,2092)	1:20:A:LEU:HB3	1:23:A:GLY:H	9	0.26
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	12	0.26
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	12	0.26
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	12	0.26
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	18	0.26
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	18	0.26
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	18	0.26
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	18	0.26
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	18	0.26
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	18	0.26
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	7	0.26
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	8	0.26
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	18	0.26
(2,1724)	1:154:A:LEU:H	1:154:A:LEU:HB3	1	0.26
(2,1693)	1:62:A:LYS:HD2	1:112:A:ALA:H	2	0.26
(2,1693)	1:62:A:LYS:HD3	1:112:A:ALA:H	2	0.26
(2,1693)	1:62:A:LYS:HD2	1:112:A:ALA:H	3	0.26
(2,1693)	1:62:A:LYS:HD3	1:112:A:ALA:H	3	0.26
(2,1693)	1:62:A:LYS:HD2	1:112:A:ALA:H	17	0.26
(2,1693)	1:62:A:LYS:HD3	1:112:A:ALA:H	17	0.26
(2,1672)	1:115:A:LYS:HE2	1:116:A:SER:H	13	0.26
(2,1672)	1:115:A:LYS:HE3	1:116:A:SER:H	13	0.26
(2,1662)	1:54:A:SER:HB2	1:66:A:LEU:H	15	0.26
(2,1662)	1:54:A:SER:HB3	1:66:A:LEU:H	15	0.26
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	1	0.26
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	12	0.26
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	16	0.26
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	8	0.26
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	8	0.26
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	8	0.26
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	18	0.26
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	18	0.26
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	18	0.26
(2,1242)	1:20:A:LEU:H	1:23:A:GLY:H	19	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	10	0.26
(2,876)	1:62:A:LYS:HD2	1:115:A:LYS:HA	4	0.26
(2,876)	1:62:A:LYS:HD3	1:115:A:LYS:HA	4	0.26
(2,876)	1:62:A:LYS:HD2	1:115:A:LYS:HA	9	0.26
(2,876)	1:62:A:LYS:HD3	1:115:A:LYS:HA	9	0.26
(2,369)	1:17:A:PHE:HA	1:20:A:LEU:HA	11	0.26
(2,303)	1:8:A:GLN:HA	1:9:A:ASN:HD21	10	0.26
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	9	0.26
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	9	0.26
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	9	0.26
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	15	0.26
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	15	0.26
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	15	0.26
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	16	0.26
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	16	0.26
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	16	0.26
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	8	0.26
(2,230)	1:55:A:ARG:H	1:108:A:LEU:HB3	11	0.26
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	11	0.26
(2,128)	1:63:A:LEU:HD11	1:123:A:LYS:HA	13	0.26
(2,128)	1:63:A:LEU:HD12	1:123:A:LYS:HA	13	0.26
(2,128)	1:63:A:LEU:HD13	1:123:A:LYS:HA	13	0.26
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	8	0.26
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	10	0.26
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	9	0.26
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	15	0.26
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	19	0.26
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	20	0.26
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	4	0.26
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	11	0.26
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	13	0.26
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	20	0.26
(1,64)	1:62:A:LYS:O	1:66:A:LEU:H	13	0.26
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	18	0.26
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	9	0.26
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	11	0.26
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	13	0.26
(2,2312)	1:141:A:TYR:HB2	1:142:A:LEU:H	10	0.25
(2,2312)	1:141:A:TYR:HB3	1:142:A:LEU:H	10	0.25
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	7	0.25
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	7	0.25
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	14	0.25
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD21	11	0.25
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD22	11	0.25
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD23	11	0.25
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	2	0.25
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	12	0.25
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	12	0.25
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	12	0.25
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	2	0.25
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	2	0.25
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	2	0.25
(2,1662)	1:54:A:SER:HB2	1:66:A:LEU:H	8	0.25
(2,1662)	1:54:A:SER:HB3	1:66:A:LEU:H	8	0.25
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	6	0.25
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	11	0.25
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	15	0.25
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	15	0.25
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	4	0.25
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	4	0.25
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	4	0.25
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	7	0.25
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	7	0.25
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	7	0.25
(2,1494)	1:96:A:HIS:H	1:99:A:ASN:HD22	4	0.25
(2,1242)	1:20:A:LEU:H	1:23:A:GLY:H	1	0.25
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	16	0.25
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	16	0.25
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	5	0.25
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	5	0.25
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	5	0.25
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	17	0.25
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	17	0.25
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	17	0.25
(2,996)	1:152:A:MET:H	1:152:A:MET:HG3	2	0.25
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG21	19	0.25
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG22	19	0.25
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG23	19	0.25
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	15	0.25
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	15	0.25
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	17	0.25
(2,568)	1:49:A:LEU:HG	1:53:A:TYR:HA	4	0.25
(2,397)	1:14:A:LEU:HD11	1:53:A:TYR:H	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,397)	1:14:A:LEU:HD12	1:53:A:TYR:H	12	0.25
(2,397)	1:14:A:LEU:HD13	1:53:A:TYR:H	12	0.25
(2,381)	1:24:A:ILE:H	1:24:A:ILE:HD11	17	0.25
(2,381)	1:24:A:ILE:H	1:24:A:ILE:HD12	17	0.25
(2,381)	1:24:A:ILE:H	1:24:A:ILE:HD13	17	0.25
(2,303)	1:8:A:GLN:HA	1:9:A:ASN:HD21	18	0.25
(2,303)	1:8:A:GLN:HA	1:9:A:ASN:HD21	19	0.25
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	1	0.25
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	1	0.25
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	1	0.25
(2,30)	1:8:A:GLN:HG2	1:12:A:ALA:H	18	0.25
(2,30)	1:8:A:GLN:HG3	1:12:A:ALA:H	18	0.25
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	7	0.25
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	18	0.25
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	19	0.25
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	2	0.25
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	5	0.25
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	15	0.25
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	16	0.25
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	11	0.25
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	13	0.25
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	16	0.25
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	14	0.25
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	1	0.25
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	3	0.25
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	6	0.25
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	9	0.25
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	10	0.25
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	13	0.25
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	16	0.25
(1,65)	1:63:A:LEU:O	1:67:A:TYR:N	9	0.25
(1,64)	1:62:A:LYS:O	1:66:A:LEU:H	5	0.25
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	13	0.25
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	2	0.25
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	10	0.25
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	7	0.25
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	16	0.25
(2,2286)	1:122:A:GLU:H	1:122:A:GLU:HG2	15	0.24
(2,2286)	1:122:A:GLU:H	1:122:A:GLU:HG3	15	0.24
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB2	10	0.24
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB3	10	0.24
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB2	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB3	10	0.24
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	17	0.24
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	17	0.24
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	17	0.24
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	14	0.24
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	14	0.24
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	14	0.24
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	3	0.24
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	11	0.24
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD11	2	0.24
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD12	2	0.24
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD13	2	0.24
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	19	0.24
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	19	0.24
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	19	0.24
(2,1693)	1:62:A:LYS:HD2	1:112:A:ALA:H	13	0.24
(2,1693)	1:62:A:LYS:HD3	1:112:A:ALA:H	13	0.24
(2,1693)	1:62:A:LYS:HD2	1:112:A:ALA:H	19	0.24
(2,1693)	1:62:A:LYS:HD3	1:112:A:ALA:H	19	0.24
(2,1628)	1:148:A:LYS:HB2	1:149:A:CYS:H	7	0.24
(2,1628)	1:148:A:LYS:HB3	1:149:A:CYS:H	7	0.24
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	6	0.24
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	7	0.24
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	11	0.24
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	13	0.24
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	12	0.24
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	12	0.24
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	12	0.24
(2,1494)	1:96:A:HIS:H	1:99:A:ASN:HD22	20	0.24
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB2	1	0.24
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB3	1	0.24
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB2	7	0.24
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB3	7	0.24
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB2	9	0.24
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB3	9	0.24
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB2	10	0.24
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB3	10	0.24
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB2	13	0.24
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB3	13	0.24
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB2	18	0.24
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB3	18	0.24
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB2	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1136)	1:5:A:ASP:H	1:5:A:ASP:HB3	19	0.24
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	2	0.24
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	2	0.24
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	11	0.24
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	11	0.24
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD11	5	0.24
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD12	5	0.24
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD13	5	0.24
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD11	5	0.24
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD12	5	0.24
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD13	5	0.24
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD11	5	0.24
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD12	5	0.24
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD13	5	0.24
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	18	0.24
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	18	0.24
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	18	0.24
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	17	0.24
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	17	0.24
(2,961)	1:123:A:LYS:HA	1:126:A:MET:HB3	15	0.24
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG21	12	0.24
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG22	12	0.24
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG23	12	0.24
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG21	12	0.24
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG22	12	0.24
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG23	12	0.24
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG21	12	0.24
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG22	12	0.24
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG23	12	0.24
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	19	0.24
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	13	0.24
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	13	0.24
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	13	0.24
(2,252)	1:153:A:ASP:HB3	1:154:A:LEU:HB3	12	0.24
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	12	0.24
(2,197)	1:153:A:ASP:HA	1:155:A:GLU:HB2	15	0.24
(2,197)	1:153:A:ASP:HA	1:155:A:GLU:HB3	15	0.24
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	15	0.24
(2,111)	1:43:A:GLU:H	1:44:A:SER:HB2	8	0.24
(2,30)	1:8:A:GLN:HG2	1:12:A:ALA:H	10	0.24
(2,30)	1:8:A:GLN:HG3	1:12:A:ALA:H	10	0.24
(2,30)	1:8:A:GLN:HG2	1:12:A:ALA:H	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,30)	1:8:A:GLN:HG3	1:12:A:ALA:H	19	0.24
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	4	0.24
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	14	0.24
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	9	0.24
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	19	0.24
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	12	0.24
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	5	0.24
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	8	0.24
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	16	0.24
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	18	0.24
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	20	0.24
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	16	0.24
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	3	0.24
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	11	0.24
(1,64)	1:62:A:LYS:O	1:66:A:LEU:H	7	0.24
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	18	0.24
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	11	0.24
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	17	0.24
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	15	0.24
(1,16)	1:14:A:LEU:O	1:18:A:LYS:H	19	0.24
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	1	0.24
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	14	0.24
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD11	4	0.23
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD12	4	0.23
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD13	4	0.23
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD21	4	0.23
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD22	4	0.23
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD23	4	0.23
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD11	9	0.23
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD12	9	0.23
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD13	9	0.23
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD21	9	0.23
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD22	9	0.23
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD23	9	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	1	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	1	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	1	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	1	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	1	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	1	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	1	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	1	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	1	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	1	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	1	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	10	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	10	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	10	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	10	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	10	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	10	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	10	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	10	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	10	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	10	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	10	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	10	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	16	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	16	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	16	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	16	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	16	0.23
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	16	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	16	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	16	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	16	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	16	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	16	0.23
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	16	0.23
(2,2180)	1:55:A:ARG:HD2	1:56:A:LEU:HG	3	0.23
(2,2180)	1:55:A:ARG:HD3	1:56:A:LEU:HG	3	0.23
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	2	0.23
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	2	0.23
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	2	0.23
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	5	0.23
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	5	0.23
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	5	0.23
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	16	0.23
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	16	0.23
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	16	0.23
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	17	0.23
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	1	0.23
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1829)	1:62:A:LYS:HB2	1:113:A:ILE:H	14	0.23
(2,1829)	1:62:A:LYS:HB3	1:113:A:ILE:H	14	0.23
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	13	0.23
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	13	0.23
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	13	0.23
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	8	0.23
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	8	0.23
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	8	0.23
(2,1730)	1:155:A:GLU:H	1:156:A:HIS:H	2	0.23
(2,1730)	1:155:A:GLU:H	1:156:A:HIS:H	3	0.23
(2,1672)	1:115:A:LYS:HE2	1:116:A:SER:H	2	0.23
(2,1672)	1:115:A:LYS:HE3	1:116:A:SER:H	2	0.23
(2,1573)	1:113:A:ILE:H	1:115:A:LYS:H	5	0.23
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	20	0.23
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	14	0.23
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	14	0.23
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	14	0.23
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	16	0.23
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	16	0.23
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	16	0.23
(2,1494)	1:96:A:HIS:H	1:99:A:ASN:HD22	11	0.23
(2,1385)	1:52:A:ASP:H	1:53:A:TYR:HB2	19	0.23
(2,1322)	1:41:A:ASP:H	1:93:A:THR:HG21	8	0.23
(2,1322)	1:41:A:ASP:H	1:93:A:THR:HG22	8	0.23
(2,1322)	1:41:A:ASP:H	1:93:A:THR:HG23	8	0.23
(2,1242)	1:20:A:LEU:H	1:23:A:GLY:H	6	0.23
(2,1242)	1:20:A:LEU:H	1:23:A:GLY:H	17	0.23
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	14	0.23
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	14	0.23
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	14	0.23
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	5	0.23
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	5	0.23
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	7	0.23
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	7	0.23
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	8	0.23
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	8	0.23
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	12	0.23
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	12	0.23
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	20	0.23
(2,879)	1:63:A:LEU:HB2	1:123:A:LYS:HB2	3	0.23
(2,879)	1:63:A:LEU:HB2	1:123:A:LYS:HB3	3	0.23
(2,854)	1:109:A:LEU:HD21	1:128:A:LEU:HA	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,854)	1:109:A:LEU:HD22	1:128:A:LEU:HA	8	0.23
(2,854)	1:109:A:LEU:HD23	1:128:A:LEU:HA	8	0.23
(2,742)	1:76:A:TYR:HA	1:94:A:CYS:HA	7	0.23
(2,568)	1:49:A:LEU:HG	1:53:A:TYR:HA	9	0.23
(2,369)	1:17:A:PHE:HA	1:20:A:LEU:HA	1	0.23
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD21	11	0.23
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD22	11	0.23
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD23	11	0.23
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	1	0.23
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	14	0.23
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	12	0.23
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	17	0.23
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	6	0.23
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	10	0.23
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	2	0.23
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	4	0.23
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	9	0.23
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	15	0.23
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	3	0.23
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	2	0.23
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	7	0.23
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	17	0.23
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	19	0.23
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	5	0.23
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	11	0.23
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	5	0.23
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	1	0.23
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	4	0.23
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	9	0.23
(1,68)	1:64:A:GLY:O	1:68:A:ILE:H	4	0.23
(1,68)	1:64:A:GLY:O	1:68:A:ILE:H	20	0.23
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	15	0.23
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	6	0.23
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	10	0.23
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	18	0.23
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD11	16	0.22
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD12	16	0.22
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD13	16	0.22
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD21	16	0.22
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD22	16	0.22
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD23	16	0.22
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	5	0.22
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	5	0.22
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	5	0.22
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	5	0.22
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	5	0.22
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	5	0.22
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	5	0.22
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	5	0.22
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	5	0.22
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	5	0.22
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	5	0.22
(2,2180)	1:55:A:ARG:HD2	1:56:A:LEU:HG	2	0.22
(2,2180)	1:55:A:ARG:HD3	1:56:A:LEU:HG	2	0.22
(2,2180)	1:55:A:ARG:HD2	1:56:A:LEU:HG	17	0.22
(2,2180)	1:55:A:ARG:HD3	1:56:A:LEU:HG	17	0.22
(2,2093)	1:20:A:LEU:HB2	1:24:A:ILE:H	17	0.22
(2,2093)	1:20:A:LEU:HB3	1:24:A:ILE:H	17	0.22
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB2	1	0.22
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB3	1	0.22
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB2	18	0.22
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB3	18	0.22
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB2	19	0.22
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB3	19	0.22
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	8	0.22
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	8	0.22
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	8	0.22
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	4	0.22
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	4	0.22
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	4	0.22
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	10	0.22
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	10	0.22
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	10	0.22
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	19	0.22
(2,1906)	1:23:A:GLY:H	1:24:A:ILE:HG12	6	0.22
(2,1906)	1:23:A:GLY:H	1:24:A:ILE:HG13	6	0.22
(2,1902)	1:62:A:LYS:HD2	1:115:A:LYS:H	14	0.22
(2,1902)	1:62:A:LYS:HD3	1:115:A:LYS:H	14	0.22
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	7	0.22
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	6	0.22
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	8	0.22
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	13	0.22
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD11	13	0.22
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD12	13	0.22
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD13	13	0.22
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	5	0.22
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	5	0.22
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	5	0.22
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	17	0.22
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	17	0.22
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	17	0.22
(2,1730)	1:155:A:GLU:H	1:156:A:HIS:H	5	0.22
(2,1730)	1:155:A:GLU:H	1:156:A:HIS:H	10	0.22
(2,1730)	1:155:A:GLU:H	1:156:A:HIS:H	17	0.22
(2,1724)	1:154:A:LEU:H	1:154:A:LEU:HB3	5	0.22
(2,1662)	1:54:A:SER:HB2	1:66:A:LEU:H	17	0.22
(2,1662)	1:54:A:SER:HB3	1:66:A:LEU:H	17	0.22
(2,1629)	1:142:A:LEU:H	1:146:A:ARG:HA	5	0.22
(2,1628)	1:148:A:LYS:HB2	1:149:A:CYS:H	14	0.22
(2,1628)	1:148:A:LYS:HB3	1:149:A:CYS:H	14	0.22
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	17	0.22
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD21	4	0.22
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD22	4	0.22
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD23	4	0.22
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD21	13	0.22
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD22	13	0.22
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD23	13	0.22
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD21	18	0.22
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD22	18	0.22
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD23	18	0.22
(2,1494)	1:96:A:HIS:H	1:99:A:ASN:HD22	18	0.22
(2,1242)	1:20:A:LEU:H	1:23:A:GLY:H	9	0.22
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	8	0.22
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	8	0.22
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	17	0.22
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	17	0.22
(2,1004)	1:149:A:CYS:HA	1:153:A:ASP:HA	4	0.22
(2,1004)	1:149:A:CYS:HA	1:153:A:ASP:HA	20	0.22
(2,996)	1:152:A:MET:H	1:152:A:MET:HG3	5	0.22
(2,996)	1:152:A:MET:H	1:152:A:MET:HG3	15	0.22
(2,996)	1:152:A:MET:H	1:152:A:MET:HG3	17	0.22
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	2	0.22
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	2	0.22
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	3	0.22
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	11	0.22
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	11	0.22
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG21	5	0.22
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG22	5	0.22
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG23	5	0.22
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG21	5	0.22
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG22	5	0.22
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG23	5	0.22
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG21	5	0.22
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG22	5	0.22
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG23	5	0.22
(2,742)	1:76:A:TYR:HA	1:94:A:CYS:HA	9	0.22
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG21	7	0.22
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG22	7	0.22
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG23	7	0.22
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	18	0.22
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	18	0.22
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	18	0.22
(2,568)	1:49:A:LEU:HG	1:53:A:TYR:HA	6	0.22
(2,369)	1:17:A:PHE:HA	1:20:A:LEU:HA	7	0.22
(2,369)	1:17:A:PHE:HA	1:20:A:LEU:HA	13	0.22
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	18	0.22
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	18	0.22
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	18	0.22
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	18	0.22
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	18	0.22
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	18	0.22
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	19	0.22
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	19	0.22
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	19	0.22
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	19	0.22
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	19	0.22
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	19	0.22
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	10	0.22
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	10	0.22
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	10	0.22
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	10	0.22
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	10	0.22
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	10	0.22
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	10	0.22
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	10	0.22
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB2	18	0.22
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB3	18	0.22
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB2	18	0.22
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB3	18	0.22
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB2	18	0.22
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB3	18	0.22
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	10	0.22
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	18	0.22
(2,281)	1:128:A:LEU:HD11	1:129:A:ASP:H	19	0.22
(2,281)	1:128:A:LEU:HD12	1:129:A:ASP:H	19	0.22
(2,281)	1:128:A:LEU:HD13	1:129:A:ASP:H	19	0.22
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	2	0.22
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	2	0.22
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	2	0.22
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	4	0.22
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	4	0.22
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	4	0.22
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	8	0.22
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	8	0.22
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	8	0.22
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	14	0.22
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	14	0.22
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	14	0.22
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	6	0.22
(2,167)	1:63:A:LEU:HD11	1:67:A:TYR:HB2	13	0.22
(2,167)	1:63:A:LEU:HD12	1:67:A:TYR:HB2	13	0.22
(2,167)	1:63:A:LEU:HD13	1:67:A:TYR:HB2	13	0.22
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG2	16	0.22
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG3	16	0.22
(2,128)	1:63:A:LEU:HD11	1:123:A:LYS:HA	20	0.22
(2,128)	1:63:A:LEU:HD12	1:123:A:LYS:HA	20	0.22
(2,128)	1:63:A:LEU:HD13	1:123:A:LYS:HA	20	0.22
(1,148)	1:143:A:ASN:O	1:147:A:SER:H	6	0.22
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	7	0.22
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	8	0.22
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	18	0.22
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	19	0.22
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	20	0.22
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	3	0.22
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	16	0.22
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	6	0.22
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	8	0.22
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	12	0.22
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	15	0.22
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	14	0.22
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	15	0.22
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	13	0.22
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	14	0.22
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	18	0.22
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	20	0.22
(1,68)	1:64:A:GLY:O	1:68:A:ILE:H	1	0.22
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	10	0.22
(1,64)	1:62:A:LYS:O	1:66:A:LEU:H	12	0.22
(1,63)	1:62:A:LYS:O	1:66:A:LEU:N	2	0.22
(1,59)	1:60:A:SER:O	1:64:A:GLY:N	18	0.22
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	4	0.22
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	10	0.22
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	18	0.22
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	12	0.22
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	16	0.22
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	4	0.22
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	9	0.22
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	13	0.22
(1,14)	1:13:A:THR:O	1:17:A:PHE:H	14	0.22
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD11	13	0.21
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD12	13	0.21
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD13	13	0.21
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD21	13	0.21
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD22	13	0.21
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD23	13	0.21
(2,2286)	1:122:A:GLU:H	1:122:A:GLU:HG2	17	0.21
(2,2286)	1:122:A:GLU:H	1:122:A:GLU:HG3	17	0.21
(2,2178)	1:55:A:ARG:HG2	1:56:A:LEU:H	10	0.21
(2,2178)	1:55:A:ARG:HG3	1:56:A:LEU:H	10	0.21
(2,2178)	1:55:A:ARG:HG2	1:56:A:LEU:H	19	0.21
(2,2178)	1:55:A:ARG:HG3	1:56:A:LEU:H	19	0.21
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD11	4	0.21
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD12	4	0.21
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD13	4	0.21
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD21	4	0.21
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD22	4	0.21
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD23	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB2	7	0.21
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB3	7	0.21
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB2	9	0.21
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB3	9	0.21
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB2	13	0.21
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB3	13	0.21
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	4	0.21
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	4	0.21
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	4	0.21
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	14	0.21
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	14	0.21
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	14	0.21
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	1	0.21
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	1	0.21
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	1	0.21
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	9	0.21
(2,1931)	1:141:A:TYR:H	1:142:A:LEU:H	20	0.21
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD21	17	0.21
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD22	17	0.21
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD23	17	0.21
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	8	0.21
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	12	0.21
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	16	0.21
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	16	0.21
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	16	0.21
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	18	0.21
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	18	0.21
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	18	0.21
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	3	0.21
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	3	0.21
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	3	0.21
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	15	0.21
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	15	0.21
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	15	0.21
(2,1693)	1:62:A:LYS:HD2	1:112:A:ALA:H	7	0.21
(2,1693)	1:62:A:LYS:HD3	1:112:A:ALA:H	7	0.21
(2,1693)	1:62:A:LYS:HD2	1:112:A:ALA:H	8	0.21
(2,1693)	1:62:A:LYS:HD3	1:112:A:ALA:H	8	0.21
(2,1662)	1:54:A:SER:HB2	1:66:A:LEU:H	5	0.21
(2,1662)	1:54:A:SER:HB3	1:66:A:LEU:H	5	0.21
(2,1662)	1:54:A:SER:HB2	1:66:A:LEU:H	7	0.21
(2,1662)	1:54:A:SER:HB3	1:66:A:LEU:H	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1573)	1:113:A:ILE:H	1:115:A:LYS:H	14	0.21
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	3	0.21
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	5	0.21
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	14	0.21
(2,1385)	1:52:A:ASP:H	1:53:A:TYR:HB2	3	0.21
(2,1341)	1:43:A:GLU:HG2	1:44:A:SER:H	8	0.21
(2,1341)	1:43:A:GLU:HG3	1:44:A:SER:H	8	0.21
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	15	0.21
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	15	0.21
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	15	0.21
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD11	1	0.21
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD12	1	0.21
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD13	1	0.21
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD11	1	0.21
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD12	1	0.21
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD13	1	0.21
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD11	1	0.21
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD12	1	0.21
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD13	1	0.21
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD11	18	0.21
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD12	18	0.21
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD13	18	0.21
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD11	18	0.21
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD12	18	0.21
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD13	18	0.21
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD11	18	0.21
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD12	18	0.21
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD13	18	0.21
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	5	0.21
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	5	0.21
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	5	0.21
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	15	0.21
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	15	0.21
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	15	0.21
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG21	8	0.21
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG22	8	0.21
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG23	8	0.21
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG21	20	0.21
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG22	20	0.21
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG23	20	0.21
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	4	0.21
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	4	0.21
(2,369)	1:17:A:PHE:HA	1:20:A:LEU:HA	16	0.21
(2,369)	1:17:A:PHE:HA	1:20:A:LEU:HA	19	0.21
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	4	0.21
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	4	0.21
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	4	0.21
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	4	0.21
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	4	0.21
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	4	0.21
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	4	0.21
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	4	0.21
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	4	0.21
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	14	0.21
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	14	0.21
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	14	0.21
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	14	0.21
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	14	0.21
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	14	0.21
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	14	0.21
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	14	0.21
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	14	0.21
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	1	0.21
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	9	0.21
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	12	0.21
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	18	0.21
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	19	0.21
(2,128)	1:63:A:LEU:HD11	1:123:A:LYS:HA	1	0.21
(2,128)	1:63:A:LEU:HD12	1:123:A:LYS:HA	1	0.21
(2,128)	1:63:A:LEU:HD13	1:123:A:LYS:HA	1	0.21
(2,128)	1:63:A:LEU:HD11	1:123:A:LYS:HA	4	0.21
(2,128)	1:63:A:LEU:HD12	1:123:A:LYS:HA	4	0.21
(2,128)	1:63:A:LEU:HD13	1:123:A:LYS:HA	4	0.21
(2,16)	2:1009:B:PRO:HA	1:74:A:ARG:HE	6	0.21
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	9	0.21
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	18	0.21
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	14	0.21
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	11	0.21
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	20	0.21
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	5	0.21
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	17	0.21
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	13	0.21
(1,122)	1:118:A:GLN:O	1:122:A:GLU:H	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	1	0.21
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	20	0.21
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	17	0.21
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	16	0.21
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	5	0.21
(1,64)	1:62:A:LYS:O	1:66:A:LEU:H	11	0.21
(1,63)	1:62:A:LYS:O	1:66:A:LEU:N	19	0.21
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	20	0.21
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	1	0.21
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	2	0.21
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	16	0.21
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	19	0.21
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	1	0.21
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	7	0.21
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	20	0.21
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	18	0.21
(2,2352)	1:105:A:ILE:HD11	1:137:A:PHE:HD1	11	0.2
(2,2352)	1:105:A:ILE:HD11	1:137:A:PHE:HD2	11	0.2
(2,2352)	1:105:A:ILE:HD12	1:137:A:PHE:HD1	11	0.2
(2,2352)	1:105:A:ILE:HD12	1:137:A:PHE:HD2	11	0.2
(2,2352)	1:105:A:ILE:HD13	1:137:A:PHE:HD1	11	0.2
(2,2352)	1:105:A:ILE:HD13	1:137:A:PHE:HD2	11	0.2
(2,2341)	1:105:A:ILE:HD11	1:137:A:PHE:HD1	11	0.2
(2,2341)	1:105:A:ILE:HD11	1:137:A:PHE:HD2	11	0.2
(2,2341)	1:105:A:ILE:HD12	1:137:A:PHE:HD1	11	0.2
(2,2341)	1:105:A:ILE:HD12	1:137:A:PHE:HD2	11	0.2
(2,2341)	1:105:A:ILE:HD13	1:137:A:PHE:HD1	11	0.2
(2,2341)	1:105:A:ILE:HD13	1:137:A:PHE:HD2	11	0.2
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD11	10	0.2
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD12	10	0.2
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD13	10	0.2
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD21	10	0.2
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD22	10	0.2
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD23	10	0.2
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD11	14	0.2
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD12	14	0.2
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD13	14	0.2
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD21	14	0.2
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD22	14	0.2
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD23	14	0.2
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD11	9	0.2
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD12	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD13	9	0.2
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD21	9	0.2
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD22	9	0.2
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD23	9	0.2
(2,2286)	1:122:A:GLU:H	1:122:A:GLU:HG2	12	0.2
(2,2286)	1:122:A:GLU:H	1:122:A:GLU:HG3	12	0.2
(2,2101)	1:24:A:ILE:HG12	1:64:A:GLY:HA2	7	0.2
(2,2101)	1:24:A:ILE:HG12	1:64:A:GLY:HA3	7	0.2
(2,2101)	1:24:A:ILE:HG13	1:64:A:GLY:HA2	7	0.2
(2,2101)	1:24:A:ILE:HG13	1:64:A:GLY:HA3	7	0.2
(2,2093)	1:20:A:LEU:HB2	1:24:A:ILE:H	6	0.2
(2,2093)	1:20:A:LEU:HB3	1:24:A:ILE:H	6	0.2
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB2	6	0.2
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB3	6	0.2
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB2	6	0.2
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB3	6	0.2
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB2	10	0.2
(2,2073)	1:5:A:ASP:H	1:6:A:ASP:HB3	10	0.2
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	3	0.2
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	3	0.2
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	3	0.2
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	6	0.2
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	6	0.2
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	6	0.2
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	11	0.2
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	11	0.2
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	11	0.2
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD21	3	0.2
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD22	3	0.2
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD23	3	0.2
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	4	0.2
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	13	0.2
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	13	0.2
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	13	0.2
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD11	18	0.2
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD12	18	0.2
(2,1758)	1:151:A:ALA:H	1:154:A:LEU:HD13	18	0.2
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	11	0.2
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	11	0.2
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	11	0.2
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	12	0.2
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	12	0.2
(2,1724)	1:154:A:LEU:H	1:154:A:LEU:HB3	16	0.2
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	13	0.2
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	8	0.2
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	10	0.2
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	10	0.2
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	10	0.2
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	5	0.2
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	5	0.2
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	5	0.2
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD11	19	0.2
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD12	19	0.2
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD13	19	0.2
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD11	19	0.2
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD12	19	0.2
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD13	19	0.2
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD11	19	0.2
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD12	19	0.2
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD13	19	0.2
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	12	0.2
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	12	0.2
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	12	0.2
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	14	0.2
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	14	0.2
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD11	1	0.2
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD12	1	0.2
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD13	1	0.2
(2,961)	1:123:A:LYS:HA	1:126:A:MET:HB3	11	0.2
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	18	0.2
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	18	0.2
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	18	0.2
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	6	0.2
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	12	0.2
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	13	0.2
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	18	0.2
(2,854)	1:109:A:LEU:HD21	1:128:A:LEU:HA	4	0.2
(2,854)	1:109:A:LEU:HD22	1:128:A:LEU:HA	4	0.2
(2,854)	1:109:A:LEU:HD23	1:128:A:LEU:HA	4	0.2
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG21	4	0.2
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG22	4	0.2
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG23	4	0.2
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	20	0.2
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	20	0.2
(2,568)	1:49:A:LEU:HG	1:53:A:TYR:HA	14	0.2
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	10	0.2
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	10	0.2
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	10	0.2
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	10	0.2
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	10	0.2
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	10	0.2
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	1	0.2
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	1	0.2
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	1	0.2
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	1	0.2
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	1	0.2
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	1	0.2
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	1	0.2
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	1	0.2
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	1	0.2
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	18	0.2
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	18	0.2
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	18	0.2
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	18	0.2
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	18	0.2
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	18	0.2
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	18	0.2
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	18	0.2
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	18	0.2
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB2	10	0.2
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB3	10	0.2
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB2	10	0.2
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB3	10	0.2
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB2	10	0.2
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB3	10	0.2
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	5	0.2
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	5	0.2
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	5	0.2
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	7	0.2
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	7	0.2
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	7	0.2
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	12	0.2
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	12	0.2
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	17	0.2
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	17	0.2
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	17	0.2
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	17	0.2
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	4	0.2
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	7	0.2
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	10	0.2
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	11	0.2
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	14	0.2
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	16	0.2
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	17	0.2
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	20	0.2
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	3	0.2
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	19	0.2
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	16	0.2
(2,31)	1:8:A:GLN:HG2	1:9:A:ASN:HD21	10	0.2
(2,31)	1:8:A:GLN:HG3	1:9:A:ASN:HD21	10	0.2
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	12	0.2
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	14	0.2
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	19	0.2
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	7	0.2
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	8	0.2
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	17	0.2
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	2	0.2
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	6	0.2
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	18	0.2
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	9	0.2
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	6	0.2
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	3	0.2
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	5	0.2
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	10	0.2
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	16	0.2
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	18	0.2
(1,124)	1:119:A:ASP:O	1:123:A:LYS:H	7	0.2
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	1	0.2
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	11	0.2
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	6	0.2
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	13	0.2
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	15	0.2
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	20	0.2
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	1	0.2
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	7	0.2
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	9	0.2
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	11	0.2
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	6	0.2
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	10	0.2
(1,68)	1:64:A:GLY:O	1:68:A:ILE:H	6	0.2
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	11	0.2
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	13	0.2
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	16	0.2
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	4	0.2
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	5	0.2
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	9	0.2
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	20	0.2
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	3	0.2
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	8	0.2
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	15	0.2
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	2	0.2
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	4	0.2
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	11	0.2
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	10	0.2
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	18	0.2
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD11	2	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD12	2	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD13	2	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD21	2	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD22	2	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD23	2	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD11	3	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD12	3	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD13	3	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD21	3	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD22	3	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD23	3	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD11	5	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD12	5	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD13	5	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD21	5	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD22	5	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD23	5	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD11	6	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD12	6	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD13	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD21	6	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD22	6	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD23	6	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD11	8	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD12	8	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD13	8	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD21	8	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD22	8	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD23	8	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD11	11	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD12	11	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD13	11	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD21	11	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD22	11	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD23	11	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD11	15	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD12	15	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD13	15	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD21	15	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD22	15	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD23	15	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD11	17	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD12	17	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD13	17	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD21	17	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD22	17	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD23	17	0.19
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD11	12	0.19
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD12	12	0.19
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD13	12	0.19
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD21	12	0.19
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD22	12	0.19
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD23	12	0.19
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD11	18	0.19
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD12	18	0.19
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD13	18	0.19
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD21	18	0.19
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD22	18	0.19
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD23	18	0.19
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	15	0.19
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	15	0.19
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	15	0.19
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	15	0.19
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	15	0.19
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	15	0.19
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	15	0.19
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	15	0.19
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	15	0.19
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	15	0.19
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	15	0.19
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	20	0.19
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	20	0.19
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	20	0.19
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	20	0.19
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	20	0.19
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	20	0.19
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	20	0.19
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	20	0.19
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	20	0.19
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	20	0.19
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	20	0.19
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	20	0.19
(2,2198)	1:59:A:ASP:HB2	1:61:A:HIS:H	4	0.19
(2,2198)	1:59:A:ASP:HB3	1:61:A:HIS:H	4	0.19
(2,2180)	1:55:A:ARG:HD2	1:56:A:LEU:HG	7	0.19
(2,2180)	1:55:A:ARG:HD3	1:56:A:LEU:HG	7	0.19
(2,2178)	1:55:A:ARG:HG2	1:56:A:LEU:H	4	0.19
(2,2178)	1:55:A:ARG:HG3	1:56:A:LEU:H	4	0.19
(2,2178)	1:55:A:ARG:HG2	1:56:A:LEU:H	8	0.19
(2,2178)	1:55:A:ARG:HG3	1:56:A:LEU:H	8	0.19
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD11	13	0.19
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD12	13	0.19
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD13	13	0.19
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD21	13	0.19
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD22	13	0.19
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD23	13	0.19
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	1	0.19
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	1	0.19
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	1	0.19
(2,1977)	1:110:A:SER:H	1:145:A:ILE:HG21	9	0.19
(2,1977)	1:110:A:SER:H	1:145:A:ILE:HG22	9	0.19
(2,1977)	1:110:A:SER:H	1:145:A:ILE:HG23	9	0.19
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	8	0.19
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	8	0.19
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	9	0.19
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	9	0.19
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	9	0.19
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	12	0.19
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	12	0.19
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	12	0.19
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	13	0.19
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	13	0.19
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	13	0.19
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	4	0.19
(2,1931)	1:141:A:TYR:H	1:142:A:LEU:H	4	0.19
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD21	2	0.19
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD22	2	0.19
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD23	2	0.19
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD21	7	0.19
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD22	7	0.19
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD23	7	0.19
(2,1876)	1:7:A:PHE:H	1:9:A:ASN:H	10	0.19
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	20	0.19
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	1	0.19
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	1	0.19
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	1	0.19
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	6	0.19
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	6	0.19
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	6	0.19
(2,1790)	1:142:A:LEU:H	1:142:A:LEU:HG	5	0.19
(2,1790)	1:142:A:LEU:H	1:142:A:LEU:HG	9	0.19
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	13	0.19
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	13	0.19
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	13	0.19
(2,1724)	1:154:A:LEU:H	1:154:A:LEU:HB3	2	0.19
(2,1672)	1:115:A:LYS:HE2	1:116:A:SER:H	12	0.19
(2,1672)	1:115:A:LYS:HE3	1:116:A:SER:H	12	0.19
(2,1672)	1:115:A:LYS:HE2	1:116:A:SER:H	15	0.19
(2,1672)	1:115:A:LYS:HE3	1:116:A:SER:H	15	0.19
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	1	0.19
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	2	0.19
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	10	0.19
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	19	0.19
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	3	0.19
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	3	0.19
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	5	0.19
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	5	0.19
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	5	0.19
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD21	20	0.19
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD22	20	0.19
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD23	20	0.19
(2,1431)	1:63:A:LEU:HD11	1:66:A:LEU:H	19	0.19
(2,1431)	1:63:A:LEU:HD12	1:66:A:LEU:H	19	0.19
(2,1431)	1:63:A:LEU:HD13	1:66:A:LEU:H	19	0.19
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD1	7	0.19
(2,1117)	1:17:A:PHE:HB2	1:53:A:TYR:HD2	7	0.19
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	3	0.19
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	3	0.19
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	3	0.19
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	20	0.19
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	20	0.19
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	20	0.19
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	2	0.19
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	2	0.19
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	2	0.19
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	8	0.19
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	8	0.19
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	8	0.19
(2,1004)	1:149:A:CYS:HA	1:153:A:ASP:HA	13	0.19
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	9	0.19
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	9	0.19
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	18	0.19
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	18	0.19
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG21	11	0.19
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG22	11	0.19
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG23	11	0.19
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG21	11	0.19
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG22	11	0.19
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG23	11	0.19
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG21	11	0.19
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG22	11	0.19
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG23	11	0.19
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	11	0.19
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	11	0.19
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,886)	1:113:A:ILE:HD11	1:151:A:ALA:H	15	0.19
(2,886)	1:113:A:ILE:HD12	1:151:A:ALA:H	15	0.19
(2,886)	1:113:A:ILE:HD13	1:151:A:ALA:H	15	0.19
(2,854)	1:109:A:LEU:HD21	1:128:A:LEU:HA	19	0.19
(2,854)	1:109:A:LEU:HD22	1:128:A:LEU:HA	19	0.19
(2,854)	1:109:A:LEU:HD23	1:128:A:LEU:HA	19	0.19
(2,742)	1:76:A:TYR:HA	1:94:A:CYS:HA	11	0.19
(2,742)	1:76:A:TYR:HA	1:94:A:CYS:HA	18	0.19
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG21	11	0.19
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG22	11	0.19
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG23	11	0.19
(2,568)	1:49:A:LEU:HG	1:53:A:TYR:HA	1	0.19
(2,568)	1:49:A:LEU:HG	1:53:A:TYR:HA	10	0.19
(2,369)	1:17:A:PHE:HA	1:20:A:LEU:HA	10	0.19
(2,369)	1:17:A:PHE:HA	1:20:A:LEU:HA	15	0.19
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	6	0.19
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	6	0.19
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	6	0.19
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	20	0.19
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	20	0.19
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	20	0.19
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	20	0.19
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	20	0.19
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	20	0.19
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	20	0.19
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	20	0.19
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	20	0.19
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	2	0.19
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	3	0.19
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD21	5	0.19
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD22	5	0.19
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD23	5	0.19
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD21	20	0.19
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD22	20	0.19
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD23	20	0.19
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	2	0.19
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	3	0.19
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	5	0.19
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	6	0.19
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	13	0.19
(2,223)	1:44:A:SER:HB3	1:45:A:LYS:HE3	15	0.19
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	17	0.19
(2,190)	1:66:A:LEU:HD11	1:112:A:ALA:H	14	0.19
(2,190)	1:66:A:LEU:HD12	1:112:A:ALA:H	14	0.19
(2,190)	1:66:A:LEU:HD13	1:112:A:ALA:H	14	0.19
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	3	0.19
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	9	0.19
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	10	0.19
(2,106)	1:23:A:GLY:H	1:24:A:ILE:HA	6	0.19
(2,31)	1:8:A:GLN:HG2	1:9:A:ASN:HD21	18	0.19
(2,31)	1:8:A:GLN:HG3	1:9:A:ASN:HD21	18	0.19
(1,158)	2:1008:B:ASN:O	2:1011:B:THR:N	7	0.19
(1,150)	1:148:A:LYS:O	1:152:A:MET:H	20	0.19
(1,144)	1:129:A:ASP:O	1:133:A:ARG:H	11	0.19
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	2	0.19
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	4	0.19
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	13	0.19
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	6	0.19
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	10	0.19
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	15	0.19
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	16	0.19
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	5	0.19
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	14	0.19
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	15	0.19
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	16	0.19
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	8	0.19
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	17	0.19
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	13	0.19
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	8	0.19
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	5	0.19
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	8	0.19
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	12	0.19
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	14	0.19
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	17	0.19
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	18	0.19
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	1	0.19
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	4	0.19
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	9	0.19
(1,67)	1:64:A:GLY:O	1:68:A:ILE:N	4	0.19
(1,67)	1:64:A:GLY:O	1:68:A:ILE:N	20	0.19
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	4	0.19
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	6	0.19
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:51:A:ILE:O	1:55:A:ARG:N	1	0.19
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	11	0.19
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	17	0.19
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	14	0.19
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	3	0.19
(1,14)	1:13:A:THR:O	1:17:A:PHE:H	10	0.19
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	1	0.19
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	14	0.19
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	19	0.19
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	20	0.19
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD11	1	0.18
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD12	1	0.18
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD13	1	0.18
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD21	1	0.18
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD22	1	0.18
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD23	1	0.18
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD11	16	0.18
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD12	16	0.18
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD13	16	0.18
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD21	16	0.18
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD22	16	0.18
(2,2332)	1:154:A:LEU:HA	1:154:A:LEU:HD23	16	0.18
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD11	7	0.18
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD12	7	0.18
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD13	7	0.18
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD21	7	0.18
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD22	7	0.18
(2,2330)	1:153:A:ASP:H	1:154:A:LEU:HD23	7	0.18
(2,2315)	1:149:A:CYS:HB2	1:150:A:PHE:H	14	0.18
(2,2315)	1:149:A:CYS:HB3	1:150:A:PHE:H	14	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	6	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	6	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	6	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	6	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	6	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	6	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	6	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	6	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	6	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	6	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	6	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	17	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	17	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	17	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	17	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	17	0.18
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	17	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	17	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	17	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	17	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	17	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	17	0.18
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	17	0.18
(2,2178)	1:55:A:ARG:HG2	1:56:A:LEU:H	11	0.18
(2,2178)	1:55:A:ARG:HG3	1:56:A:LEU:H	11	0.18
(2,2178)	1:55:A:ARG:HG2	1:56:A:LEU:H	14	0.18
(2,2178)	1:55:A:ARG:HG3	1:56:A:LEU:H	14	0.18
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD2	3	0.18
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD3	3	0.18
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD2	17	0.18
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD3	17	0.18
(2,2101)	1:24:A:ILE:HG12	1:64:A:GLY:HA2	17	0.18
(2,2101)	1:24:A:ILE:HG12	1:64:A:GLY:HA3	17	0.18
(2,2101)	1:24:A:ILE:HG13	1:64:A:GLY:HA2	17	0.18
(2,2101)	1:24:A:ILE:HG13	1:64:A:GLY:HA3	17	0.18
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	20	0.18
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	20	0.18
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	20	0.18
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	16	0.18
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	16	0.18
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	16	0.18
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	10	0.18
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	15	0.18
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	16	0.18
(2,1858)	1:148:A:LYS:HB2	1:150:A:PHE:H	7	0.18
(2,1858)	1:148:A:LYS:HB3	1:150:A:PHE:H	7	0.18
(2,1858)	1:148:A:LYS:HB2	1:150:A:PHE:H	14	0.18
(2,1858)	1:148:A:LYS:HB3	1:150:A:PHE:H	14	0.18
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	2	0.18
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	3	0.18
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	4	0.18
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	4	0.18
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	14	0.18
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	14	0.18
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	14	0.18
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	9	0.18
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	9	0.18
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	9	0.18
(2,1730)	1:155:A:GLU:H	1:156:A:HIS:H	1	0.18
(2,1724)	1:154:A:LEU:H	1:154:A:LEU:HB3	17	0.18
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	4	0.18
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	7	0.18
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	8	0.18
(2,1629)	1:142:A:LEU:H	1:146:A:ARG:HA	2	0.18
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	7	0.18
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	7	0.18
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	8	0.18
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	8	0.18
(2,1573)	1:113:A:ILE:H	1:115:A:LYS:H	8	0.18
(2,1573)	1:113:A:ILE:H	1:115:A:LYS:H	12	0.18
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD21	12	0.18
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD22	12	0.18
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD23	12	0.18
(2,1533)	1:104:A:VAL:H	1:106:A:GLN:HG2	18	0.18
(2,1428)	1:53:A:TYR:HD1	1:65:A:SER:H	13	0.18
(2,1428)	1:53:A:TYR:HD2	1:65:A:SER:H	13	0.18
(2,1385)	1:52:A:ASP:H	1:53:A:TYR:HB2	7	0.18
(2,1216)	1:15:A:GLU:HB2	1:17:A:PHE:H	14	0.18
(2,1216)	1:15:A:GLU:HB3	1:17:A:PHE:H	14	0.18
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	2	0.18
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	2	0.18
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	2	0.18
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	6	0.18
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	6	0.18
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	6	0.18
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	9	0.18
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	9	0.18
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	9	0.18
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	19	0.18
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	19	0.18
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	19	0.18
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD11	2	0.18
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD12	2	0.18
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD13	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD11	2	0.18
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD12	2	0.18
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD13	2	0.18
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD11	2	0.18
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD12	2	0.18
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD13	2	0.18
(2,1004)	1:149:A:CYS:HA	1:153:A:ASP:HA	9	0.18
(2,1004)	1:149:A:CYS:HA	1:153:A:ASP:HA	12	0.18
(2,1004)	1:149:A:CYS:HA	1:153:A:ASP:HA	18	0.18
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG21	6	0.18
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG22	6	0.18
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG23	6	0.18
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD11	11	0.18
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD12	11	0.18
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD13	11	0.18
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	4	0.18
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG21	5	0.18
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG22	5	0.18
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG23	5	0.18
(2,716)	1:77:A:LEU:H	1:77:A:LEU:HD11	17	0.18
(2,716)	1:77:A:LEU:H	1:77:A:LEU:HD12	17	0.18
(2,716)	1:77:A:LEU:H	1:77:A:LEU:HD13	17	0.18
(2,599)	1:46:A:ILE:HG21	1:51:A:ILE:H	19	0.18
(2,599)	1:46:A:ILE:HG22	1:51:A:ILE:H	19	0.18
(2,599)	1:46:A:ILE:HG23	1:51:A:ILE:H	19	0.18
(2,397)	1:14:A:LEU:HD11	1:53:A:TYR:H	5	0.18
(2,397)	1:14:A:LEU:HD12	1:53:A:TYR:H	5	0.18
(2,397)	1:14:A:LEU:HD13	1:53:A:TYR:H	5	0.18
(2,397)	1:14:A:LEU:HD11	1:53:A:TYR:H	11	0.18
(2,397)	1:14:A:LEU:HD12	1:53:A:TYR:H	11	0.18
(2,397)	1:14:A:LEU:HD13	1:53:A:TYR:H	11	0.18
(2,369)	1:17:A:PHE:HA	1:20:A:LEU:HA	17	0.18
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	14	0.18
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	14	0.18
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	14	0.18
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	5	0.18
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	5	0.18
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	5	0.18
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	5	0.18
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	5	0.18
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	5	0.18
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	5	0.18
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	5	0.18
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	9	0.18
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	9	0.18
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	9	0.18
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	9	0.18
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	9	0.18
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	9	0.18
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	9	0.18
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	9	0.18
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	9	0.18
(2,322)	1:8:A:GLN:HA	1:11:A:VAL:HG11	18	0.18
(2,322)	1:8:A:GLN:HA	1:11:A:VAL:HG12	18	0.18
(2,322)	1:8:A:GLN:HA	1:11:A:VAL:HG13	18	0.18
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	1	0.18
(2,295)	1:6:A:ASP:HA	1:7:A:PHE:HA	4	0.18
(2,295)	1:6:A:ASP:HA	1:7:A:PHE:HA	11	0.18
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	5	0.18
(2,230)	1:55:A:ARG:H	1:108:A:LEU:HB3	3	0.18
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	5	0.18
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	13	0.18
(2,128)	1:63:A:LEU:HD11	1:123:A:LYS:HA	11	0.18
(2,128)	1:63:A:LEU:HD12	1:123:A:LYS:HA	11	0.18
(2,128)	1:63:A:LEU:HD13	1:123:A:LYS:HA	11	0.18
(2,128)	1:63:A:LEU:HD11	1:123:A:LYS:HA	15	0.18
(2,128)	1:63:A:LEU:HD12	1:123:A:LYS:HA	15	0.18
(2,128)	1:63:A:LEU:HD13	1:123:A:LYS:HA	15	0.18
(2,106)	1:23:A:GLY:H	1:24:A:ILE:HA	17	0.18
(2,27)	2:1001:B:ASP:HB2	1:21:A:LYS:HE2	4	0.18
(2,27)	2:1001:B:ASP:HB2	1:21:A:LYS:HE3	4	0.18
(2,27)	2:1001:B:ASP:HB3	1:21:A:LYS:HE2	4	0.18
(2,27)	2:1001:B:ASP:HB3	1:21:A:LYS:HE3	4	0.18
(2,15)	1:126:A:MET:HE2	2:1009:B:PRO:HG2	12	0.18
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG21	9	0.18
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG22	9	0.18
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG23	9	0.18
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG21	9	0.18
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG22	9	0.18
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG23	9	0.18
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG21	9	0.18
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG22	9	0.18
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG23	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:143:A:ASN:O	1:147:A:SER:N	6	0.18
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	5	0.18
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	7	0.18
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	2	0.18
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	3	0.18
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	11	0.18
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	1	0.18
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	12	0.18
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	13	0.18
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	17	0.18
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	18	0.18
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	2	0.18
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	19	0.18
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	2	0.18
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	10	0.18
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	15	0.18
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	18	0.18
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	4	0.18
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	12	0.18
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	11	0.18
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	13	0.18
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	14	0.18
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	15	0.18
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	17	0.18
(1,92)	1:76:A:TYR:O	1:80:A:THR:H	5	0.18
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	2	0.18
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	4	0.18
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	19	0.18
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	14	0.18
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	18	0.18
(1,68)	1:64:A:GLY:O	1:68:A:ILE:H	16	0.18
(1,67)	1:64:A:GLY:O	1:68:A:ILE:N	1	0.18
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	14	0.18
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	18	0.18
(1,65)	1:63:A:LEU:O	1:67:A:TYR:N	10	0.18
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	6	0.18
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	7	0.18
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	8	0.18
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	12	0.18
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	14	0.18
(1,18)	1:15:A:GLU:O	1:19:A:ASP:H	19	0.18
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	11	0.18
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	17	0.18
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	7	0.18
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	16	0.18
(2,2354)	1:102:A:GLY:H	1:137:A:PHE:HD1	13	0.17
(2,2354)	1:102:A:GLY:H	1:137:A:PHE:HD2	13	0.17
(2,2343)	1:102:A:GLY:H	1:137:A:PHE:HD1	13	0.17
(2,2343)	1:102:A:GLY:H	1:137:A:PHE:HD2	13	0.17
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	2	0.17
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	2	0.17
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	2	0.17
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	2	0.17
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	2	0.17
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	2	0.17
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	2	0.17
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	2	0.17
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	2	0.17
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	2	0.17
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	2	0.17
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	2	0.17
(2,2198)	1:59:A:ASP:HB2	1:61:A:HIS:H	16	0.17
(2,2198)	1:59:A:ASP:HB3	1:61:A:HIS:H	16	0.17
(2,2198)	1:59:A:ASP:HB2	1:61:A:HIS:H	20	0.17
(2,2198)	1:59:A:ASP:HB3	1:61:A:HIS:H	20	0.17
(2,2181)	1:55:A:ARG:HD2	1:108:A:LEU:HD21	18	0.17
(2,2181)	1:55:A:ARG:HD2	1:108:A:LEU:HD22	18	0.17
(2,2181)	1:55:A:ARG:HD2	1:108:A:LEU:HD23	18	0.17
(2,2181)	1:55:A:ARG:HD3	1:108:A:LEU:HD21	18	0.17
(2,2181)	1:55:A:ARG:HD3	1:108:A:LEU:HD22	18	0.17
(2,2181)	1:55:A:ARG:HD3	1:108:A:LEU:HD23	18	0.17
(2,2178)	1:55:A:ARG:HG2	1:56:A:LEU:H	6	0.17
(2,2178)	1:55:A:ARG:HG3	1:56:A:LEU:H	6	0.17
(2,2178)	1:55:A:ARG:HG2	1:56:A:LEU:H	9	0.17
(2,2178)	1:55:A:ARG:HG3	1:56:A:LEU:H	9	0.17
(2,2178)	1:55:A:ARG:HG2	1:56:A:LEU:H	16	0.17
(2,2178)	1:55:A:ARG:HG3	1:56:A:LEU:H	16	0.17
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD2	2	0.17
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD3	2	0.17
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD11	14	0.17
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD12	14	0.17
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD13	14	0.17
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD21	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD22	14	0.17
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD23	14	0.17
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	9	0.17
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	9	0.17
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	9	0.17
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	3	0.17
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	3	0.17
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	3	0.17
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	7	0.17
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	7	0.17
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	7	0.17
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	1	0.17
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	6	0.17
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD21	8	0.17
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD22	8	0.17
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD23	8	0.17
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD21	12	0.17
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD22	12	0.17
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD23	12	0.17
(2,1876)	1:7:A:PHE:H	1:9:A:ASN:H	19	0.17
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	5	0.17
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	17	0.17
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	9	0.17
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	9	0.17
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	9	0.17
(2,1790)	1:142:A:LEU:H	1:142:A:LEU:HG	3	0.17
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	4	0.17
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	4	0.17
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	4	0.17
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	16	0.17
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	16	0.17
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	16	0.17
(2,1727)	1:151:A:ALA:H	1:154:A:LEU:H	3	0.17
(2,1724)	1:154:A:LEU:H	1:154:A:LEU:HB3	10	0.17
(2,1662)	1:54:A:SER:HB2	1:66:A:LEU:H	11	0.17
(2,1662)	1:54:A:SER:HB3	1:66:A:LEU:H	11	0.17
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	5	0.17
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	18	0.17
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	20	0.17
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	2	0.17
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	2	0.17
(2,1573)	1:113:A:ILE:H	1:115:A:LYS:H	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1573)	1:113:A:ILE:H	1:115:A:LYS:H	17	0.17
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	15	0.17
(2,1533)	1:104:A:VAL:H	1:106:A:GLN:HG2	6	0.17
(2,1385)	1:52:A:ASP:H	1:53:A:TYR:HB2	2	0.17
(2,1060)	1:62:A:LYS:HG2	1:115:A:LYS:HE2	13	0.17
(2,1060)	1:62:A:LYS:HG2	1:115:A:LYS:HE3	13	0.17
(2,1060)	1:62:A:LYS:HG3	1:115:A:LYS:HE2	13	0.17
(2,1060)	1:62:A:LYS:HG3	1:115:A:LYS:HE3	13	0.17
(2,1060)	1:62:A:LYS:HG2	1:115:A:LYS:HE2	18	0.17
(2,1060)	1:62:A:LYS:HG2	1:115:A:LYS:HE3	18	0.17
(2,1060)	1:62:A:LYS:HG3	1:115:A:LYS:HE2	18	0.17
(2,1060)	1:62:A:LYS:HG3	1:115:A:LYS:HE3	18	0.17
(2,1054)	1:24:A:ILE:HD11	1:63:A:LEU:HD21	3	0.17
(2,1054)	1:24:A:ILE:HD11	1:63:A:LEU:HD22	3	0.17
(2,1054)	1:24:A:ILE:HD11	1:63:A:LEU:HD23	3	0.17
(2,1054)	1:24:A:ILE:HD12	1:63:A:LEU:HD21	3	0.17
(2,1054)	1:24:A:ILE:HD12	1:63:A:LEU:HD22	3	0.17
(2,1054)	1:24:A:ILE:HD12	1:63:A:LEU:HD23	3	0.17
(2,1054)	1:24:A:ILE:HD13	1:63:A:LEU:HD21	3	0.17
(2,1054)	1:24:A:ILE:HD13	1:63:A:LEU:HD22	3	0.17
(2,1054)	1:24:A:ILE:HD13	1:63:A:LEU:HD23	3	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	2	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	2	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	2	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	8	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	8	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	8	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	12	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	12	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	12	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	14	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	14	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	14	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	15	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	15	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	15	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	16	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	16	0.17
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	16	0.17
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	14	0.17
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	14	0.17
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	20	0.17
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	20	0.17
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	20	0.17
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	6	0.17
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	6	0.17
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	10	0.17
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	10	0.17
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	13	0.17
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	13	0.17
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG21	13	0.17
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG22	13	0.17
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG23	13	0.17
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG21	13	0.17
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG22	13	0.17
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG23	13	0.17
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG21	13	0.17
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG22	13	0.17
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG23	13	0.17
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	1	0.17
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	1	0.17
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	1	0.17
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	5	0.17
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	5	0.17
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	5	0.17
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	9	0.17
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	9	0.17
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	9	0.17
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	13	0.17
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	13	0.17
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	13	0.17
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	19	0.17
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	19	0.17
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	19	0.17
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	15	0.17
(2,875)	1:113:A:ILE:HB	1:114:A:ALA:HB1	5	0.17
(2,875)	1:113:A:ILE:HB	1:114:A:ALA:HB2	5	0.17
(2,875)	1:113:A:ILE:HB	1:114:A:ALA:HB3	5	0.17
(2,865)	1:112:A:ALA:HA	1:115:A:LYS:HB3	15	0.17
(2,854)	1:109:A:LEU:HD21	1:128:A:LEU:HA	7	0.17
(2,854)	1:109:A:LEU:HD22	1:128:A:LEU:HA	7	0.17
(2,854)	1:109:A:LEU:HD23	1:128:A:LEU:HA	7	0.17
(2,854)	1:109:A:LEU:HD21	1:128:A:LEU:HA	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,854)	1:109:A:LEU:HD22	1:128:A:LEU:HA	11	0.17
(2,854)	1:109:A:LEU:HD23	1:128:A:LEU:HA	11	0.17
(2,854)	1:109:A:LEU:HD21	1:128:A:LEU:HA	20	0.17
(2,854)	1:109:A:LEU:HD22	1:128:A:LEU:HA	20	0.17
(2,854)	1:109:A:LEU:HD23	1:128:A:LEU:HA	20	0.17
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG21	9	0.17
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG22	9	0.17
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG23	9	0.17
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG21	13	0.17
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG22	13	0.17
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG23	13	0.17
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG21	18	0.17
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG22	18	0.17
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG23	18	0.17
(2,568)	1:49:A:LEU:HG	1:53:A:TYR:HA	16	0.17
(2,397)	1:14:A:LEU:HD11	1:53:A:TYR:H	13	0.17
(2,397)	1:14:A:LEU:HD12	1:53:A:TYR:H	13	0.17
(2,397)	1:14:A:LEU:HD13	1:53:A:TYR:H	13	0.17
(2,381)	1:24:A:ILE:H	1:24:A:ILE:HD11	14	0.17
(2,381)	1:24:A:ILE:H	1:24:A:ILE:HD12	14	0.17
(2,381)	1:24:A:ILE:H	1:24:A:ILE:HD13	14	0.17
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	5	0.17
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	5	0.17
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	5	0.17
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	5	0.17
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	5	0.17
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	5	0.17
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	2	0.17
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	2	0.17
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	2	0.17
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	2	0.17
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	2	0.17
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	2	0.17
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	2	0.17
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	2	0.17
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	2	0.17
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	6	0.17
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	6	0.17
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	6	0.17
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	6	0.17
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	6	0.17
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	6	0.17
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	6	0.17
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	6	0.17
(2,322)	1:8:A:GLN:HA	1:11:A:VAL:HG11	10	0.17
(2,322)	1:8:A:GLN:HA	1:11:A:VAL:HG12	10	0.17
(2,322)	1:8:A:GLN:HA	1:11:A:VAL:HG13	10	0.17
(2,322)	1:8:A:GLN:HA	1:11:A:VAL:HG11	19	0.17
(2,322)	1:8:A:GLN:HA	1:11:A:VAL:HG12	19	0.17
(2,322)	1:8:A:GLN:HA	1:11:A:VAL:HG13	19	0.17
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	2	0.17
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	4	0.17
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	6	0.17
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	6	0.17
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	6	0.17
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB1	18	0.17
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB2	18	0.17
(2,276)	1:125:A:ARG:HB2	1:151:A:ALA:HB3	18	0.17
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	10	0.17
(2,231)	1:109:A:LEU:HD11	1:144:A:ALA:HB1	20	0.17
(2,231)	1:109:A:LEU:HD11	1:144:A:ALA:HB2	20	0.17
(2,231)	1:109:A:LEU:HD11	1:144:A:ALA:HB3	20	0.17
(2,231)	1:109:A:LEU:HD12	1:144:A:ALA:HB1	20	0.17
(2,231)	1:109:A:LEU:HD12	1:144:A:ALA:HB2	20	0.17
(2,231)	1:109:A:LEU:HD12	1:144:A:ALA:HB3	20	0.17
(2,231)	1:109:A:LEU:HD13	1:144:A:ALA:HB1	20	0.17
(2,231)	1:109:A:LEU:HD13	1:144:A:ALA:HB2	20	0.17
(2,231)	1:109:A:LEU:HD13	1:144:A:ALA:HB3	20	0.17
(2,230)	1:55:A:ARG:H	1:108:A:LEU:HB3	5	0.17
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	7	0.17
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	10	0.17
(2,197)	1:153:A:ASP:HA	1:155:A:GLU:HB2	12	0.17
(2,197)	1:153:A:ASP:HA	1:155:A:GLU:HB3	12	0.17
(2,190)	1:66:A:LEU:HD11	1:112:A:ALA:H	7	0.17
(2,190)	1:66:A:LEU:HD12	1:112:A:ALA:H	7	0.17
(2,190)	1:66:A:LEU:HD13	1:112:A:ALA:H	7	0.17
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG2	1	0.17
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG3	1	0.17
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG2	8	0.17
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG3	8	0.17
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	7	0.17
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	14	0.17
(2,31)	1:8:A:GLN:HG2	1:9:A:ASN:HD21	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,31)	1:8:A:GLN:HG3	1:9:A:ASN:HD21	19	0.17
(1,150)	1:148:A:LYS:O	1:152:A:MET:H	15	0.17
(1,143)	1:129:A:ASP:O	1:133:A:ARG:N	11	0.17
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	1	0.17
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	8	0.17
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	10	0.17
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	9	0.17
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	18	0.17
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	20	0.17
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	12	0.17
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	7	0.17
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	7	0.17
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	20	0.17
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	16	0.17
(1,129)	1:122:A:GLU:O	1:126:A:MET:N	6	0.17
(1,126)	1:120:A:HIS:O	1:124:A:ILE:H	7	0.17
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	4	0.17
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	9	0.17
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	4	0.17
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	6	0.17
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	18	0.17
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	9	0.17
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	18	0.17
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	8	0.17
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	20	0.17
(1,92)	1:76:A:TYR:O	1:80:A:THR:H	17	0.17
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	16	0.17
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	20	0.17
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	1	0.17
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	3	0.17
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	6	0.17
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	5	0.17
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	10	0.17
(1,68)	1:64:A:GLY:O	1:68:A:ILE:H	13	0.17
(1,65)	1:63:A:LEU:O	1:67:A:TYR:N	5	0.17
(1,63)	1:62:A:LYS:O	1:66:A:LEU:N	3	0.17
(1,63)	1:62:A:LYS:O	1:66:A:LEU:N	8	0.17
(1,63)	1:62:A:LYS:O	1:66:A:LEU:N	15	0.17
(1,63)	1:62:A:LYS:O	1:66:A:LEU:N	17	0.17
(1,52)	1:50:A:ILE:O	1:54:A:SER:H	14	0.17
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	3	0.17
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:28:A:ARG:O	1:32:A:LEU:H	2	0.17
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	15	0.17
(1,15)	1:14:A:LEU:O	1:18:A:LYS:N	19	0.17
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	2	0.17
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	7	0.17
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	9	0.17
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	4	0.17
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	3	0.16
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	3	0.16
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	3	0.16
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	3	0.16
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	3	0.16
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	3	0.16
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	3	0.16
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	3	0.16
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	3	0.16
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	3	0.16
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	3	0.16
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	3	0.16
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	18	0.16
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	18	0.16
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	18	0.16
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	18	0.16
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	18	0.16
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	18	0.16
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	18	0.16
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	18	0.16
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	18	0.16
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	18	0.16
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	18	0.16
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	18	0.16
(2,2267)	1:110:A:SER:HA	1:154:A:LEU:HD11	10	0.16
(2,2267)	1:110:A:SER:HA	1:154:A:LEU:HD12	10	0.16
(2,2267)	1:110:A:SER:HA	1:154:A:LEU:HD13	10	0.16
(2,2267)	1:110:A:SER:HA	1:154:A:LEU:HD21	10	0.16
(2,2267)	1:110:A:SER:HA	1:154:A:LEU:HD22	10	0.16
(2,2267)	1:110:A:SER:HA	1:154:A:LEU:HD23	10	0.16
(2,2206)	1:62:A:LYS:HD2	1:111:A:ASP:HB2	17	0.16
(2,2206)	1:62:A:LYS:HD2	1:111:A:ASP:HB3	17	0.16
(2,2206)	1:62:A:LYS:HD3	1:111:A:ASP:HB2	17	0.16
(2,2206)	1:62:A:LYS:HD3	1:111:A:ASP:HB3	17	0.16
(2,2198)	1:59:A:ASP:HB2	1:61:A:HIS:H	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2198)	1:59:A:ASP:HB3	1:61:A:HIS:H	18	0.16
(2,2180)	1:55:A:ARG:HD2	1:56:A:LEU:HG	5	0.16
(2,2180)	1:55:A:ARG:HD3	1:56:A:LEU:HG	5	0.16
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD11	15	0.16
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD12	15	0.16
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD13	15	0.16
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD21	15	0.16
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD22	15	0.16
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD23	15	0.16
(2,2092)	1:20:A:LEU:HB2	1:23:A:GLY:H	17	0.16
(2,2092)	1:20:A:LEU:HB3	1:23:A:GLY:H	17	0.16
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB2	4	0.16
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB3	4	0.16
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB2	4	0.16
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB3	4	0.16
(2,2009)	1:35:A:TYR:HD1	1:38:A:ASP:H	4	0.16
(2,2009)	1:35:A:TYR:HD2	1:38:A:ASP:H	4	0.16
(2,2009)	1:35:A:TYR:HD1	1:38:A:ASP:H	18	0.16
(2,2009)	1:35:A:TYR:HD2	1:38:A:ASP:H	18	0.16
(2,1934)	1:147:A:SER:H	1:150:A:PHE:H	13	0.16
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD21	15	0.16
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD22	15	0.16
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD23	15	0.16
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	10	0.16
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	11	0.16
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	12	0.16
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	2	0.16
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	2	0.16
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	2	0.16
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	19	0.16
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	19	0.16
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	19	0.16
(2,1782)	1:69:A:ILE:HG21	1:74:A:ARG:H	16	0.16
(2,1782)	1:69:A:ILE:HG22	1:74:A:ARG:H	16	0.16
(2,1782)	1:69:A:ILE:HG23	1:74:A:ARG:H	16	0.16
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	18	0.16
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	18	0.16
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	18	0.16
(2,1724)	1:154:A:LEU:H	1:154:A:LEU:HB3	3	0.16
(2,1724)	1:154:A:LEU:H	1:154:A:LEU:HB3	6	0.16
(2,1724)	1:154:A:LEU:H	1:154:A:LEU:HB3	11	0.16
(2,1724)	1:154:A:LEU:H	1:154:A:LEU:HB3	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	16	0.16
(2,1629)	1:142:A:LEU:H	1:146:A:ARG:HA	8	0.16
(2,1629)	1:142:A:LEU:H	1:146:A:ARG:HA	14	0.16
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	9	0.16
(2,1533)	1:104:A:VAL:H	1:106:A:GLN:HG2	1	0.16
(2,1533)	1:104:A:VAL:H	1:106:A:GLN:HG2	4	0.16
(2,1533)	1:104:A:VAL:H	1:106:A:GLN:HG2	14	0.16
(2,1533)	1:104:A:VAL:H	1:106:A:GLN:HG2	16	0.16
(2,1533)	1:104:A:VAL:H	1:106:A:GLN:HG2	19	0.16
(2,1431)	1:63:A:LEU:HD11	1:66:A:LEU:H	2	0.16
(2,1431)	1:63:A:LEU:HD12	1:66:A:LEU:H	2	0.16
(2,1431)	1:63:A:LEU:HD13	1:66:A:LEU:H	2	0.16
(2,1385)	1:52:A:ASP:H	1:53:A:TYR:HB2	15	0.16
(2,1242)	1:20:A:LEU:H	1:23:A:GLY:H	14	0.16
(2,1216)	1:15:A:GLU:HB2	1:17:A:PHE:H	10	0.16
(2,1216)	1:15:A:GLU:HB3	1:17:A:PHE:H	10	0.16
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD11	17	0.16
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD12	17	0.16
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD13	17	0.16
(2,1063)	1:105:A:ILE:HG12	1:109:A:LEU:HG	20	0.16
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG12	15	0.16
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG13	15	0.16
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG12	15	0.16
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG13	15	0.16
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG12	15	0.16
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG13	15	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	1	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	1	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	1	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	4	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	4	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	4	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	10	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	10	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	10	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	11	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	11	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	11	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	17	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	17	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	17	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	18	0.16
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	18	0.16
(2,1004)	1:149:A:CYS:HA	1:153:A:ASP:HA	5	0.16
(2,982)	1:128:A:LEU:HD11	1:145:A:ILE:HB	9	0.16
(2,982)	1:128:A:LEU:HD12	1:145:A:ILE:HB	9	0.16
(2,982)	1:128:A:LEU:HD13	1:145:A:ILE:HB	9	0.16
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD11	3	0.16
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD12	3	0.16
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD13	3	0.16
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	7	0.16
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	7	0.16
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	7	0.16
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	14	0.16
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	14	0.16
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	14	0.16
(2,854)	1:109:A:LEU:HD21	1:128:A:LEU:HA	2	0.16
(2,854)	1:109:A:LEU:HD22	1:128:A:LEU:HA	2	0.16
(2,854)	1:109:A:LEU:HD23	1:128:A:LEU:HA	2	0.16
(2,854)	1:109:A:LEU:HD21	1:128:A:LEU:HA	17	0.16
(2,854)	1:109:A:LEU:HD22	1:128:A:LEU:HA	17	0.16
(2,854)	1:109:A:LEU:HD23	1:128:A:LEU:HA	17	0.16
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	1	0.16
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	1	0.16
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	1	0.16
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	5	0.16
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	5	0.16
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	5	0.16
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	15	0.16
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	15	0.16
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	15	0.16
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	17	0.16
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	17	0.16
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	17	0.16
(2,506)	1:40:A:ILE:HA	1:43:A:GLU:HG2	5	0.16
(2,506)	1:40:A:ILE:HA	1:43:A:GLU:HG3	5	0.16
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	5	0.16
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	5	0.16
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	5	0.16
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	9	0.16
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	9	0.16
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	9	0.16
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	10	0.16
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	10	0.16
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	11	0.16
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	11	0.16
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	11	0.16
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	18	0.16
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	18	0.16
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	18	0.16
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	20	0.16
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	20	0.16
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	20	0.16
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	8	0.16
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	8	0.16
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	8	0.16
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	8	0.16
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	8	0.16
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	8	0.16
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	12	0.16
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	12	0.16
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	12	0.16
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	12	0.16
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	12	0.16
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	12	0.16
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	7	0.16
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	7	0.16
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	7	0.16
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	7	0.16
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	7	0.16
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	7	0.16
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	7	0.16
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	7	0.16
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	7	0.16
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	16	0.16
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	16	0.16
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	16	0.16
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	16	0.16
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	16	0.16
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	16	0.16
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	16	0.16
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	16	0.16
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	16	0.16
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD21	7	0.16
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD22	7	0.16
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD23	7	0.16
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD21	12	0.16
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD22	12	0.16
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD23	12	0.16
(2,230)	1:55:A:ARG:H	1:108:A:LEU:HB3	7	0.16
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	4	0.16
(2,190)	1:66:A:LEU:HD11	1:112:A:ALA:H	18	0.16
(2,190)	1:66:A:LEU:HD12	1:112:A:ALA:H	18	0.16
(2,190)	1:66:A:LEU:HD13	1:112:A:ALA:H	18	0.16
(2,169)	1:26:A:GLY:HA2	1:28:A:ARG:HB2	3	0.16
(2,169)	1:26:A:GLY:HA2	1:28:A:ARG:HB2	18	0.16
(2,167)	1:63:A:LEU:HD11	1:67:A:TYR:HB2	7	0.16
(2,167)	1:63:A:LEU:HD12	1:67:A:TYR:HB2	7	0.16
(2,167)	1:63:A:LEU:HD13	1:67:A:TYR:HB2	7	0.16
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG2	17	0.16
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG3	17	0.16
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	4	0.16
(2,128)	1:63:A:LEU:HD11	1:123:A:LYS:HA	9	0.16
(2,128)	1:63:A:LEU:HD12	1:123:A:LYS:HA	9	0.16
(2,128)	1:63:A:LEU:HD13	1:123:A:LYS:HA	9	0.16
(2,105)	1:15:A:GLU:HB2	1:16:A:SER:HB2	11	0.16
(2,105)	1:15:A:GLU:HB3	1:16:A:SER:HB2	11	0.16
(2,15)	1:126:A:MET:HE3	2:1009:B:PRO:HD2	20	0.16
(1,157)	2:1008:B:ASN:OD1	2:1010:B:TYR:N	7	0.16
(1,150)	1:148:A:LYS:O	1:152:A:MET:H	1	0.16
(1,150)	1:148:A:LYS:O	1:152:A:MET:H	12	0.16
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	17	0.16
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	14	0.16
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	14	0.16
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	18	0.16
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	8	0.16
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	15	0.16
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	17	0.16
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	4	0.16
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	8	0.16
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	6	0.16
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	18	0.16
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	2	0.16
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	1	0.16
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	17	0.16
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	9	0.16
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	16	0.16
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	19	0.16
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	7	0.16
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	19	0.16
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	6	0.16
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	5	0.16
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	9	0.16
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	18	0.16
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	11	0.16
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	13	0.16
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	19	0.16
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	6	0.16
(1,67)	1:64:A:GLY:O	1:68:A:ILE:N	6	0.16
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	1	0.16
(1,65)	1:63:A:LEU:O	1:67:A:TYR:N	11	0.16
(1,65)	1:63:A:LEU:O	1:67:A:TYR:N	16	0.16
(1,63)	1:62:A:LYS:O	1:66:A:LEU:N	5	0.16
(1,44)	1:46:A:ILE:O	1:50:A:ILE:H	13	0.16
(1,24)	1:28:A:ARG:O	1:32:A:LEU:H	12	0.16
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	12	0.16
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	16	0.16
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	20	0.16
(1,14)	1:13:A:THR:O	1:17:A:PHE:H	7	0.16
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	6	0.16
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	13	0.16
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	11	0.16
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	20	0.16
(2,2198)	1:59:A:ASP:HB2	1:61:A:HIS:H	6	0.15
(2,2198)	1:59:A:ASP:HB3	1:61:A:HIS:H	6	0.15
(2,2198)	1:59:A:ASP:HB2	1:61:A:HIS:H	10	0.15
(2,2198)	1:59:A:ASP:HB3	1:61:A:HIS:H	10	0.15
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD2	12	0.15
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD3	12	0.15
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD2	18	0.15
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD3	18	0.15
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD11	5	0.15
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD12	5	0.15
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD13	5	0.15
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD21	5	0.15
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD22	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2113)	1:34:A:THR:HB	1:37:A:LEU:HD23	5	0.15
(2,2100)	1:24:A:ILE:HB	1:64:A:GLY:HA2	17	0.15
(2,2100)	1:24:A:ILE:HB	1:64:A:GLY:HA3	17	0.15
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB2	9	0.15
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB3	9	0.15
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB2	9	0.15
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB3	9	0.15
(2,2009)	1:35:A:TYR:HD1	1:38:A:ASP:H	15	0.15
(2,2009)	1:35:A:TYR:HD2	1:38:A:ASP:H	15	0.15
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	6	0.15
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	6	0.15
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	6	0.15
(2,1942)	1:74:A:ARG:HD2	1:75:A:ALA:H	1	0.15
(2,1942)	1:74:A:ARG:HD3	1:75:A:ALA:H	1	0.15
(2,1906)	1:23:A:GLY:H	1:24:A:ILE:HG12	14	0.15
(2,1906)	1:23:A:GLY:H	1:24:A:ILE:HG13	14	0.15
(2,1876)	1:7:A:PHE:H	1:9:A:ASN:H	18	0.15
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	16	0.15
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	10	0.15
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	10	0.15
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	10	0.15
(2,1760)	1:37:A:LEU:HA	1:40:A:ILE:H	4	0.15
(2,1760)	1:37:A:LEU:HA	1:40:A:ILE:H	15	0.15
(2,1730)	1:155:A:GLU:H	1:156:A:HIS:H	20	0.15
(2,1727)	1:151:A:ALA:H	1:154:A:LEU:H	8	0.15
(2,1727)	1:151:A:ALA:H	1:154:A:LEU:H	16	0.15
(2,1724)	1:154:A:LEU:H	1:154:A:LEU:HB3	8	0.15
(2,1662)	1:54:A:SER:HB2	1:66:A:LEU:H	12	0.15
(2,1662)	1:54:A:SER:HB3	1:66:A:LEU:H	12	0.15
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	3	0.15
(2,1630)	1:151:A:ALA:H	1:153:A:ASP:H	9	0.15
(2,1629)	1:142:A:LEU:H	1:146:A:ARG:HA	6	0.15
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	3	0.15
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	3	0.15
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	13	0.15
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	13	0.15
(2,1573)	1:113:A:ILE:H	1:115:A:LYS:H	11	0.15
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD21	11	0.15
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD22	11	0.15
(2,1559)	1:109:A:LEU:H	1:109:A:LEU:HD23	11	0.15
(2,1431)	1:63:A:LEU:HD11	1:66:A:LEU:H	8	0.15
(2,1431)	1:63:A:LEU:HD12	1:66:A:LEU:H	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1431)	1:63:A:LEU:HD13	1:66:A:LEU:H	8	0.15
(2,1431)	1:63:A:LEU:HD11	1:66:A:LEU:H	12	0.15
(2,1431)	1:63:A:LEU:HD12	1:66:A:LEU:H	12	0.15
(2,1431)	1:63:A:LEU:HD13	1:66:A:LEU:H	12	0.15
(2,1428)	1:53:A:TYR:HD1	1:65:A:SER:H	7	0.15
(2,1428)	1:53:A:TYR:HD2	1:65:A:SER:H	7	0.15
(2,1418)	1:58:A:PRO:HA	1:62:A:LYS:H	11	0.15
(2,1411)	1:59:A:ASP:H	1:61:A:HIS:H	1	0.15
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	2	0.15
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	3	0.15
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	5	0.15
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	10	0.15
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	19	0.15
(2,1216)	1:15:A:GLU:HB2	1:17:A:PHE:H	1	0.15
(2,1216)	1:15:A:GLU:HB3	1:17:A:PHE:H	1	0.15
(2,1216)	1:15:A:GLU:HB2	1:17:A:PHE:H	6	0.15
(2,1216)	1:15:A:GLU:HB3	1:17:A:PHE:H	6	0.15
(2,1216)	1:15:A:GLU:HB2	1:17:A:PHE:H	12	0.15
(2,1216)	1:15:A:GLU:HB3	1:17:A:PHE:H	12	0.15
(2,1158)	1:5:A:ASP:HA	1:9:A:ASN:H	19	0.15
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD11	2	0.15
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD12	2	0.15
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD13	2	0.15
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD11	5	0.15
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD12	5	0.15
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD13	5	0.15
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD11	18	0.15
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD12	18	0.15
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD13	18	0.15
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	7	0.15
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	7	0.15
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	7	0.15
(2,1019)	1:105:A:ILE:HD11	1:108:A:LEU:HB3	11	0.15
(2,1019)	1:105:A:ILE:HD12	1:108:A:LEU:HB3	11	0.15
(2,1019)	1:105:A:ILE:HD13	1:108:A:LEU:HB3	11	0.15
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD11	14	0.15
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD12	14	0.15
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD13	14	0.15
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD11	14	0.15
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD12	14	0.15
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD13	14	0.15
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD11	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD12	14	0.15
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD13	14	0.15
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	6	0.15
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	6	0.15
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	6	0.15
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	9	0.15
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	9	0.15
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	9	0.15
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	11	0.15
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	11	0.15
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	11	0.15
(2,994)	1:125:A:ARG:HA	1:151:A:ALA:HB1	9	0.15
(2,994)	1:125:A:ARG:HA	1:151:A:ALA:HB2	9	0.15
(2,994)	1:125:A:ARG:HA	1:151:A:ALA:HB3	9	0.15
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD11	7	0.15
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD12	7	0.15
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD13	7	0.15
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD11	9	0.15
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD12	9	0.15
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD13	9	0.15
(2,962)	1:126:A:MET:HB3	1:126:A:MET:HE1	19	0.15
(2,962)	1:126:A:MET:HB3	1:126:A:MET:HE2	19	0.15
(2,962)	1:126:A:MET:HB3	1:126:A:MET:HE3	19	0.15
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	8	0.15
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	8	0.15
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	8	0.15
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	14	0.15
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	16	0.15
(2,876)	1:62:A:LYS:HD2	1:115:A:LYS:HA	18	0.15
(2,876)	1:62:A:LYS:HD3	1:115:A:LYS:HA	18	0.15
(2,643)	1:65:A:SER:HA	1:67:A:TYR:HB2	15	0.15
(2,599)	1:46:A:ILE:HG21	1:51:A:ILE:H	10	0.15
(2,599)	1:46:A:ILE:HG22	1:51:A:ILE:H	10	0.15
(2,599)	1:46:A:ILE:HG23	1:51:A:ILE:H	10	0.15
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	6	0.15
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	6	0.15
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	6	0.15
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	8	0.15
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	8	0.15
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	8	0.15
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	9	0.15
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	9	0.15
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	10	0.15
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	10	0.15
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	10	0.15
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	1	0.15
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	1	0.15
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	1	0.15
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	9	0.15
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	9	0.15
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	9	0.15
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	9	0.15
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	9	0.15
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	9	0.15
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	3	0.15
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	3	0.15
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	3	0.15
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	3	0.15
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	3	0.15
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	3	0.15
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	3	0.15
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	3	0.15
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	3	0.15
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	19	0.15
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	19	0.15
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	19	0.15
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	19	0.15
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	19	0.15
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	19	0.15
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	19	0.15
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	19	0.15
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	19	0.15
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB2	6	0.15
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB3	6	0.15
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB2	6	0.15
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB3	6	0.15
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB2	6	0.15
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB3	6	0.15
(2,301)	1:11:A:VAL:HG21	1:49:A:LEU:HB2	14	0.15
(2,301)	1:11:A:VAL:HG22	1:49:A:LEU:HB2	14	0.15
(2,301)	1:11:A:VAL:HG23	1:49:A:LEU:HB2	14	0.15
(2,298)	1:11:A:VAL:HG21	1:15:A:GLU:H	14	0.15
(2,298)	1:11:A:VAL:HG22	1:15:A:GLU:H	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,298)	1:11:A:VAL:HG23	1:15:A:GLU:H	14	0.15
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	11	0.15
(2,274)	1:112:A:ALA:HA	1:115:A:LYS:HE2	18	0.15
(2,274)	1:112:A:ALA:HA	1:115:A:LYS:HE3	18	0.15
(2,230)	1:55:A:ARG:H	1:108:A:LEU:HB3	8	0.15
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	5	0.15
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	13	0.15
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	16	0.15
(2,167)	1:63:A:LEU:HD11	1:67:A:TYR:HB2	15	0.15
(2,167)	1:63:A:LEU:HD12	1:67:A:TYR:HB2	15	0.15
(2,167)	1:63:A:LEU:HD13	1:67:A:TYR:HB2	15	0.15
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG2	2	0.15
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG3	2	0.15
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG2	7	0.15
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG3	7	0.15
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG2	10	0.15
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG3	10	0.15
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	8	0.15
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	12	0.15
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	17	0.15
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	20	0.15
(2,128)	1:63:A:LEU:HD11	1:123:A:LYS:HA	12	0.15
(2,128)	1:63:A:LEU:HD12	1:123:A:LYS:HA	12	0.15
(2,128)	1:63:A:LEU:HD13	1:123:A:LYS:HA	12	0.15
(2,128)	1:63:A:LEU:HD11	1:123:A:LYS:HA	17	0.15
(2,128)	1:63:A:LEU:HD12	1:123:A:LYS:HA	17	0.15
(2,128)	1:63:A:LEU:HD13	1:123:A:LYS:HA	17	0.15
(2,17)	2:1010:B:TYR:HA	1:74:A:ARG:HE	5	0.15
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG21	6	0.15
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG22	6	0.15
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG23	6	0.15
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG21	6	0.15
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG22	6	0.15
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG23	6	0.15
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG21	6	0.15
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG22	6	0.15
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG23	6	0.15
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	12	0.15
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	2	0.15
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	4	0.15
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	5	0.15
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	19	0.15
(1,140)	1:127:A:LEU:O	1:131:A:TRP:H	4	0.15
(1,140)	1:127:A:LEU:O	1:131:A:TRP:H	19	0.15
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	6	0.15
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	13	0.15
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	2	0.15
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	10	0.15
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	11	0.15
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	2	0.15
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	5	0.15
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	14	0.15
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	15	0.15
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	8	0.15
(1,129)	1:122:A:GLU:O	1:126:A:MET:N	18	0.15
(1,128)	1:121:A:LYS:O	1:125:A:ARG:H	9	0.15
(1,128)	1:121:A:LYS:O	1:125:A:ARG:H	10	0.15
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	3	0.15
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	5	0.15
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	14	0.15
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	12	0.15
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	14	0.15
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	17	0.15
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	20	0.15
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	6	0.15
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	3	0.15
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	9	0.15
(1,92)	1:76:A:TYR:O	1:80:A:THR:H	12	0.15
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	1	0.15
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	4	0.15
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	14	0.15
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	16	0.15
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	18	0.15
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	4	0.15
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	5	0.15
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	14	0.15
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	15	0.15
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	2	0.15
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	17	0.15
(1,65)	1:63:A:LEU:O	1:67:A:TYR:N	13	0.15
(1,65)	1:63:A:LEU:O	1:67:A:TYR:N	14	0.15
(1,65)	1:63:A:LEU:O	1:67:A:TYR:N	20	0.15
(1,63)	1:62:A:LYS:O	1:66:A:LEU:N	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:50:A:ILE:O	1:54:A:SER:H	1	0.15
(1,52)	1:50:A:ILE:O	1:54:A:SER:H	6	0.15
(1,52)	1:50:A:ILE:O	1:54:A:SER:H	9	0.15
(1,24)	1:28:A:ARG:O	1:32:A:LEU:H	19	0.15
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	3	0.15
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	7	0.15
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	8	0.15
(1,14)	1:13:A:THR:O	1:17:A:PHE:H	1	0.15
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	3	0.15
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	5	0.15
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	12	0.15
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	15	0.15
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	1	0.15
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	16	0.15
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	19	0.15
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG2	1	0.14
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG3	1	0.14
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG2	2	0.14
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG3	2	0.14
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG2	8	0.14
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG3	8	0.14
(2,2206)	1:62:A:LYS:HD2	1:111:A:ASP:HB2	12	0.14
(2,2206)	1:62:A:LYS:HD2	1:111:A:ASP:HB3	12	0.14
(2,2206)	1:62:A:LYS:HD3	1:111:A:ASP:HB2	12	0.14
(2,2206)	1:62:A:LYS:HD3	1:111:A:ASP:HB3	12	0.14
(2,2181)	1:55:A:ARG:HD2	1:108:A:LEU:HD21	12	0.14
(2,2181)	1:55:A:ARG:HD2	1:108:A:LEU:HD22	12	0.14
(2,2181)	1:55:A:ARG:HD2	1:108:A:LEU:HD23	12	0.14
(2,2181)	1:55:A:ARG:HD3	1:108:A:LEU:HD21	12	0.14
(2,2181)	1:55:A:ARG:HD3	1:108:A:LEU:HD22	12	0.14
(2,2181)	1:55:A:ARG:HD3	1:108:A:LEU:HD23	12	0.14
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD2	7	0.14
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD3	7	0.14
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD2	15	0.14
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD3	15	0.14
(2,2092)	1:20:A:LEU:HB2	1:23:A:GLY:H	6	0.14
(2,2092)	1:20:A:LEU:HB3	1:23:A:GLY:H	6	0.14
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB2	14	0.14
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB3	14	0.14
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB2	14	0.14
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB3	14	0.14
(2,2010)	1:122:A:GLU:H	1:123:A:LYS:H	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2009)	1:35:A:TYR:HD1	1:38:A:ASP:H	10	0.14
(2,2009)	1:35:A:TYR:HD2	1:38:A:ASP:H	10	0.14
(2,2009)	1:35:A:TYR:HD1	1:38:A:ASP:H	11	0.14
(2,2009)	1:35:A:TYR:HD2	1:38:A:ASP:H	11	0.14
(2,2009)	1:35:A:TYR:HD1	1:38:A:ASP:H	17	0.14
(2,2009)	1:35:A:TYR:HD2	1:38:A:ASP:H	17	0.14
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	2	0.14
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	2	0.14
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	2	0.14
(2,1942)	1:74:A:ARG:HD2	1:75:A:ALA:H	5	0.14
(2,1942)	1:74:A:ARG:HD3	1:75:A:ALA:H	5	0.14
(2,1942)	1:74:A:ARG:HD2	1:75:A:ALA:H	19	0.14
(2,1942)	1:74:A:ARG:HD3	1:75:A:ALA:H	19	0.14
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD21	9	0.14
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD22	9	0.14
(2,1928)	1:54:A:SER:H	1:108:A:LEU:HD23	9	0.14
(2,1927)	1:50:A:ILE:HA	1:53:A:TYR:H	13	0.14
(2,1858)	1:148:A:LYS:HB2	1:150:A:PHE:H	10	0.14
(2,1858)	1:148:A:LYS:HB3	1:150:A:PHE:H	10	0.14
(2,1858)	1:148:A:LYS:HB2	1:150:A:PHE:H	11	0.14
(2,1858)	1:148:A:LYS:HB3	1:150:A:PHE:H	11	0.14
(2,1840)	1:38:A:ASP:HA	1:40:A:ILE:H	5	0.14
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	8	0.14
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	8	0.14
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	8	0.14
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	17	0.14
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	17	0.14
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	17	0.14
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	20	0.14
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	20	0.14
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	20	0.14
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD11	8	0.14
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD12	8	0.14
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD13	8	0.14
(2,1760)	1:37:A:LEU:HA	1:40:A:ILE:H	13	0.14
(2,1760)	1:37:A:LEU:HA	1:40:A:ILE:H	14	0.14
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	7	0.14
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	7	0.14
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	7	0.14
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	20	0.14
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	20	0.14
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1727)	1:151:A:ALA:H	1:154:A:LEU:H	6	0.14
(2,1724)	1:154:A:LEU:H	1:154:A:LEU:HB3	14	0.14
(2,1681)	1:129:A:ASP:H	1:130:A:ILE:HD11	3	0.14
(2,1681)	1:129:A:ASP:H	1:130:A:ILE:HD12	3	0.14
(2,1681)	1:129:A:ASP:H	1:130:A:ILE:HD13	3	0.14
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	17	0.14
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	19	0.14
(2,1629)	1:142:A:LEU:H	1:146:A:ARG:HA	11	0.14
(2,1629)	1:142:A:LEU:H	1:146:A:ARG:HA	18	0.14
(2,1629)	1:142:A:LEU:H	1:146:A:ARG:HA	19	0.14
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	14	0.14
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	14	0.14
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	18	0.14
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	18	0.14
(2,1573)	1:113:A:ILE:H	1:115:A:LYS:H	3	0.14
(2,1564)	1:110:A:SER:H	1:113:A:ILE:HG13	18	0.14
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD21	7	0.14
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD22	7	0.14
(2,1552)	1:151:A:ALA:H	1:154:A:LEU:HD23	7	0.14
(2,1431)	1:63:A:LEU:HD11	1:66:A:LEU:H	7	0.14
(2,1431)	1:63:A:LEU:HD12	1:66:A:LEU:H	7	0.14
(2,1431)	1:63:A:LEU:HD13	1:66:A:LEU:H	7	0.14
(2,1428)	1:53:A:TYR:HD1	1:65:A:SER:H	11	0.14
(2,1428)	1:53:A:TYR:HD2	1:65:A:SER:H	11	0.14
(2,1411)	1:59:A:ASP:H	1:61:A:HIS:H	10	0.14
(2,1385)	1:52:A:ASP:H	1:53:A:TYR:HB2	17	0.14
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	1	0.14
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	4	0.14
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	6	0.14
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	12	0.14
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	13	0.14
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	14	0.14
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	16	0.14
(2,1216)	1:15:A:GLU:HB2	1:17:A:PHE:H	7	0.14
(2,1216)	1:15:A:GLU:HB3	1:17:A:PHE:H	7	0.14
(2,1216)	1:15:A:GLU:HB2	1:17:A:PHE:H	18	0.14
(2,1216)	1:15:A:GLU:HB3	1:17:A:PHE:H	18	0.14
(2,1216)	1:15:A:GLU:HB2	1:17:A:PHE:H	20	0.14
(2,1216)	1:15:A:GLU:HB3	1:17:A:PHE:H	20	0.14
(2,1158)	1:5:A:ASP:HA	1:9:A:ASN:H	18	0.14
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	20	0.14
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	20	0.14
(2,1019)	1:105:A:ILE:HD11	1:108:A:LEU:HB3	20	0.14
(2,1019)	1:105:A:ILE:HD12	1:108:A:LEU:HB3	20	0.14
(2,1019)	1:105:A:ILE:HD13	1:108:A:LEU:HB3	20	0.14
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	3	0.14
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	3	0.14
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	3	0.14
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	4	0.14
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	4	0.14
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	4	0.14
(2,1002)	1:154:A:LEU:H	1:154:A:LEU:HB2	11	0.14
(2,1002)	1:154:A:LEU:H	1:154:A:LEU:HB2	14	0.14
(2,1002)	1:154:A:LEU:H	1:154:A:LEU:HB2	15	0.14
(2,999)	1:152:A:MET:HA	1:152:A:MET:HG3	20	0.14
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG21	1	0.14
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG22	1	0.14
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG23	1	0.14
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG21	16	0.14
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG22	16	0.14
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG23	16	0.14
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	4	0.14
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	4	0.14
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	16	0.14
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	16	0.14
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD11	2	0.14
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD12	2	0.14
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD13	2	0.14
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	3	0.14
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	3	0.14
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	3	0.14
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	4	0.14
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	4	0.14
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	4	0.14
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	9	0.14
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	11	0.14
(2,869)	1:113:A:ILE:HB	1:151:A:ALA:HB1	20	0.14
(2,869)	1:113:A:ILE:HB	1:151:A:ALA:HB2	20	0.14
(2,869)	1:113:A:ILE:HB	1:151:A:ALA:HB3	20	0.14
(2,744)	1:93:A:THR:HG21	1:94:A:CYS:HA	7	0.14
(2,744)	1:93:A:THR:HG22	1:94:A:CYS:HA	7	0.14
(2,744)	1:93:A:THR:HG23	1:94:A:CYS:HA	7	0.14
(2,742)	1:76:A:TYR:HA	1:94:A:CYS:HA	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG21	17	0.14
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG22	17	0.14
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG23	17	0.14
(2,599)	1:46:A:ILE:HG21	1:51:A:ILE:H	2	0.14
(2,599)	1:46:A:ILE:HG22	1:51:A:ILE:H	2	0.14
(2,599)	1:46:A:ILE:HG23	1:51:A:ILE:H	2	0.14
(2,599)	1:46:A:ILE:HG21	1:51:A:ILE:H	5	0.14
(2,599)	1:46:A:ILE:HG22	1:51:A:ILE:H	5	0.14
(2,599)	1:46:A:ILE:HG23	1:51:A:ILE:H	5	0.14
(2,599)	1:46:A:ILE:HG21	1:51:A:ILE:H	15	0.14
(2,599)	1:46:A:ILE:HG22	1:51:A:ILE:H	15	0.14
(2,599)	1:46:A:ILE:HG23	1:51:A:ILE:H	15	0.14
(2,599)	1:46:A:ILE:HG21	1:51:A:ILE:H	16	0.14
(2,599)	1:46:A:ILE:HG22	1:51:A:ILE:H	16	0.14
(2,599)	1:46:A:ILE:HG23	1:51:A:ILE:H	16	0.14
(2,599)	1:46:A:ILE:HG21	1:51:A:ILE:H	17	0.14
(2,599)	1:46:A:ILE:HG22	1:51:A:ILE:H	17	0.14
(2,599)	1:46:A:ILE:HG23	1:51:A:ILE:H	17	0.14
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	3	0.14
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	3	0.14
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	3	0.14
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	11	0.14
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	11	0.14
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	11	0.14
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	12	0.14
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	12	0.14
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	12	0.14
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	4	0.14
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	4	0.14
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	4	0.14
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	7	0.14
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	7	0.14
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	7	0.14
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	13	0.14
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	13	0.14
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	13	0.14
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	13	0.14
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	13	0.14
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	13	0.14
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	20	0.14
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	20	0.14
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	20	0.14
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	20	0.14
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	20	0.14
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	11	0.14
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	11	0.14
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	11	0.14
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	11	0.14
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	11	0.14
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	11	0.14
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	11	0.14
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	11	0.14
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	11	0.14
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	15	0.14
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	15	0.14
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	15	0.14
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	15	0.14
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	15	0.14
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	15	0.14
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	15	0.14
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	15	0.14
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	15	0.14
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	17	0.14
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	17	0.14
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	17	0.14
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	17	0.14
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	17	0.14
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	17	0.14
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	17	0.14
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	17	0.14
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	17	0.14
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB2	14	0.14
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB3	14	0.14
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB2	14	0.14
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB3	14	0.14
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB2	14	0.14
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB3	14	0.14
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	5	0.14
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	8	0.14
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	11	0.14
(2,301)	1:11:A:VAL:HG21	1:49:A:LEU:HB2	6	0.14
(2,301)	1:11:A:VAL:HG22	1:49:A:LEU:HB2	6	0.14
(2,301)	1:11:A:VAL:HG23	1:49:A:LEU:HB2	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,301)	1:11:A:VAL:HG21	1:49:A:LEU:HB2	10	0.14
(2,301)	1:11:A:VAL:HG22	1:49:A:LEU:HB2	10	0.14
(2,301)	1:11:A:VAL:HG23	1:49:A:LEU:HB2	10	0.14
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD21	10	0.14
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD22	10	0.14
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD23	10	0.14
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD21	14	0.14
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD22	14	0.14
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD23	14	0.14
(2,252)	1:153:A:ASP:HB3	1:154:A:LEU:HB3	5	0.14
(2,252)	1:153:A:ASP:HB3	1:154:A:LEU:HB3	7	0.14
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	9	0.14
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	11	0.14
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	18	0.14
(2,190)	1:66:A:LEU:HD11	1:112:A:ALA:H	17	0.14
(2,190)	1:66:A:LEU:HD12	1:112:A:ALA:H	17	0.14
(2,190)	1:66:A:LEU:HD13	1:112:A:ALA:H	17	0.14
(2,15)	1:126:A:MET:HE2	2:1009:B:PRO:HG2	18	0.14
(1,158)	2:1008:B:ASN:O	2:1011:B:THR:N	3	0.14
(1,158)	2:1008:B:ASN:O	2:1011:B:THR:N	19	0.14
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	11	0.14
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	1	0.14
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	7	0.14
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	10	0.14
(1,140)	1:127:A:LEU:O	1:131:A:TRP:H	15	0.14
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	1	0.14
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	4	0.14
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	3	0.14
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	12	0.14
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	13	0.14
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	17	0.14
(1,132)	1:123:A:LYS:O	1:127:A:LEU:H	19	0.14
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	1	0.14
(1,129)	1:122:A:GLU:O	1:126:A:MET:N	16	0.14
(1,128)	1:121:A:LYS:O	1:125:A:ARG:H	18	0.14
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	8	0.14
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	3	0.14
(1,112)	1:107:A:GLU:O	1:111:A:ASP:H	5	0.14
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	8	0.14
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	17	0.14
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	4	0.14
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	12	0.14
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	19	0.14
(1,92)	1:76:A:TYR:O	1:80:A:THR:H	14	0.14
(1,92)	1:76:A:TYR:O	1:80:A:THR:H	19	0.14
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	15	0.14
(1,76)	1:68:A:ILE:O	1:72:A:ILE:H	10	0.14
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	16	0.14
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	12	0.14
(1,67)	1:64:A:GLY:O	1:68:A:ILE:N	16	0.14
(1,65)	1:63:A:LEU:O	1:67:A:TYR:N	4	0.14
(1,65)	1:63:A:LEU:O	1:67:A:TYR:N	18	0.14
(1,52)	1:50:A:ILE:O	1:54:A:SER:H	10	0.14
(1,52)	1:50:A:ILE:O	1:54:A:SER:H	18	0.14
(1,43)	1:46:A:ILE:O	1:50:A:ILE:N	10	0.14
(1,34)	1:33:A:THR:O	1:37:A:LEU:H	16	0.14
(1,24)	1:28:A:ARG:O	1:32:A:LEU:H	18	0.14
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	1	0.14
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	15	0.14
(1,14)	1:13:A:THR:O	1:17:A:PHE:H	12	0.14
(1,14)	1:13:A:THR:O	1:17:A:PHE:H	20	0.14
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	17	0.14
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	2	0.14
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	14	0.14
(3,7)	2:1004:B:GLU:HB2	1:30:A:LYS:HE2	7	0.13
(3,7)	2:1004:B:GLU:HB2	1:30:A:LYS:HE3	7	0.13
(3,7)	2:1004:B:GLU:HB3	1:30:A:LYS:HE2	7	0.13
(3,7)	2:1004:B:GLU:HB3	1:30:A:LYS:HE3	7	0.13
(2,2352)	1:105:A:ILE:HD11	1:137:A:PHE:HD1	13	0.13
(2,2352)	1:105:A:ILE:HD11	1:137:A:PHE:HD2	13	0.13
(2,2352)	1:105:A:ILE:HD12	1:137:A:PHE:HD1	13	0.13
(2,2352)	1:105:A:ILE:HD12	1:137:A:PHE:HD2	13	0.13
(2,2352)	1:105:A:ILE:HD13	1:137:A:PHE:HD1	13	0.13
(2,2352)	1:105:A:ILE:HD13	1:137:A:PHE:HD2	13	0.13
(2,2341)	1:105:A:ILE:HD11	1:137:A:PHE:HD1	13	0.13
(2,2341)	1:105:A:ILE:HD11	1:137:A:PHE:HD2	13	0.13
(2,2341)	1:105:A:ILE:HD12	1:137:A:PHE:HD1	13	0.13
(2,2341)	1:105:A:ILE:HD12	1:137:A:PHE:HD2	13	0.13
(2,2341)	1:105:A:ILE:HD13	1:137:A:PHE:HD1	13	0.13
(2,2341)	1:105:A:ILE:HD13	1:137:A:PHE:HD2	13	0.13
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG2	7	0.13
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG3	7	0.13
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG2	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG3	19	0.13
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	8	0.13
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	8	0.13
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	8	0.13
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	8	0.13
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	8	0.13
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	8	0.13
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	8	0.13
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	8	0.13
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	8	0.13
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	8	0.13
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	8	0.13
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	8	0.13
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	9	0.13
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	9	0.13
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	9	0.13
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	9	0.13
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	9	0.13
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	9	0.13
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	9	0.13
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	9	0.13
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	9	0.13
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	9	0.13
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	9	0.13
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	9	0.13
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB2	17	0.13
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB3	17	0.13
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB2	17	0.13
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB3	17	0.13
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD2	13	0.13
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD3	13	0.13
(2,2009)	1:35:A:TYR:HD1	1:38:A:ASP:H	5	0.13
(2,2009)	1:35:A:TYR:HD2	1:38:A:ASP:H	5	0.13
(2,2000)	1:113:A:ILE:HD11	1:125:A:ARG:H	10	0.13
(2,2000)	1:113:A:ILE:HD12	1:125:A:ARG:H	10	0.13
(2,2000)	1:113:A:ILE:HD13	1:125:A:ARG:H	10	0.13
(2,1966)	1:70:A:ASP:H	1:127:A:LEU:HD21	20	0.13
(2,1966)	1:70:A:ASP:H	1:127:A:LEU:HD22	20	0.13
(2,1966)	1:70:A:ASP:H	1:127:A:LEU:HD23	20	0.13
(2,1959)	1:109:A:LEU:HD21	1:145:A:ILE:H	5	0.13
(2,1959)	1:109:A:LEU:HD22	1:145:A:ILE:H	5	0.13
(2,1959)	1:109:A:LEU:HD23	1:145:A:ILE:H	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1942)	1:74:A:ARG:HD2	1:75:A:ALA:H	7	0.13
(2,1942)	1:74:A:ARG:HD3	1:75:A:ALA:H	7	0.13
(2,1942)	1:74:A:ARG:HD2	1:75:A:ALA:H	11	0.13
(2,1942)	1:74:A:ARG:HD3	1:75:A:ALA:H	11	0.13
(2,1942)	1:74:A:ARG:HD2	1:75:A:ALA:H	12	0.13
(2,1942)	1:74:A:ARG:HD3	1:75:A:ALA:H	12	0.13
(2,1942)	1:74:A:ARG:HD2	1:75:A:ALA:H	20	0.13
(2,1942)	1:74:A:ARG:HD3	1:75:A:ALA:H	20	0.13
(2,1927)	1:50:A:ILE:HA	1:53:A:TYR:H	5	0.13
(2,1895)	1:67:A:TYR:H	1:70:A:ASP:HB2	2	0.13
(2,1895)	1:67:A:TYR:H	1:70:A:ASP:HB2	8	0.13
(2,1865)	1:106:A:GLN:H	1:144:A:ALA:HA	10	0.13
(2,1858)	1:148:A:LYS:HB2	1:150:A:PHE:H	20	0.13
(2,1858)	1:148:A:LYS:HB3	1:150:A:PHE:H	20	0.13
(2,1840)	1:38:A:ASP:HA	1:40:A:ILE:H	1	0.13
(2,1840)	1:38:A:ASP:HA	1:40:A:ILE:H	13	0.13
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	7	0.13
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	7	0.13
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	7	0.13
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	11	0.13
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	11	0.13
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	11	0.13
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	15	0.13
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	15	0.13
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	15	0.13
(2,1774)	1:39:A:HIS:HB2	1:41:A:ASP:H	5	0.13
(2,1774)	1:39:A:HIS:HB2	1:41:A:ASP:H	7	0.13
(2,1774)	1:39:A:HIS:HB2	1:41:A:ASP:H	12	0.13
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	1	0.13
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	1	0.13
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	1	0.13
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	6	0.13
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	6	0.13
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	6	0.13
(2,1727)	1:151:A:ALA:H	1:154:A:LEU:H	11	0.13
(2,1727)	1:151:A:ALA:H	1:154:A:LEU:H	14	0.13
(2,1629)	1:142:A:LEU:H	1:146:A:ARG:HA	4	0.13
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	9	0.13
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	9	0.13
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	10	0.13
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	10	0.13
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	11	0.13
(2,1541)	1:105:A:ILE:H	1:106:A:GLN:HB3	2	0.13
(2,1533)	1:104:A:VAL:H	1:106:A:GLN:HG2	17	0.13
(2,1533)	1:104:A:VAL:H	1:106:A:GLN:HG2	20	0.13
(2,1454)	1:77:A:LEU:HG	1:78:A:ASP:H	17	0.13
(2,1431)	1:63:A:LEU:HD11	1:66:A:LEU:H	17	0.13
(2,1431)	1:63:A:LEU:HD12	1:66:A:LEU:H	17	0.13
(2,1431)	1:63:A:LEU:HD13	1:66:A:LEU:H	17	0.13
(2,1411)	1:59:A:ASP:H	1:61:A:HIS:H	4	0.13
(2,1411)	1:59:A:ASP:H	1:61:A:HIS:H	20	0.13
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	7	0.13
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	11	0.13
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	15	0.13
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	17	0.13
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	20	0.13
(2,1216)	1:15:A:GLU:HB2	1:17:A:PHE:H	8	0.13
(2,1216)	1:15:A:GLU:HB3	1:17:A:PHE:H	8	0.13
(2,1216)	1:15:A:GLU:HB2	1:17:A:PHE:H	16	0.13
(2,1216)	1:15:A:GLU:HB3	1:17:A:PHE:H	16	0.13
(2,1157)	1:9:A:ASN:H	1:35:A:TYR:HE1	10	0.13
(2,1157)	1:9:A:ASN:H	1:35:A:TYR:HE2	10	0.13
(2,1153)	1:14:A:LEU:HG	1:15:A:GLU:H	11	0.13
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	3	0.13
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	3	0.13
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	3	0.13
(2,1114)	1:113:A:ILE:HD11	1:150:A:PHE:HA	6	0.13
(2,1114)	1:113:A:ILE:HD12	1:150:A:PHE:HA	6	0.13
(2,1114)	1:113:A:ILE:HD13	1:150:A:PHE:HA	6	0.13
(2,1105)	1:138:A:GLN:HA	1:139:A:LYS:HA	4	0.13
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD11	7	0.13
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD12	7	0.13
(2,1091)	1:24:A:ILE:HB	1:24:A:ILE:HD13	7	0.13
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG12	10	0.13
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG13	10	0.13
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG12	10	0.13
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG13	10	0.13
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG12	10	0.13
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG13	10	0.13
(2,1042)	1:63:A:LEU:HA	1:124:A:ILE:HG12	8	0.13
(2,1042)	1:63:A:LEU:HA	1:124:A:ILE:HG13	8	0.13
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD11	20	0.13
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD12	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD13	20	0.13
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD11	20	0.13
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD12	20	0.13
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD13	20	0.13
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD11	20	0.13
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD12	20	0.13
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD13	20	0.13
(2,1002)	1:154:A:LEU:H	1:154:A:LEU:HB2	2	0.13
(2,1002)	1:154:A:LEU:H	1:154:A:LEU:HB2	3	0.13
(2,1002)	1:154:A:LEU:H	1:154:A:LEU:HB2	5	0.13
(2,1002)	1:154:A:LEU:H	1:154:A:LEU:HB2	6	0.13
(2,1002)	1:154:A:LEU:H	1:154:A:LEU:HB2	8	0.13
(2,1002)	1:154:A:LEU:H	1:154:A:LEU:HB2	10	0.13
(2,1002)	1:154:A:LEU:H	1:154:A:LEU:HB2	16	0.13
(2,1002)	1:154:A:LEU:H	1:154:A:LEU:HB2	17	0.13
(2,942)	1:66:A:LEU:HD11	1:109:A:LEU:HD21	14	0.13
(2,942)	1:66:A:LEU:HD11	1:109:A:LEU:HD22	14	0.13
(2,942)	1:66:A:LEU:HD11	1:109:A:LEU:HD23	14	0.13
(2,942)	1:66:A:LEU:HD12	1:109:A:LEU:HD21	14	0.13
(2,942)	1:66:A:LEU:HD12	1:109:A:LEU:HD22	14	0.13
(2,942)	1:66:A:LEU:HD12	1:109:A:LEU:HD23	14	0.13
(2,942)	1:66:A:LEU:HD13	1:109:A:LEU:HD21	14	0.13
(2,942)	1:66:A:LEU:HD13	1:109:A:LEU:HD22	14	0.13
(2,942)	1:66:A:LEU:HD13	1:109:A:LEU:HD23	14	0.13
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG21	7	0.13
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG22	7	0.13
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG23	7	0.13
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG21	7	0.13
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG22	7	0.13
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG23	7	0.13
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG21	7	0.13
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG22	7	0.13
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG23	7	0.13
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	15	0.13
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	15	0.13
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	15	0.13
(2,933)	1:124:A:ILE:HG21	1:128:A:LEU:HD11	14	0.13
(2,933)	1:124:A:ILE:HG21	1:128:A:LEU:HD12	14	0.13
(2,933)	1:124:A:ILE:HG21	1:128:A:LEU:HD13	14	0.13
(2,933)	1:124:A:ILE:HG22	1:128:A:LEU:HD11	14	0.13
(2,933)	1:124:A:ILE:HG22	1:128:A:LEU:HD12	14	0.13
(2,933)	1:124:A:ILE:HG22	1:128:A:LEU:HD13	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,933)	1:124:A:ILE:HG23	1:128:A:LEU:HD11	14	0.13
(2,933)	1:124:A:ILE:HG23	1:128:A:LEU:HD12	14	0.13
(2,933)	1:124:A:ILE:HG23	1:128:A:LEU:HD13	14	0.13
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	3	0.13
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	8	0.13
(2,886)	1:113:A:ILE:HD11	1:151:A:ALA:H	3	0.13
(2,886)	1:113:A:ILE:HD12	1:151:A:ALA:H	3	0.13
(2,886)	1:113:A:ILE:HD13	1:151:A:ALA:H	3	0.13
(2,854)	1:109:A:LEU:HD21	1:128:A:LEU:HA	15	0.13
(2,854)	1:109:A:LEU:HD22	1:128:A:LEU:HA	15	0.13
(2,854)	1:109:A:LEU:HD23	1:128:A:LEU:HA	15	0.13
(2,807)	1:104:A:VAL:HA	1:107:A:GLU:HB3	20	0.13
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG21	15	0.13
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG22	15	0.13
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG23	15	0.13
(2,716)	1:77:A:LEU:H	1:77:A:LEU:HD11	7	0.13
(2,716)	1:77:A:LEU:H	1:77:A:LEU:HD12	7	0.13
(2,716)	1:77:A:LEU:H	1:77:A:LEU:HD13	7	0.13
(2,599)	1:46:A:ILE:HG21	1:51:A:ILE:H	3	0.13
(2,599)	1:46:A:ILE:HG22	1:51:A:ILE:H	3	0.13
(2,599)	1:46:A:ILE:HG23	1:51:A:ILE:H	3	0.13
(2,599)	1:46:A:ILE:HG21	1:51:A:ILE:H	11	0.13
(2,599)	1:46:A:ILE:HG22	1:51:A:ILE:H	11	0.13
(2,599)	1:46:A:ILE:HG23	1:51:A:ILE:H	11	0.13
(2,599)	1:46:A:ILE:HG21	1:51:A:ILE:H	18	0.13
(2,599)	1:46:A:ILE:HG22	1:51:A:ILE:H	18	0.13
(2,599)	1:46:A:ILE:HG23	1:51:A:ILE:H	18	0.13
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	2	0.13
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	2	0.13
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	2	0.13
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	13	0.13
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	13	0.13
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	13	0.13
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	16	0.13
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	16	0.13
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	16	0.13
(2,506)	1:40:A:ILE:HA	1:43:A:GLU:HG2	18	0.13
(2,506)	1:40:A:ILE:HA	1:43:A:GLU:HG3	18	0.13
(2,397)	1:14:A:LEU:HD11	1:53:A:TYR:H	16	0.13
(2,397)	1:14:A:LEU:HD12	1:53:A:TYR:H	16	0.13
(2,397)	1:14:A:LEU:HD13	1:53:A:TYR:H	16	0.13
(2,387)	1:24:A:ILE:HD11	1:64:A:GLY:HA3	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,387)	1:24:A:ILE:HD12	1:64:A:GLY:HA3	6	0.13
(2,387)	1:24:A:ILE:HD13	1:64:A:GLY:HA3	6	0.13
(2,378)	1:20:A:LEU:HD11	1:25:A:SER:HA	10	0.13
(2,378)	1:20:A:LEU:HD12	1:25:A:SER:HA	10	0.13
(2,378)	1:20:A:LEU:HD13	1:25:A:SER:HA	10	0.13
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	2	0.13
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	2	0.13
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	2	0.13
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	3	0.13
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	3	0.13
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	3	0.13
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	8	0.13
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	8	0.13
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	8	0.13
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	12	0.13
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	12	0.13
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	12	0.13
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	13	0.13
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	13	0.13
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	13	0.13
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	16	0.13
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	16	0.13
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	16	0.13
(2,334)	1:11:A:VAL:HA	1:14:A:LEU:HA	14	0.13
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	3	0.13
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	3	0.13
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	3	0.13
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	3	0.13
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	3	0.13
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	3	0.13
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	6	0.13
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	6	0.13
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	6	0.13
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	6	0.13
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	6	0.13
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	6	0.13
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	7	0.13
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	7	0.13
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	7	0.13
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	7	0.13
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	7	0.13
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	16	0.13
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	16	0.13
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	16	0.13
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	16	0.13
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	16	0.13
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	16	0.13
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	17	0.13
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	17	0.13
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	17	0.13
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	17	0.13
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	17	0.13
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	17	0.13
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	8	0.13
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	8	0.13
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	8	0.13
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	8	0.13
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	8	0.13
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	8	0.13
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	8	0.13
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	8	0.13
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	8	0.13
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	12	0.13
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	12	0.13
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	12	0.13
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	12	0.13
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	12	0.13
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	12	0.13
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	12	0.13
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	12	0.13
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	12	0.13
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	13	0.13
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	14	0.13
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	16	0.13
(2,283)	1:53:A:TYR:HD1	1:56:A:LEU:HD11	7	0.13
(2,283)	1:53:A:TYR:HD1	1:56:A:LEU:HD12	7	0.13
(2,283)	1:53:A:TYR:HD1	1:56:A:LEU:HD13	7	0.13
(2,283)	1:53:A:TYR:HD2	1:56:A:LEU:HD11	7	0.13
(2,283)	1:53:A:TYR:HD2	1:56:A:LEU:HD12	7	0.13
(2,283)	1:53:A:TYR:HD2	1:56:A:LEU:HD13	7	0.13
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD21	4	0.13
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD22	4	0.13
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD23	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD21	16	0.13
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD22	16	0.13
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD23	16	0.13
(2,230)	1:55:A:ARG:H	1:108:A:LEU:HB3	2	0.13
(2,230)	1:55:A:ARG:H	1:108:A:LEU:HB3	14	0.13
(2,230)	1:55:A:ARG:H	1:108:A:LEU:HB3	19	0.13
(2,227)	1:116:A:SER:H	1:120:A:HIS:HB2	10	0.13
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	20	0.13
(2,203)	1:99:A:ASN:HB2	1:100:A:THR:H	4	0.13
(2,203)	1:99:A:ASN:HB2	1:100:A:THR:H	5	0.13
(2,203)	1:99:A:ASN:HB2	1:100:A:THR:H	12	0.13
(2,203)	1:99:A:ASN:HB2	1:100:A:THR:H	20	0.13
(2,167)	1:63:A:LEU:HD11	1:67:A:TYR:HB2	8	0.13
(2,167)	1:63:A:LEU:HD12	1:67:A:TYR:HB2	8	0.13
(2,167)	1:63:A:LEU:HD13	1:67:A:TYR:HB2	8	0.13
(2,166)	1:69:A:ILE:HB	1:108:A:LEU:HD11	10	0.13
(2,166)	1:69:A:ILE:HB	1:108:A:LEU:HD12	10	0.13
(2,166)	1:69:A:ILE:HB	1:108:A:LEU:HD13	10	0.13
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG2	3	0.13
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG3	3	0.13
(2,128)	1:63:A:LEU:HD11	1:123:A:LYS:HA	16	0.13
(2,128)	1:63:A:LEU:HD12	1:123:A:LYS:HA	16	0.13
(2,128)	1:63:A:LEU:HD13	1:123:A:LYS:HA	16	0.13
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG21	20	0.13
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG22	20	0.13
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG23	20	0.13
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG21	20	0.13
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG22	20	0.13
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG23	20	0.13
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG21	20	0.13
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG22	20	0.13
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG23	20	0.13
(1,155)	2:1007:B:TYR:OH	1:74:A:ARG:NH2	13	0.13
(1,154)	2:1009:B:PRO:HA	1:74:A:ARG:NH2	8	0.13
(1,153)	2:1009:B:PRO:O	1:74:A:ARG:HE	16	0.13
(1,150)	1:148:A:LYS:O	1:152:A:MET:H	16	0.13
(1,150)	1:148:A:LYS:O	1:152:A:MET:H	18	0.13
(1,149)	1:148:A:LYS:O	1:152:A:MET:N	1	0.13
(1,144)	1:129:A:ASP:O	1:133:A:ARG:H	7	0.13
(1,144)	1:129:A:ASP:O	1:133:A:ARG:H	16	0.13
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	8	0.13
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	12	0.13
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	18	0.13
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	1	0.13
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	7	0.13
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	20	0.13
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	7	0.13
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	10	0.13
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	14	0.13
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	15	0.13
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	17	0.13
(1,129)	1:122:A:GLU:O	1:126:A:MET:N	2	0.13
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	8	0.13
(1,112)	1:107:A:GLU:O	1:111:A:ASP:H	11	0.13
(1,112)	1:107:A:GLU:O	1:111:A:ASP:H	19	0.13
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	10	0.13
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	3	0.13
(1,92)	1:76:A:TYR:O	1:80:A:THR:H	2	0.13
(1,92)	1:76:A:TYR:O	1:80:A:THR:H	3	0.13
(1,88)	1:74:A:ARG:O	1:78:A:ASP:H	16	0.13
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	6	0.13
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	19	0.13
(1,81)	1:71:A:SER:O	1:75:A:ALA:N	1	0.13
(1,81)	1:71:A:SER:O	1:75:A:ALA:N	4	0.13
(1,81)	1:71:A:SER:O	1:75:A:ALA:N	5	0.13
(1,81)	1:71:A:SER:O	1:75:A:ALA:N	14	0.13
(1,81)	1:71:A:SER:O	1:75:A:ALA:N	18	0.13
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	17	0.13
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	20	0.13
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	3	0.13
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	15	0.13
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	5	0.13
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	11	0.13
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	19	0.13
(1,68)	1:64:A:GLY:O	1:68:A:ILE:H	9	0.13
(1,68)	1:64:A:GLY:O	1:68:A:ILE:H	18	0.13
(1,65)	1:63:A:LEU:O	1:67:A:TYR:N	6	0.13
(1,43)	1:46:A:ILE:O	1:50:A:ILE:N	18	0.13
(1,34)	1:33:A:THR:O	1:37:A:LEU:H	14	0.13
(1,24)	1:28:A:ARG:O	1:32:A:LEU:H	1	0.13
(1,24)	1:28:A:ARG:O	1:32:A:LEU:H	10	0.13
(1,24)	1:28:A:ARG:O	1:32:A:LEU:H	11	0.13
(1,24)	1:28:A:ARG:O	1:32:A:LEU:H	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:28:A:ARG:O	1:32:A:LEU:N	2	0.13
(1,22)	1:27:A:SER:O	1:31:A:LYS:H	6	0.13
(1,22)	1:27:A:SER:O	1:31:A:LYS:H	13	0.13
(1,20)	1:26:A:GLY:O	1:30:A:LYS:H	14	0.13
(1,14)	1:13:A:THR:O	1:17:A:PHE:H	16	0.13
(1,14)	1:13:A:THR:O	1:17:A:PHE:H	18	0.13
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	7	0.13
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	9	0.13
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	13	0.13
(3,7)	2:1004:B:GLU:HB2	1:30:A:LYS:HE2	14	0.12
(3,7)	2:1004:B:GLU:HB2	1:30:A:LYS:HE3	14	0.12
(3,7)	2:1004:B:GLU:HB3	1:30:A:LYS:HE2	14	0.12
(3,7)	2:1004:B:GLU:HB3	1:30:A:LYS:HE3	14	0.12
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD11	19	0.12
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD12	19	0.12
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD13	19	0.12
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD21	19	0.12
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD22	19	0.12
(2,2320)	1:151:A:ALA:H	1:154:A:LEU:HD23	19	0.12
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG2	5	0.12
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG3	5	0.12
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG2	10	0.12
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG3	10	0.12
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB2	7	0.12
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB3	7	0.12
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB2	7	0.12
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB3	7	0.12
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD2	5	0.12
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD3	5	0.12
(2,2100)	1:24:A:ILE:HB	1:64:A:GLY:HA2	5	0.12
(2,2100)	1:24:A:ILE:HB	1:64:A:GLY:HA3	5	0.12
(2,2094)	1:20:A:LEU:HG	1:23:A:GLY:HA2	13	0.12
(2,2094)	1:20:A:LEU:HG	1:23:A:GLY:HA3	13	0.12
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB2	3	0.12
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB3	3	0.12
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB2	3	0.12
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB3	3	0.12
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB2	7	0.12
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB3	7	0.12
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB2	7	0.12
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB3	7	0.12
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB2	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB3	11	0.12
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB2	11	0.12
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB3	11	0.12
(2,2018)	1:132:A:ASP:H	1:134:A:SER:H	11	0.12
(2,2010)	1:122:A:GLU:H	1:123:A:LYS:H	12	0.12
(2,2010)	1:122:A:GLU:H	1:123:A:LYS:H	15	0.12
(2,2009)	1:35:A:TYR:HD1	1:38:A:ASP:H	2	0.12
(2,2009)	1:35:A:TYR:HD2	1:38:A:ASP:H	2	0.12
(2,2001)	1:157:A:HIS:HB2	1:158:A:HIS:H	12	0.12
(2,2001)	1:157:A:HIS:HB3	1:158:A:HIS:H	12	0.12
(2,1942)	1:74:A:ARG:HD2	1:75:A:ALA:H	17	0.12
(2,1942)	1:74:A:ARG:HD3	1:75:A:ALA:H	17	0.12
(2,1927)	1:50:A:ILE:HA	1:53:A:TYR:H	12	0.12
(2,1895)	1:67:A:TYR:H	1:70:A:ASP:HB2	5	0.12
(2,1895)	1:67:A:TYR:H	1:70:A:ASP:HB2	9	0.12
(2,1895)	1:67:A:TYR:H	1:70:A:ASP:HB2	20	0.12
(2,1858)	1:148:A:LYS:HB2	1:150:A:PHE:H	19	0.12
(2,1858)	1:148:A:LYS:HB3	1:150:A:PHE:H	19	0.12
(2,1840)	1:38:A:ASP:HA	1:40:A:ILE:H	11	0.12
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	5	0.12
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	5	0.12
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	5	0.12
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB1	12	0.12
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB2	12	0.12
(2,1798)	1:72:A:ILE:H	1:75:A:ALA:HB3	12	0.12
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD11	9	0.12
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD12	9	0.12
(2,1791)	1:142:A:LEU:H	1:142:A:LEU:HD13	9	0.12
(2,1782)	1:69:A:ILE:HG21	1:74:A:ARG:H	4	0.12
(2,1782)	1:69:A:ILE:HG22	1:74:A:ARG:H	4	0.12
(2,1782)	1:69:A:ILE:HG23	1:74:A:ARG:H	4	0.12
(2,1782)	1:69:A:ILE:HG21	1:74:A:ARG:H	10	0.12
(2,1782)	1:69:A:ILE:HG22	1:74:A:ARG:H	10	0.12
(2,1782)	1:69:A:ILE:HG23	1:74:A:ARG:H	10	0.12
(2,1760)	1:37:A:LEU:HA	1:40:A:ILE:H	7	0.12
(2,1727)	1:151:A:ALA:H	1:154:A:LEU:H	2	0.12
(2,1672)	1:115:A:LYS:HE2	1:116:A:SER:H	16	0.12
(2,1672)	1:115:A:LYS:HE3	1:116:A:SER:H	16	0.12
(2,1672)	1:115:A:LYS:HE2	1:116:A:SER:H	17	0.12
(2,1672)	1:115:A:LYS:HE3	1:116:A:SER:H	17	0.12
(2,1662)	1:54:A:SER:HB2	1:66:A:LEU:H	16	0.12
(2,1662)	1:54:A:SER:HB3	1:66:A:LEU:H	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	10	0.12
(2,1636)	1:153:A:ASP:HA	1:155:A:GLU:H	16	0.12
(2,1629)	1:142:A:LEU:H	1:146:A:ARG:HA	20	0.12
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	1	0.12
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	1	0.12
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	5	0.12
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	5	0.12
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	16	0.12
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	16	0.12
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	17	0.12
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	17	0.12
(2,1577)	1:115:A:LYS:H	1:115:A:LYS:HB3	15	0.12
(2,1573)	1:113:A:ILE:H	1:115:A:LYS:H	15	0.12
(2,1573)	1:113:A:ILE:H	1:115:A:LYS:H	19	0.12
(2,1541)	1:105:A:ILE:H	1:106:A:GLN:HB3	1	0.12
(2,1541)	1:105:A:ILE:H	1:106:A:GLN:HB3	4	0.12
(2,1431)	1:63:A:LEU:HD11	1:66:A:LEU:H	15	0.12
(2,1431)	1:63:A:LEU:HD12	1:66:A:LEU:H	15	0.12
(2,1431)	1:63:A:LEU:HD13	1:66:A:LEU:H	15	0.12
(2,1428)	1:53:A:TYR:HD1	1:65:A:SER:H	5	0.12
(2,1428)	1:53:A:TYR:HD2	1:65:A:SER:H	5	0.12
(2,1428)	1:53:A:TYR:HD1	1:65:A:SER:H	15	0.12
(2,1428)	1:53:A:TYR:HD2	1:65:A:SER:H	15	0.12
(2,1411)	1:59:A:ASP:H	1:61:A:HIS:H	9	0.12
(2,1411)	1:59:A:ASP:H	1:61:A:HIS:H	14	0.12
(2,1411)	1:59:A:ASP:H	1:61:A:HIS:H	16	0.12
(2,1385)	1:52:A:ASP:H	1:53:A:TYR:HB2	8	0.12
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	9	0.12
(2,1216)	1:15:A:GLU:HB2	1:17:A:PHE:H	2	0.12
(2,1216)	1:15:A:GLU:HB3	1:17:A:PHE:H	2	0.12
(2,1157)	1:9:A:ASN:H	1:35:A:TYR:HE1	18	0.12
(2,1157)	1:9:A:ASN:H	1:35:A:TYR:HE2	18	0.12
(2,1153)	1:14:A:LEU:HG	1:15:A:GLU:H	13	0.12
(2,1130)	1:117:A:ASN:HA	1:117:A:ASN:HD21	9	0.12
(2,1105)	1:138:A:GLN:HA	1:139:A:LYS:HA	6	0.12
(2,1080)	1:51:A:ILE:HD11	1:101:A:LEU:H	14	0.12
(2,1080)	1:51:A:ILE:HD12	1:101:A:LEU:H	14	0.12
(2,1080)	1:51:A:ILE:HD13	1:101:A:LEU:H	14	0.12
(2,1063)	1:105:A:ILE:HG12	1:109:A:LEU:HG	4	0.12
(2,1063)	1:105:A:ILE:HG12	1:109:A:LEU:HG	12	0.12
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG12	17	0.12
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG13	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG12	17	0.12
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG13	17	0.12
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG12	17	0.12
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG13	17	0.12
(2,1042)	1:63:A:LEU:HA	1:124:A:ILE:HG12	14	0.12
(2,1042)	1:63:A:LEU:HA	1:124:A:ILE:HG13	14	0.12
(2,1037)	1:127:A:LEU:H	1:127:A:LEU:HD11	8	0.12
(2,1037)	1:127:A:LEU:H	1:127:A:LEU:HD12	8	0.12
(2,1037)	1:127:A:LEU:H	1:127:A:LEU:HD13	8	0.12
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD11	6	0.12
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD12	6	0.12
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD13	6	0.12
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD11	6	0.12
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD12	6	0.12
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD13	6	0.12
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD11	6	0.12
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD12	6	0.12
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD13	6	0.12
(2,1004)	1:149:A:CYS:HA	1:153:A:ASP:HA	7	0.12
(2,1004)	1:149:A:CYS:HA	1:153:A:ASP:HA	17	0.12
(2,1002)	1:154:A:LEU:H	1:154:A:LEU:HB2	1	0.12
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	19	0.12
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	19	0.12
(2,969)	1:125:A:ARG:HG2	1:128:A:LEU:HD11	19	0.12
(2,969)	1:125:A:ARG:HG2	1:128:A:LEU:HD12	19	0.12
(2,969)	1:125:A:ARG:HG2	1:128:A:LEU:HD13	19	0.12
(2,968)	1:109:A:LEU:HD11	1:128:A:LEU:HD21	15	0.12
(2,968)	1:109:A:LEU:HD11	1:128:A:LEU:HD22	15	0.12
(2,968)	1:109:A:LEU:HD11	1:128:A:LEU:HD23	15	0.12
(2,968)	1:109:A:LEU:HD12	1:128:A:LEU:HD21	15	0.12
(2,968)	1:109:A:LEU:HD12	1:128:A:LEU:HD22	15	0.12
(2,968)	1:109:A:LEU:HD12	1:128:A:LEU:HD23	15	0.12
(2,968)	1:109:A:LEU:HD13	1:128:A:LEU:HD21	15	0.12
(2,968)	1:109:A:LEU:HD13	1:128:A:LEU:HD22	15	0.12
(2,968)	1:109:A:LEU:HD13	1:128:A:LEU:HD23	15	0.12
(2,968)	1:109:A:LEU:HD11	1:128:A:LEU:HD21	17	0.12
(2,968)	1:109:A:LEU:HD11	1:128:A:LEU:HD22	17	0.12
(2,968)	1:109:A:LEU:HD11	1:128:A:LEU:HD23	17	0.12
(2,968)	1:109:A:LEU:HD12	1:128:A:LEU:HD21	17	0.12
(2,968)	1:109:A:LEU:HD12	1:128:A:LEU:HD22	17	0.12
(2,968)	1:109:A:LEU:HD12	1:128:A:LEU:HD23	17	0.12
(2,968)	1:109:A:LEU:HD13	1:128:A:LEU:HD21	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,968)	1:109:A:LEU:HD13	1:128:A:LEU:HD22	17	0.12
(2,968)	1:109:A:LEU:HD13	1:128:A:LEU:HD23	17	0.12
(2,962)	1:126:A:MET:HB3	1:126:A:MET:HE1	12	0.12
(2,962)	1:126:A:MET:HB3	1:126:A:MET:HE2	12	0.12
(2,962)	1:126:A:MET:HB3	1:126:A:MET:HE3	12	0.12
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG21	1	0.12
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG22	1	0.12
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG23	1	0.12
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG21	1	0.12
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG22	1	0.12
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG23	1	0.12
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG21	1	0.12
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG22	1	0.12
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG23	1	0.12
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG21	16	0.12
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG22	16	0.12
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG23	16	0.12
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG21	16	0.12
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG22	16	0.12
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG23	16	0.12
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG21	16	0.12
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG22	16	0.12
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG23	16	0.12
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG21	17	0.12
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG22	17	0.12
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG23	17	0.12
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG21	17	0.12
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG22	17	0.12
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG23	17	0.12
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG21	17	0.12
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG22	17	0.12
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG23	17	0.12
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	12	0.12
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	12	0.12
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	12	0.12
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	5	0.12
(2,922)	1:122:A:GLU:HA	1:125:A:ARG:HG3	7	0.12
(2,886)	1:113:A:ILE:HD11	1:151:A:ALA:H	6	0.12
(2,886)	1:113:A:ILE:HD12	1:151:A:ALA:H	6	0.12
(2,886)	1:113:A:ILE:HD13	1:151:A:ALA:H	6	0.12
(2,854)	1:109:A:LEU:HD21	1:128:A:LEU:HA	6	0.12
(2,854)	1:109:A:LEU:HD22	1:128:A:LEU:HA	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,854)	1:109:A:LEU:HD23	1:128:A:LEU:HA	6	0.12
(2,854)	1:109:A:LEU:HD21	1:128:A:LEU:HA	13	0.12
(2,854)	1:109:A:LEU:HD22	1:128:A:LEU:HA	13	0.12
(2,854)	1:109:A:LEU:HD23	1:128:A:LEU:HA	13	0.12
(2,756)	1:80:A:THR:HG21	1:95:A:ALA:H	12	0.12
(2,756)	1:80:A:THR:HG22	1:95:A:ALA:H	12	0.12
(2,756)	1:80:A:THR:HG23	1:95:A:ALA:H	12	0.12
(2,742)	1:76:A:TYR:HA	1:94:A:CYS:HA	15	0.12
(2,742)	1:76:A:TYR:HA	1:94:A:CYS:HA	17	0.12
(2,716)	1:77:A:LEU:H	1:77:A:LEU:HD11	13	0.12
(2,716)	1:77:A:LEU:H	1:77:A:LEU:HD12	13	0.12
(2,716)	1:77:A:LEU:H	1:77:A:LEU:HD13	13	0.12
(2,714)	1:76:A:TYR:HA	1:97:A:ALA:HB1	12	0.12
(2,714)	1:76:A:TYR:HA	1:97:A:ALA:HB2	12	0.12
(2,714)	1:76:A:TYR:HA	1:97:A:ALA:HB3	12	0.12
(2,613)	1:47:A:ILE:HG21	1:97:A:ALA:HB1	10	0.12
(2,613)	1:47:A:ILE:HG21	1:97:A:ALA:HB2	10	0.12
(2,613)	1:47:A:ILE:HG21	1:97:A:ALA:HB3	10	0.12
(2,613)	1:47:A:ILE:HG22	1:97:A:ALA:HB1	10	0.12
(2,613)	1:47:A:ILE:HG22	1:97:A:ALA:HB2	10	0.12
(2,613)	1:47:A:ILE:HG22	1:97:A:ALA:HB3	10	0.12
(2,613)	1:47:A:ILE:HG23	1:97:A:ALA:HB1	10	0.12
(2,613)	1:47:A:ILE:HG23	1:97:A:ALA:HB2	10	0.12
(2,613)	1:47:A:ILE:HG23	1:97:A:ALA:HB3	10	0.12
(2,599)	1:46:A:ILE:HG21	1:51:A:ILE:H	9	0.12
(2,599)	1:46:A:ILE:HG22	1:51:A:ILE:H	9	0.12
(2,599)	1:46:A:ILE:HG23	1:51:A:ILE:H	9	0.12
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	7	0.12
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	7	0.12
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	7	0.12
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	14	0.12
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	14	0.12
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	14	0.12
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG21	19	0.12
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG22	19	0.12
(2,584)	1:48:A:SER:HA	1:100:A:THR:HG23	19	0.12
(2,568)	1:49:A:LEU:HG	1:53:A:TYR:HA	3	0.12
(2,506)	1:40:A:ILE:HA	1:43:A:GLU:HG2	20	0.12
(2,506)	1:40:A:ILE:HA	1:43:A:GLU:HG3	20	0.12
(2,488)	1:40:A:ILE:HG21	1:41:A:ASP:H	7	0.12
(2,488)	1:40:A:ILE:HG22	1:41:A:ASP:H	7	0.12
(2,488)	1:40:A:ILE:HG23	1:41:A:ASP:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	16	0.12
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	18	0.12
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	19	0.12
(2,387)	1:24:A:ILE:HD11	1:64:A:GLY:HA3	9	0.12
(2,387)	1:24:A:ILE:HD12	1:64:A:GLY:HA3	9	0.12
(2,387)	1:24:A:ILE:HD13	1:64:A:GLY:HA3	9	0.12
(2,369)	1:17:A:PHE:HA	1:20:A:LEU:HA	14	0.12
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	17	0.12
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	17	0.12
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	17	0.12
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	14	0.12
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	14	0.12
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	14	0.12
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	14	0.12
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	14	0.12
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	14	0.12
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	15	0.12
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	15	0.12
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	15	0.12
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	15	0.12
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	15	0.12
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	15	0.12
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD21	13	0.12
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD22	13	0.12
(2,325)	1:11:A:VAL:HG11	1:49:A:LEU:HD23	13	0.12
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD21	13	0.12
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD22	13	0.12
(2,325)	1:11:A:VAL:HG12	1:49:A:LEU:HD23	13	0.12
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD21	13	0.12
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD22	13	0.12
(2,325)	1:11:A:VAL:HG13	1:49:A:LEU:HD23	13	0.12
(2,301)	1:11:A:VAL:HG21	1:49:A:LEU:HB2	1	0.12
(2,301)	1:11:A:VAL:HG22	1:49:A:LEU:HB2	1	0.12
(2,301)	1:11:A:VAL:HG23	1:49:A:LEU:HB2	1	0.12
(2,301)	1:11:A:VAL:HG21	1:49:A:LEU:HB2	4	0.12
(2,301)	1:11:A:VAL:HG22	1:49:A:LEU:HB2	4	0.12
(2,301)	1:11:A:VAL:HG23	1:49:A:LEU:HB2	4	0.12
(2,298)	1:11:A:VAL:HG21	1:15:A:GLU:H	6	0.12
(2,298)	1:11:A:VAL:HG22	1:15:A:GLU:H	6	0.12
(2,298)	1:11:A:VAL:HG23	1:15:A:GLU:H	6	0.12
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	7	0.12
(2,252)	1:153:A:ASP:HB3	1:154:A:LEU:HB3	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,252)	1:153:A:ASP:HB3	1:154:A:LEU:HB3	17	0.12
(2,230)	1:55:A:ARG:H	1:108:A:LEU:HB3	9	0.12
(2,230)	1:55:A:ARG:H	1:108:A:LEU:HB3	17	0.12
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	2	0.12
(2,190)	1:66:A:LEU:HD11	1:112:A:ALA:H	8	0.12
(2,190)	1:66:A:LEU:HD12	1:112:A:ALA:H	8	0.12
(2,190)	1:66:A:LEU:HD13	1:112:A:ALA:H	8	0.12
(2,187)	1:104:A:VAL:HG11	1:105:A:ILE:H	4	0.12
(2,187)	1:104:A:VAL:HG12	1:105:A:ILE:H	4	0.12
(2,187)	1:104:A:VAL:HG13	1:105:A:ILE:H	4	0.12
(2,169)	1:26:A:GLY:HA2	1:28:A:ARG:HB2	20	0.12
(2,167)	1:63:A:LEU:HD11	1:67:A:TYR:HB2	20	0.12
(2,167)	1:63:A:LEU:HD12	1:67:A:TYR:HB2	20	0.12
(2,167)	1:63:A:LEU:HD13	1:67:A:TYR:HB2	20	0.12
(2,166)	1:69:A:ILE:HB	1:108:A:LEU:HD11	14	0.12
(2,166)	1:69:A:ILE:HB	1:108:A:LEU:HD12	14	0.12
(2,166)	1:69:A:ILE:HB	1:108:A:LEU:HD13	14	0.12
(2,166)	1:69:A:ILE:HB	1:108:A:LEU:HD11	18	0.12
(2,166)	1:69:A:ILE:HB	1:108:A:LEU:HD12	18	0.12
(2,166)	1:69:A:ILE:HB	1:108:A:LEU:HD13	18	0.12
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	18	0.12
(1,155)	2:1007:B:TYR:OH	1:74:A:ARG:NH2	2	0.12
(1,155)	2:1007:B:TYR:OH	1:74:A:ARG:NH2	8	0.12
(1,154)	2:1009:B:PRO:HA	1:74:A:ARG:NH2	10	0.12
(1,153)	2:1009:B:PRO:O	1:74:A:ARG:HE	13	0.12
(1,150)	1:148:A:LYS:O	1:152:A:MET:H	2	0.12
(1,150)	1:148:A:LYS:O	1:152:A:MET:H	13	0.12
(1,142)	1:128:A:LEU:O	1:132:A:ASP:H	15	0.12
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	12	0.12
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	17	0.12
(1,140)	1:127:A:LEU:O	1:131:A:TRP:H	9	0.12
(1,140)	1:127:A:LEU:O	1:131:A:TRP:H	18	0.12
(1,140)	1:127:A:LEU:O	1:131:A:TRP:H	20	0.12
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	6	0.12
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	13	0.12
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	14	0.12
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	3	0.12
(1,136)	1:125:A:ARG:O	1:129:A:ASP:H	19	0.12
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	4	0.12
(1,135)	1:125:A:ARG:O	1:129:A:ASP:N	8	0.12
(1,132)	1:123:A:LYS:O	1:127:A:LEU:H	8	0.12
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	12	0.12
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	19	0.12
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	20	0.12
(1,129)	1:122:A:GLU:O	1:126:A:MET:N	8	0.12
(1,128)	1:121:A:LYS:O	1:125:A:ARG:H	20	0.12
(1,127)	1:121:A:LYS:O	1:125:A:ARG:N	10	0.12
(1,125)	1:120:A:HIS:O	1:124:A:ILE:N	7	0.12
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	5	0.12
(1,123)	1:119:A:ASP:O	1:123:A:LYS:N	7	0.12
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	4	0.12
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	5	0.12
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	14	0.12
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	15	0.12
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	18	0.12
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	9	0.12
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	12	0.12
(1,81)	1:71:A:SER:O	1:75:A:ALA:N	16	0.12
(1,80)	1:70:A:ASP:O	1:74:A:ARG:H	3	0.12
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	2	0.12
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	7	0.12
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	8	0.12
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	10	0.12
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	19	0.12
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	13	0.12
(1,67)	1:64:A:GLY:O	1:68:A:ILE:N	13	0.12
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	7	0.12
(1,65)	1:63:A:LEU:O	1:67:A:TYR:N	1	0.12
(1,63)	1:62:A:LYS:O	1:66:A:LEU:N	11	0.12
(1,63)	1:62:A:LYS:O	1:66:A:LEU:N	12	0.12
(1,63)	1:62:A:LYS:O	1:66:A:LEU:N	13	0.12
(1,52)	1:50:A:ILE:O	1:54:A:SER:H	3	0.12
(1,52)	1:50:A:ILE:O	1:54:A:SER:H	16	0.12
(1,43)	1:46:A:ILE:O	1:50:A:ILE:N	2	0.12
(1,43)	1:46:A:ILE:O	1:50:A:ILE:N	19	0.12
(1,34)	1:33:A:THR:O	1:37:A:LEU:H	6	0.12
(1,34)	1:33:A:THR:O	1:37:A:LEU:H	12	0.12
(1,34)	1:33:A:THR:O	1:37:A:LEU:H	20	0.12
(1,23)	1:28:A:ARG:O	1:32:A:LEU:N	12	0.12
(1,22)	1:27:A:SER:O	1:31:A:LYS:H	10	0.12
(1,17)	1:15:A:GLU:O	1:19:A:ASP:N	19	0.12
(1,14)	1:13:A:THR:O	1:17:A:PHE:H	11	0.12
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,5)	2:1007:B:TYR:O	1:67:A:TYR:HE1	1	0.11
(2,2354)	1:102:A:GLY:H	1:137:A:PHE:HD1	6	0.11
(2,2354)	1:102:A:GLY:H	1:137:A:PHE:HD2	6	0.11
(2,2354)	1:102:A:GLY:H	1:137:A:PHE:HD1	10	0.11
(2,2354)	1:102:A:GLY:H	1:137:A:PHE:HD2	10	0.11
(2,2343)	1:102:A:GLY:H	1:137:A:PHE:HD1	6	0.11
(2,2343)	1:102:A:GLY:H	1:137:A:PHE:HD2	6	0.11
(2,2343)	1:102:A:GLY:H	1:137:A:PHE:HD1	10	0.11
(2,2343)	1:102:A:GLY:H	1:137:A:PHE:HD2	10	0.11
(2,2328)	1:152:A:MET:HB2	1:153:A:ASP:HA	2	0.11
(2,2328)	1:152:A:MET:HB3	1:153:A:ASP:HA	2	0.11
(2,2328)	1:152:A:MET:HB2	1:153:A:ASP:HA	5	0.11
(2,2328)	1:152:A:MET:HB3	1:153:A:ASP:HA	5	0.11
(2,2328)	1:152:A:MET:HB2	1:153:A:ASP:HA	15	0.11
(2,2328)	1:152:A:MET:HB3	1:153:A:ASP:HA	15	0.11
(2,2328)	1:152:A:MET:HB2	1:153:A:ASP:HA	17	0.11
(2,2328)	1:152:A:MET:HB3	1:153:A:ASP:HA	17	0.11
(2,2287)	1:122:A:GLU:HA	1:125:A:ARG:HD2	17	0.11
(2,2287)	1:122:A:GLU:HA	1:125:A:ARG:HD3	17	0.11
(2,2286)	1:122:A:GLU:H	1:122:A:GLU:HG2	2	0.11
(2,2286)	1:122:A:GLU:H	1:122:A:GLU:HG3	2	0.11
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG2	9	0.11
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG3	9	0.11
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG2	13	0.11
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG3	13	0.11
(2,2274)	1:113:A:ILE:HG13	1:150:A:PHE:HB2	18	0.11
(2,2274)	1:113:A:ILE:HG13	1:150:A:PHE:HB3	18	0.11
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD11	4	0.11
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD12	4	0.11
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD13	4	0.11
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD21	4	0.11
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD22	4	0.11
(2,2268)	1:110:A:SER:HB2	1:154:A:LEU:HD23	4	0.11
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD11	4	0.11
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD12	4	0.11
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD13	4	0.11
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD21	4	0.11
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD22	4	0.11
(2,2268)	1:110:A:SER:HB3	1:154:A:LEU:HD23	4	0.11
(2,2237)	1:94:A:CYS:HB2	1:95:A:ALA:HA	5	0.11
(2,2237)	1:94:A:CYS:HB3	1:95:A:ALA:HA	5	0.11
(2,2237)	1:94:A:CYS:HB2	1:95:A:ALA:HA	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2237)	1:94:A:CYS:HB3	1:95:A:ALA:HA	17	0.11
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB2	19	0.11
(2,2205)	1:62:A:LYS:HG2	1:115:A:LYS:HB3	19	0.11
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB2	19	0.11
(2,2205)	1:62:A:LYS:HG3	1:115:A:LYS:HB3	19	0.11
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD2	1	0.11
(2,2168)	1:54:A:SER:H	1:55:A:ARG:HD3	1	0.11
(2,2137)	1:39:A:HIS:HB2	1:42:A:ILE:H	7	0.11
(2,2137)	1:39:A:HIS:HB3	1:42:A:ILE:H	7	0.11
(2,2137)	1:39:A:HIS:HB2	1:42:A:ILE:H	13	0.11
(2,2137)	1:39:A:HIS:HB3	1:42:A:ILE:H	13	0.11
(2,2100)	1:24:A:ILE:HB	1:64:A:GLY:HA2	2	0.11
(2,2100)	1:24:A:ILE:HB	1:64:A:GLY:HA3	2	0.11
(2,2100)	1:24:A:ILE:HB	1:64:A:GLY:HA2	4	0.11
(2,2100)	1:24:A:ILE:HB	1:64:A:GLY:HA3	4	0.11
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB2	20	0.11
(2,2082)	1:9:A:ASN:HB2	1:31:A:LYS:HB3	20	0.11
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB2	20	0.11
(2,2082)	1:9:A:ASN:HB3	1:31:A:LYS:HB3	20	0.11
(2,2009)	1:35:A:TYR:HD1	1:38:A:ASP:H	1	0.11
(2,2009)	1:35:A:TYR:HD2	1:38:A:ASP:H	1	0.11
(2,2009)	1:35:A:TYR:HD1	1:38:A:ASP:H	14	0.11
(2,2009)	1:35:A:TYR:HD2	1:38:A:ASP:H	14	0.11
(2,2009)	1:35:A:TYR:HD1	1:38:A:ASP:H	16	0.11
(2,2009)	1:35:A:TYR:HD2	1:38:A:ASP:H	16	0.11
(2,2009)	1:35:A:TYR:HD1	1:38:A:ASP:H	19	0.11
(2,2009)	1:35:A:TYR:HD2	1:38:A:ASP:H	19	0.11
(2,1987)	1:111:A:ASP:H	1:111:A:ASP:HB3	10	0.11
(2,1942)	1:74:A:ARG:HD2	1:75:A:ALA:H	4	0.11
(2,1942)	1:74:A:ARG:HD3	1:75:A:ALA:H	4	0.11
(2,1942)	1:74:A:ARG:HD2	1:75:A:ALA:H	13	0.11
(2,1942)	1:74:A:ARG:HD3	1:75:A:ALA:H	13	0.11
(2,1902)	1:62:A:LYS:HD2	1:115:A:LYS:H	18	0.11
(2,1902)	1:62:A:LYS:HD3	1:115:A:LYS:H	18	0.11
(2,1895)	1:67:A:TYR:H	1:70:A:ASP:HB2	1	0.11
(2,1895)	1:67:A:TYR:H	1:70:A:ASP:HB2	14	0.11
(2,1840)	1:38:A:ASP:HA	1:40:A:ILE:H	8	0.11
(2,1840)	1:38:A:ASP:HA	1:40:A:ILE:H	10	0.11
(2,1803)	1:104:A:VAL:HG21	1:106:A:GLN:H	4	0.11
(2,1803)	1:104:A:VAL:HG22	1:106:A:GLN:H	4	0.11
(2,1803)	1:104:A:VAL:HG23	1:106:A:GLN:H	4	0.11
(2,1782)	1:69:A:ILE:HG21	1:74:A:ARG:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1782)	1:69:A:ILE:HG22	1:74:A:ARG:H	1	0.11
(2,1782)	1:69:A:ILE:HG23	1:74:A:ARG:H	1	0.11
(2,1782)	1:69:A:ILE:HG21	1:74:A:ARG:H	18	0.11
(2,1782)	1:69:A:ILE:HG22	1:74:A:ARG:H	18	0.11
(2,1782)	1:69:A:ILE:HG23	1:74:A:ARG:H	18	0.11
(2,1776)	1:116:A:SER:HB2	1:117:A:ASN:H	5	0.11
(2,1774)	1:39:A:HIS:HB2	1:41:A:ASP:H	13	0.11
(2,1760)	1:37:A:LEU:HA	1:40:A:ILE:H	5	0.11
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG21	14	0.11
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG22	14	0.11
(2,1738)	1:50:A:ILE:H	1:68:A:ILE:HG23	14	0.11
(2,1672)	1:115:A:LYS:HE2	1:116:A:SER:H	6	0.11
(2,1672)	1:115:A:LYS:HE3	1:116:A:SER:H	6	0.11
(2,1667)	1:94:A:CYS:H	1:97:A:ALA:H	11	0.11
(2,1662)	1:54:A:SER:HB2	1:66:A:LEU:H	13	0.11
(2,1662)	1:54:A:SER:HB3	1:66:A:LEU:H	13	0.11
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	2	0.11
(2,1649)	1:54:A:SER:H	1:56:A:LEU:HG	14	0.11
(2,1645)	1:43:A:GLU:H	1:93:A:THR:H	12	0.11
(2,1630)	1:151:A:ALA:H	1:153:A:ASP:H	18	0.11
(2,1629)	1:142:A:LEU:H	1:146:A:ARG:HA	7	0.11
(2,1620)	1:147:A:SER:H	1:147:A:SER:HB2	10	0.11
(2,1620)	1:147:A:SER:H	1:147:A:SER:HB3	10	0.11
(2,1573)	1:113:A:ILE:H	1:115:A:LYS:H	13	0.11
(2,1561)	1:108:A:LEU:H	1:110:A:SER:H	10	0.11
(2,1541)	1:105:A:ILE:H	1:106:A:GLN:HB3	3	0.11
(2,1541)	1:105:A:ILE:H	1:106:A:GLN:HB3	6	0.11
(2,1541)	1:105:A:ILE:H	1:106:A:GLN:HB3	14	0.11
(2,1541)	1:105:A:ILE:H	1:106:A:GLN:HB3	17	0.11
(2,1541)	1:105:A:ILE:H	1:106:A:GLN:HB3	18	0.11
(2,1533)	1:104:A:VAL:H	1:106:A:GLN:HG2	8	0.11
(2,1442)	1:74:A:ARG:H	1:74:A:ARG:HD2	5	0.11
(2,1442)	1:74:A:ARG:H	1:74:A:ARG:HD3	5	0.11
(2,1428)	1:53:A:TYR:HD1	1:65:A:SER:H	2	0.11
(2,1428)	1:53:A:TYR:HD2	1:65:A:SER:H	2	0.11
(2,1418)	1:58:A:PRO:HA	1:62:A:LYS:H	7	0.11
(2,1346)	1:45:A:LYS:H	1:45:A:LYS:HE2	18	0.11
(2,1276)	1:113:A:ILE:H	1:124:A:ILE:HG12	19	0.11
(2,1276)	1:113:A:ILE:H	1:124:A:ILE:HG13	19	0.11
(2,1242)	1:20:A:LEU:H	1:23:A:GLY:H	10	0.11
(2,1216)	1:15:A:GLU:HB2	1:17:A:PHE:H	19	0.11
(2,1216)	1:15:A:GLU:HB3	1:17:A:PHE:H	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1192)	1:11:A:VAL:HG11	1:13:A:THR:H	2	0.11
(2,1192)	1:11:A:VAL:HG12	1:13:A:THR:H	2	0.11
(2,1192)	1:11:A:VAL:HG13	1:13:A:THR:H	2	0.11
(2,1192)	1:11:A:VAL:HG11	1:13:A:THR:H	5	0.11
(2,1192)	1:11:A:VAL:HG12	1:13:A:THR:H	5	0.11
(2,1192)	1:11:A:VAL:HG13	1:13:A:THR:H	5	0.11
(2,1192)	1:11:A:VAL:HG11	1:13:A:THR:H	8	0.11
(2,1192)	1:11:A:VAL:HG12	1:13:A:THR:H	8	0.11
(2,1192)	1:11:A:VAL:HG13	1:13:A:THR:H	8	0.11
(2,1192)	1:11:A:VAL:HG11	1:13:A:THR:H	20	0.11
(2,1192)	1:11:A:VAL:HG12	1:13:A:THR:H	20	0.11
(2,1192)	1:11:A:VAL:HG13	1:13:A:THR:H	20	0.11
(2,1157)	1:9:A:ASN:H	1:35:A:TYR:HE1	19	0.11
(2,1157)	1:9:A:ASN:H	1:35:A:TYR:HE2	19	0.11
(2,1143)	1:7:A:PHE:H	1:10:A:PHE:HB3	5	0.11
(2,1133)	1:141:A:TYR:H	1:142:A:LEU:HD11	13	0.11
(2,1133)	1:141:A:TYR:H	1:142:A:LEU:HD12	13	0.11
(2,1133)	1:141:A:TYR:H	1:142:A:LEU:HD13	13	0.11
(2,1130)	1:117:A:ASN:HA	1:117:A:ASN:HD21	19	0.11
(2,1105)	1:138:A:GLN:HA	1:139:A:LYS:HA	19	0.11
(2,1062)	1:43:A:GLU:HA	1:47:A:ILE:HG12	18	0.11
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG12	1	0.11
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG13	1	0.11
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG12	1	0.11
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG13	1	0.11
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG12	1	0.11
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG13	1	0.11
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG12	6	0.11
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG13	6	0.11
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG12	6	0.11
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG13	6	0.11
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG12	6	0.11
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG13	6	0.11
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG12	8	0.11
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG13	8	0.11
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG12	8	0.11
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG13	8	0.11
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG12	8	0.11
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG13	8	0.11
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD11	13	0.11
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD12	13	0.11
(2,1020)	1:130:A:ILE:HA	1:130:A:ILE:HD13	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD11	8	0.11
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD12	8	0.11
(2,1016)	1:113:A:ILE:HD11	1:145:A:ILE:HD13	8	0.11
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD11	8	0.11
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD12	8	0.11
(2,1016)	1:113:A:ILE:HD12	1:145:A:ILE:HD13	8	0.11
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD11	8	0.11
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD12	8	0.11
(2,1016)	1:113:A:ILE:HD13	1:145:A:ILE:HD13	8	0.11
(2,1012)	1:151:A:ALA:HA	1:155:A:GLU:HB2	1	0.11
(2,1012)	1:151:A:ALA:HA	1:155:A:GLU:HB3	1	0.11
(2,1009)	1:154:A:LEU:HA	1:155:A:GLU:H	7	0.11
(2,1009)	1:154:A:LEU:HA	1:155:A:GLU:H	9	0.11
(2,1009)	1:154:A:LEU:HA	1:155:A:GLU:H	19	0.11
(2,1004)	1:149:A:CYS:HA	1:153:A:ASP:HA	2	0.11
(2,1004)	1:149:A:CYS:HA	1:153:A:ASP:HA	10	0.11
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG21	18	0.11
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG22	18	0.11
(2,981)	1:110:A:SER:HA	1:145:A:ILE:HG23	18	0.11
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB2	1	0.11
(2,976)	1:146:A:ARG:HG3	1:147:A:SER:HB3	1	0.11
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD11	8	0.11
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD12	8	0.11
(2,973)	1:144:A:ALA:HA	1:145:A:ILE:HD13	8	0.11
(2,968)	1:109:A:LEU:HD11	1:128:A:LEU:HD21	20	0.11
(2,968)	1:109:A:LEU:HD11	1:128:A:LEU:HD22	20	0.11
(2,968)	1:109:A:LEU:HD11	1:128:A:LEU:HD23	20	0.11
(2,968)	1:109:A:LEU:HD12	1:128:A:LEU:HD21	20	0.11
(2,968)	1:109:A:LEU:HD12	1:128:A:LEU:HD22	20	0.11
(2,968)	1:109:A:LEU:HD12	1:128:A:LEU:HD23	20	0.11
(2,968)	1:109:A:LEU:HD13	1:128:A:LEU:HD21	20	0.11
(2,968)	1:109:A:LEU:HD13	1:128:A:LEU:HD22	20	0.11
(2,968)	1:109:A:LEU:HD13	1:128:A:LEU:HD23	20	0.11
(2,942)	1:66:A:LEU:HD11	1:109:A:LEU:HD21	18	0.11
(2,942)	1:66:A:LEU:HD11	1:109:A:LEU:HD22	18	0.11
(2,942)	1:66:A:LEU:HD11	1:109:A:LEU:HD23	18	0.11
(2,942)	1:66:A:LEU:HD12	1:109:A:LEU:HD21	18	0.11
(2,942)	1:66:A:LEU:HD12	1:109:A:LEU:HD22	18	0.11
(2,942)	1:66:A:LEU:HD12	1:109:A:LEU:HD23	18	0.11
(2,942)	1:66:A:LEU:HD13	1:109:A:LEU:HD21	18	0.11
(2,942)	1:66:A:LEU:HD13	1:109:A:LEU:HD22	18	0.11
(2,942)	1:66:A:LEU:HD13	1:109:A:LEU:HD23	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	17	0.11
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	17	0.11
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	17	0.11
(2,933)	1:124:A:ILE:HG21	1:128:A:LEU:HD11	1	0.11
(2,933)	1:124:A:ILE:HG21	1:128:A:LEU:HD12	1	0.11
(2,933)	1:124:A:ILE:HG21	1:128:A:LEU:HD13	1	0.11
(2,933)	1:124:A:ILE:HG22	1:128:A:LEU:HD11	1	0.11
(2,933)	1:124:A:ILE:HG22	1:128:A:LEU:HD12	1	0.11
(2,933)	1:124:A:ILE:HG22	1:128:A:LEU:HD13	1	0.11
(2,933)	1:124:A:ILE:HG23	1:128:A:LEU:HD11	1	0.11
(2,933)	1:124:A:ILE:HG23	1:128:A:LEU:HD12	1	0.11
(2,933)	1:124:A:ILE:HG23	1:128:A:LEU:HD13	1	0.11
(2,933)	1:124:A:ILE:HG21	1:128:A:LEU:HD11	18	0.11
(2,933)	1:124:A:ILE:HG21	1:128:A:LEU:HD12	18	0.11
(2,933)	1:124:A:ILE:HG21	1:128:A:LEU:HD13	18	0.11
(2,933)	1:124:A:ILE:HG22	1:128:A:LEU:HD11	18	0.11
(2,933)	1:124:A:ILE:HG22	1:128:A:LEU:HD12	18	0.11
(2,933)	1:124:A:ILE:HG22	1:128:A:LEU:HD13	18	0.11
(2,933)	1:124:A:ILE:HG23	1:128:A:LEU:HD11	18	0.11
(2,933)	1:124:A:ILE:HG23	1:128:A:LEU:HD12	18	0.11
(2,933)	1:124:A:ILE:HG23	1:128:A:LEU:HD13	18	0.11
(2,901)	1:126:A:MET:HA	1:129:A:ASP:HA	5	0.11
(2,886)	1:113:A:ILE:HD11	1:151:A:ALA:H	8	0.11
(2,886)	1:113:A:ILE:HD12	1:151:A:ALA:H	8	0.11
(2,886)	1:113:A:ILE:HD13	1:151:A:ALA:H	8	0.11
(2,875)	1:113:A:ILE:HB	1:114:A:ALA:HB1	14	0.11
(2,875)	1:113:A:ILE:HB	1:114:A:ALA:HB2	14	0.11
(2,875)	1:113:A:ILE:HB	1:114:A:ALA:HB3	14	0.11
(2,854)	1:109:A:LEU:HD21	1:128:A:LEU:HA	5	0.11
(2,854)	1:109:A:LEU:HD22	1:128:A:LEU:HA	5	0.11
(2,854)	1:109:A:LEU:HD23	1:128:A:LEU:HA	5	0.11
(2,854)	1:109:A:LEU:HD21	1:128:A:LEU:HA	12	0.11
(2,854)	1:109:A:LEU:HD22	1:128:A:LEU:HA	12	0.11
(2,854)	1:109:A:LEU:HD23	1:128:A:LEU:HA	12	0.11
(2,772)	1:29:A:ILE:HG21	1:71:A:SER:H	15	0.11
(2,772)	1:29:A:ILE:HG22	1:71:A:SER:H	15	0.11
(2,772)	1:29:A:ILE:HG23	1:71:A:SER:H	15	0.11
(2,756)	1:80:A:THR:HG21	1:95:A:ALA:H	6	0.11
(2,756)	1:80:A:THR:HG22	1:95:A:ALA:H	6	0.11
(2,756)	1:80:A:THR:HG23	1:95:A:ALA:H	6	0.11
(2,756)	1:80:A:THR:HG21	1:95:A:ALA:H	16	0.11
(2,756)	1:80:A:THR:HG22	1:95:A:ALA:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,756)	1:80:A:THR:HG23	1:95:A:ALA:H	16	0.11
(2,744)	1:93:A:THR:HG21	1:94:A:CYS:HA	17	0.11
(2,744)	1:93:A:THR:HG22	1:94:A:CYS:HA	17	0.11
(2,744)	1:93:A:THR:HG23	1:94:A:CYS:HA	17	0.11
(2,735)	1:80:A:THR:HG21	1:94:A:CYS:HA	5	0.11
(2,735)	1:80:A:THR:HG22	1:94:A:CYS:HA	5	0.11
(2,735)	1:80:A:THR:HG23	1:94:A:CYS:HA	5	0.11
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG21	10	0.11
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG22	10	0.11
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG23	10	0.11
(2,716)	1:77:A:LEU:H	1:77:A:LEU:HD11	15	0.11
(2,716)	1:77:A:LEU:H	1:77:A:LEU:HD12	15	0.11
(2,716)	1:77:A:LEU:H	1:77:A:LEU:HD13	15	0.11
(2,613)	1:47:A:ILE:HG21	1:97:A:ALA:HB1	14	0.11
(2,613)	1:47:A:ILE:HG21	1:97:A:ALA:HB2	14	0.11
(2,613)	1:47:A:ILE:HG21	1:97:A:ALA:HB3	14	0.11
(2,613)	1:47:A:ILE:HG22	1:97:A:ALA:HB1	14	0.11
(2,613)	1:47:A:ILE:HG22	1:97:A:ALA:HB2	14	0.11
(2,613)	1:47:A:ILE:HG22	1:97:A:ALA:HB3	14	0.11
(2,613)	1:47:A:ILE:HG23	1:97:A:ALA:HB1	14	0.11
(2,613)	1:47:A:ILE:HG23	1:97:A:ALA:HB2	14	0.11
(2,613)	1:47:A:ILE:HG23	1:97:A:ALA:HB3	14	0.11
(2,599)	1:46:A:ILE:HG21	1:51:A:ILE:H	1	0.11
(2,599)	1:46:A:ILE:HG22	1:51:A:ILE:H	1	0.11
(2,599)	1:46:A:ILE:HG23	1:51:A:ILE:H	1	0.11
(2,599)	1:46:A:ILE:HG21	1:51:A:ILE:H	12	0.11
(2,599)	1:46:A:ILE:HG22	1:51:A:ILE:H	12	0.11
(2,599)	1:46:A:ILE:HG23	1:51:A:ILE:H	12	0.11
(2,599)	1:46:A:ILE:HG21	1:51:A:ILE:H	14	0.11
(2,599)	1:46:A:ILE:HG22	1:51:A:ILE:H	14	0.11
(2,599)	1:46:A:ILE:HG23	1:51:A:ILE:H	14	0.11
(2,568)	1:49:A:LEU:HG	1:53:A:TYR:HA	17	0.11
(2,568)	1:49:A:LEU:HG	1:53:A:TYR:HA	18	0.11
(2,568)	1:49:A:LEU:HG	1:53:A:TYR:HA	20	0.11
(2,491)	1:40:A:ILE:HG21	1:41:A:ASP:HA	7	0.11
(2,491)	1:40:A:ILE:HG22	1:41:A:ASP:HA	7	0.11
(2,491)	1:40:A:ILE:HG23	1:41:A:ASP:HA	7	0.11
(2,491)	1:40:A:ILE:HG21	1:41:A:ASP:HA	12	0.11
(2,491)	1:40:A:ILE:HG22	1:41:A:ASP:HA	12	0.11
(2,491)	1:40:A:ILE:HG23	1:41:A:ASP:HA	12	0.11
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	2	0.11
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	6	0.11
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	8	0.11
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	10	0.11
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	11	0.11
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	12	0.11
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	14	0.11
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	15	0.11
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	17	0.11
(2,397)	1:14:A:LEU:HD11	1:53:A:TYR:H	17	0.11
(2,397)	1:14:A:LEU:HD12	1:53:A:TYR:H	17	0.11
(2,397)	1:14:A:LEU:HD13	1:53:A:TYR:H	17	0.11
(2,369)	1:17:A:PHE:HA	1:20:A:LEU:HA	5	0.11
(2,361)	1:11:A:VAL:HG21	1:15:A:GLU:HG3	15	0.11
(2,361)	1:11:A:VAL:HG22	1:15:A:GLU:HG3	15	0.11
(2,361)	1:11:A:VAL:HG23	1:15:A:GLU:HG3	15	0.11
(2,334)	1:11:A:VAL:HA	1:14:A:LEU:HA	6	0.11
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB1	1	0.11
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB2	1	0.11
(2,330)	1:8:A:GLN:HB2	1:12:A:ALA:HB3	1	0.11
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB1	1	0.11
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB2	1	0.11
(2,330)	1:8:A:GLN:HB3	1:12:A:ALA:HB3	1	0.11
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB2	5	0.11
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB3	5	0.11
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB2	5	0.11
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB3	5	0.11
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB2	5	0.11
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB3	5	0.11
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB2	9	0.11
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB3	9	0.11
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB2	9	0.11
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB3	9	0.11
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB2	9	0.11
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB3	9	0.11
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB2	19	0.11
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB3	19	0.11
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB2	19	0.11
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB3	19	0.11
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB2	19	0.11
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB3	19	0.11
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	6	0.11
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	9	0.11
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	12	0.11
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	19	0.11
(2,281)	1:128:A:LEU:HD11	1:129:A:ASP:H	15	0.11
(2,281)	1:128:A:LEU:HD12	1:129:A:ASP:H	15	0.11
(2,281)	1:128:A:LEU:HD13	1:129:A:ASP:H	15	0.11
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD21	1	0.11
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD22	1	0.11
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD23	1	0.11
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD21	6	0.11
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD22	6	0.11
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD23	6	0.11
(2,252)	1:153:A:ASP:HB3	1:154:A:LEU:HB3	9	0.11
(2,190)	1:66:A:LEU:HD11	1:112:A:ALA:H	3	0.11
(2,190)	1:66:A:LEU:HD12	1:112:A:ALA:H	3	0.11
(2,190)	1:66:A:LEU:HD13	1:112:A:ALA:H	3	0.11
(2,169)	1:26:A:GLY:HA2	1:28:A:ARG:HB2	4	0.11
(2,169)	1:26:A:GLY:HA2	1:28:A:ARG:HB2	8	0.11
(2,167)	1:63:A:LEU:HD11	1:67:A:TYR:HB2	16	0.11
(2,167)	1:63:A:LEU:HD12	1:67:A:TYR:HB2	16	0.11
(2,167)	1:63:A:LEU:HD13	1:67:A:TYR:HB2	16	0.11
(2,157)	1:118:A:GLN:HA	1:121:A:LYS:HD2	15	0.11
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG2	4	0.11
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG3	4	0.11
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG2	5	0.11
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG3	5	0.11
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG2	6	0.11
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG3	6	0.11
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG2	14	0.11
(2,132)	1:123:A:LYS:HA	1:126:A:MET:HG3	14	0.11
(2,128)	1:63:A:LEU:HD11	1:123:A:LYS:HA	6	0.11
(2,128)	1:63:A:LEU:HD12	1:123:A:LYS:HA	6	0.11
(2,128)	1:63:A:LEU:HD13	1:123:A:LYS:HA	6	0.11
(2,128)	1:63:A:LEU:HD11	1:123:A:LYS:HA	19	0.11
(2,128)	1:63:A:LEU:HD12	1:123:A:LYS:HA	19	0.11
(2,128)	1:63:A:LEU:HD13	1:123:A:LYS:HA	19	0.11
(2,98)	1:24:A:ILE:HB	1:67:A:TYR:HE1	2	0.11
(2,98)	1:24:A:ILE:HB	1:67:A:TYR:HE2	2	0.11
(2,28)	2:1004:B:GLU:HB2	1:27:A:SER:H	12	0.11
(2,28)	2:1004:B:GLU:HB3	1:27:A:SER:H	12	0.11
(2,27)	2:1001:B:ASP:HB2	1:21:A:LYS:HE2	14	0.11
(2,27)	2:1001:B:ASP:HB2	1:21:A:LYS:HE3	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	2:1001:B:ASP:HB3	1:21:A:LYS:HE2	14	0.11
(2,27)	2:1001:B:ASP:HB3	1:21:A:LYS:HE3	14	0.11
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG21	16	0.11
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG22	16	0.11
(2,1)	1:130:A:ILE:HD11	2:1011:B:THR:HG23	16	0.11
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG21	16	0.11
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG22	16	0.11
(2,1)	1:130:A:ILE:HD12	2:1011:B:THR:HG23	16	0.11
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG21	16	0.11
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG22	16	0.11
(2,1)	1:130:A:ILE:HD13	2:1011:B:THR:HG23	16	0.11
(1,158)	2:1008:B:ASN:O	2:1011:B:THR:N	12	0.11
(1,157)	2:1008:B:ASN:OD1	2:1010:B:TYR:N	3	0.11
(1,154)	2:1009:B:PRO:HA	1:74:A:ARG:NH2	2	0.11
(1,150)	1:148:A:LYS:O	1:152:A:MET:H	8	0.11
(1,144)	1:129:A:ASP:O	1:133:A:ARG:H	13	0.11
(1,144)	1:129:A:ASP:O	1:133:A:ARG:H	15	0.11
(1,143)	1:129:A:ASP:O	1:133:A:ARG:N	7	0.11
(1,143)	1:129:A:ASP:O	1:133:A:ARG:N	16	0.11
(1,141)	1:128:A:LEU:O	1:132:A:ASP:N	11	0.11
(1,140)	1:127:A:LEU:O	1:131:A:TRP:H	11	0.11
(1,140)	1:127:A:LEU:O	1:131:A:TRP:H	14	0.11
(1,138)	1:126:A:MET:O	1:130:A:ILE:H	9	0.11
(1,134)	1:124:A:ILE:O	1:128:A:LEU:H	20	0.11
(1,132)	1:123:A:LYS:O	1:127:A:LEU:H	12	0.11
(1,132)	1:123:A:LYS:O	1:127:A:LEU:H	17	0.11
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	13	0.11
(1,129)	1:122:A:GLU:O	1:126:A:MET:N	1	0.11
(1,129)	1:122:A:GLU:O	1:126:A:MET:N	10	0.11
(1,129)	1:122:A:GLU:O	1:126:A:MET:N	14	0.11
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	3	0.11
(1,100)	1:95:A:ALA:O	1:99:A:ASN:H	1	0.11
(1,96)	1:78:A:ASP:O	1:82:A:SER:H	14	0.11
(1,92)	1:76:A:TYR:O	1:80:A:THR:H	15	0.11
(1,88)	1:74:A:ARG:O	1:78:A:ASP:H	10	0.11
(1,88)	1:74:A:ARG:O	1:78:A:ASP:H	14	0.11
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	2	0.11
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	10	0.11
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	17	0.11
(1,81)	1:71:A:SER:O	1:75:A:ALA:N	15	0.11
(1,81)	1:71:A:SER:O	1:75:A:ALA:N	19	0.11
(1,75)	1:68:A:ILE:O	1:72:A:ILE:N	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	7	0.11
(1,74)	1:67:A:TYR:O	1:71:A:SER:H	8	0.11
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	2	0.11
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	12	0.11
(1,73)	1:67:A:TYR:O	1:71:A:SER:N	17	0.11
(1,68)	1:64:A:GLY:O	1:68:A:ILE:H	14	0.11
(1,64)	1:62:A:LYS:O	1:66:A:LEU:H	10	0.11
(1,52)	1:50:A:ILE:O	1:54:A:SER:H	4	0.11
(1,52)	1:50:A:ILE:O	1:54:A:SER:H	20	0.11
(1,43)	1:46:A:ILE:O	1:50:A:ILE:N	1	0.11
(1,43)	1:46:A:ILE:O	1:50:A:ILE:N	4	0.11
(1,43)	1:46:A:ILE:O	1:50:A:ILE:N	5	0.11
(1,43)	1:46:A:ILE:O	1:50:A:ILE:N	11	0.11
(1,43)	1:46:A:ILE:O	1:50:A:ILE:N	16	0.11
(1,34)	1:33:A:THR:O	1:37:A:LEU:H	2	0.11
(1,34)	1:33:A:THR:O	1:37:A:LEU:H	17	0.11
(1,34)	1:33:A:THR:O	1:37:A:LEU:H	18	0.11
(1,34)	1:33:A:THR:O	1:37:A:LEU:H	19	0.11
(1,24)	1:28:A:ARG:O	1:32:A:LEU:H	8	0.11
(1,24)	1:28:A:ARG:O	1:32:A:LEU:H	15	0.11
(1,23)	1:28:A:ARG:O	1:32:A:LEU:N	19	0.11
(1,22)	1:27:A:SER:O	1:31:A:LYS:H	3	0.11
(1,8)	1:10:A:PHE:O	1:14:A:LEU:H	8	0.11
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	3	0.11
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	5	0.11
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	12	0.11
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	15	0.11
(2,2287)	1:122:A:GLU:HA	1:125:A:ARG:HD2	18	0.1
(2,2287)	1:122:A:GLU:HA	1:125:A:ARG:HD3	18	0.1
(2,2286)	1:122:A:GLU:H	1:122:A:GLU:HG2	8	0.1
(2,2286)	1:122:A:GLU:H	1:122:A:GLU:HG3	8	0.1
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG2	3	0.1
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG3	3	0.1
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG2	20	0.1
(2,2285)	1:121:A:LYS:H	1:122:A:GLU:HG3	20	0.1
(2,2100)	1:24:A:ILE:HB	1:64:A:GLY:HA2	7	0.1
(2,2100)	1:24:A:ILE:HB	1:64:A:GLY:HA3	7	0.1
(2,2094)	1:20:A:LEU:HG	1:23:A:GLY:HA2	1	0.1
(2,2094)	1:20:A:LEU:HG	1:23:A:GLY:HA3	1	0.1
(2,2083)	1:9:A:ASN:HB2	1:31:A:LYS:HG2	14	0.1
(2,2083)	1:9:A:ASN:HB2	1:31:A:LYS:HG3	14	0.1
(2,2083)	1:9:A:ASN:HB3	1:31:A:LYS:HG2	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2083)	1:9:A:ASN:HB3	1:31:A:LYS:HG3	14	0.1
(2,2074)	1:5:A:ASP:HA	1:9:A:ASN:HB2	11	0.1
(2,2074)	1:5:A:ASP:HA	1:9:A:ASN:HB3	11	0.1
(2,1987)	1:111:A:ASP:H	1:111:A:ASP:HB3	1	0.1
(2,1987)	1:111:A:ASP:H	1:111:A:ASP:HB3	16	0.1
(2,1987)	1:111:A:ASP:H	1:111:A:ASP:HB3	19	0.1
(2,1987)	1:111:A:ASP:H	1:111:A:ASP:HB3	20	0.1
(2,1895)	1:67:A:TYR:H	1:70:A:ASP:HB2	3	0.1
(2,1847)	1:151:A:ALA:H	1:155:A:GLU:H	15	0.1
(2,1840)	1:38:A:ASP:HA	1:40:A:ILE:H	7	0.1
(2,1819)	1:37:A:LEU:H	1:37:A:LEU:HD21	6	0.1
(2,1819)	1:37:A:LEU:H	1:37:A:LEU:HD22	6	0.1
(2,1819)	1:37:A:LEU:H	1:37:A:LEU:HD23	6	0.1
(2,1782)	1:69:A:ILE:HG21	1:74:A:ARG:H	3	0.1
(2,1782)	1:69:A:ILE:HG22	1:74:A:ARG:H	3	0.1
(2,1782)	1:69:A:ILE:HG23	1:74:A:ARG:H	3	0.1
(2,1775)	1:117:A:ASN:H	1:119:A:ASP:H	12	0.1
(2,1759)	1:40:A:ILE:H	1:42:A:ILE:H	8	0.1
(2,1672)	1:115:A:LYS:HE2	1:116:A:SER:H	18	0.1
(2,1672)	1:115:A:LYS:HE3	1:116:A:SER:H	18	0.1
(2,1645)	1:43:A:GLU:H	1:93:A:THR:H	18	0.1
(2,1630)	1:151:A:ALA:H	1:153:A:ASP:H	7	0.1
(2,1630)	1:151:A:ALA:H	1:153:A:ASP:H	12	0.1
(2,1630)	1:151:A:ALA:H	1:153:A:ASP:H	13	0.1
(2,1622)	1:145:A:ILE:HB	1:147:A:SER:H	18	0.1
(2,1611)	1:67:A:TYR:HE1	1:127:A:LEU:H	19	0.1
(2,1611)	1:67:A:TYR:HE2	1:127:A:LEU:H	19	0.1
(2,1577)	1:115:A:LYS:H	1:115:A:LYS:HB3	2	0.1
(2,1541)	1:105:A:ILE:H	1:106:A:GLN:HB3	9	0.1
(2,1541)	1:105:A:ILE:H	1:106:A:GLN:HB3	10	0.1
(2,1541)	1:105:A:ILE:H	1:106:A:GLN:HB3	16	0.1
(2,1541)	1:105:A:ILE:H	1:106:A:GLN:HB3	19	0.1
(2,1533)	1:104:A:VAL:H	1:106:A:GLN:HG2	3	0.1
(2,1533)	1:104:A:VAL:H	1:106:A:GLN:HG2	11	0.1
(2,1431)	1:63:A:LEU:HD11	1:66:A:LEU:H	3	0.1
(2,1431)	1:63:A:LEU:HD12	1:66:A:LEU:H	3	0.1
(2,1431)	1:63:A:LEU:HD13	1:66:A:LEU:H	3	0.1
(2,1216)	1:15:A:GLU:HB2	1:17:A:PHE:H	13	0.1
(2,1216)	1:15:A:GLU:HB3	1:17:A:PHE:H	13	0.1
(2,1167)	1:10:A:PHE:H	1:11:A:VAL:HG11	11	0.1
(2,1167)	1:10:A:PHE:H	1:11:A:VAL:HG12	11	0.1
(2,1167)	1:10:A:PHE:H	1:11:A:VAL:HG13	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1143)	1:7:A:PHE:H	1:10:A:PHE:HB3	20	0.1
(2,1062)	1:43:A:GLU:HA	1:47:A:ILE:HG12	19	0.1
(2,1060)	1:62:A:LYS:HG2	1:115:A:LYS:HE2	20	0.1
(2,1060)	1:62:A:LYS:HG2	1:115:A:LYS:HE3	20	0.1
(2,1060)	1:62:A:LYS:HG3	1:115:A:LYS:HE2	20	0.1
(2,1060)	1:62:A:LYS:HG3	1:115:A:LYS:HE3	20	0.1
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG12	4	0.1
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG13	4	0.1
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG12	4	0.1
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG13	4	0.1
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG12	4	0.1
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG13	4	0.1
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG12	13	0.1
(2,1044)	1:109:A:LEU:HD21	1:124:A:ILE:HG13	13	0.1
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG12	13	0.1
(2,1044)	1:109:A:LEU:HD22	1:124:A:ILE:HG13	13	0.1
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG12	13	0.1
(2,1044)	1:109:A:LEU:HD23	1:124:A:ILE:HG13	13	0.1
(2,1019)	1:105:A:ILE:HD11	1:108:A:LEU:HB3	4	0.1
(2,1019)	1:105:A:ILE:HD12	1:108:A:LEU:HB3	4	0.1
(2,1019)	1:105:A:ILE:HD13	1:108:A:LEU:HB3	4	0.1
(2,1011)	1:142:A:LEU:HD21	1:144:A:ALA:HA	19	0.1
(2,1011)	1:142:A:LEU:HD22	1:144:A:ALA:HA	19	0.1
(2,1011)	1:142:A:LEU:HD23	1:144:A:ALA:HA	19	0.1
(2,962)	1:126:A:MET:HB3	1:126:A:MET:HE1	10	0.1
(2,962)	1:126:A:MET:HB3	1:126:A:MET:HE2	10	0.1
(2,962)	1:126:A:MET:HB3	1:126:A:MET:HE3	10	0.1
(2,942)	1:66:A:LEU:HD11	1:109:A:LEU:HD21	13	0.1
(2,942)	1:66:A:LEU:HD11	1:109:A:LEU:HD22	13	0.1
(2,942)	1:66:A:LEU:HD11	1:109:A:LEU:HD23	13	0.1
(2,942)	1:66:A:LEU:HD12	1:109:A:LEU:HD21	13	0.1
(2,942)	1:66:A:LEU:HD12	1:109:A:LEU:HD22	13	0.1
(2,942)	1:66:A:LEU:HD12	1:109:A:LEU:HD23	13	0.1
(2,942)	1:66:A:LEU:HD13	1:109:A:LEU:HD21	13	0.1
(2,942)	1:66:A:LEU:HD13	1:109:A:LEU:HD22	13	0.1
(2,942)	1:66:A:LEU:HD13	1:109:A:LEU:HD23	13	0.1
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG21	4	0.1
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG22	4	0.1
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG23	4	0.1
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG21	4	0.1
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG22	4	0.1
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG23	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG21	4	0.1
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG22	4	0.1
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG23	4	0.1
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG21	9	0.1
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG22	9	0.1
(2,940)	1:14:A:LEU:HD21	1:68:A:ILE:HG23	9	0.1
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG21	9	0.1
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG22	9	0.1
(2,940)	1:14:A:LEU:HD22	1:68:A:ILE:HG23	9	0.1
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG21	9	0.1
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG22	9	0.1
(2,940)	1:14:A:LEU:HD23	1:68:A:ILE:HG23	9	0.1
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	10	0.1
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	10	0.1
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	10	0.1
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD11	16	0.1
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD12	16	0.1
(2,934)	1:109:A:LEU:HB2	1:113:A:ILE:HD13	16	0.1
(2,927)	1:125:A:ARG:HG2	1:126:A:MET:HA	19	0.1
(2,901)	1:126:A:MET:HA	1:129:A:ASP:HA	8	0.1
(2,901)	1:126:A:MET:HA	1:129:A:ASP:HA	16	0.1
(2,894)	1:77:A:LEU:HA	1:78:A:ASP:HB2	13	0.1
(2,807)	1:104:A:VAL:HA	1:107:A:GLU:HB3	10	0.1
(2,807)	1:104:A:VAL:HA	1:107:A:GLU:HB3	13	0.1
(2,735)	1:80:A:THR:HG21	1:94:A:CYS:HA	17	0.1
(2,735)	1:80:A:THR:HG22	1:94:A:CYS:HA	17	0.1
(2,735)	1:80:A:THR:HG23	1:94:A:CYS:HA	17	0.1
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG21	2	0.1
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG22	2	0.1
(2,726)	1:42:A:ILE:H	1:93:A:THR:HG23	2	0.1
(2,714)	1:76:A:TYR:HA	1:97:A:ALA:HB1	1	0.1
(2,714)	1:76:A:TYR:HA	1:97:A:ALA:HB2	1	0.1
(2,714)	1:76:A:TYR:HA	1:97:A:ALA:HB3	1	0.1
(2,714)	1:76:A:TYR:HA	1:97:A:ALA:HB1	10	0.1
(2,714)	1:76:A:TYR:HA	1:97:A:ALA:HB2	10	0.1
(2,714)	1:76:A:TYR:HA	1:97:A:ALA:HB3	10	0.1
(2,714)	1:76:A:TYR:HA	1:97:A:ALA:HB1	14	0.1
(2,714)	1:76:A:TYR:HA	1:97:A:ALA:HB2	14	0.1
(2,714)	1:76:A:TYR:HA	1:97:A:ALA:HB3	14	0.1
(2,708)	1:33:A:THR:HG21	1:75:A:ALA:H	3	0.1
(2,708)	1:33:A:THR:HG22	1:75:A:ALA:H	3	0.1
(2,708)	1:33:A:THR:HG23	1:75:A:ALA:H	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,674)	1:39:A:HIS:H	1:46:A:ILE:HD11	14	0.1
(2,674)	1:39:A:HIS:H	1:46:A:ILE:HD12	14	0.1
(2,674)	1:39:A:HIS:H	1:46:A:ILE:HD13	14	0.1
(2,491)	1:40:A:ILE:HG21	1:41:A:ASP:HA	18	0.1
(2,491)	1:40:A:ILE:HG22	1:41:A:ASP:HA	18	0.1
(2,491)	1:40:A:ILE:HG23	1:41:A:ASP:HA	18	0.1
(2,488)	1:40:A:ILE:HG21	1:41:A:ASP:H	5	0.1
(2,488)	1:40:A:ILE:HG22	1:41:A:ASP:H	5	0.1
(2,488)	1:40:A:ILE:HG23	1:41:A:ASP:H	5	0.1
(2,488)	1:40:A:ILE:HG21	1:41:A:ASP:H	10	0.1
(2,488)	1:40:A:ILE:HG22	1:41:A:ASP:H	10	0.1
(2,488)	1:40:A:ILE:HG23	1:41:A:ASP:H	10	0.1
(2,488)	1:40:A:ILE:HG21	1:41:A:ASP:H	18	0.1
(2,488)	1:40:A:ILE:HG22	1:41:A:ASP:H	18	0.1
(2,488)	1:40:A:ILE:HG23	1:41:A:ASP:H	18	0.1
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	1	0.1
(2,451)	1:34:A:THR:HB	1:35:A:TYR:H	7	0.1
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB2	17	0.1
(2,323)	1:11:A:VAL:HG11	1:15:A:GLU:HB3	17	0.1
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB2	17	0.1
(2,323)	1:11:A:VAL:HG12	1:15:A:GLU:HB3	17	0.1
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB2	17	0.1
(2,323)	1:11:A:VAL:HG13	1:15:A:GLU:HB3	17	0.1
(2,316)	1:11:A:VAL:HA	1:49:A:LEU:HB2	3	0.1
(2,301)	1:11:A:VAL:HG21	1:49:A:LEU:HB2	18	0.1
(2,301)	1:11:A:VAL:HG22	1:49:A:LEU:HB2	18	0.1
(2,301)	1:11:A:VAL:HG23	1:49:A:LEU:HB2	18	0.1
(2,298)	1:11:A:VAL:HG21	1:15:A:GLU:H	9	0.1
(2,298)	1:11:A:VAL:HG22	1:15:A:GLU:H	9	0.1
(2,298)	1:11:A:VAL:HG23	1:15:A:GLU:H	9	0.1
(2,281)	1:128:A:LEU:HD11	1:129:A:ASP:H	17	0.1
(2,281)	1:128:A:LEU:HD12	1:129:A:ASP:H	17	0.1
(2,281)	1:128:A:LEU:HD13	1:129:A:ASP:H	17	0.1
(2,277)	1:47:A:ILE:HB	1:76:A:TYR:HE1	6	0.1
(2,277)	1:47:A:ILE:HB	1:76:A:TYR:HE2	6	0.1
(2,275)	1:151:A:ALA:HA	1:155:A:GLU:HA	9	0.1
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD21	15	0.1
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD22	15	0.1
(2,258)	1:104:A:VAL:HA	1:108:A:LEU:HD23	15	0.1
(2,252)	1:153:A:ASP:HB3	1:154:A:LEU:HB3	2	0.1
(2,216)	1:42:A:ILE:HA	1:45:A:LYS:HB2	8	0.1
(2,203)	1:99:A:ASN:HB2	1:100:A:THR:H	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,187)	1:104:A:VAL:HG11	1:105:A:ILE:H	6	0.1
(2,187)	1:104:A:VAL:HG12	1:105:A:ILE:H	6	0.1
(2,187)	1:104:A:VAL:HG13	1:105:A:ILE:H	6	0.1
(2,167)	1:63:A:LEU:HD11	1:67:A:TYR:HB2	4	0.1
(2,167)	1:63:A:LEU:HD12	1:67:A:TYR:HB2	4	0.1
(2,167)	1:63:A:LEU:HD13	1:67:A:TYR:HB2	4	0.1
(2,157)	1:118:A:GLN:HA	1:121:A:LYS:HD2	7	0.1
(2,147)	1:146:A:ARG:HB2	1:147:A:SER:HB2	10	0.1
(2,147)	1:146:A:ARG:HB2	1:147:A:SER:HB3	10	0.1
(2,147)	1:146:A:ARG:HB3	1:147:A:SER:HB2	10	0.1
(2,147)	1:146:A:ARG:HB3	1:147:A:SER:HB3	10	0.1
(2,131)	1:122:A:GLU:HA	1:125:A:ARG:HB2	6	0.1
(2,128)	1:63:A:LEU:HD11	1:123:A:LYS:HA	5	0.1
(2,128)	1:63:A:LEU:HD12	1:123:A:LYS:HA	5	0.1
(2,128)	1:63:A:LEU:HD13	1:123:A:LYS:HA	5	0.1
(2,98)	1:24:A:ILE:HB	1:67:A:TYR:HE1	14	0.1
(2,98)	1:24:A:ILE:HB	1:67:A:TYR:HE2	14	0.1
(2,98)	1:24:A:ILE:HB	1:67:A:TYR:HE1	20	0.1
(2,98)	1:24:A:ILE:HB	1:67:A:TYR:HE2	20	0.1
(1,155)	2:1007:B:TYR:OH	1:74:A:ARG:NH2	18	0.1
(1,144)	1:129:A:ASP:O	1:133:A:ARG:H	9	0.1
(1,137)	1:126:A:MET:O	1:130:A:ILE:N	1	0.1
(1,134)	1:124:A:ILE:O	1:128:A:LEU:H	11	0.1
(1,132)	1:123:A:LYS:O	1:127:A:LEU:H	2	0.1
(1,132)	1:123:A:LYS:O	1:127:A:LEU:H	16	0.1
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	3	0.1
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	5	0.1
(1,130)	1:122:A:GLU:O	1:126:A:MET:H	9	0.1
(1,129)	1:122:A:GLU:O	1:126:A:MET:N	7	0.1
(1,128)	1:121:A:LYS:O	1:125:A:ARG:H	11	0.1
(1,127)	1:121:A:LYS:O	1:125:A:ARG:N	9	0.1
(1,127)	1:121:A:LYS:O	1:125:A:ARG:N	18	0.1
(1,110)	1:106:A:GLN:O	1:110:A:SER:H	12	0.1
(1,104)	1:97:A:ALA:O	1:101:A:LEU:H	14	0.1
(1,99)	1:95:A:ALA:O	1:99:A:ASN:N	10	0.1
(1,96)	1:78:A:ASP:O	1:82:A:SER:H	6	0.1
(1,96)	1:78:A:ASP:O	1:82:A:SER:H	16	0.1
(1,92)	1:76:A:TYR:O	1:80:A:THR:H	16	0.1
(1,87)	1:74:A:ARG:O	1:78:A:ASP:N	16	0.1
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	11	0.1
(1,82)	1:71:A:SER:O	1:75:A:ALA:H	20	0.1
(1,81)	1:71:A:SER:O	1:75:A:ALA:N	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:71:A:SER:O	1:75:A:ALA:N	12	0.1
(1,72)	1:66:A:LEU:O	1:70:A:ASP:H	15	0.1
(1,67)	1:64:A:GLY:O	1:68:A:ILE:N	9	0.1
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	3	0.1
(1,66)	1:63:A:LEU:O	1:67:A:TYR:H	12	0.1
(1,64)	1:62:A:LYS:O	1:66:A:LEU:H	14	0.1
(1,52)	1:50:A:ILE:O	1:54:A:SER:H	19	0.1
(1,34)	1:33:A:THR:O	1:37:A:LEU:H	9	0.1
(1,24)	1:28:A:ARG:O	1:32:A:LEU:H	3	0.1
(1,24)	1:28:A:ARG:O	1:32:A:LEU:H	5	0.1
(1,23)	1:28:A:ARG:O	1:32:A:LEU:N	16	0.1
(1,23)	1:28:A:ARG:O	1:32:A:LEU:N	18	0.1
(1,22)	1:27:A:SER:O	1:31:A:LYS:H	4	0.1
(1,22)	1:27:A:SER:O	1:31:A:LYS:H	9	0.1
(1,21)	1:27:A:SER:O	1:31:A:LYS:N	6	0.1
(1,14)	1:13:A:THR:O	1:17:A:PHE:H	8	0.1
(1,7)	1:10:A:PHE:O	1:14:A:LEU:N	17	0.1

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

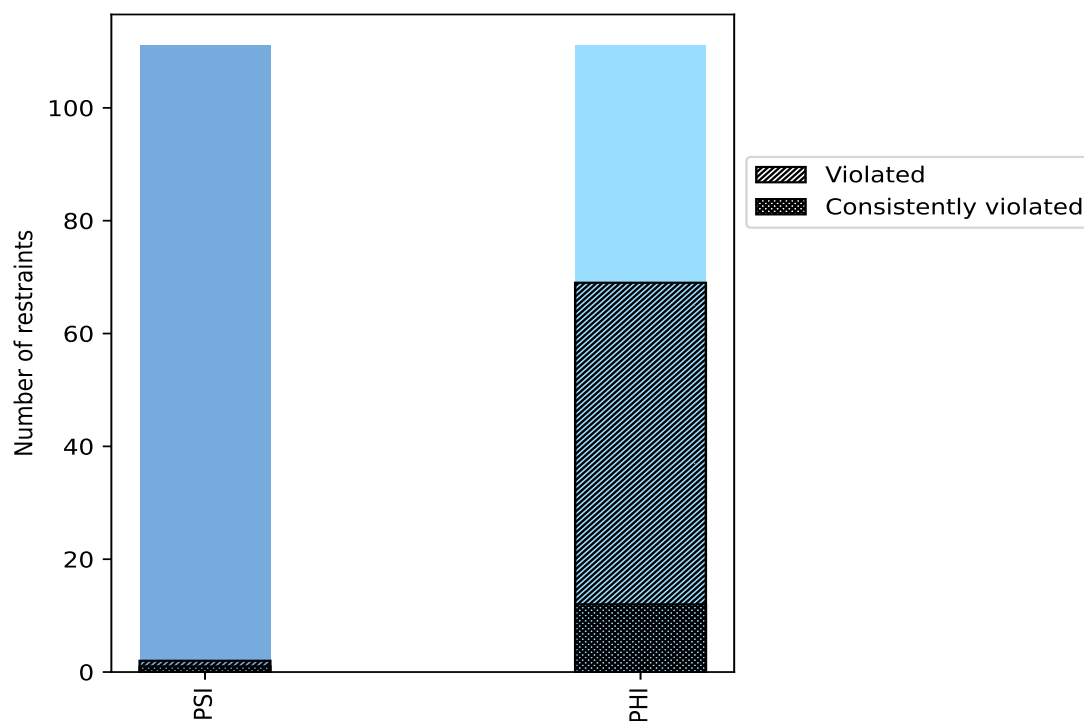
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	111	50.0	2	1.8	0.9	1	0.9	0.5
PHI	111	50.0	69	62.2	31.1	12	10.8	5.4
Total	222	100.0	71	32.0	32.0	13	5.9	5.9

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

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



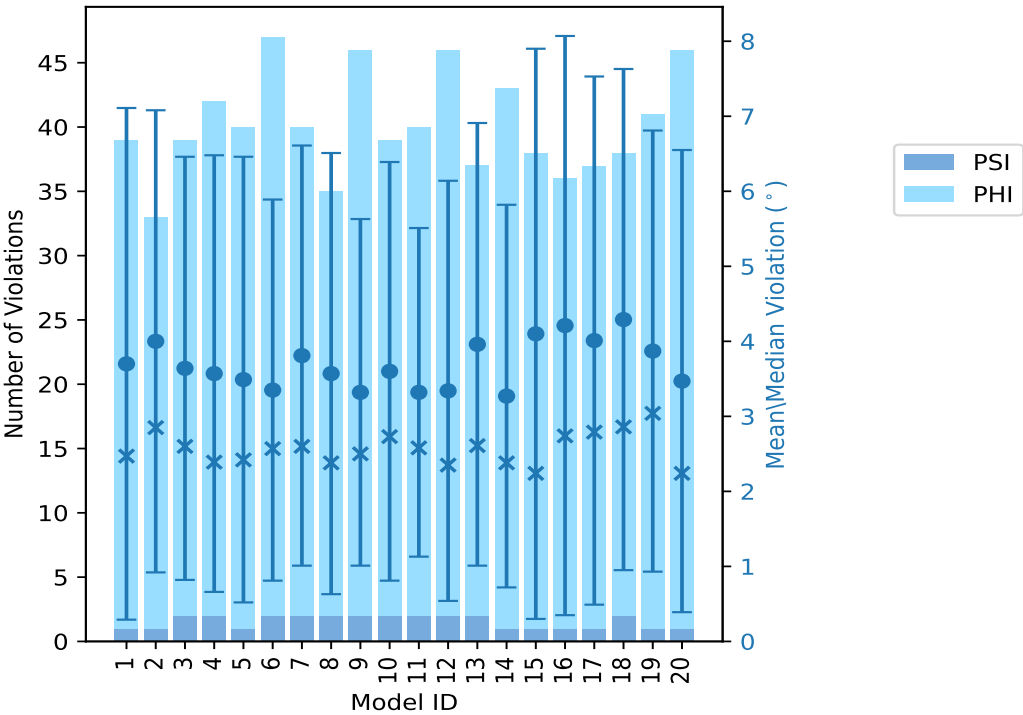
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	1	38	39	3.7	15.53	3.41	2.47
2	1	32	33	4.0	13.34	3.08	2.85
3	2	37	39	3.64	13.95	2.82	2.6
4	2	40	42	3.57	12.55	2.91	2.39
5	1	39	40	3.49	13.15	2.97	2.42
6	2	45	47	3.35	11.96	2.54	2.57
7	2	38	40	3.81	12.9	2.8	2.6
8	2	33	35	3.57	13.63	2.94	2.38
9	2	44	46	3.32	11.82	2.31	2.5
10	2	37	39	3.6	13.85	2.79	2.73
11	2	38	40	3.32	9.66	2.19	2.58
12	2	44	46	3.34	12.07	2.8	2.35
13	2	35	37	3.96	11.81	2.95	2.61
14	1	42	43	3.27	11.89	2.55	2.38
15	1	37	38	4.1	16.1	3.8	2.24
16	1	35	36	4.21	16.93	3.86	2.74
17	1	36	37	4.01	13.56	3.52	2.79
18	2	36	38	4.29	14.57	3.34	2.86
19	1	40	41	3.87	13.33	2.94	3.04
20	1	45	46	3.47	16.15	3.08	2.24

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	5	5	1	5.0
0	4	4	2	10.0
0	1	1	3	15.0
0	6	6	4	20.0
0	1	1	5	25.0
0	7	7	6	30.0
0	2	2	7	35.0
0	6	6	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
1	4	5	11	55.0

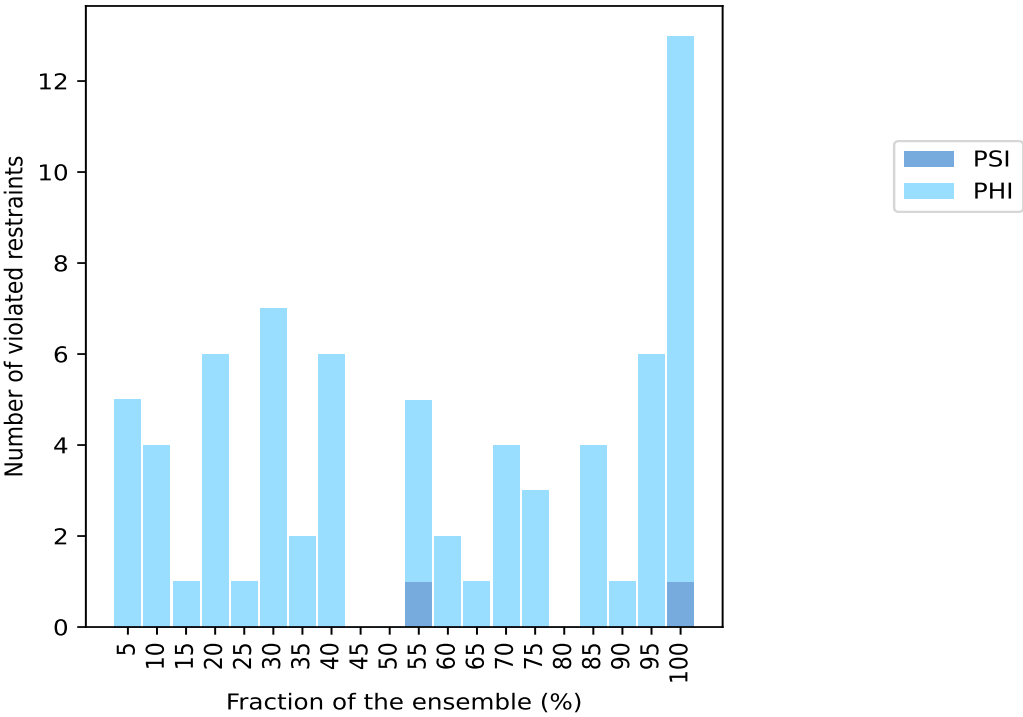
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	2	2	12	60.0
0	1	1	13	65.0
0	4	4	14	70.0
0	3	3	15	75.0
0	0	0	16	80.0
0	4	4	17	85.0
0	1	1	18	90.0
0	6	6	19	95.0
1	12	13	20	100.0

¹ Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

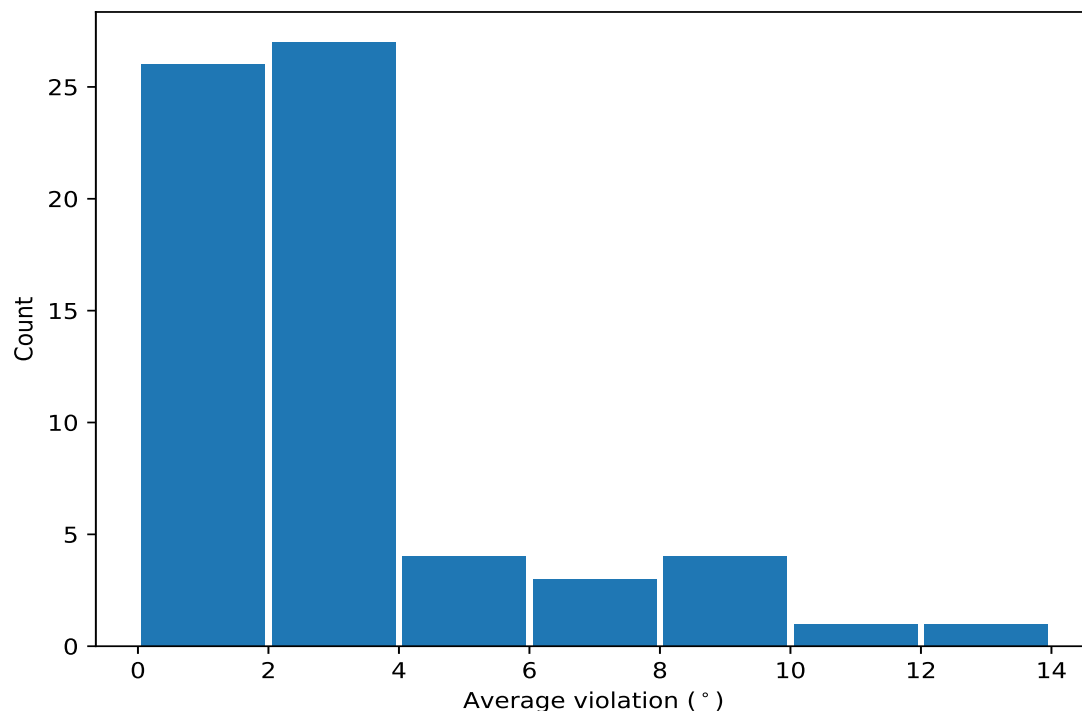


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle 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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	20	12.36	2.03	12.6
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	20	10.1	2.64	10.06
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	20	8.87	2.52	10.05
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	20	8.44	1.16	8.36
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	20	7.63	0.39	7.68
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	20	6.2	0.62	6.34
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	20	3.72	0.57	3.65
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	20	3.15	0.72	3.16
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	20	2.69	0.45	2.64
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	20	2.66	0.55	2.76
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	20	2.47	0.46	2.4
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	20	2.43	0.38	2.48
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	20	2.43	0.66	2.31
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	19	4.51	1.43	4.07
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	19	3.55	0.63	3.65
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	19	3.28	1.27	2.95
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	19	2.65	1.53	2.34
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	19	2.62	0.74	2.76
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	19	2.3	0.32	2.36
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	18	2.37	0.72	2.44

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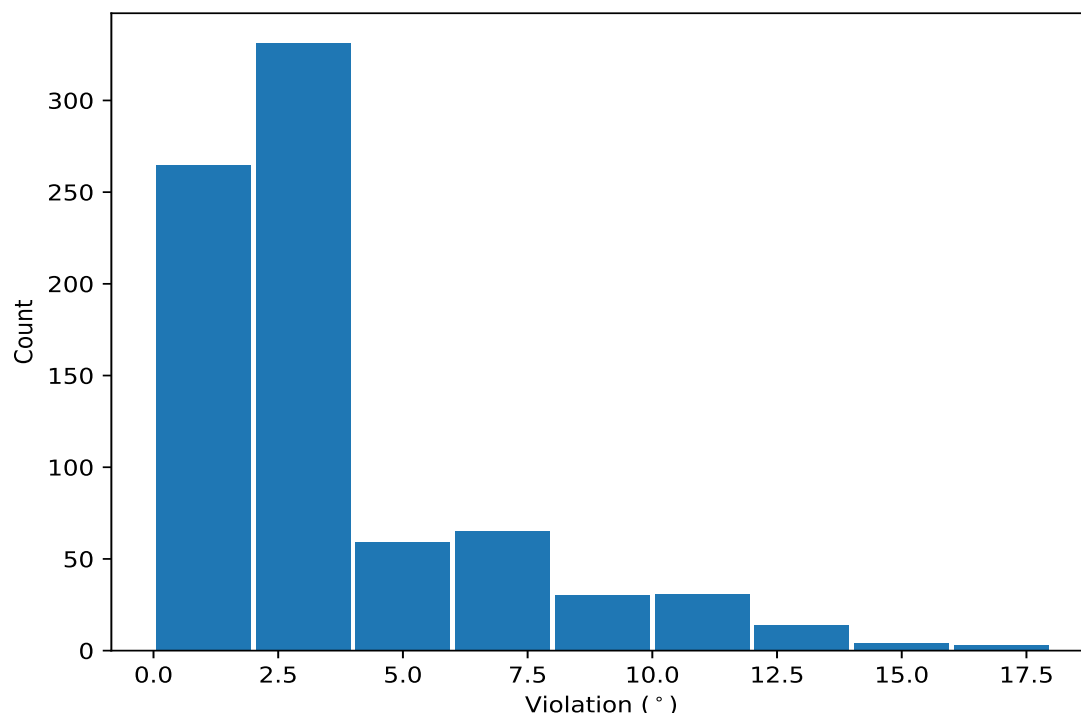
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	17	5.68	2.27	5.9
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	17	2.77	0.38	2.79
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	17	2.3	0.79	2.33
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	17	2.16	0.58	2.14
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	15	8.45	4.47	6.04
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	15	1.66	0.35	1.68
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	15	1.56	0.34	1.53
(1,21)	1:16:A:SER:C	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	14	2.07	0.7	2.01
(1,19)	1:15:A:GLU:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	14	2.02	0.91	1.88
(1,71)	1:51:A:ILE:C	1:52:A:ASP:N	1:52:A:ASP:CA	1:52:A:ASP:C	14	1.86	0.65	1.86
(1,99)	1:67:A:TYR:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	14	1.78	0.38	1.86
(1,23)	1:17:A:PHE:C	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	13	2.32	1.22	1.93
(1,215)	1:149:A:CYS:C	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	12	2.82	0.98	2.77
(1,151)	1:106:A:GLN:C	1:107:A:GLU:N	1:107:A:GLU:CA	1:107:A:GLU:C	12	1.4	0.27	1.4
(1,216)	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	1:151:A:ALA:N	11	6.41	4.28	9.51
(1,79)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	11	5.45	1.82	5.8
(1,25)	1:18:A:LYS:C	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:C	11	2.13	1.21	1.45
(1,101)	1:68:A:ILE:C	1:69:A:ILE:N	1:69:A:ILE:CA	1:69:A:ILE:C	11	1.77	0.51	1.7
(1,59)	1:45:A:LYS:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	11	1.52	0.28	1.41
(1,219)	1:151:A:ALA:C	1:152:A:MET:N	1:152:A:MET:CA	1:152:A:MET:C	8	4.89	1.54	5.24
(1,105)	1:70:A:ASP:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	8	1.58	0.16	1.64
(1,69)	1:50:A:ILE:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	8	1.53	0.29	1.4
(1,137)	1:97:A:ALA:C	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	8	1.45	0.36	1.34
(1,139)	1:98:A:ILE:C	1:99:A:ASN:N	1:99:A:ASN:CA	1:99:A:ASN:C	8	1.34	0.22	1.32
(1,15)	1:13:A:THR:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	8	1.33	0.19	1.35
(1,201)	1:133:A:ARG:C	1:134:A:SER:N	1:134:A:SER:CA	1:134:A:SER:C	7	2.25	0.9	2.07
(1,121)	1:78:A:ASP:C	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	7	1.77	1.29	1.26
(1,77)	1:54:A:SER:C	1:55:A:ARG:N	1:55:A:ARG:CA	1:55:A:ARG:C	6	2.7	1.25	2.42
(1,83)	1:59:A:ASP:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	6	2.6	0.84	2.42
(1,113)	1:74:A:ARG:C	1:75:A:ALA:N	1:75:A:ALA:CA	1:75:A:ALA:C	6	1.95	1.41	1.2
(1,135)	1:96:A:HIS:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	6	1.87	0.37	1.69
(1,153)	1:107:A:GLU:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	6	1.5	0.26	1.49
(1,141)	1:99:A:ASN:C	1:100:A:THR:N	1:100:A:THR:CA	1:100:A:THR:C	6	1.46	0.27	1.5
(1,35)	1:29:A:ILE:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	6	1.2	0.13	1.22
(1,7)	1:9:A:ASN:C	1:10:A:PHE:N	1:10:A:PHE:CA	1:10:A:PHE:C	5	1.21	0.15	1.18
(1,217)	1:150:A:PHE:C	1:151:A:ALA:N	1:151:A:ALA:CA	1:151:A:ALA:C	4	8.5	3.91	8.8
(1,1)	1:6:A:ASP:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	4	2.08	0.61	2.16
(1,203)	1:142:A:LEU:C	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	4	2.01	0.64	1.78
(1,163)	1:112:A:ALA:C	1:113:A:ILE:N	1:113:A:ILE:CA	1:113:A:ILE:C	4	1.79	0.89	1.38
(1,161)	1:111:A:ASP:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	4	1.65	0.44	1.72
(1,185)	1:125:A:ARG:C	1:126:A:MET:N	1:126:A:MET:CA	1:126:A:MET:C	4	1.64	0.3	1.73
(1,27)	1:25:A:SER:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	3	1.39	0.25	1.51
(1,3)	1:7:A:PHE:C	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	2	2.36	0.23	2.36
(1,73)	1:52:A:ASP:C	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	2	1.6	0.01	1.6
(1,199)	1:132:A:ASP:C	1:133:A:ARG:N	1:133:A:ARG:CA	1:133:A:ARG:C	2	1.54	0.36	1.54
(1,197)	1:131:A:TRP:C	1:132:A:ASP:N	1:132:A:ASP:CA	1:132:A:ASP:C	2	1.22	0.04	1.22

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	16	16.93
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	20	16.15
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	15	16.1
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	1	15.53
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	15	14.84
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	18	14.57
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	16	14.32
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	3	13.95
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	10	13.85
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	8	13.63
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	17	13.56
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	2	13.34
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	19	13.33
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	5	13.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	7	12.9
(1,217)	1:150:A:PHE:C	1:151:A:ALA:N	1:151:A:ALA:CA	1:151:A:ALA:C	16	12.87
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	17	12.8
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	15	12.74
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	19	12.64
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	4	12.55
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	12	12.07
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	6	11.96
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	14	11.89
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	9	11.82
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	14	11.82
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	13	11.81
(1,217)	1:150:A:PHE:C	1:151:A:ALA:N	1:151:A:ALA:CA	1:151:A:ALA:C	1	11.73
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	5	11.62
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	2	11.49
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	18	11.48
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	17	11.16
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	16	11.14
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	13	11.13
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	20	11.01
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	17	10.98
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	18	10.98
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	18	10.97
(1,216)	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	1:151:A:ALA:N	13	10.97
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	1	10.94
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	1	10.92
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	12	10.63
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	4	10.59
(1,216)	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	1:151:A:ALA:N	4	10.53
(1,216)	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	1:151:A:ALA:N	12	10.49
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	6	10.46
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	20	10.45
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	19	10.34
(1,216)	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	1:151:A:ALA:N	18	10.23
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	4	10.23
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	15	10.12
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	3	10.09
(1,216)	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	1:151:A:ALA:N	7	10.08
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	10	9.98
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	20	9.89
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	17	9.82
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	11	9.66
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	12	9.56
(1,216)	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	1:151:A:ALA:N	9	9.51
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	5	9.24
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	10	9.22
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	2	9.03
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	7	8.86
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	17	8.83
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	19	8.82
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	15	8.81

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	11	8.79
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	1	8.73
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	2	8.69
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	3	8.68
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	6	8.66
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	16	8.6
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	13	8.58
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	14	8.53
(1,207)	1:144:A:ALA:C	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	8	8.45
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	9	8.4
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	13	8.33
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	4	8.33
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	5	8.25
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	6	8.14
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	5	8.07
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	3	8.06
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	3	8.04
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	6	7.94
(1,79)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	5	7.94
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	7	7.93
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	17	7.92
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	8	7.9
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	10	7.89
(1,79)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	7	7.87
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	2	7.85
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	8	7.84
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	7	7.82
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	15	7.77
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	4	7.71
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	8	7.7
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	20	7.69
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	8	7.68
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	8	7.66
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	18	7.63
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	14	7.58
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	2	7.54
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	16	7.53
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	15	7.53
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	12	7.51
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	11	7.44
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	7	7.38
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	18	7.33
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	9	7.32
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	11	7.25
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	12	7.24
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	13	7.22
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	10	7.22
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	9	7.2
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	19	7.09
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	19	7.01
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1	7.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,75)	1:53:A:TYR:C	1:54:A:SER:N	1:54:A:SER:CA	1:54:A:SER:C	14	7.01
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	10	6.97
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	7	6.92
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	13	6.84
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	11	6.82
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	5	6.78
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	20	6.77
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	5	6.74
(1,171)	1:118:A:GLN:C	1:119:A:ASP:N	1:119:A:ASP:CA	1:119:A:ASP:C	1	6.74
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	15	6.68
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	16	6.58
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	8	6.51
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	3	6.51
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	4	6.47
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	14	6.47
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	11	6.46
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	19	6.43
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	3	6.39
(1,219)	1:151:A:ALA:C	1:152:A:MET:N	1:152:A:MET:CA	1:152:A:MET:C	18	6.34
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	20	6.3
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	11	6.3
(1,79)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	12	6.29
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	13	6.25
(1,23)	1:17:A:PHE:C	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	6	6.22
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	18	6.21
(1,221)	1:152:A:MET:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	9	6.19
(1,79)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	13	6.17
(1,79)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	15	6.17
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	2	6.1
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	18	6.06
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	10	6.04
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	16	5.99
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	4	5.98
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	10	5.9
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	19	5.9
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	2	5.89
(1,217)	1:150:A:PHE:C	1:151:A:ALA:N	1:151:A:ALA:CA	1:151:A:ALA:C	19	5.88
(1,219)	1:151:A:ALA:C	1:152:A:MET:N	1:152:A:MET:CA	1:152:A:MET:C	12	5.87
(1,219)	1:151:A:ALA:C	1:152:A:MET:N	1:152:A:MET:CA	1:152:A:MET:C	13	5.87
(1,79)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	2	5.8
(1,79)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	3	5.75
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	6	5.66
(1,79)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	17	5.66
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	6	5.65
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	6	5.47
(1,219)	1:151:A:ALA:C	1:152:A:MET:N	1:152:A:MET:CA	1:152:A:MET:C	19	5.46
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	11	5.43
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	17	5.39
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	7	5.32
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	7	5.28
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	12	5.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,77)	1:54:A:SER:C	1:55:A:ARG:N	1:55:A:ARG:CA	1:55:A:ARG:C	18	5.16
(1,219)	1:151:A:ALA:C	1:152:A:MET:N	1:152:A:MET:CA	1:152:A:MET:C	7	5.03
(1,113)	1:74:A:ARG:C	1:75:A:ALA:N	1:75:A:ALA:CA	1:75:A:ALA:C	3	5.02
(1,215)	1:149:A:CYS:C	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	20	5.01
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	8	4.98
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	9	4.98
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	9	4.89
(1,121)	1:78:A:ASP:C	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	6	4.88
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	3	4.86
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1	4.83
(1,219)	1:151:A:ALA:C	1:152:A:MET:N	1:152:A:MET:CA	1:152:A:MET:C	4	4.8
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	12	4.73
(1,177)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	15	4.71
(1,219)	1:151:A:ALA:C	1:152:A:MET:N	1:152:A:MET:CA	1:152:A:MET:C	9	4.68
(1,19)	1:15:A:GLU:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	6	4.63
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	14	4.61
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	4	4.6
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	18	4.55
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	14	4.54
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	1	4.48
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	20	4.46
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	12	4.44
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	7	4.39
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	7	4.36
(1,83)	1:59:A:ASP:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	10	4.33
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	20	4.33
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	12	4.22
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	20	4.21
(1,25)	1:18:A:LYS:C	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:C	9	4.2
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	10	4.19
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	3	4.18
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	20	4.16
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	16	4.14
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	20	4.11
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	6	4.09
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	9	4.08
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	13	4.07
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	6	4.01
(1,25)	1:18:A:LYS:C	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:C	17	4.0
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	18	3.99
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	9	3.98
(1,25)	1:18:A:LYS:C	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:C	6	3.97
(1,215)	1:149:A:CYS:C	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	9	3.96
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	17	3.93
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	2	3.91
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	16	3.89
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	1	3.88
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	9	3.87
(1,201)	1:133:A:ARG:C	1:134:A:SER:N	1:134:A:SER:CA	1:134:A:SER:C	11	3.85
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1	3.82
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	12	3.76

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	19	3.74
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	19	3.74
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	17	3.73
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	15	3.71
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	2	3.7
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	15	3.68
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	11	3.68
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	14	3.67
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	9	3.66
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	14	3.66
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	10	3.65
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	1	3.65
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	19	3.61
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	3	3.61
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	8	3.59
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	14	3.58
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	13	3.58
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	13	3.57
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	3	3.55
(1,71)	1:51:A:ILE:C	1:52:A:ASP:N	1:52:A:ASP:CA	1:52:A:ASP:C	15	3.55
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	20	3.53
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	16	3.53
(1,217)	1:150:A:PHE:C	1:151:A:ALA:N	1:151:A:ALA:CA	1:151:A:ALA:C	20	3.52
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	16	3.51
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	5	3.49
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	16	3.49
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	8	3.48
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	19	3.47
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	17	3.46
(1,215)	1:149:A:CYS:C	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	7	3.45
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	6	3.42
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	2	3.4
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	1	3.4
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	18	3.4
(1,21)	1:16:A:SER:C	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	7	3.4
(1,206)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ILE:N	9	3.39
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	13	3.38
(1,79)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	11	3.36
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	14	3.35
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	11	3.33
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	2	3.33
(1,163)	1:112:A:ALA:C	1:113:A:ILE:N	1:113:A:ILE:CA	1:113:A:ILE:C	5	3.31
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	11	3.3
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	8	3.3
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	15	3.27
(1,215)	1:149:A:CYS:C	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	19	3.25
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	8	3.25
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	12	3.25
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	13	3.24
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	19	3.24
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	7	3.23

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	16	3.23
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	11	3.22
(1,87)	1:61:A:HIS:C	1:62:A:LYS:N	1:62:A:LYS:CA	1:62:A:LYS:C	14	3.2
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	5	3.2
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	6	3.2
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	10	3.19
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	5	3.18
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	18	3.17
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	8	3.16
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	2	3.16
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	10	3.16
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	10	3.16
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	3	3.14
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	7	3.14
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	11	3.14
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	18	3.13
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	6	3.12
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	11	3.11
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	7	3.11
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1	3.1
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	3	3.1
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	5	3.09
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	19	3.09
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	19	3.08
(1,21)	1:16:A:SER:C	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	10	3.08
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	13	3.07
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	15	3.07
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	11	3.07
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	19	3.07
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	15	3.07
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	13	3.07
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	17	3.07
(1,203)	1:142:A:LEU:C	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	19	3.06
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	14	3.06
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	12	3.06
(1,81)	1:58:A:PRO:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	4	3.04
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	11	3.04
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	17	3.04
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	19	3.04
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	1	3.03
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	6	3.02
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	19	3.01
(1,77)	1:54:A:SER:C	1:55:A:ARG:N	1:55:A:ARG:CA	1:55:A:ARG:C	6	3.01
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	17	3.0
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	14	3.0
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	4	2.99
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	3	2.97
(1,19)	1:15:A:GLU:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	18	2.97
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	18	2.95
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	19	2.95
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	5	2.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	2	2.95
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	9	2.94
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	18	2.93
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	14	2.93
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	13	2.93
(1,21)	1:16:A:SER:C	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	14	2.93
(1,77)	1:54:A:SER:C	1:55:A:ARG:N	1:55:A:ARG:CA	1:55:A:ARG:C	14	2.92
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	12	2.91
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	10	2.91
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	17	2.91
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	11	2.91
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	9	2.9
(1,215)	1:149:A:CYS:C	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	12	2.89
(1,201)	1:133:A:ARG:C	1:134:A:SER:N	1:134:A:SER:CA	1:134:A:SER:C	7	2.89
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	4	2.87
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1	2.87
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	2	2.87
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	12	2.87
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	10	2.86
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	17	2.86
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	2	2.85
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	5	2.85
(1,215)	1:149:A:CYS:C	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	4	2.83
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	2	2.83
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	10	2.83
(1,23)	1:17:A:PHE:C	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	9	2.83
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	6	2.82
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	16	2.82
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	4	2.82
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	6	2.81
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	15	2.81
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	6	2.81
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	9	2.8
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	16	2.79
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	17	2.79
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	4	2.79
(1,1)	1:6:A:ASP:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	18	2.79
(1,201)	1:133:A:ARG:C	1:134:A:SER:N	1:134:A:SER:CA	1:134:A:SER:C	16	2.78
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	9	2.78
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	9	2.78
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	16	2.78
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	8	2.77
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	4	2.76
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	17	2.76
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	3	2.75
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	10	2.75
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	19	2.75
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	2	2.75
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	10	2.73
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	14	2.72
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	14	2.72

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,215)	1:149:A:CYS:C	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	10	2.71
(1,19)	1:15:A:GLU:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	10	2.7
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	17	2.69
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	16	2.69
(1,83)	1:59:A:ASP:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	20	2.68
(1,79)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	8	2.68
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	16	2.68
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	9	2.67
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	4	2.64
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	19	2.64
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	3	2.64
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	4	2.64
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	12	2.64
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	3	2.63
(1,215)	1:149:A:CYS:C	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	13	2.61
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	13	2.61
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	5	2.61
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	7	2.61
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	5	2.61
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	3	2.6
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	12	2.6
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	14	2.6
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	2	2.6
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	7	2.6
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	1	2.59
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	6	2.59
(1,23)	1:17:A:PHE:C	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	4	2.59
(1,21)	1:16:A:SER:C	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	16	2.59
(1,3)	1:7:A:PHE:C	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	11	2.59
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1	2.58
(1,71)	1:51:A:ILE:C	1:52:A:ASP:N	1:52:A:ASP:CA	1:52:A:ASP:C	6	2.57
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	11	2.57
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	18	2.55
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	19	2.55
(1,23)	1:17:A:PHE:C	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	18	2.55
(1,135)	1:96:A:HIS:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	11	2.54
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	13	2.54
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	18	2.54
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	16	2.54
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	11	2.54
(1,101)	1:68:A:ILE:C	1:69:A:ILE:N	1:69:A:ILE:CA	1:69:A:ILE:C	20	2.53
(1,55)	1:43:A:GLU:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	7	2.52
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	20	2.52
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	12	2.51
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	5	2.51
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	12	2.51
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	6	2.5
(1,23)	1:17:A:PHE:C	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	20	2.5
(1,1)	1:6:A:ASP:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	19	2.5
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	5	2.49
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	1	2.49

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,145)	1:101:A:LEU:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	11	2.47
(1,89)	1:62:A:LYS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	1	2.47
(1,83)	1:59:A:ASP:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	16	2.47
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	20	2.47
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	11	2.46
(1,101)	1:68:A:ILE:C	1:69:A:ILE:N	1:69:A:ILE:CA	1:69:A:ILE:C	16	2.46
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	5	2.46
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	20	2.46
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	8	2.44
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	1	2.43
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	18	2.43
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	20	2.43
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	12	2.42
(1,99)	1:67:A:TYR:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	18	2.41
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	2	2.4
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	4	2.4
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	7	2.4
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	7	2.39
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	10	2.39
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	13	2.39
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	2	2.38
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	4	2.38
(1,83)	1:59:A:ASP:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	14	2.38
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	8	2.38
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	14	2.37
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	5	2.37
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	14	2.37
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	19	2.37
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	8	2.37
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	18	2.36
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	4	2.36
(1,101)	1:68:A:ILE:C	1:69:A:ILE:N	1:69:A:ILE:CA	1:69:A:ILE:C	15	2.35
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	17	2.35
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	16	2.34
(1,215)	1:149:A:CYS:C	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	18	2.33
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	9	2.33
(1,137)	1:97:A:ALA:C	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	20	2.33
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	10	2.33
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	2	2.33
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	9	2.33
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	8	2.32
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	18	2.32
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	3	2.3
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	12	2.28
(1,71)	1:51:A:ILE:C	1:52:A:ASP:N	1:52:A:ASP:CA	1:52:A:ASP:C	7	2.28
(1,19)	1:15:A:GLU:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	9	2.28
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	13	2.27
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	4	2.27
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	9	2.27
(1,21)	1:16:A:SER:C	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	15	2.27
(1,109)	1:72:A:ILE:C	1:73:A:GLY:N	1:73:A:GLY:CA	1:73:A:GLY:C	3	2.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	7	2.26
(1,216)	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	1:151:A:ALA:N	10	2.25
(1,99)	1:67:A:TYR:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	14	2.24
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	16	2.24
(1,79)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	19	2.22
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	4	2.21
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	15	2.21
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	13	2.2
(1,135)	1:96:A:HIS:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	4	2.2
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	10	2.18
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	10	2.17
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	17	2.17
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	9	2.16
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	11	2.16
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	3	2.15
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	20	2.15
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	15	2.15
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	9	2.14
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	16	2.14
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	13	2.13
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	13	2.13
(1,99)	1:67:A:TYR:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	9	2.13
(1,71)	1:51:A:ILE:C	1:52:A:ASP:N	1:52:A:ASP:CA	1:52:A:ASP:C	17	2.13
(1,21)	1:16:A:SER:C	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	1	2.13
(1,21)	1:16:A:SER:C	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	19	2.13
(1,101)	1:68:A:ILE:C	1:69:A:ILE:N	1:69:A:ILE:CA	1:69:A:ILE:C	1	2.12
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	14	2.12
(1,71)	1:51:A:ILE:C	1:52:A:ASP:N	1:52:A:ASP:CA	1:52:A:ASP:C	19	2.12
(1,3)	1:7:A:PHE:C	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	4	2.12
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	5	2.11
(1,25)	1:18:A:LYS:C	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:C	7	2.11
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	15	2.1
(1,161)	1:111:A:ASP:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	14	2.09
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	20	2.09
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	7	2.08
(1,99)	1:67:A:TYR:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	4	2.08
(1,19)	1:15:A:GLU:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	20	2.08
(1,201)	1:133:A:ARG:C	1:134:A:SER:N	1:134:A:SER:CA	1:134:A:SER:C	15	2.07
(1,179)	1:122:A:GLU:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	20	2.07
(1,161)	1:111:A:ASP:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	11	2.07
(1,59)	1:45:A:LYS:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	14	2.07
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	3	2.07
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	3	2.07
(1,216)	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	1:151:A:ALA:N	3	2.06
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	5	2.06
(1,113)	1:74:A:ARG:C	1:75:A:ALA:N	1:75:A:ALA:CA	1:75:A:ALA:C	18	2.06
(1,151)	1:106:A:GLN:C	1:107:A:GLU:N	1:107:A:GLU:CA	1:107:A:GLU:C	20	2.05
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	8	2.05
(1,85)	1:60:A:SER:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	3	2.05
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	13	2.05
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	9	2.05

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	17	2.05
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	15	2.04
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	18	2.04
(1,71)	1:51:A:ILE:C	1:52:A:ASP:N	1:52:A:ASP:CA	1:52:A:ASP:C	3	2.02
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	13	2.02
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	15	2.01
(1,99)	1:67:A:TYR:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	10	2.01
(1,69)	1:50:A:ILE:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	16	2.01
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	11	2.01
(1,203)	1:142:A:LEU:C	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	6	2.0
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	7	2.0
(1,83)	1:59:A:ASP:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	18	2.0
(1,23)	1:17:A:PHE:C	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	5	2.0
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	4	1.99
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	7	1.99
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	15	1.99
(1,19)	1:15:A:GLU:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	14	1.98
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	2	1.98
(1,99)	1:67:A:TYR:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	20	1.97
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	1	1.97
(1,69)	1:50:A:ILE:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	4	1.95
(1,59)	1:45:A:LYS:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	6	1.95
(1,185)	1:125:A:ARG:C	1:126:A:MET:N	1:126:A:MET:CA	1:126:A:MET:C	9	1.93
(1,23)	1:17:A:PHE:C	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	2	1.93
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	19	1.92
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	10	1.91
(1,77)	1:54:A:SER:C	1:55:A:ARG:N	1:55:A:ARG:CA	1:55:A:ARG:C	10	1.91
(1,71)	1:51:A:ILE:C	1:52:A:ASP:N	1:52:A:ASP:CA	1:52:A:ASP:C	9	1.91
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	12	1.91
(1,19)	1:15:A:GLU:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	4	1.91
(1,199)	1:132:A:ASP:C	1:133:A:ARG:N	1:133:A:ARG:CA	1:133:A:ARG:C	11	1.9
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	13	1.9
(1,21)	1:16:A:SER:C	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	13	1.9
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	9	1.89
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	5	1.88
(1,101)	1:68:A:ILE:C	1:69:A:ILE:N	1:69:A:ILE:CA	1:69:A:ILE:C	4	1.88
(1,99)	1:67:A:TYR:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	6	1.88
(1,185)	1:125:A:ARG:C	1:126:A:MET:N	1:126:A:MET:CA	1:126:A:MET:C	20	1.87
(1,19)	1:15:A:GLU:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	5	1.86
(1,23)	1:17:A:PHE:C	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	12	1.84
(1,21)	1:16:A:SER:C	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	3	1.84
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	4	1.84
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	8	1.83
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	8	1.83
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	14	1.83
(1,153)	1:107:A:GLU:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	14	1.83
(1,99)	1:67:A:TYR:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	13	1.83
(1,105)	1:70:A:ASP:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	14	1.82
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	6	1.82
(1,71)	1:51:A:ILE:C	1:52:A:ASP:N	1:52:A:ASP:CA	1:52:A:ASP:C	12	1.82
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	20	1.82

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1)	1:6:A:ASP:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	11	1.82
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	5	1.81
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	5	1.8
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	20	1.79
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	20	1.79
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	1	1.78
(1,153)	1:107:A:GLU:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	6	1.78
(1,77)	1:54:A:SER:C	1:55:A:ARG:N	1:55:A:ARG:CA	1:55:A:ARG:C	20	1.78
(1,215)	1:149:A:CYS:C	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	11	1.77
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	20	1.77
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	12	1.77
(1,23)	1:17:A:PHE:C	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	3	1.77
(1,141)	1:99:A:ASN:C	1:100:A:THR:N	1:100:A:THR:CA	1:100:A:THR:C	5	1.76
(1,99)	1:67:A:TYR:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	1	1.76
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	15	1.75
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	6	1.75
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	4	1.75
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	6	1.75
(1,19)	1:15:A:GLU:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	2	1.75
(1,141)	1:99:A:ASN:C	1:100:A:THR:N	1:100:A:THR:CA	1:100:A:THR:C	4	1.73
(1,135)	1:96:A:HIS:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	18	1.73
(1,93)	1:64:A:GLY:C	1:65:A:SER:N	1:65:A:SER:CA	1:65:A:SER:C	9	1.73
(1,151)	1:106:A:GLN:C	1:107:A:GLU:N	1:107:A:GLU:CA	1:107:A:GLU:C	9	1.72
(1,105)	1:70:A:ASP:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	15	1.72
(1,83)	1:59:A:ASP:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	4	1.72
(1,59)	1:45:A:LYS:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	3	1.72
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	5	1.71
(1,101)	1:68:A:ILE:C	1:69:A:ILE:N	1:69:A:ILE:CA	1:69:A:ILE:C	9	1.7
(1,65)	1:48:A:SER:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1	1.7
(1,121)	1:78:A:ASP:C	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	15	1.69
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	15	1.69
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	15	1.69
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	6	1.69
(1,13)	1:12:A:ALA:C	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	11	1.69
(1,69)	1:50:A:ILE:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	10	1.68
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	14	1.68
(1,23)	1:17:A:PHE:C	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	1	1.68
(1,215)	1:149:A:CYS:C	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	17	1.67
(1,139)	1:98:A:ILE:C	1:99:A:ASN:N	1:99:A:ASN:CA	1:99:A:ASN:C	9	1.67
(1,135)	1:96:A:HIS:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	20	1.66
(1,105)	1:70:A:ASP:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	12	1.66
(1,105)	1:70:A:ASP:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	20	1.65
(1,193)	1:129:A:ASP:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	11	1.64
(1,105)	1:70:A:ASP:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	6	1.64
(1,137)	1:97:A:ALA:C	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	5	1.63
(1,141)	1:99:A:ASN:C	1:100:A:THR:N	1:100:A:THR:CA	1:100:A:THR:C	12	1.62
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	18	1.61
(1,73)	1:52:A:ASP:C	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	6	1.61
(1,27)	1:25:A:SER:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	14	1.61
(1,201)	1:133:A:ARG:C	1:134:A:SER:N	1:134:A:SER:CA	1:134:A:SER:C	3	1.6
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	2	1.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,153)	1:107:A:GLU:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	18	1.6
(1,73)	1:52:A:ASP:C	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	9	1.6
(1,49)	1:36:A:ALA:C	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	7	1.6
(1,45)	1:34:A:THR:C	1:35:A:TYR:N	1:35:A:TYR:CA	1:35:A:TYR:C	14	1.6
(1,15)	1:13:A:THR:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	15	1.6
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	2	1.59
(1,185)	1:125:A:ARG:C	1:126:A:MET:N	1:126:A:MET:CA	1:126:A:MET:C	1	1.59
(1,135)	1:96:A:HIS:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	12	1.59
(1,53)	1:42:A:ILE:C	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	20	1.59
(1,216)	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	1:151:A:ALA:N	6	1.58
(1,139)	1:98:A:ILE:C	1:99:A:ASN:N	1:99:A:ASN:CA	1:99:A:ASN:C	15	1.58
(1,71)	1:51:A:ILE:C	1:52:A:ASP:N	1:52:A:ASP:CA	1:52:A:ASP:C	5	1.58
(1,203)	1:142:A:LEU:C	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	4	1.56
(1,59)	1:45:A:LYS:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	9	1.56
(1,59)	1:45:A:LYS:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	12	1.56
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	16	1.55
(1,151)	1:106:A:GLN:C	1:107:A:GLU:N	1:107:A:GLU:CA	1:107:A:GLU:C	12	1.55
(1,101)	1:68:A:ILE:C	1:69:A:ILE:N	1:69:A:ILE:CA	1:69:A:ILE:C	17	1.55
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	7	1.53
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	18	1.53
(1,139)	1:98:A:ILE:C	1:99:A:ASN:N	1:99:A:ASN:CA	1:99:A:ASN:C	13	1.52
(1,25)	1:18:A:LYS:C	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:C	15	1.52
(1,23)	1:17:A:PHE:C	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	16	1.52
(1,21)	1:16:A:SER:C	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	12	1.52
(1,21)	1:16:A:SER:C	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	20	1.52
(1,101)	1:68:A:ILE:C	1:69:A:ILE:N	1:69:A:ILE:CA	1:69:A:ILE:C	6	1.51
(1,41)	1:32:A:LEU:C	1:33:A:THR:N	1:33:A:THR:CA	1:33:A:THR:C	3	1.51
(1,27)	1:25:A:SER:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	1	1.51
(1,15)	1:13:A:THR:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	19	1.51
(1,135)	1:96:A:HIS:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	5	1.5
(1,23)	1:17:A:PHE:C	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	8	1.5
(1,216)	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	1:151:A:ALA:N	11	1.49
(1,163)	1:112:A:ALA:C	1:113:A:ILE:N	1:113:A:ILE:CA	1:113:A:ILE:C	10	1.49
(1,63)	1:47:A:ILE:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	8	1.48
(1,19)	1:15:A:GLU:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	13	1.48
(1,15)	1:13:A:THR:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	7	1.48
(1,99)	1:67:A:TYR:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	19	1.47
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	17	1.46
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	6	1.45
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	12	1.45
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	3	1.45
(1,25)	1:18:A:LYS:C	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:C	19	1.45
(1,7)	1:9:A:ASN:C	1:10:A:PHE:N	1:10:A:PHE:CA	1:10:A:PHE:C	6	1.45
(1,151)	1:106:A:GLN:C	1:107:A:GLU:N	1:107:A:GLU:CA	1:107:A:GLU:C	3	1.44
(1,151)	1:106:A:GLN:C	1:107:A:GLU:N	1:107:A:GLU:CA	1:107:A:GLU:C	14	1.44
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	7	1.44
(1,25)	1:18:A:LYS:C	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:C	12	1.44
(1,203)	1:142:A:LEU:C	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	12	1.43
(1,105)	1:70:A:ASP:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	9	1.43
(1,69)	1:50:A:ILE:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	3	1.43
(1,201)	1:133:A:ARG:C	1:134:A:SER:N	1:134:A:SER:CA	1:134:A:SER:C	20	1.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,77)	1:54:A:SER:C	1:55:A:ARG:N	1:55:A:ARG:CA	1:55:A:ARG:C	9	1.42
(1,151)	1:106:A:GLN:C	1:107:A:GLU:N	1:107:A:GLU:CA	1:107:A:GLU:C	6	1.41
(1,99)	1:67:A:TYR:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	12	1.41
(1,59)	1:45:A:LYS:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	19	1.41
(1,215)	1:149:A:CYS:C	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	5	1.4
(1,59)	1:45:A:LYS:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	7	1.4
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	6	1.4
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	18	1.4
(1,35)	1:29:A:ILE:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	11	1.4
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	8	1.39
(1,105)	1:70:A:ASP:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	5	1.39
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	20	1.39
(1,99)	1:67:A:TYR:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	17	1.39
(1,71)	1:51:A:ILE:C	1:52:A:ASP:N	1:52:A:ASP:CA	1:52:A:ASP:C	2	1.39
(1,161)	1:111:A:ASP:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	3	1.38
(1,153)	1:107:A:GLU:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	13	1.38
(1,151)	1:106:A:GLN:C	1:107:A:GLU:N	1:107:A:GLU:CA	1:107:A:GLU:C	8	1.38
(1,141)	1:99:A:ASN:C	1:100:A:THR:N	1:100:A:THR:CA	1:100:A:THR:C	20	1.38
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	10	1.38
(1,25)	1:18:A:LYS:C	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:C	16	1.38
(1,21)	1:16:A:SER:C	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	5	1.38
(1,15)	1:13:A:THR:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	6	1.38
(1,216)	1:150:A:PHE:N	1:150:A:PHE:CA	1:150:A:PHE:C	1:151:A:ALA:N	8	1.37
(1,137)	1:97:A:ALA:C	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	13	1.37
(1,69)	1:50:A:ILE:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	5	1.37
(1,139)	1:98:A:ILE:C	1:99:A:ASN:N	1:99:A:ASN:CA	1:99:A:ASN:C	7	1.36
(1,105)	1:70:A:ASP:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	19	1.36
(1,69)	1:50:A:ILE:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	9	1.35
(1,19)	1:15:A:GLU:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1	1.35
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	8	1.34
(1,137)	1:97:A:ALA:C	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	7	1.34
(1,69)	1:50:A:ILE:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	6	1.34
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	15	1.33
(1,137)	1:97:A:ALA:C	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	12	1.33
(1,71)	1:51:A:ILE:C	1:52:A:ASP:N	1:52:A:ASP:CA	1:52:A:ASP:C	14	1.33
(1,59)	1:45:A:LYS:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	16	1.33
(1,121)	1:78:A:ASP:C	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	19	1.32
(1,15)	1:13:A:THR:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	3	1.32
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	18	1.31
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	10	1.31
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	17	1.3
(1,59)	1:45:A:LYS:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1	1.3
(1,35)	1:29:A:ILE:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	14	1.3
(1,137)	1:97:A:ALA:C	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	15	1.29
(1,101)	1:68:A:ILE:C	1:69:A:ILE:N	1:69:A:ILE:CA	1:69:A:ILE:C	12	1.29
(1,139)	1:98:A:ILE:C	1:99:A:ASN:N	1:99:A:ASN:CA	1:99:A:ASN:C	17	1.28
(1,7)	1:9:A:ASN:C	1:10:A:PHE:N	1:10:A:PHE:CA	1:10:A:PHE:C	5	1.28
(1,163)	1:112:A:ALA:C	1:113:A:ILE:N	1:113:A:ILE:CA	1:113:A:ILE:C	14	1.27
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	6	1.27
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	16	1.27
(1,197)	1:131:A:TRP:C	1:132:A:ASP:N	1:132:A:ASP:CA	1:132:A:ASP:C	19	1.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,121)	1:78:A:ASP:C	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	4	1.26
(1,35)	1:29:A:ILE:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	16	1.26
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	14	1.25
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	7	1.24
(1,153)	1:107:A:GLU:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	15	1.24
(1,151)	1:106:A:GLN:C	1:107:A:GLU:N	1:107:A:GLU:CA	1:107:A:GLU:C	18	1.24
(1,141)	1:99:A:ASN:C	1:100:A:THR:N	1:100:A:THR:CA	1:100:A:THR:C	14	1.24
(1,59)	1:45:A:LYS:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	5	1.23
(1,1)	1:6:A:ASP:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	10	1.23
(1,113)	1:74:A:ARG:C	1:75:A:ALA:N	1:75:A:ALA:CA	1:75:A:ALA:C	8	1.22
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	10	1.22
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	11	1.21
(1,139)	1:98:A:ILE:C	1:99:A:ASN:N	1:99:A:ASN:CA	1:99:A:ASN:C	1	1.21
(1,99)	1:67:A:TYR:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	16	1.21
(1,71)	1:51:A:ILE:C	1:52:A:ASP:N	1:52:A:ASP:CA	1:52:A:ASP:C	1	1.21
(1,25)	1:18:A:LYS:C	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:C	1	1.21
(1,15)	1:13:A:THR:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	9	1.2
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	1	1.19
(1,159)	1:110:A:SER:C	1:111:A:ASP:N	1:111:A:ASP:CA	1:111:A:ASP:C	6	1.19
(1,113)	1:74:A:ARG:C	1:75:A:ALA:N	1:75:A:ALA:CA	1:75:A:ALA:C	20	1.19
(1,199)	1:132:A:ASP:C	1:133:A:ARG:N	1:133:A:ARG:CA	1:133:A:ARG:C	12	1.18
(1,197)	1:131:A:TRP:C	1:132:A:ASP:N	1:132:A:ASP:CA	1:132:A:ASP:C	7	1.18
(1,185)	1:125:A:ARG:C	1:126:A:MET:N	1:126:A:MET:CA	1:126:A:MET:C	8	1.18
(1,181)	1:123:A:LYS:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	19	1.18
(1,151)	1:106:A:GLN:C	1:107:A:GLU:N	1:107:A:GLU:CA	1:107:A:GLU:C	4	1.18
(1,59)	1:45:A:LYS:C	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	17	1.18
(1,35)	1:29:A:ILE:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	20	1.18
(1,23)	1:17:A:PHE:C	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	13	1.18
(1,7)	1:9:A:ASN:C	1:10:A:PHE:N	1:10:A:PHE:CA	1:10:A:PHE:C	8	1.18
(1,137)	1:97:A:ALA:C	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	9	1.17
(1,151)	1:106:A:GLN:C	1:107:A:GLU:N	1:107:A:GLU:CA	1:107:A:GLU:C	7	1.16
(1,151)	1:106:A:GLN:C	1:107:A:GLU:N	1:107:A:GLU:CA	1:107:A:GLU:C	10	1.16
(1,121)	1:78:A:ASP:C	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	2	1.16
(1,21)	1:16:A:SER:C	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	4	1.16
(1,205)	1:143:A:ASN:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1	1.15
(1,189)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	12	1.15
(1,137)	1:97:A:ALA:C	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	4	1.15
(1,99)	1:67:A:TYR:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	11	1.15
(1,19)	1:15:A:GLU:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	8	1.15
(1,153)	1:107:A:GLU:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	2	1.14
(1,69)	1:50:A:ILE:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	17	1.14
(1,25)	1:18:A:LYS:C	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:C	10	1.14
(1,15)	1:13:A:THR:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	17	1.14
(1,113)	1:74:A:ARG:C	1:75:A:ALA:N	1:75:A:ALA:CA	1:75:A:ALA:C	10	1.13
(1,19)	1:15:A:GLU:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	12	1.13
(1,201)	1:133:A:ARG:C	1:134:A:SER:N	1:134:A:SER:CA	1:134:A:SER:C	12	1.11
(1,71)	1:51:A:ILE:C	1:52:A:ASP:N	1:52:A:ASP:CA	1:52:A:ASP:C	16	1.11
(1,165)	1:113:A:ILE:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	2	1.1
(1,163)	1:112:A:ALA:C	1:113:A:ILE:N	1:113:A:ILE:CA	1:113:A:ILE:C	9	1.1
(1,97)	1:66:A:LEU:C	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	1	1.1
(1,21)	1:16:A:SER:C	1:17:A:PHE:N	1:17:A:PHE:CA	1:17:A:PHE:C	8	1.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,7)	1:9:A:ASN:C	1:10:A:PHE:N	1:10:A:PHE:CA	1:10:A:PHE:C	17	1.09
(1,219)	1:151:A:ALA:C	1:152:A:MET:N	1:152:A:MET:CA	1:152:A:MET:C	20	1.08
(1,113)	1:74:A:ARG:C	1:75:A:ALA:N	1:75:A:ALA:CA	1:75:A:ALA:C	2	1.08
(1,101)	1:68:A:ILE:C	1:69:A:ILE:N	1:69:A:ILE:CA	1:69:A:ILE:C	11	1.08
(1,161)	1:111:A:ASP:C	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	17	1.07
(1,139)	1:98:A:ILE:C	1:99:A:ASN:N	1:99:A:ASN:CA	1:99:A:ASN:C	19	1.07
(1,19)	1:15:A:GLU:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	3	1.07
(1,121)	1:78:A:ASP:C	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	14	1.05
(1,103)	1:69:A:ILE:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	4	1.05
(1,51)	1:37:A:LEU:C	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	1	1.05
(1,39)	1:31:A:LYS:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	14	1.05
(1,35)	1:29:A:ILE:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	12	1.05
(1,35)	1:29:A:ILE:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	6	1.04
(1,27)	1:25:A:SER:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	13	1.04
(1,141)	1:99:A:ASN:C	1:100:A:THR:N	1:100:A:THR:CA	1:100:A:THR:C	11	1.03
(1,139)	1:98:A:ILE:C	1:99:A:ASN:N	1:99:A:ASN:CA	1:99:A:ASN:C	6	1.03
(1,121)	1:78:A:ASP:C	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	17	1.03
(1,101)	1:68:A:ILE:C	1:69:A:ILE:N	1:69:A:ILE:CA	1:69:A:ILE:C	5	1.03
(1,7)	1:9:A:ASN:C	1:10:A:PHE:N	1:10:A:PHE:CA	1:10:A:PHE:C	12	1.03
(1,151)	1:106:A:GLN:C	1:107:A:GLU:N	1:107:A:GLU:CA	1:107:A:GLU:C	15	1.02
(1,71)	1:51:A:ILE:C	1:52:A:ASP:N	1:52:A:ASP:CA	1:52:A:ASP:C	8	1.02
(1,25)	1:18:A:LYS:C	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:C	11	1.02
(1,15)	1:13:A:THR:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	20	1.0